COE 332: Software Engineering & Design

Texas Advanced Computing Center

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The objective of this course is to introduce students to advanced computing concepts in software engineering, software systems design, cloud computing, distributed systems, and computational engineering. Through a series of assignments spanning the course of the semester, students will build a cloud-based, computational system to interact with a time series dataset and provide a web-accessible interface to their system.

COURSE SCHEDULE: 1

2 COURSE SCHEDULE:

UNIT 1: ONBOARDING AND ESSENTIAL SKILLS

We will use the first few days of class to set expectations and describe requirements for the upcoming semester. We will begin to set up some necessary accounts and onboard students to the TACC / class ecosystem. We will also quickly review essential Linux, Python, and Version Control (Git) skills that will be necessary for the rest of this course.

1.1 Class Introduction

Welcome to:

COE 332 – Software Engineering & Design, Spring 2024 Department of Aerospace Engineering and Engineering Mechanics The University of Texas at Austin

Unique Number: 14410

Instructors:

- Joe Allen, wallen@tacc.utexas.edu
- Charlie Dey, charlie@tacc.utexas.edu
- Joe Stubbs, jstubbs@tacc.utexas.edu

Time: Tues/Thur 11:00am - 12:30pm Location: ASE 1.112 A (in person) Teaching Assistant: Aditya Anekar

Important Links:

- Canvas: https://utexas.instructure.com/courses/1380167
- Class Repo: https://coe-332-sp24.readthedocs.io/
- Slack: https://tacc-learn.slack.com/ (#coe332-sp24)

Catalog Description:

Covers methods and tools for planning, designing, implementing, validating and maintaining large software systems. May include project work to build a software system as a team, using appropriate software engineering tools and techniques.

Prerequisites:

Computational Engineering 322 with a grade of at least C-.

Knowledge, Skills, and Abilities Students Should Have Before Entering This Course:

This course assumes familiarity with the Python programming language and strong working knowledge of basic, high-level language programming concepts including data structures, conditionals, loops, and functions. We also assume a basic, working knowledge of the Linux command line. We will briefly review programming concepts in Linux and Python during the first week of class, the first homework assignment will be based on these topics, and we will make every effort to help students who are less familiar with these concepts. Ultimately, each student is expected to and responsible for mastering this material. This is not an introductory programming class and we will not have time to give a comprehensive treatment of all of these topics.

Knowledge, Skills, and Abilities Students Gain from this Course (Learning Outcomes):

The objective of this course is to introduce students to advanced computing concepts in software engineering, software systems design, cloud computing, distributed systems, and computational engineering. Through a series of assignments spanning the course of the semester, students will build a cloud-based, computational system to interact with a time series data set and provide a web-accessible interface to their system.

Relationship of Course to Program Outcomes:

This course contributes to the ABET Criterion 3 student outcomes that took effect with the Fall 2019 semester. For more information, see Criteria for Accrediting Engineering Programs, 2020-2021 at https://www.abet.org/accreditation/accreditation-criteria/criteria-for-accrediting-engineering-programs-2020-2021/

STUDENT OUTCOME

- 1. an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics
- 2. an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors
- 3. an ability to communicate effectively with a range of audiences
- 4. an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts
- 5. an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives
- 6. an ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions
- 7. an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

ABET Program Criteria Achieved:

Program criteria are unique to each degree program and are to be compiled from the program criteria given for each degree program and listed in table format below. The faculty should check which of the program criteria are achieved in the course.

Criterion	Criterion	Criterion
A. Aerodynamics	G. Orbital Mechanics	M. Preliminary/Conceptual Design
B. Aerospace Materials	H. Space Environment	N. Other Design Content
C. Structures	I. Attitude Determination and Control	O. Professionalism
D. Propulsion	J. Telecommunications	P. Computer Usage
E. Flight Mechanics	K. Space Structures	
F. Stability and Control	L. Rocket Propulsion	

Topics (subject to change):

- Software engineering and design practices in Python (d=28) (outcomes=1,2,3,4,5,6,7; criteria=M,N,O,P)
- Version control with Git (d=1)(outcomes=2,3,5; criteria=N,O,P)
- Unit testing, integration testing, continuous integration (d=4) (outcomes=1,2,6; criteria=M,N,O,P)
- Linux containers with Docker, container orchestration (d=4) (outcomes=1,2,7; criteria=M,N,O,P)
- HTTP and RESTful web services (d=5) (outcomes=1,2,6, criteria=M,N,P)
- Application programming interfaces (d=2) (outcomes=1,2,3; criteria=M,N,O,P)
- Virtualization with Kubernetes (d=4) (outcomes=1,2,7; criteria=M,N,P)
- Databases and Queues (d=4) (outcomes=1,2,6; criteria=M,N,P)
- Asynchronous programming patterns in distributed systems (d=2) (outcomes=1,2,5,6,7; criteria=M,N,P)
- Other advanced topics as time permits

Please note: In the course of learning and working through the above topics, students will be exposed to data sets from a variety of sources (e.g. https://data.nasa.gov/browse) representing other select Criterion (A-L) relevant to the ABET program accreditation. The exact data sets and types of data will depend on individual student interests.

Professionalism Topics:

Throughout the course, students will be taught to communicate professionally in the documentation of their software and in their software engineering & design projects. Effective communication in software projects is necessary to inform other engineers about the purpose or function of the project, and how to use it. Students will form teams to work together on the Final Projects (see description below) and will be required to address ethical and professional responsibilities in the course of working on their project.

Design Assignments (Final Project Description):

The Final Project will be a culmination of all materials covered in the class. Students will build a cloud-based, computational system to interact with a time series data set and provide a web-accessible interface to their system. Prior to working on the Final Project, students will form teams to work through a "design" phase where they must identify a primary data set to work on, describe API endpoints, diagram architecture components, and draft other major documentation components. In addition, students will be required to write in their own words what they think their ethical

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and professional responsibilities are as an engineer and how that relates to the Final Project. The project design will be pitched to the instructors and given feedback / subject to approval. The Final Project will be due at the end of the semester in the form of a written report (e.g. pdf) and a GitHub repository containing the software and all support files. The full Final Project description will be posted on the class webpage.

Computer:

The entire course will be computer based. The instructors will provide a remote server for students to work on. Students are expected to have access to a personal / lab computer with a web browser and a terminal (or SSH client).

Text:

No textbook will be used for this course.

Class Format:

The class will be delivered in person in a computer lab setting. Most class meetings will be comprised of lectures/demonstrations and hands-on labs. Students are expected to attend every lecture and actively participate in the hands-on labs during the class. The hands-on portions will often solve parts of homework assignments. Lecture materials with worked examples will be posted to the class website right before the class meeting. Additionally, there will be a class Slack channel for discussing ideas about the course with your fellow students.

Class Schedule (approximate, subject to change):

- Week 1: Onboarding, Linux, Python Review
- Week 2: Version Control, Working with JSON, CSV, XML, YAML
- Week 3: Code Organization, Documentation, Exception Handling, Unit Testing
- Week 4: Concepts in Software Design, REST APIs, Intro to Flask
- Week 5: Advanced Flask
- Week 6: Intro to Containerization and Automation
- Week 7: Advanced Containers, Docker Compose
- Week 8: Databases, Persistence in REST, Midterm Project Due
- Week of March 11 Spring Break
- Week 9: Virtualization: Container Orchestration and Kubernetes
- Week 10: Virtualization: Container Orchestration and Kubernetes, cont.
- Week 11: Asynchronous Programming, Concurrency
- Week 12: Messaging Systems, Queues
- Week 13: Continuous Integration, Integration Testing
- Week 14: Special Topics Final Week of Class
- Final Exam Day / Time: Friday, May 3, 1pm-3pm (subject to change), Final Project Due

Disability and Access (D&A):

The university is committed to creating an accessible and inclusive learning environment consistent with university policy and federal and state law. Please let me know if you experience any barriers to learning so I can work with you to ensure you have equal opportunity to participate fully in this course. If you are a student with a disability, or think you may have a disability, and need accommodations please contact Disability and Access (D&A). Please refer to D&A's website for contact and more information: http://diversity.utexas.edu/disability/. If you are already registered with D&A, please deliver your Accommodation Letter to me as early as possible in the semester so we can discuss your approved accommodations and needs in this course.

Grading:

Grades for the course will be based on the following:

- 50% Homework Approximately 8-10 coding / software design assignments to be submitted via GitHub.
- 20% Midterm A midterm design project will include concepts from the first half of the semester and build on the first 4-5 homework assignments. A written component will also be required.
- 30% Final Project Students will form groups to work on a final class project consisting of a distributed, web-accessible, cloud system to interact with a time series data set. The project will draw from and build upon work done throughout the semester in homework assignments. The project will need to be pitched to the instructors for approval, and a written component will also be required.

(See syllabus for letter grade cutoffs)

Homework Policy:

We encourage collaboration on homework assignments. Engaging in discussions and comparing notes with other students about the homework assignments can be a valuable learning experience. However, each student is expected to complete and turn in their own homework assignment. We do not allow students to copy directly from others.

All homework assignments will be turned in as Git repositories on GitHub. Homework repositories should be set to private, and shared with the course instructor. The course instructor will pull homework from the repositories at the posted due date / time. Instructions on setting up the repositories and sharing them with the course instructor will be covered in class.

Attendance:

Regular attendance is expected but absences will not count against the student's grades. We expect students to give us a week notice in advance of their absence if known ahead of time.

Office Hours:

Office hours will be for 1 hour immediately following the class and/or by appointment. We plan to use Slack for general communications and to help with the materials. https://tacc-learn.slack.com/

Important Dates:

Please refer to UT's academic calendar for important dates: https://registrar.utexas.edu/calendars/23-24

Special Notes:

The University of Texas at Austin provides upon request appropriate academic adjustments for qualified students with disabilities. For more information, contact the Office of the Dean of Students at 471-6259, 471-4641 TDD or the Cockrell School of Engineering Director of Students with Disabilities at 471-4321.

Evaluation:

The Measurement and Evaluation Center forms for the Cockrell School of Engineering will be used during the last week of class to evaluate the course and the instructor.

Honor Code:

The University of Texas at Austin strives to create a dynamic and engaging community of teaching and learning where students feel intellectually challenged; build knowledge and skills; and develop critical thinking, creativity, and intellectual curiosity. As a part of this community, it is important to engage in assignments, exams, and other work for your classes with openness, integrity, and a willingness to make mistakes and learn from them. The UT Austin honor code champions these principles:

• I pledge, as a member of the University of Texas community, to do my work honestly, respectfully, and through the intentional pursuit of learning and scholarship.

The honor code affirmation includes three additional principles that elaborate on the core theme:

• I pledge to be honest about what I create and to acknowledge what I use that belongs to others.

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- I pledge to value the process of learning in addition to the outcome, while celebrating and learning from mistakes.
- This code encompasses all of the academic and scholarly endeavors of the university community.

The honor code is more than a set of rules, it reflects the values that are foundational to your academic community. By affirming and embracing the honor code, you are both upholding the integrity of your work and contributing to a campus culture of trust and respect.

Academic Integrity Expectations:

Students who violate University rules on academic misconduct are subject to the student conduct process. A student found responsible for academic misconduct may be assigned both a status sanction and a grade impact for the course. The grade impact could range from a zero on the assignment in question up to a failing grade in the course. A status sanction can range from a written warning, probation, deferred suspension and/or dismissal from the University. To learn more about academic integrity standards, tips for avoiding a potential academic misconduct violation, and the overall conduct process, please visit the Student Conduct and Academic Integrity website at: http://deanofstudents.utexas.edu/conduct.

Artificial Intelligence:

The creation of artificial intelligence tools for widespread use is an exciting innovation. These tools have both appropriate and inappropriate uses in classwork. The use of artificial intelligence tools (such as ChatGPT) in this class shall be permitted on a limited basis. You will be informed as to the assignments for which AI may be utilized. You are also welcome to seek my prior-approval to use AI writing tools on any assignment. In either instance, AI writing tools should be used with caution and proper citation, as the use of AI should be properly attributed. Using AI writing tools without my permission or authorization, or failing to properly cite AI even where permitted, shall constitute a violation of UT Austin's Institutional Rules on academic integrity. If you are considering the use of AI writing tools but are unsure if you are allowed or the extent to which they may be utilized appropriately, please ask.

Religious Holy Days:

By UT Austin policy, you must notify me of your pending absence for a religious holy day as far in advance as possible of the date of observance. If you must miss a class, an examination, a work assignment, or a project in order to observe a religious holy day, you will be given an opportunity to complete the missed work within a reasonable time after the absence.

Names and Pronouns:

Class rosters are provided to the instructor with the student's legal name, unless they have added a chosen name with the registrar's office. If you have not yet done so, I will gladly honor your request to address you with the name and pronouns that you prefer for me to use for you. It is helpful to advise me of any changes or needs regarding your name and pronouns early in the semester so that I may make appropriate updates to my records and be informed about how to support you in this class.

- For instructions on how to add your pronouns to Canvas, visit this site.
- If you would like to update your chosen name with the registrar's office, you can do so here, and reference this guide.
- For additional guidelines prepared by the Gender and Sexuality Center for changing your name on various campus systems, see the Resources page under UT Resources here.

TITLE IX DISCLOSURE

Beginning January 1, 2020, Texas Education Code, Section 51.252 (formerly known as Senate Bill 212) requires all employees of Texas universities, including faculty, to report to the Title IX Office any information regarding incidents of sexual harassment, sexual assault, dating violence, or stalking that is disclosed to them. Texas law requires that all employees who witness or receive information about incidents of this type (including, but not limited to, written forms, applications, one-on-one conversations, class assignments, class discussions, or third-party reports) must report it to the Title IX Coordinator. Before talking with me, or with any faculty or staff member about a Title IX-related incident, please remember that I will be required to report this information.

Although graduate teaching and research assistants are not subject to Texas Education Code, Section 51.252, they are mandatory reporters under federal Title IX regulations and are required to report a wide range of behaviors we refer to as sexual misconduct, including the types of misconduct covered under Texas Education Code, Section 51.252. Title IX of the Education Amendments of 1972 is a federal civil rights law that prohibits discrimination on the basis of sex - including pregnancy and parental status - in educational programs and activities. The Title IX Office has developed supportive ways and compiled campus resources to support all impacted by a Title IX matter.

If you would like to speak with a case manager, who can provide support, resources, or academic accommodations, in the Title IX Office, please email: supportandresources@austin.utexas.edu. Case managers can also provide support, resources, and accommodations for pregnant, nursing, and parenting students.

For more information about reporting options and resources, please visit: https://titleix.utexas.edu, contact the Title IX Office via email at: titleix@austin.utexas.edu, or call 512-471-0419.

Campus Safety

The following are recommendations regarding emergency evacuation from the Office of Emergency Management, 512-232-2114:

- Students should sign up for Campus Emergency Text Alerts at the page linked above.
- Occupants of buildings on The University of Texas at Austin campus must evacuate buildings when a fire alarm is activated. Alarm activation or announcement requires exiting and assembling outside.
- Familiarize yourself with all exit doors of each classroom and building you may occupy. Remember that the nearest exit door may not be the one you used when entering the building.
- Students requiring assistance in evacuation shall inform their instructor in writing during the first week of class.
- In the event of an evacuation, follow the instruction of faculty or class instructors. Do not re-enter a building unless given instructions by the following: Austin Fire Department, The University of Texas at Austin Police Department, or Fire Prevention Services office.
- For more information, please visit the Office of Emergency Management.

University Resources

For a list of university resources that may be helpful to you as you engage with and navigate your courses and the university, see the University Resources Students Canvas page.

1.1.1 Additional Help

Our main goal for this class is your success. Please contact us if you need help:

- Joe Allen, wallen@tacc.utexas.edu
- Joe Stubbs, jstubbs@tacc.utexas.edu
- Charlie Dey, charlie@tacc.utexas.edu

Important links:

- Canvas: https://utexas.instructure.com/courses/1380167
- Class Repo: https://coe-332-sp24.readthedocs.io/
- Slack: https://tacc-learn.slack.com/ (#coe332-sp24)

1.2 Onboarding to TACC

The Texas Advanced Computing Center (TACC) at UT Austin designs and operates some of the world's most powerful computing resources. The center's mission is to enable discoveries that advance science and society through the application of advanced computing technologies.

We will be using cloud resources at TACC as our development environment. We will access the cloud resources via our SSH clients and TACC account credentials. You will need a TACC username, password, and multifactor token for this class.

Attention: Everyone please apply for a TACC account now using this link. If you already have a TACC account, you can just use that. Send your TACC username to the course instructors via Slack or e-mail as soon as possible (see below).

1.2.1 About TACC

TACC is a Research Center, part of UT Austin, and located at the JJ Pickle Research Campus.

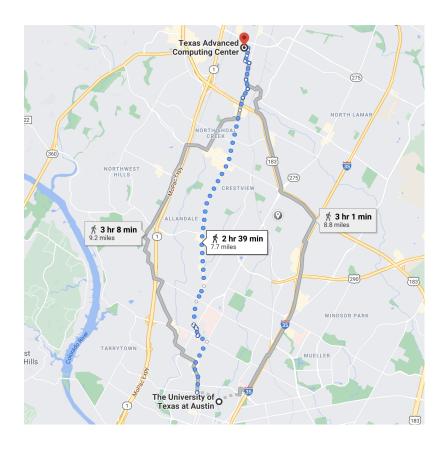
TACC at a Glance

Other TACC Activities

- · Portals and gateways
- · Web service APIs
- · Rich software stacks
- Consulting
- Curation and analysis
- Code optimization
- · Training and outreach
- => Learn more

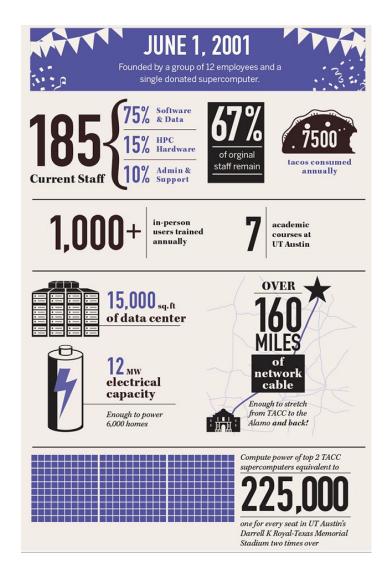
TACC Partnerships

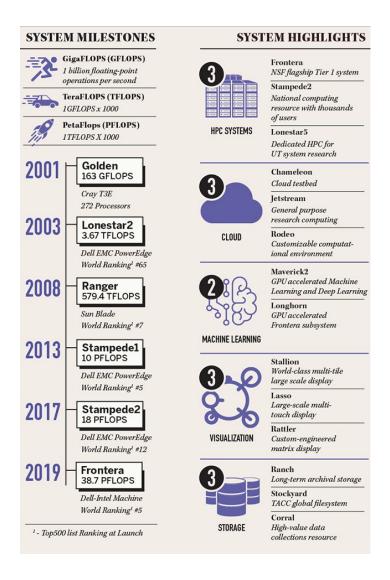
- NSF: Leadership Class Computing Facility (LCCF)
- NSF: Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)
- UT System Research Cyberinfrastructure (UTRC)
- TX Lonestar Education and Research Network (LEARN)
- Industry, STAR Program

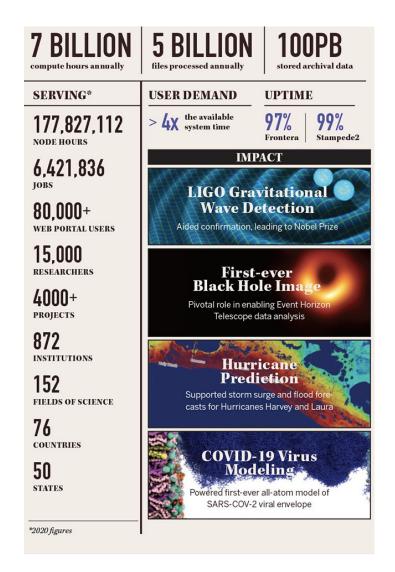


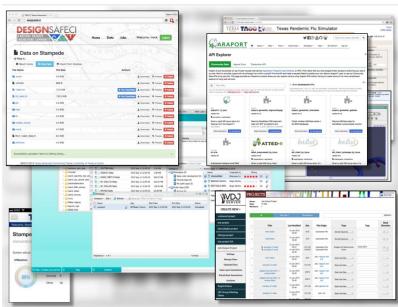












- International, The International Collaboratory for Emerging Technologies
- => Learn more

Attention: Did you already e-mail your information to the course instructors?

Which brings us to the question: Why are we here teaching this class?

1.2.2 Engineering Complex Systems in the Cloud

The Tapis Framework, developed at TACC, is a great example of a complex assembly of code with many moving parts, engineered to help researchers interact with high performance computing systems in streamlined and automated ways. Tapis empowers its users to:

- Authenticate using TACC (or other) credentials
- Manage, move, share, and publish data sets
- · Run scientific code in batch jobs on clusters
- Set up event-driven processes
- · Many other things!

The above description of Tapis and the below schematic diagram are both intentionally left a little bit vague as we will cover more of the specifics of Tapis later on in the semester.

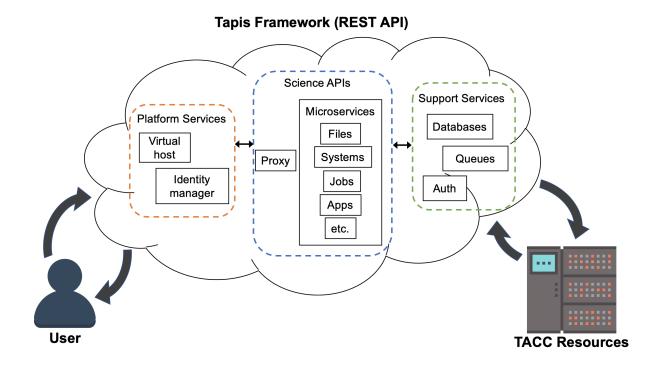
Tip: Astute observers may notice that most, if not all, tools, technologies, and concepts that form the Tapis ecosystem show up somewhere in the agenda for COE 332.

So what can you do with Tapis?

Why would I want to build something similar?

Why should I learn how to use all of these tools and technologies?

Without concrete examples, it can seem rather esoteric. The vignette below hopefully illustrate how a carefully designed framework can be employed to tackle a real-world problem.



Application in Biomedical Engineering: Real-Time Quantitative MRI

Problem: Quantitative analysis of MR images is typically performed after the patient has left the scanner. Corrupted or poor quality images can result in patient call backs, delaying disease intervention.

Importance: Real-time analytics of MRI scans can enable same-session quality control, reducing patient call backs, and it can enable precision medicine.

Approach: Faculty and staff from UTHealth - Houston and TACC used the Tapis framework to help develop an automated platform for real-time MRI.

Result: Scan data can now be automatically processed on high performance computing resources in real-time with no human intervention.

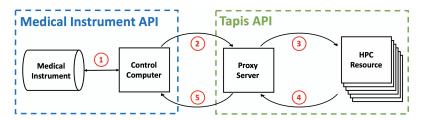


Fig. 1: Diagram of computer systems and APIs employed.

Source: https://dx.doi.org/10.1109/JBHI.2017.2771299

Attention: If you already e-mailed your TACC account to the instructors, please go ahead and try the exercise below.

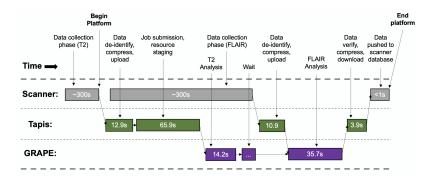


Fig. 2: Sample platform workflow for combining two images into one enhanced image.

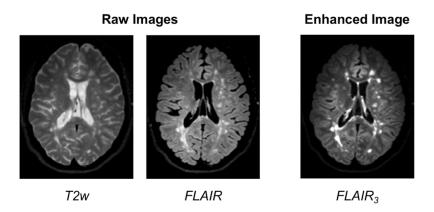


Fig. 3: Final image shows enhanced MS lesions.

Application in Aerospace Engineering: Ingenuity Helicopter

On April 19, 2021, the helicopter *Ingenuity* (part of NASA's Mars 2020 mission along with the rover *Perseverance*) completed the first ever "powered controlled extraterrestrial flight by an aircraft". As of January 2023, it has made ~38 flights recording pictures, sound, position, and other data during flight.

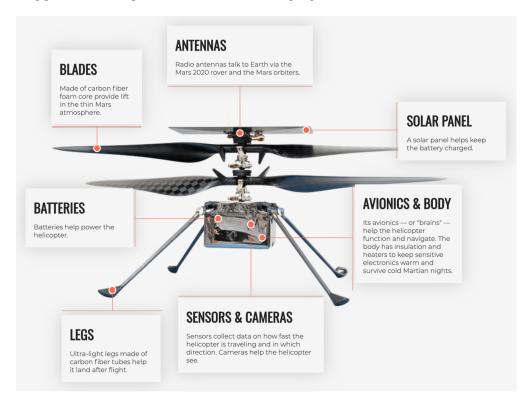


Fig. 4: Source: https://en.wikipedia.org/wiki/File:Anatomy_of_the_Mars_Helicopter.png

How do *Perseverance* and *Ingenuity* communicate to carry out missions and return that sensor data? NASA JPL credited a long list of open source code repositories on GitHub that the helicopter project depends on.

Included in the list are a lot of libraries and tools that we will be using this semester to build our cloud systems including: Linux, curl, pycurl, yaml, flask, click, pytest, jinja, requests, urllib3, werkzeug, (and many others). Looking at the packages, it seems pretty likely that the rover communicates with the helicopter through something similar to a REST API! We will all be building similar systems this semester.

Read more here: https://github.com/readme/featured/nasa-ingenuity-helicopter

1.2.3 Bringing it All Together

Hopefully these examples start to show you what kind of software projects we will be working on this semester. Each week will be introducing a new concept, tool, or technology that will slowly be building to a larger overall framework with many moving parts.

1.2.4 For Next Time

Using your SSH client, please try to log in to the class server before the next class period:

```
[local]$ ssh username@student-login.tacc.utexas.edu
(username@student-login.tacc.utexas.edu) Password:
(username@student-login.tacc.utexas.edu) TACC_Token:
Welcome to Ubuntu 20.04.6 LTS (GNU/Linux 5.4.0-153-generic x86_64)
* Documentation: https://help.ubuntu.com
* Management: https://landscape.canonical.com
* Support:
                 https://ubuntu.com/advantage
 System information as of Mon 15 Jan 2024 09:58:37 PM CST
 System load: 0.0
                                  Processes:
                                                           249
 Usage of /: 93.2% of 17.12GB Users logged in:
                                                          1
 Memory usage: 22%
                                  IPv4 address for ens192: 129.114.4.186
 Swap usage: 1%
Welcome to the Texas Advanced Computing Center
  at The University of Texas at Austin
** Unauthorized use/access is prohibited. **
If you log on to this computer system, you acknowledge your awareness
of and concurrence with the UT Austin Acceptable Use Policy. The
University will prosecute violators to the full extent of the law.
TACC Usage Policies:
http://www.tacc.utexas.edu/user-services/usage-policies/
TACC Support:
https://portal.tacc.utexas.edu/tacc-consulting
Last login: Wed Jan 10 15:33:13 2024 from 146.6.176.142
[student-login]$ hostname -f
student-login.tacc.utexas.edu
```

Note: In the above, replace 'username' with your TACC username.

1.3 Student Goals

When asked about their area of concentration, students responded:

- Computational Engineering 18
- Aerospace 7
- Biomedical / Health 5
- Data Science / AI / ML 5
- Software 3
- Math 2
- Parallel Processing 2
- Climate 1
- Electrical and Computer Engineering 1
- Energy 1
- Natural Sciences 1
- Physics 1
- Quantum Computing 1
- Space Exploration 1
- Trading Analysis 1

When asked what their goals were for the course, students responded (most of these were edited for typos and readability):

Programming

- Become a better programmer
- · Learn more about python
- · Learn how to write python code effectively
- Gain more experience with python
- · Get better at cython for fun
- · Learn parallel processing in python
- Get quicker at solving coding problems
- Be a stronger software developer
- Better understand parallel computing at the supercomputer level
- Learn to use Python more professionally to enhance skills to utilize in the real world
- · Learn more Object Oriented Programming
- Develop a better workflow and headspace for coding
- · Learn python

Software Engineering

- Develop a good understanding of computational applications in software engineering
- Learn virtualization and other advanced topics

- Learn more about software engineering
- Advance my software development skills in the area of cloud based systems
- · Hone my abilities in software engineering
- Grasp knowledge of cloud computing as it relates to Aerospace
- Get a lot better at cloud development
- · Learn things useful for both software engineering and software engineering technical interviews
- · Learn more about software development and design
- Learn more about different aspects of software engineering in general

Technologies / Applications

- Understand how to build containers
- Learning Kubernetes
- Learn some unique utilities in technologies like git or bash
- Learn and understand APIs well enough to explain them to other people
- Learn more about Flask and learn how to apply it to my code
- Learn Kubernetes, FLASK, and APIs
- Learn the fundamentals of databases
- · Learn the fundamentals of creating web applications
- Have a better understanding of webdev so that I would be capable of finishing cloud-integrated projects on my own
- Learn emacs
- · Better understand containerization
- · Learn more about containers

Professional Development

- Familiarize myself with processing datasets that may be relevant to a future job
- Be able to use the material learned in this course and apply them in a career setting
- Use the material learned in this course to start a career in software programming or computation
- Develop computational skills
- Increase my confidence within the field to make myself a more valuable talent for future hires
- Use the learning to get an internship
- Connect with the Professor to potentially get an internship at TACC this Summer
- Explore job opportunities, working at TACC for the summer
- Be prepared for an internship or a research opportunity
- Land a summer internship through the powerful connections available to me
- · Develop technical industry skills
- · Land an internship
- Find an internship/research for the summer

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- Be prepared for interviews
- Be able to put coding skills on my resume

Data Science / Research

- · Learn how to do scientific computation
- Learn to develop tools to solve problems
- Gain relevant experience working with large datasets
- · Get familiar with programming languages/scientific programming so I can use this for my research interests
- Applying and enhancing my current knowledge of cloud computing, software engineering, and data science through real-world projects
- Incorporate my data sets from research I participate in
- Want to learn more about Quantitative Analysis
- · Learn things in terms of aerospace and other aspects

1.4 Linux Essentials

To be successful in this class, students should be able to:

- · Describe basic functions of essential Linux commands
- Use Linux commands to navigate a file system and manipulate files
- Transfer data to / from a remote Linux file system
- Edit files directly on a Linux system using a command line utility (e.g. vim, nano, emacs)

Topics covered in this module include:

- Creating and navigating folders (pwd, 1s, mkdir, cd, rmdir)
- Creating and manipulating files (touch, rm, mv, cp)
- Looking at the contents of files (cat, more, less, head, tail, grep)
- Network and file transfers (hostname, whoami, logout, ssh, scp, rsync)
- Text editing with vim (insert mode, normal mode, navigating, saving, quitting)

1.4.1 Log in to the Class Server

To log in to student-login.tacc.utexas.edu, follow the instructions for your operating system or ssh client below.

Note: Replace username with your TACC username.

Mac / Linux

```
Open the application 'Terminal'
type: ssh username@student-login.tacc.utexas.edu
(enter password)
(enter token)
```

Windows (use WSL2 or an SSH client like PuTTY)

```
Open the application 'Terminal' or 'PuTTY'
enter Host Name: student-login.tacc.utexas.edu
(click 'Open')
(enter username)
(enter password)
(enter token)
```

If you can't access the class server yet, a local or web-based Linux environment will work for this guide. However, you will need to access the class server for future lectures.

Try this Linux environment in a browser.

1.4.2 Creating and Navigating Folders

On a Windows or Mac desktop, our present location determines what files and folders we can access. I can "see" my present location visually with the help of the graphic interface - I could be looking at my Desktop, or the contents of a folder, for example. In a Linux command-line interface, we lack the same visual queues to tell us what our location is. Instead, we use a command - pwd (print working directory) - to tell us our present location. Try executing this command in the terminal:

```
$ pwd
/home/username
```

This home location on the Linux filesystem is unique for each user, and it is roughly analogous to C:\Users\username on Windows, or /Users\username on Mac.

To see what files and folders are available at this location, use the 1s (list) command:

```
$ 1s
```

I have no files or folders in my home directory yet, so I do not get a response. We can create some folders using the mkdir (make directory) command. The words 'folder' and 'directory' are interchangeable:

```
$ mkdir folder1
$ mkdir folder2
$ mkdir folder3
```

```
$ ls
folder1 folder2 folder3
```

Now we have some folders to work with. To "open" a folder, navigate into that folder using the cd (change directory) command. This process is analogous to double-clicking a folder on Windows or Mac:

```
$ pwd
/home/username/
$ cd folder1
$ pwd
/home/username/folder1
```

Now that we are inside folder1, make a few sub-folders:

```
$ mkdir subfolderA
$ mkdir subfolderB
(continues on next page)
```

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(continued from previous page)

```
$ mkdir subfolderC
$ ls
subfolderA subfolderB subfolderC
```

Use cd to Navigate into subfolderA, then use 1s to list the contents. What do you expect to see?

```
$ cd subfolderA
$ pwd
/home/username/folder1/subfolderA
$ ls
```

There is nothing there because we have not made anything yet. Next, we will navigate back to the home directory. So far we have seen how to navigate "down" into folders, but how do we navigate back "up" to the parent folder? There are different ways to do it. For example, we could specify the complete path of where we want to go:

```
$ pwd
/home/username/folder1/subfolderA
$ cd /home/username/folder1
$ pwd
/home/username/folder1/
```

Or, we could use a shortcut, ..., which refers to the **parent folder** - one level higher than the present location:

```
$ pwd
/home/username/folder1
$ cd ..
$ pwd
/home/username
```

We are back in our home directory. Finally, use the rmdir (remove directory) command to remove folders. This will not work on folders that have any contents (more on this later):

```
$ mkdir junkfolder
$ ls
folder1 folder2 folder3 junkfolder
$ rmdir junkfolder
$ ls
folder1 folder2 folder3
```

Before we move on, let's remove the directories we have made, using rm -r to remove our parent folder folder1 and its subfolders. The -r command line option recursively removes subfolders and files located "down" the parent directory. -r is required for non-empty folders.

```
$ rm -r folder1
$ ls
folder2 folder3
```

Which command should we use to remove folder2 and folder3?

```
$ rmdir folder2
$ rmdir folder3
$ ls
```

1.4.3 Creating and Manipulating Files

We have seen how to navigate around the filesystem and perform operations with folders. But, what about files? Just like on Windows or Mac, we can easily create new files, copy files, rename files, and move files to different locations. First, we will navigate to the home directory and create a few new folders and files with the mkdir and touch commands:

```
$ cd  # cd on an empty line will automatically take you back to the home directory
$ pwd
/home/username
$ mkdir folder1
$ mkdir folder2
$ mkdir folder3
$ touch file_a
$ touch file_b
$ touch file_c
$ ls
file_a file_b file_c folder1 folder2 folder3
```

These files we have created are all empty. Removing a file is done with the rm (remove) command. Please note that on Linux file systems, there is no "Recycle Bin". Any file or folder removed is gone forever and often un-recoverable:

```
$ touch junkfile
$ rm junkfile
```

Moving files with the mv command and copying files with the cp command works similarly to how you would expect on a Windows or Mac machine. The context around the move or copy operation determines what the result will be. For example, we could move and/or copy files into folders:

```
$ mv file_a folder1/
$ mv file_b folder2/
$ cp file_c folder3/
```

Before listing the results with 1s, try to guess what the result will be.

```
$ ls
file_c folder1 folder2 folder3
$ ls folder1
file_a
$ ls folder2
file_b
$ ls folder3
file_c
```

Two files have been moved into folders, and file_c has been copied - so there is still a copy of file_c in the home directory. Move and copy commands can also be used to change the name of a file:

```
$ cp file_c file_c_copy
$ mv file_c file_c_new_name
```

By now, you may have found that Linux is very unforgiving with typos. Generous use of the <Tab> key to autocomplete file and folder names, as well as the <UpArrow> to cycle back through command history, will greatly improve the experience. As a general rule, try not to use spaces or strange characters in files or folder names. Stick to:

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```
A-Z # capital letters
a-z # lowercase letters
0-9 # digits
- # hyphen
_ # underscore
. # period
```

Before we move on, let's clean up once again by removing the files and folders we have created. Do you remember the command for removing non-empty folders?

```
$ rm -r folder1
$ rm -r folder2
$ rm -r folder3
```

How do we remove file_c_copy and file_c_new_name?

```
$ rm file_c_copy
$ rm file_c_new_name
```

1.4.4 Looking at the Contents of Files

Everything we have seen so far has been with empty files and folders. We will now start looking at some real data. Navigate to your home directory, then issue the following cp command to copy a public file on the server to your local space:

```
$ cd ~ # the tilde ~ is also a shortcut referring to your home directory
$ pwd
/home/username
$ cp /usr/share/dict/words .
$ ls
words
```

Try to use <Tab> to autocomplete the name of the file. Also, please notice the single dot. at the end of the copy command, which indicates that you want to cp the file to., this present location (your home directory).

This words file is a standard file that can be found on most Linux operating systems. This version contains 654,895 words, each word on its own line. To see the contents of a file, use the cat command to print it to screen:

```
$ cat words
A
A'asia
A's
AATech
AATech's
AAEE
AAeE
AAeE
AAer's
AAgr
AAgr
```

This is a long file! Printing everything to screen is much too fast and not very useful. We can use a few other commands to look at the contents of the file with more control:

```
$ more words
```

Press the <Enter> key to scroll through line-by-line, or the <Space> key to scroll through page-by-page. Press q to quit the view, or <Ctrl+c> to force a quit if things freeze up. A % indicator at the bottom of the screen shows your progress through the file. This is still a little bit messy and fills up the screen. The less command has the same effect, but is a little bit cleaner:

```
$ less words
```

Scrolling through the data is the same, but now we can also search the data. Press the / forward slash key, and type a word that you would like to search for. The screen will jump down to the first match of that word. The n key will cycle through other matches, if they exist.

Finally, you can view just the beginning or the end of a file with the head and tail commands. For example:

```
$ head words
$ tail words
```

The > and >> shortcuts in Linux indicate that you would like to redirect the output of one of the commands above. Instead of printing to screen, the output can be redirected into a file:

```
$ cat words > words_new.txt
$ head words > first_10_lines.txt
```

A single greater than sign > will redirect and **overwrite** any contents in the target file. A double greater than sign >> will redirect and **append** any output to the end of the target file.

One final useful way to look at the contents of files is with the grep command. grep searches a file for a specific pattern, and returns all lines that match the pattern. For example:

```
$ grep "banana" words
banana
banana's
bananaquit
bananas
cassabanana
```

Although it is not always necessary, it is safe to put the search term in quotes.

1.4.5 Network and File Transfers

In order to login or transfer files to a remote Linux file system, you must know the hostname (unique network identifier) and the username. If you are already on a Linux file system, those are easy to determine using the following commands:

```
[student-login]$ whoami
username
[student-login]$ hostname -f
student-login.tacc.utexas.edu
```

Given that information, a user would remotely login to this Linux machine using ssh in a Terminal:

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```
(enter token)
[student-login]$
```

Logging out of a remote system is done using the logout command, or the shortcut <Ctrl+d>:

```
[student-login]$ logout
[local]$
```

Copying files from your local computer to your home folder on the class server would require the scp command:

```
[local]$ scp my_file username@student-login.tacc.utexas.edu:/home/username/
(enter password)
(enter token)
```

In this command, you specify the name of the file you want to transfer (my_file), your username (username), the hostname (student-login.tacc.utexas.edu), and the path you want to put the file (/home/username/). Take careful notice of the separators including spaces, the @ symbol, and the colon:

Copy files from the class server to your local computer using the following:

```
[local]$ scp username@student-login.tacc.utexas.edu:/home/username/my_file ./
(enter password)
(enter token)
```

Instead of files, full directories can be copied using the "recursive" flag (scp -r ...). The rsync tool is an advanced copy tool that is useful for synching data between two sites. Although we will not go into depth here, example rsync usage is as follows:

```
$ rsync -azv local remote
$ rsync -azv remote local
```

This is just the basics of copying files. See example scp usage and example rsync usage for more info.

1.4.6 Text Editing with VIM

VIM is a text editor used on Linux file systems.

Open a file (or create a new file if it does not exist):

```
$ vim file_name
```

There are two "modes" in VIM that we will need to know. They are called "insert mode" and "normal mode". In insert mode, the user is typing text into a file as seen through the terminal (think about typing text into TextEdit or Notepad). In normal mode, the user can perform other functions like save, quit, cut and paste, find and replace, etc. (think about clicking the menu options in TextEdit or Notepad). The two main keys to remember to toggle between the modes are i and Esc.

Entering VIM insert mode:

```
> i
```

Entering VIM normal mode:

```
> Esc
```

A summary of the most important keys to know for normal mode are:

```
# Navigating the file:
                  move up, down, left, right
arrow keys
    Ctrl+u
                  page up
    Ctrl+d
                  page down
                  move to beginning of line
         0
                  move to end of line
                  move to beginning of file
        gg
                  move to end of file
         G
        :N
                  move to line N
# Saving and quitting:
                  quit editing the file
        :q
        :q!
                  quit editing the file without saving
                  save the file, continue editing
        :w
                  save and quit
        :wq
```

1.4.7 Review of Topics Covered

Part 1: Creating and navigating folders

Command	Effect
pwd	print working directory
ls	list files and directories
ls -1	list files in column format
mkdir dir_name/	make a new directory
cd dir_name/	navigate into a directory
<pre>rmdir dir_name/</pre>	remove an empty directory
rm -r dir_name/	remove a directory and its contents
. or ./	refers to the present location
or/	refers to the parent directory

Part 2: Creating and manipulating files

Command	Effect
touch file_name	create a new file
rm file_name	remove a file
rm -r dir_name/	remove a directory and its contents
<pre>mv file_name dir_name/</pre>	move a file into a directory
<pre>mv old_file new_file</pre>	change the name of a file
<pre>mv old_dir/ new_dir/</pre>	change the name of a directory
<pre>cp old_file new_file</pre>	copy a file
<pre>cp -r old_dir/ new_dir/</pre>	copy a directory
<tab></tab>	autocomplete file or folder names
<uparrow></uparrow>	cycle through command history

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Part 3: Looking at the contents of files

Command	Effect
cat file_name	print file contents to screen
<pre>cat file_name >> new_file</pre>	redirect output to new file
more file_name	scroll through file contents
less file_name	scroll through file contents
head file_name	output beginning of file
tail file_name	output end of a file
grep pattern file_name	search for 'pattern' in a file
~/	shortcut for home directory
<ctrl+c></ctrl+c>	force interrupt
>	redirect and overwrite
>>	redirect and append

Part 4: Network and file transfers

Command	Effect
hostname -f	print hostname
whoami	print username
ssh username@hostname	remote login
logout	logout
scp local remote	copy a file from local to remote
scp remote local	copy a file from remote to local
rsync -azv local remote	sync files between local and remote
rsync -azv remote local	sync files between remote and local
<ctrl+d></ctrl+d>	logout of host

Part 5: Text editing with VIM

Command	Effect
vim file.txt	open "file.txt" and edit with vim
i	toggle to insert mode
<esc></esc>	toggle to normal mode
<arrow keys=""></arrow>	navigate the file
:q	quit ending the file
:q!	quit editing the file without saving
: W	save the file, continue editing
:wq	save and quit

1.4.8 Additional Resources

- · Practice Linux commands safely in a web-based emulator
- Practice VIM in a web browser
- Practice VIM on the command line by typing vimtutor

1.5 Python Refresher

To be successful in this class, students should be able to:

- Write and execute Python code on the class server
- Use variables, lists, and dictionaries in Python
- Write conditionals using a variety of comparison operators
- Write useful while and for loops
- Arrange code into clean, well organized functions
- Read input from and write output to a file
- Import and use standard and non-standard Python libraries

Topics covered in this module include:

- Data types and variables (integers, floats, booleans, strings, type(), print())
- Arithmetic operations (+, -, *, /, **, %, //)
- Lists and dictionaries (creating, interpreting, appending)
- Conditionals and control loops (comparison operators, if/elif/else, while, for, break, continue, pass)
- Functions (defining, passing arguments, returning values)
- File handling (open, with, read(), readline(), strip(), write())
- Importing libraries (import, random, names, pip)

1.5.1 Log in to the Class Server

To log in to student-login.tacc.utexas.edu, follow the instructions for your operating system or ssh client below.

Note: Replace username with your TACC username.

Mac / Linux

```
Open the application 'Terminal'
type: ssh username@student-login.tacc.utexas.edu
(enter password)
(enter token)
```

Windows (use WSL2 or an SSH client like PuTTY)

```
Open the application 'Terminal' or 'PuTTY'
enter Host Name: student-login.tacc.utexas.edu
(click 'Open')
(enter username)
(enter password)
(enter token)
```

If you can't access the class server yet, a local or web-based Python 3 environment will work for this guide. However, you will need to access the class server for future lectures.

Try this Python 3 environment in a browser.

Note: For the first few sections below, we will be using the Python interpreter in *interactive mode* to try out different things. Later on when we get to more complex code, we will be saving the code in files (scripts) and invoking the interpreter non-interactively.

1.5.2 Data Types and Variables

Start up the interactive Python interpreter:

```
[student-login]$ python3
Python 3.8.10 (default, Nov 22 2023, 10:22:35)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Tip: To exit the interpreter, type quit().

The most common data types in Python are similar to other programming languages. For this class, we probably only need to worry about **integers**, **floats**, **booleans**, and **strings**.

Assign some values to variables by doing the following:

```
>>> my_int = 5
>>> my_float = 5.0
>>> my_bool = True  # or False, notice the first letter is capitalized
>>> my_string = 'Hello, world!'
```

In Python, you don't have to declare type. Python figures out the type automatically. Check using the type() function:

```
>>> type(my_int)
<class 'int'>
>>> type(my_float)
<class 'float'>
>>> type(my_bool)
<class 'bool'>
>>> type(my_string)
<class 'str'>
```

Print the values of each variable using the print() function:

```
>>> print(my_int)
5
>>> print('my_int')
my_int
```

(Try printing the others as well). And, notice what happens when we print with and without single quotes? What is the difference between my_int and 'my_int'?

You can convert between types using a few different functions. For example, when you read in data from a file, numbers are often read as strings. Thus, you may want to convert the string to integer or float as appropriate:

```
>>> str(my_int)  # convert int to string
>>> str(my_float)  # convert float to string
>>> int(my_string)  # convert string to int
>>> float(my_string)  # convert string to float
>>>
>>> value = 5
>>> print(value)
5
>>> type(value)
<class 'int'>
>>> new_value = str(value)
>>> print(new_value)
'5'
>>> type(new_value)
<class 'str'>
```

1.5.3 Arithmetic Operations

Next, we will look at some basic arithmetic. You are probably familiar with the standard operations from other languages:

```
Operator
           Function
                              Example
                                         Result
           Addition
                                         2
                               1+1
           Subtraction
                               9-5
                                         4
*
           Multiplication
                              2*2
                                         4
           Division
                               8/4
                                         2
                               3**2
           Exponentiation
                                         9
%
           Modulus
                               5%2
                                         1
           Floor division
//
                               5//2
                                         2
```

Try a few things to see how they work:

```
>>> print(2+2)
>>> print(355/113)
>>> print(10%9)
>>> print(3+5*2)
>>> print('hello' + 'world')
>>> print('some' + 1)
>>> print('number' * 5)
```

Also, carefully consider how arithmetic options may affect type:

```
>>> number1 = 5.0/2
>>> type(number1)
<class 'float'>
>>> print(number1)
2.5
>>> number2 = 5/2
>>> type(number2)
<class 'float'>
>>> print(number2)
2.5
>>> print(number2)
2.5
>>> print(int(number2))
2
```

1.5.4 Lists and Dictionaries

Lists are a data structure in Python that can contain multiple elements. They are ordered, they can contain duplicate values, and they can be modified. Declare a list with square brackets as follows:

```
>>> my_shape_list = ['circle', 'heart', 'triangle', 'square']
>>> type(my_shape_list)
<class 'list'>
>>> print(my_shape_list)
['circle', 'heart', 'triangle', 'square']
```

Access individual list elements:

```
>>> print(my_shape_list[0])
circle
>>> type(my_shape_list[0])
<class 'str'>
>>> print(my_shape_list[2])
triangle
```

Create an empty list and add things to it:

```
>>> my_number_list = []
>>> my_number_list.append(5)  # 'append()' is a method of the list class
>>> my_number_list.append(6)
>>> my_number_list.append(2)
>>> my_number_list.append(2**2)
>>> print(my_number_list)
[5, 6, 2, 4]
>>> type(my_number_list)
<class 'list'>
>>> type(my_number_list[1])
<class 'int'>
```

Lists are not restricted to containing one data type. Combine the lists together to demonstrate:

```
>>> my_big_list = my_shape_list + my_number_list
>>> print(my_big_list)
['circle', 'heart', 'triangle', 'square', 5, 6, 2, 4]
```

Another way to access the contents of lists is by slicing. Slicing supports a start index, stop index, and step taking the form: mylist[start:stop:step]. Only the first colon is required. If you omit the start, stop, or :step, it is assumed you mean the beginning, end, and a step of 1, respectively. Here are some examples of slicing:

```
>>> mylist = ['thing1', 'thing2', 'thing3', 'thing4', 'thing5']
>>> print(mylist[0:2])
                           # returns the first two things
['thing1', 'thing2']
>>> print(mylist[:2])
                           # if you omit the start index, it assumes the beginning
['thing1', 'thing2']
>>> print(mylist[-2:])
                           # returns the last two things (omit the stop index and it.
\rightarrow assumes the end)
['thing4', 'thing5']
>>> print(mylist[:])
                           # returns the entire list
['thing1', 'thing2', 'thing3', 'thing4', 'thing5']
>>> print(mylist[::2])
                           # return every other thing (step = 2)
['thing1', 'thing3', 'thing5']
```

Note: If you slice from a list, it returns an object of type list. If you access a list element by its index, it returns an object of whatever type that element is. The choice of whether to slice from a list, or iterate over a list by index, will depend on what you want to do with the data.

Dictionaries are another data structure in Python that contain key:value pairs. They are always unordered, they cannot contain duplicate keys, and they can be modified. Create a new dictionary using curly brackets:

As your preferences change over time, so too can values stored in dictionaries:

```
>>> my_shape_dict['most_favorite'] = 'rectangle'
>>> print(my_shape_dict['most_favorite'])
rectangle
```

Add new key:value pairs to the dictionary as follows:

```
>>> my_shape_dict['funniest'] = 'squircle'
>>> print(my_shape_dict['funniest'])
squircle
```

Many other methods exist to access, manipulate, interpolate, copy, etc., lists and dictionaries. We will learn more about them out as we encounter them later in this course.

1.5.5 Conditionals and Control Loops

Python **comparison operators** allow you to add conditions into your code in the form of if/elif/else statements. Valid comparison operators include:

```
Operator
           Comparison
                                        Example
                                                  Result
           Equal
                                        1==2
                                                   False
                                        1!=2
           Not equal
                                                   True
!=
>
           Greater than
                                        1>2
                                                   False
           Less than
                                        1<2
                                                   True
<
           Greater than or equal to
>=
                                       1>=2
                                                   False
           Less Than or equal to
                                                   True
<=
                                       1<=2
```

A valid conditional statement might look like:

In addition, conditional statements can be combined with logical operators. Valid logical operators include:

Operator	Description	Example
and	Returns True if both are True	a < b and $c < d$
or	Returns True if at least one is True	a < b or c < d
not	Negate the result	not(a < b)

For example, consider the following code:

```
>>> num1 = 10
>>> num2 = 20
>>>
if (num1 < 100 and num2 < 100):
... print('both are less than 100')
... else:
... print('at least one of them is not less than 100')</pre>
```

While loops also execute according to conditionals. They will continue to execute as long as a condition is True. For example:

```
>>> i = 0
>>>
>>> while (i < 10):
... print(f'i = {i}')  # literal string interpolation
... i = i + 1
```

The break statement can also be used to escape loops:

For loops in Python are useful when you need to execute the same set of instructions over and over again. They are especially great for iterating over lists:

You can also use the range() function to iterate over a range of numbers:

Note: The code is getting a little bit more complicated now. It will be better to stop running in the interpreter's interactive mode, and start writing our code in Python scripts.

1.5.6 Functions

Functions are blocks of codes that are run only when we call them. We can pass data into functions, and have functions return data to us. Functions are absolutely essential to keeping code clean and organized.

On the command line, use a text editor to start writing a Python script:

```
[student-login]$ vim function_test.py
```

Enter the following text into the script:

```
def hello_world():
    print('Hello, world!')
hello_world()
```

After saving and quitting the file, execute the script (Python code is not compiled - just run the raw script with the python3 executable):

```
[student-login]$ python3 function_test.py
Hello, world!
```

Note: Future examples from this point on will assume familiarity with using the text editor and executing the script. We will just be showing the contents of the script and console output.

More advanced functions can take parameters and return results:

```
def add5(value):
    return(value + 5)

final_number = add5(10)
print(final_number)
```

```
[15
```

Pass multiple parameters to a function:

```
def add5_after_multiplying(value1, value2):
    return( (value1 * value2) + 5)

final_number = add5_after_multiplying(10, 2)
print(final_number)
```

```
25
```

It is a good idea to put your list operations into a function in case you plan to iterate over multiple lists:

```
triangle
two
three
```

There are many more ways to call functions, including handing an arbitrary number of arguments, passing keyword / unordered arguments, assigning default values to arguments, and more.

1.5.7 File Handling

The open() function does all of the file handling in Python. It takes two arguments - the *filename* and the *mode*. The possible modes are read (r), write (w), append (a), or create (x).

For example, to read a file do the following:

```
with open('/usr/share/dict/words', 'r') as f:
    for x in range(5):
        print(f.readline())
```

```
A'asia
A's
AATech
AATech's
```

Tip: By opening the file with the with statement above, you get built in exception handling, and it automatically will close the file handle for you. It is generally recommended as the best practice for file handling.

You may have noticed in the above that there seems to be an extra space between each word. What is actually happening is that the file being read has newline characters on the end of each line (\n). When read into the Python script, the original new line is being printed, followed by another newline added by the print() function. Stripping the newline character from the original string is the easiest way to solve this problem:

```
with open('/usr/share/dict/words', 'r') as f:
    for x in range(5):
        print(f.readline().strip('\n'))
```

```
A'asia
A's
AATech
AATech's
```

Read the whole file and store it as a list:

```
words = []

with open('/usr/share/dict/words', 'r') as f:
    words = f.read().splitlines()  # careful of memory usage

for x in range(5):
    print(words[x])
```

```
A'asia
A's
AATech
AATech's
```

Write output to a new file on the file system; make sure you are attempting to write somwhere where you have permissions to write:

```
my_shapes = ['circle', 'heart', 'triangle', 'square']
with open('my_shapes.txt', 'w') as f:
    for shape in my_shapes:
        f.write(shape)
```

```
    (in my_shapes.txt)

    circlehearttrianglesquare
```

You may notice the output file is lacking in newlines this time. Try adding newline characters to your output:

```
my_shapes = ['circle', 'heart', 'triangle', 'square']

with open('my_shapes.txt', 'w') as f:
    for shape in my_shapes:
        f.write( f'{shape}\n' )
```

```
(in my_shapes.txt)
circle
heart
triangle
square
```

Now notice that the original line in the output file is gone - it has been overwritten. Be careful if you are using write (w) vs. append (a).

1.5.8 Importing Libraries

The Python built-in functions, some of which we have seen above, are useful but limited. Part of what makes Python so powerful is the huge number and variety of libraries that can be *imported*. For example, if you want to work with random numbers, you have to import the 'random' library into your code, which has a method for generating random numbers called 'random'.

```
import random

for i in range(5):
    print(random.random())
```

```
0.47115888799541383
0.5202615354150987
0.8892412583071456
0.7467080997595558
0.025668541754695906
```

More information about using the random library can be found in the Python docs

Some libraries that you might want to use are not included in the official Python distribution - called the *Python Standard Library*. Libraries written by the user community can often be found on PyPI.org and downloaded to your local environment using a tool called pip3.

For example, if you wanted to download the names library and use it in your Python code, you would do the following:

```
[student-login]$ pip3 install --user names
Collecting names
  Downloading https://files.pythonhosted.org/packages/44/4e/
  →f9cb7ef2df0250f4ba3334fbdabaa94f9c88097089763d8e85ada8092f84/names-0.3.0.tar.gz (789kB)
  100% || 798kB 1.1MB/s
Installing collected packages: names
  Running setup.py install for names ... done
Successfully installed names-0.3.0
```

Notice the library is installed above with the --user flag. The class server is a shared system and non-privileged users can not download or install packages in root locations. The --user flag instructs pip3 to install the library in your own home directory.

```
import names

for i in range(5):
    print(names.get_full_name())
```

```
Johnny Campbell
Lawrence Webb
Johnathan Holmes
Mary Wang
Jonathan Henry
```

1.5.9 Exercises

Test your understanding of the materials above by attempting the following exercises.

- 1. Write a Python script to find and print the **five** longest words in the words file from earlier in this guide. Ties go to the words that would appear first alphabetically.
- 2. Write a Python script that uses the names module to print out **five** names that are exactly **eight** characters each (**nine** characters if you include the space).
- 3. Write a Python script that uses the names module to generate a list of **five** different full names. Define a function to determine the length of a given name (in number of characters, excluding spaces). Print to screen each name followed by the length of each name as an integer.

Tip: Try passing a string into the len() function.

1.5.10 Additional Resources

- The Python Standard Library
- PEP 8 Python Style Guide
- Python3 environment in a browser
- Jupyter Notebooks in a browser

1.6 Version Control with Git: Part 1

In the next two modules, we will look at the version control system **Git**. Of the numerous version control systems available (Git, Subversion, CVS, Mercurial), Git seems to be the most popular, and we generally find that it is great for:

- · Collaborating with others on code
- Supporting multiple concurrent versions (branches)
- Tagging releases or snapshots in time
- · Restoring previous versions of files
- What it lacks in user-friendliness it makes up for in good documentation
- Intuitive web platforms available

After going through the two Git modules, students should be able to:

- · Create a new Git repository hosted on GitHub
- Clone a repository, commit and push changes to the repository
- Track the history of changes in files in a Git repository
- Demonstrate a basic understanding of forking, branching, tags, and pull requests
- Work collaboratively with others on the content in a Git repository

GitHub is a web platform where you can host and share Git repositories ("repos"). Repositories can be public or private. Much of what we will do with this section requires you to have a GitHub account.

1.6.1 The Basics of Git

Version control systems start with a base version of the document and then record changes you make each step of the way. You can think of it as a recording of your progress: you can rewind to start at the base document and play back each change you made, eventually arriving at your more recent version.

Fig. 5: Changes are saved sequentially.

Once you think of changes as separate from the document itself, you can then think about "playing back" different sets of changes on the base document, ultimately resulting in different versions of that document. For example, two users can make independent sets of changes on the same document.

Fig. 6: Different versions can be saved.

Unless there are conflicts, you can even incorporate two sets of changes into the same base document.

Fig. 7: Multiple versions can be merged.

A version control system is a tool that keeps track of these changes for us, effectively creating different versions of our files. It allows us to decide which changes will be made to the next version (each record of these changes is called a "commit", and keeps useful metadata about them. The complete history of commits for a particular project and their metadata make up a "repository". Repositories can be kept in sync across different computers, facilitating collaboration among different people.

1.6.2 Setting up Git

Log on to the class server and check which version of Git is in your PATH.

Note: Below, replace username with your TACC username.

```
[local]$ ssh username@student-login.tacc.utexas.edu
(enter password)
(enter token)

[student-login]$ which git
/usr/bin/git
[student-login]$ git --version
git version 2.25.1
```

When we use Git on a new computer for the first time, we need to configure a few things. Below are a few examples of configurations we will set as we get started with Git:

- Our name and email address,
- And that we want to use these settings globally (i.e. for every project).

On a command line, Git commands are written as git verb, where verb is what we actually want to do. Here is how we set up our environment:

```
[student-login]$ git config --global user.name "YOUR NAME HERE"
[student-login]$ git config --global user.email "YOUR@EMAIL.HERE"
```

Please use your own name and email address associated with your GitHub account. This user name and email will be connected with your subsequent Git activity, which means that any changes pushed to GitHub, Bitbucket, GitLab or another Git host server in the future will include this information.

Tip: A key benefit of Git is that it is platform agnostic. You can use it equally to interact with the same files from your laptop, from a lab computer, or from a cluster.

1.6.3 Create a New Repository on the Command Line

First, let's navigate to our home directory and create a folder for this class and for working with Git (if you haven't done it already):

```
[student-login]$ cd ~/
[student-login]$ mkdir coe-332  # you may already have a folder for this class
[student-login]$ cd coe-332
[student-login]$ mkdir my-first-git-repo
[student-login]$ cd my-first-git-repo/
[student-login]$ pwd
/home/username/coe-332/my-first-git-repo
```

Then we will use a Git command to initialize this directory as a new Git repository - or a place where Git can start to organize versions of our files.

```
[student-login]$ git init
Initialized empty Git repository in /home/username/coe-332/my-first-git-repo/.git/
```

If we use 1s -a, we can see that Git has created a hidden directory called .git:

```
[student-login]$ ls -a
./ ../ .git/
```

Use the find command to get a overview of the contents of the .git/ directory:

```
[student-login]$ find .git/
.git
.git/refs
.git/refs/heads
.git/refs/tags
.git/branches
.git/description
.git/hooks
.git/hooks/applypatch-msg.sample
.git/hooks/commit-msg.sample
.git/hooks/post-update.sample
.git/hooks/pre-applypatch.sample
.git/hooks/pre-commit.sample
.git/hooks/pre-push.sample
.git/hooks/pre-rebase.sample
.git/hooks/prepare-commit-msg.sample
.git/hooks/update.sample
.git/info
.git/info/exclude
.git/HEAD
.git/config
.git/objects
.git/objects/pack
.git/objects/info
```

Git uses this special sub-directory to store all the information about the project, including all files and sub-directories located within the project's directory. If we ever delete the .git sub-directory, we will lose the project's history. We can check that everything is set up correctly by asking Git to tell us the status of our project:

```
[student-login]$ git status
# On branch main
#
# Initial commit
nothing to commit (create/copy files and use "git add" to track)
```

As you see, there is "nothing to commit" because there are no files in here to track. To make things more interesting, let's touch / create a few new Python scripts and check the status again:

Note: If you are using a different version of git, the exact wording of the output might be slightly different.

EXERCISE

- Explore the files and folders in the .git/ directory
- Can you find any files with plain text info / meta data?

1.6.4 Tracking Changes

We will use this repository track some changes we are about to make to our example Python scripts. Above, Git mentioned that it found several "Untracked files". This means there are files in this current directory that Git isn't keeping track of. We can instruct Git to start tracking a file using git add:

```
[student-login]$ git add python_test_1.py
[student-login]$ git status
# On branch main
#
# Initial commit
#
# Changes to be committed:
# (use "git rm --cached <file>..." to unstage)
#
# new file: python_test_1.py
#
# Untracked files:
# (use "git add <file>..." to include in what will be committed)
```

```
#
# python_test_2.py
```

1.6.5 Commit Changes to the Repo

Git now knows that it's supposed to keep track of python_test_1.py, but it hasn't recorded these changes as a commit yet. To get it to do that, we need to run one more command:

```
[student-login]$ git commit -m "started tracking first Python script"
[main (root-commit) 344ec9f] started tracking first Python script
1 file changed, 29 insertions(+)
create mode 100644 python_test_1.py
```

When we run git commit, Git takes everything we have told it to save by using git add and stores a copy permanently inside the special .git directory. This permanent copy is called a "commit" (or "revision") and its short identifier is 344ec9f. Your commit may have another identifier.

We use the -m flag ("m" for "message") to record a short, descriptive, and specific comment that will help us remember later on what we did and why. Good commit messages start with a brief (<50 characters) statement about the changes made in the commit. Generally, the message should complete the sentence "If applied, this commit will" <*commit message here>*. If you want to go into more detail, add a blank line between the summary line and your additional notes. Use this additional space to explain why you made changes and/or what their impact will be.

If we run git status now:

```
[student-login]$ git status
# On branch main
# Untracked files:
# (use "git add <file>..." to include in what will be committed)
#
# python_test_2.py
nothing added to commit but untracked files present (use "git add" to track)
```

We find one remaining untracked files.

EXERCISE

Do a git add <file> followed by a git commit -m "descriptive message" for the untracked file. Also do a git status in between each command.

1.6.6 Check the Project History

If we want to know what we've done recently, we can ask Git to show us the project's history using git log:

```
[student-login]$ git log
commit 3d5d6e2c6d23aa4fb3b800b535db6a228759866e
Author: Joe Allen <wallen@tacc.utexas.edu>
Date: Wed Jan 27 23:06:03 2021 -0600
    added python_test_2.py
```

```
commit 344ec9fde550c6e009697b07298919946ff991f9
Author: Joe Allen <wallen@tacc.utexas.edu>
Date: Wed Jan 27 23:00:17 2021 -0600

started tracking first Python script
```

The command git log lists all commits made to a repository in reverse chronological order. The listing for each commit includes:

- the commit's full identifier (which starts with the same characters as the short identifier printed by the git commit command earlier),
- the commit's author.
- · when it was created,
- and the log message Git was given when the commit was created.

1.6.7 Making Further Changes

Now suppose we make a change to one of the files we are tracking. Edit the python_test_1.py script your favorite text editor and add some simple code into the script:

```
[student-login]$ vim python_test_1.py
# make some changes in the script
# save and quit
```

When we run git status now, it tells us that a file it already knows about has been modified:

```
[student-login]$ git status
# On branch main
# Changes not staged for commit:
# (use "git add <file>..." to update what will be committed)
# (use "git checkout -- <file>..." to discard changes in working directory)
#
# modified: python_test_1.py
#
no changes added to commit (use "git add" and/or "git commit -a")
```

The last line is the key phrase: "no changes added to commit". We have changed this file, but we haven't told Git we will want to save those changes (which we do with git add) nor have we saved them (which we do with git commit). So let's do that now. It is good practice to always review our changes before saving them. We do this using git diff. This shows us the differences between the current state of the file and the most recently saved version:

```
[student-login]$ git diff python_test_1.py
diff --git a/python_test_1.py b/python_test_1.py
index 5d986e9..21877cb 100644
--- a/python_test_1.py
+++ b/python_test_1.py
@@ -18,7 +18,7 @@
...
--
+# simple code inserted here
```

```
...
```

The output is cryptic because it is actually a series of commands for tools like editors and patch telling them how to reconstruct one file given the other. If we break it down into pieces:

- The first line tells us that Git is producing output similar to the Unix diff command comparing the old and new versions of the file.
- The second line tells exactly which versions of the file Git is comparing: 5d986e9 and 21877cb are unique computer-generated labels for those versions.
- The third and fourth lines once again show the name of the file being changed.
- The remaining lines are the most interesting, they show us the actual differences and the lines on which they occur. In particular, the + marker in the first column shows where we added lines.

After reviewing our change, it's time to commit it:

```
[student-login]$ git add python_test_1.py
[student-login]$ git commit -m "added a descriptive comment"
[main 8d5f563] added a descriptive comment
  1 file changed, 1 insertion(+), 1 deletion(-)
[student-login]$ git status
# On branch main
nothing to commit, working directory clean
```

Git insists that we add files to the set we want to commit before actually committing anything. This allows us to commit our changes in stages and capture changes in logical portions rather than only large batches. For example, suppose we're adding a few citations to relevant research to our thesis. We might want to commit those additions, and the corresponding bibliography entries, but *not* commit some of our work drafting the conclusion (which we haven't finished yet).

1.6.8 Directories in Git

There are a couple important facts you should know about directories in Git. First, Git does not track directories on their own, only files within them. Try it for yourself:

```
[student-login]$ mkdir directory
[student-login]$ git status
[student-login]$ git add directory
[student-login]$ git status
```

Note, our newly created empty directory does not appear in the list of untracked files even if we explicitly add it (*via* git add) to our repository.

Second, if you create a directory in your Git repository and populate it with files, you can add all files in the directory at once by:

```
[student-login]$ git add <directory-with-files>
```

Tip: A trick for tracking an empty directory with Git is to add a hidden file to the directory. People sometimes will label this .gitcanary. Adding and committing that file to the repo's history will cause the directory it is in to also be tracked.

1.6.9 Restoring Old Versions of Files

We can save changes to files and see what we've changed — now how can we restore older versions of things? Let's suppose we accidentally overwrite our file:

```
[student-login]$ echo "" > python_test_1.py
[student-login]$ cat python_test_1.py
```

Now git status tells us that the file has been changed, but those changes haven't been staged:

```
[student-login]$ git status
# On branch main
# Changes not staged for commit:
# (use "git add <file>..." to update what will be committed)
# (use "git checkout -- <file>..." to discard changes in working directory)
#
# modified: python_test_1.py
#
no changes added to commit (use "git add" and/or "git commit -a")
```

We can put things back the way they were by using git checkout and referring to the *most recent commit* of the working directory by using the identifier HEAD:

```
[student-login]$ git checkout HEAD python_test_1.py
[student-login]$ cat python_test_1.py
import random
...etc
```

As you might guess from its name, git checkout checks out (i.e., restores) an old version of a file. In this case, we're telling Git that we want to recover the version of the file recorded in HEAD, which is the last saved commit. If we want to go back even further, we can use a commit identifier instead:

```
[student-login] $ git log
commit 8d5f563fa20060f4fbe2e10ec5cbc3c22fe92559
Author: Joe Allen <wallen@tacc.utexas.edu>
       Wed Jan 27 23:15:46 2021 -0600
Date:
added a descriptive comment
commit 3d5d6e2c6d23aa4fb3b800b535db6a228759866e
Author: Joe Allen <wallen@tacc.utexas.edu>
Date:
       Wed Jan 27 23:06:03 2021 -0600
adding python_test_2.py
commit 344ec9fde550c6e009697b07298919946ff991f9
Author: Joe Allen <wallen@tacc.utexas.edu>
       Wed Jan 27 23:00:17 2021 -0600
Date:
started tracking first Python script
```

```
[student-login]$ git checkout 344ec9f python_test_1.py
# now you have a copy of python_test_1.py without that comment we added
```

Again, we can put things back the way they were by using git checkout:

```
[student-login]$ git checkout HEAD python_test_1.py
# back to the most recent version
```

1.6.10 Summing Up

To summarize the first Git module, the commands we covered were:

```
git config  # Get and set repository or global options
git init  # Create an empty Git repository or reinitialize an existing one
git status  # Show the working tree status
git add  # Add file contents to the index
git commit  # Record changes to the repository
git diff  # Show changes between commits, commit and working tree, etc
git log  # Show commit logs
git checkout  # Checkout a branch or paths to the working tree
```

The key takeaway is the general workflow of *making some changes* => git add => git commit. If you think of Git as taking snapshots of changes over the life of a project, git add specifies what will go in a snapshot (putting things in the staging area), and git commit actually takes the snapshot, and makes a permanent record of it (as a commit).

1.6.11 Additional Resources

- Some of the materials in this module were based on Software Carpentry DOI: 10.5281/zenodo.57467.
- · GitHub Glossary
- · About Branches
- About Pull Requests
- About Licenses
- · GitFlow Model
- More on different git workflows

1.7 Version Control with Git: Part 2

In the first Git module, we learned to work independently with Git repositories on the local command line. In this second part, we will focus on using the GitHub web interface and collaborating with others.

1.7.1 Link a Local Repository to GitHub

Version control really comes into its own when we begin to collaborate with other people. We already have most of the machinery we need to do this; the only thing missing is to copy changes from one repository to another.

Systems like Git allow us to move work between any two repositories. In practice, though, it's easiest to use one copy as a central hub, and to keep it on the web rather than on someone's laptop. Most programmers use hosting services like GitHub, Bitbucket, or GitLab to hold those main copies.

Let's start by sharing the changes we've made to our current project with the world. Log in to GitHub, then click on the icon in the top right corner to create a new repository:

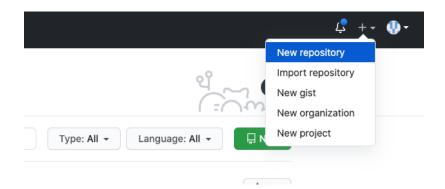


Fig. 8: Click 'New repository'.

As soon as the repository is created, GitHub displays a page with a URL and some information on how to configure your local repository. Provide a name for your new repository like python-test (or whatever you want, it doesn't have to match the name of your local folder).

Note that our local repository still contains our earlier work on python_test_1.py and other files, but the remote repository on GitHub doesn't contain any memory of python_test_1.py yet. The next step is to connect and sync the two repositories. We do this by making the GitHub repository a "remote" for the local repository. The home page of the repository on GitHub includes the string we need to identify it:

...or push an existing repository from the command line

```
git remote add origin git@github.com:wjallen/python-test.git
git branch -M main
git push -u origin main
```

Fig. 9: Follow the instructions for pushing an existing repository.

Back on class server in the local Git repo, link it to the repo on GitHub and confirm the link was created:

```
[student-login]$ git remote add origin git@github.com:wjallen/python-test.git
[student-login]$ git remote -v
origin git@github.com:wjallen/python-test.git (fetch)
origin git@github.com:wjallen/python-test.git (push)
```

Attention: Make sure to use the URL for your repository instead of the one listed here.

The name origin is a local nickname for your remote repository. We could use something else if we wanted to, but origin is by far the most common choice.

Another key step is to set up SSH keys for authentication. GitHub no longer allows simple username / password authentication from the command line. To set up SSH keys, click on:

Your account => Settings => SSH and GPG keys => New SSH key

In the "Title" box, add a memorable name for this key like "student-login". In the "Key" box, cut and paste the contents of your existing public key on the class server. You can find it by executing the command:

```
[student-login]$ cat ~/.ssh/id_rsa.pub
ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAQDF8crdmqgk2GhRmsLPcREWjzc9zb2B....
```

If you do not have an existing SSH key, it is easy to make your own. For this class, we will name the SSH key generated for GitHub slightly different than the standard key name so as not to accidentally overwrite the keys we will use later on to log in to our Jetstream VMs.

```
[student-login]$ mkdir -p ~/.ssh/ && ssh-keygen -f ~/.ssh/github_rsa -t rsa -b 3072 -N ""
[student-login]$ cat ~/.ssh/github_rsa.pub
ssh-rsa AAAAB3NzaC1yc2EAAAADAQABAAABAQDF8crdmqgk2GhRmsLPcREWjzc9zb2B....
```

One other small caveat is that we must configure our systems to use this new key when connecting to GitHub. Open up \sim /.ssh/config with your favorite text editor and add the following two lines:

```
Host github.com
IdentityFile ~/.ssh/github_rsa
```

Once the SSH key is set up, this command will push the changes from our local repository to the repository on GitHub:

```
[student-login]$ git branch -M main
[student-login]$ git push -u origin main
Warning: Permanently added the ECDSA host key for IP address '140.82.112.4' to the list

→of known hosts.
Counting objects: 3, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (2/2), done.
Writing objects: 100% (3/3), 223 bytes | 0 bytes/s, done.
Total 3 (delta 0), reused 0 (delta 0)
To git@github.com:wjallen/python-test.git

* [new branch] main -> main
Branch main set up to track remote branch main from origin.
```

Now that the repositories are synced, your development workflow has evolved to include the git push operation. From here on, if you make changes to your code, you can expect to follow the changes with the commands:

```
# Make some edits to "example_file.py"
[student-login]$ git status
[student-login]$ git add example_file.py
[student-login]$ git commit -m "description of changes"
[student-login]$ git push
```

1.7.2 Clone the Repository

Spend a few minutes browsing the web interface for GitHub. Now, anyone can make a full copy of the python-test repo including all the commit history by performing:

```
[student-login]$ git clone git@github.com:wjallen/python-test.git
Cloning into 'python-test'...
remote: Enumerating objects: 15, done.
remote: Counting objects: 100% (15/15), done.
(continues on next page)
```

```
remote: Compressing objects: 100% (10/10), done.
remote: Total 15 (delta 4), reused 15 (delta 4), pack-reused 0
Unpacking objects: 100% (15/15), done.
```

If the repository on GitHub gets ahead of your local repository, i.e. it has some changes in it that someone else pushed from somewhere else, or you pushed from a different machine, then you can try to update your local repository to pull the changes back down.

```
[student-login]$ git remote update # checks to see if there are updates in the remote
[student-login]$ git pull # pulls those updates down to local
```

Warning: If you have changes in local files that conflict with the remote repository (i.e. the repository on GitHub), the git pull will fail and you have found your way into a "merge conflict". Good luck!

1.7.3 Git / Version Control Concepts

Let's take a quick intermission to lean some important definitions (most of these things can easily be managed in the GitHub web interface):

Fork

A fork is a personal copy of another user's repository that lives on your account. Forks allow you to freely make changes to a project without affecting the original. Forks remain attached to the original, allowing you to submit a pull request to the original's author to update with your changes. You can also keep your fork up to date by pulling in updates from the original.

Branch

A branch is a parallel version of a repository. It is contained within the repository, but does not affect the primary or main branch allowing you to work freely without disrupting the "live" version. When you've made the changes you want to make, you can merge your branch back into the main branch to publish your changes. For more information, see About branches.

Tag

Git has the ability to tag specific points in history as being important. Typically people use this functionality to mark release points (v1.0, and so on).

Pull Request / Merge Request

Pull requests are proposed changes to a repository submitted by a user and accepted or rejected by a repository's collaborators. Like issues, pull requests each have their own discussion forum. For more information, see About pull requests.

1.7.4 Collaborating with Others

A public platform like GitHub makes it easier than ever to collaborate with others on the content of a repository. You can have as many local copies of a repository as you want, but there is only one "origin" repository - the repository hosted on GitHub. Other repositories may fall behind the origin, or have changes that are ahead of the origin. A common model for juggling multiple repositories where separate individuals are working on different features is the GitFlow model:

EXERCISE

Let's work on a **branch** plus **pull request** in the GitHub web interface.

- Locate and navigate to your repository
- Click on the branch / tag navigator near the top right and start typing in a new name to create a new branch
- By default, it should switch you to the new branch. Click on one of your files and edit it (e.g. add a comment) directly in the web interface
- Navigate to the "Pull requests" tab and click on "New pull request"
- Make sure to select the original branch "main" as the base, and your new branch as the downstream for comparison
- Review the code changes and make everything is as expected before choosing "Create pull request"
- Now the owner of the repository (you) can accept the pull request, merging the edits into the main branch

What are the differences between a "merge commit", "squash and merge", and "rebase and merge"? The differences are subtle. All will result in the edits getting merged into the main branch. It is mostly a stylistic thing, and the best method depends on whatever the rest of developers agree to use. More info on the differences here.

EXERCISE

Let's next work on a **fork** plus **pull request** in the GitHub web interface.

- Navigate to this repository: https://github.com/wjallen/coe-332-forking-demo
- Click the "Fork" button near the top right and fork it to your own user space
- Now you could either git clone your fork to the class server, put in a new file, then git add => git commit => git push; OR you could click "Add file" in the GitHub web interface and create a new file that way
- Navigate again to the "Pull requests" tab and click to create a "New pull request"
- Make sure the original repo (wjallen) is set as the base and your fork is set as the head
- Create the pull request and provide enough detail for the repository owner (wjallen) to know whether he should accept your pull request or not

Consult the documentation in the base repository (if documentation exists) and look out for general guidance for contributors. If you develop a new feature and it is merged back into the base, you can generally just delete your fork.

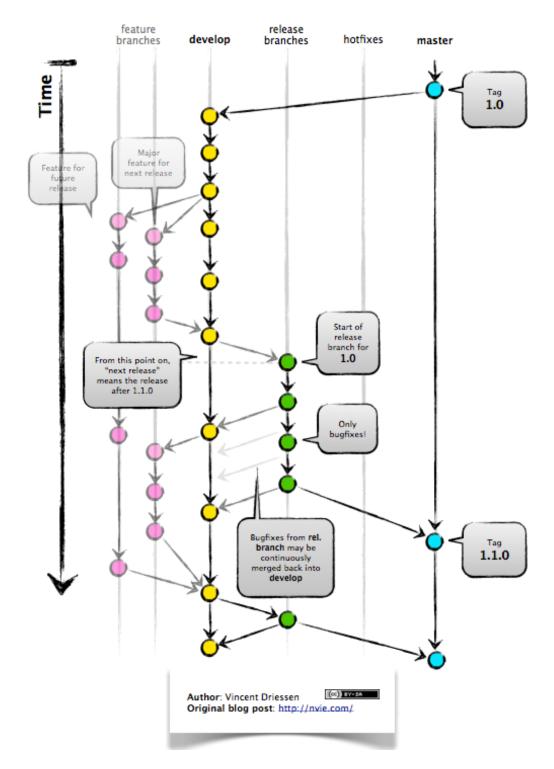


Fig. 10: GitFlow model

1.7.5 Other Considerations

Most repos will also contain a few standard files in the top directory, including:

README.md: The landing page of your repository on GitHub will display the contents of README.md, if it exists. This is a good place to describe your project and list the appropriate citations. *Please note that all of your homeworks, midterm, and final will require READMEs*.

LICENSE.txt: See if your repository needs a license.

.gitignore: Tells Git which files and directories to ignore when you make a commit.

1.7.6 Additional Resources

- Some of the materials in this module were based on Software Carpentry DOI: 10.5281/zenodo.57467.
- · GitHub Glossary
- · About Branches
- About Pull Requests
- About Licenses
- · GitFlow Model
- More on different git workflows

CHAPTER

TWO

UNIT 2: WORKING WITH COMMON DATA FORMATS

Please make sure you meet the following prerequisites before continuing past Unit 1:

- 1. You can log in to the class server, student-login.tacc.utexas.edu
- 2. You have a strong working knowledge of Linux commands
- 3. You have a strong working knowledge of the basic elements of Python3
- 4. You have a strong working knowledge of version control with Git

In Unit 2, we will begin to explore and work hands-on with essential data formats that we will use throughout the course. We will primarily be using Python3 to interact with and manipulate the data. Sample data sets for illustration purposes will be downloaded from various sources, including NASA's open data site.

2.1 Working with JSON

In this hands-on module, we will learn how to work with the JSON data format. JSON (JavaScript Object Notation) is a powerful, flexible, and lightweight data format that we see a lot throughout this course, especially when working with web apps and REST APIs.

After going through this module, students should be able to:

- · Identify and write valid JSON
- · Read JSON into an object in a Python3 script
- · Loop over and work with elements in a JSON object
- Write JSON to file from a Python3 script

2.1.1 JSON Basics

Analogous to Python3 dictionaries, JSON is typically composed of key:value pairs. The universality of this data structure makes it ideal for exchanging information between programs written in different languages and web apps. A simple, valid JSON object may look like this:

```
{
    "key1": "value1",
    "key2": "value2"
}
```

Although less common in this course, simple arrays of information (analogous to Python3 lists) are also valid JSON:

```
[ "thing1", "thing2", "thing3" ]
```

JSON offers a lot of flexibility on the placement of white space and newline characters. Types can also be mixed together, forming complex data structures:

```
"department": "COE",
   "number": 332,
   "name": "Software Engineering and Design",
   "inperson": true,
   "finalgroups": null,
   "instructors": ["Joe", "Charlie", "Joe"],
   "prerequisites": [
        {"course": "COE 322", "instructor": "Victor"},
        {"course": "SDS 322", "instructor": "Victor"}
]
```

On the class server, navigate to your home directory and make a new folder for this module:

```
[local]$ ssh username@student-login.tacc.utexas.edu
(enter password)
(enter token)
[student-login]$ cd coe-332/
[student-login]$ mkdir working-with-json && cd working-with-json
```

Download this sample JSON files into that folder using the wget command, or click this link and cut and paste the contents into a file called Meteorite_Landings.json:

Note: The Meteorite Landing data is adapted from a data set provided by The Meteoritical Society here: https://data.nasa.gov/Space-Science/Meteorite-Landings/gh4g-9sfh

EXERCISE

Plug this file (or some of the above samples) into an online JSON validator (e.g. JSONLint). Try making manual changes to some of the entries to see what breaks the JSON format.

2.1.2 Read JSON into a Python3 Script

The json Python3 library is part of the Python3 Standard Library, meaning it can be imported without having to be installed by pip. Start editing a new Python3 script using your method of choice:

```
[student-login]$ vim json_ex.py
```

Warning: Do not name your Python3 script "json.py". If you import json when there is a script called "json.py" in the same folder, it will import that instead of the actual json library.

The code you need to read in the JSON file of state names and abbreviations into a Python3 object is:

```
import json

with open('Meteorite_Landings.json', 'r') as f:
    ml_data = json.load(f)
```

Only three simple lines! We import json from the standard library so that we can work with the json class. We use the safe with open... statement to open the file we downloaded read-only into a filehandle called f. Finally, we use the load() method of the json class to load the contents of the JSON file into our new ml_data object.

EXERCISE

Try out some of these calls to the type() function on the new ml_data object that you loaded. Also print() each of these as necessary to be sure you know what each is. Be able to explain the output of each call to type() and print().

```
import json
2
   with open('Meteorite_Landings.json', 'r') as f:
       ml_data = json.load(f)
   type(ml_data)
6
   type(ml_data['meteorite_landings'])
   type(ml_data['meteorite_landings'][0])
   type(ml_data['meteorite_landings'][0]['name'])
10
   print(ml_data)
11
   print(ml_data['meteorite_landings'])
12
   print(ml_data['meteorite_landings'][0])
   print(ml_data['meteorite_landings'][0]['name'])
```

Tip: Consider doing this in the Python3 interpreter's interactive mode instead of in a script.

2.1.3 Work with JSON Data

As we have seen, the JSON object we loaded contains meteorite landing data including names, ids, classes, masses, latitudes, and longitudes. Let's write a few functions to help us explore the data.

First, write a function to calculate the average mass of all meteorites in the data set. Call that function, and have it print the average mass to screen.

```
import json

def compute_average_mass(a_list_of_dicts, a_key_string):
    total_mass = 0.
    for i in range(len(a_list_of_dicts)):
        total_mass += float(a_list_of_dicts[i][a_key_string])
    return (total_mass / len(a_list_of_dicts))

with open('Meteorite_Landings.json', 'r') as f:
    ml_data = json.load(f)

print(compute_average_mass(ml_data['meteorite_landings'], 'mass (g)'))
```

Next, write a function to check where on the globe the meteorite landing site is located. We need to check whether it is Northern or Southern hemisphere, and whether it is Western or Eastern hemisphere.

```
import json
2
   def compute_average_mass(a_list_of_dicts, a_key_string):
       total_mass = 0.
       for i in range(len(a_list_of_dicts)):
           total_mass += float(a_list_of_dicts[i][a_key_string])
       return (total_mass / len(a_list_of_dicts))
   def check_hemisphere(latitude: float, longitude: float) -> str:
                                                                          # type hints
       location = ''
10
       if (latitude > 0):
11
           location = 'Northern'
12
       else:
13
           location = 'Southern'
14
       if (longitude > 0):
15
           location = f'{location} & Eastern'
       else:
17
           location = f'{location} & Western'
       return(location)
19
   with open('Meteorite_Landings.json', 'r') as f:
21
       ml_data = json.load(f)
22
23
   print(compute_average_mass(ml_data['meteorite_landings'], 'mass (g)'))
25
   for row in ml_data['meteorite_landings']:
26
       print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
27
```

Note: Type hints in function definitions indicate what types are expected as input and output of a function, but no

checking actually happens at runtime. Think of them as documentation or annotations.

Tip: Check out Python3 ternary operators to make your if/else conditionals shorter, but perhaps a little less intuitive to read.

```
def check_hemisphere(lat, lon):
    location = 'Northern' if (lat > 0) else 'Southern'
    location = f'{location} & Eastern' if (lon > 0) else f'{location} & Western'
    return(location)
```

EXERCISE

Write a third function to count how many of each 'class' of meteorite there is in the list. The output should look something like:

```
type, number
H, 1
H4, 2
L6, 6
...etc
```

2.1.4 Write JSON to File

Finally, in a new script, we will create an object that we can write to a new JSON file.

```
import json

data = {}

data['class'] = 'COE332'

data['title'] = 'Software Engineering and Design'

data['subjects'] = []

data['subjects'].append( {'unit': 1, 'topic': ['linux', 'python3', 'git']} )

data['subjects'].append( {'unit': 2, 'topic': ['json', 'csv', 'xml', 'yaml']} )

with open('class.json', 'w') as out:
    json.dump(data, out, indent=2)
```

Notice that most of the code in the script above was simply assembling a normal Python3 dictionary. The json.dump() method only requires two arguments - the object that should be written to file, and the filehandle. The indent=2 argument is optional, but it makes the output file looks a little nicer and easier to read.

Inspect the output file and paste the contents into an online JSON validator.

EXERCISE

Write a new Python3 script to read in Meteorite_Landings.json, convert the ids, masses, latitudes, and longitudes to floats, then save it as a new JSON file called Meteorite_Landings_updated.json. Compare them side by side to make sure you can see and understand the difference.

2.1.5 Additional Resources

- · Reference for the JSON library
- Validate JSON with JSONLint
- Meteorite Landings Data

2.2 CSV Reference

This reference guide is designed to introduce you to CSV format. CSV (Comma Separated Value) is probably the most intuitive and most human-readable data format we will encounter. Many spreadsheet tools (like Excel) can read and write CSV, and many public data sets we encounter will be stored in CSV. However, there is no data typing, no support for complex data structures, and it lacks in versatility.

2.2.1 CSV Basics

CSV is usually used for simple, tabular data and generally cannot be used to represent some of the more complex data structures we will be exposed to in this class. However, CSV is a very common data format, and you will often encounter tabular CSV data that you want to transform into a list of dictionaries.

For example, consider the following valid CSV file with one header line followed by three record lines:

```
firstname,lastname,ID
joe,allen,123
charlie,day,456
joe,stubbs,789
```

The same CSV file could be represented by a **list of dictionaries** where the headers are used as the keys, and the records are used as the values:

```
]
]
```

As a slight modification of the above, you will often see that list of dictionaries stored as a **value** and assigned to a **key** with a descriptive name. We will see this exact type of data structure many times this semester:

```
"instructors": [
  {
    "firstname": "joe",
    "lastname": "allen",
    "id": 123
  },
  {
    "firstname": "charlie",
    "lastname": "dey",
    "id": 456
  },
    "firstname": "joe",
    "lastname": "stubbs",
    "id": 789
  }
]
```

The latest specification for CSV provides the following guidelines that "seem to be followed by most implementations" of CSV:

- 1. Each record is located on a separate line with a line break
- 2. The last record in the file may or may not have a line break
- 3. There maybe an optional header line appearing as the first line of the file with the same format as normal record lines
- 4. Within the header and each record, there may be one or more fields, separated by commas. Each line should contain the same number of fields throughout the file
- 5. Each field may or may not be enclosed in double quotes
- 6. Fields containing line breaks, double quotes, and commas should be enclosed in double-quotes
- 7. If double-quotes are used to enclose fields, then a double-quote appearing inside a field must be escaped by preceding it with another double quote

Source: https://datatracker.ietf.org/doc/html/rfc4180

Keep an eye out for similar formats, too. For example .tsv files generally are the exact same thing as .csv files except tab-delimited rather than comma-delimited.

Note: Check out the list of meteorite landing sites we worked with in the JSON section, but now in CSV format here.

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2.2.2 Read CSV from File

Imagine you have a CSV file with headers, e.g.:

```
name,id,recclass,mass (g),reclat,reclong,GeoLocation
Ruiz,10001,L5,21,50.775,6.08333,"(50.775, 6.08333)"
Beeler,10002,H6,720,56.18333,10.23333,"(56.18333, 10.23333)"
Brock,10003,EH4,107000,54.21667,-113,"(54.21667, -113.0)"
Hillebrand,10004,Acapulcoite,1914,16.88333,-99.9,"(16.88333, -99.9)"
Mitchell,10005,L6,780,-33.16667,-64.95,"(-33.16667, -64.95)"
... etc
```

To read it into a dictionary object, use the csv module that is part of the Python3 standard library:

```
import csv

data = {}
data['meteorite_landings'] = []

with open('Meteorite_Landings.csv', 'r') as f:
    reader = csv.DictReader(f)
    for row in reader:
        data['meteorite_landings'].append(dict(row))
```

In the above case, each row of the CSV file is iterated one by one. The keys from the header line are assigned values from the subsequent lines, then they are appended to a list of dictionaries in the data data structure.

2.2.3 Write CSV to File

Given the same data structure as in the previous example (a list of dictionaries where each dictionary has identical keys), to write that object to a CSV file, use the following:

```
import csv
import json

data = {}

with open('Meteorite_Landings.json', 'r') as f:
    data = json.load(f)

with open('Meteorite_Landings.csv', 'w') as o:
    csv_dict_writer = csv.DictWriter(o, data['meteorite_landings'][0].keys())
    csv_dict_writer.writeheader()
    csv_dict_writer.writerows(data['meteorite_landings'])
```

2.2.4 Additional Resources

- CSV Basics
- · CSV Module in the Python Standard Library

2.3 XML Reference

This reference guide is designed to introduce you to XML syntax. XML (Extensible Markup Language) was designed as a way to store, transmit, and reconstruct arbitrary data sets, particularly over the internet. You'll sometimes see it as standalone documents, or as streaming data without a definite endpoint. For this class, we will focus on the standalone documents / datasets.

2.3.1 XML Basics

Much like JSON, XML can be used to store arbitrary data sets in a dictionary-esque format of key:value pairs. However, there are a few key differences between XML and JSON:

- 1. XML is typeless, essentially everything is a string
- 2. XML documents support comments
- 3. XML documents require exactly one "root" element, so the data structure of a **dictionary with one key, whose value is a list of dictionaries** needs a slight modification in order to be valid JSON (as we will see below)

A valid XML document takes the form:

Keys always come as a pair of start-tag (<key1>) and end-tag (</key1>) markups surrounding a plain text value (value1). In the above example, the root-level key data was required to make this valid XML. Without it, the keys key1 and key2 would be at the same root level, which is invalid. The same data shown above in JSON format would appear as:

```
{
  "data": {
    "key1": "value1",
    "key2": "value2"
  }
}
```

Things get a little tricky with our favorite data structure, a **dictionary with one key, whose value is a list of dictionaries**. This is because of the way XML represents lists of dictionaries. Consider the following snippet of JSON data:

```
{
    "instructors": [
        {
            "firstname": "joe",
            "lastname": "allen",
            "id": 123
        },
        (continues on next page)
```

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```
{
    "firstname": "charlie",
    "lastname": "dey",
    "id": 456
},
    {
       "firstname": "joe",
       "lastname": "stubbs",
       "id": 789
    }
}
```

If we try to translate this directly to XML, it would take the form:

The instructors key appears multiple times at the root level, once for each element in the list. In XML, you cannot have multiple roots, even if it is the same root repeated more than once. You need exactly one root only. A simple trick to fix this is to create a new dictionary with one key, e.g. "data", whose value is the other dictionary. Doing so would slightly change the XML to a valid format:

```
<data>
    <instructors>
            <firstname>joe</firstname>
            <lastname>allen</lastname>
            <id>123</id>
    </instructors>
    <instructors>
            <firstname>charlie</firstname>
            <lastname>dey</lastname>
            <id>456</id>
    </instructors>
    <instructors>
            <firstname>joe</firstname>
            <lastname>stubbs
            <id>789</id>
    </instructors>
</data>
```

Note: Check out the list of meteorite landing sites we worked with in the JSON section, but now in XML format here.

2.3.2 Read XML from File

Here we will focus on the "document object model" for parsing XML, which means we will read in one XML document and parse the entire thing as a whole. (This works for reasonably small files that can fit in memory).

Note that the Python3 standard library has an XML module, but it does not have a method for transforming XML objects to dictionaries. Since most of what we do in this class uses JSON and dictionaries, let's instead use the xmltodict Python module which works directly in dictionary space.

```
Warning: Install the xmltodict library before proceeding:

[student-login] pip3 install --user xmltodict
```

You can read in an XML file (e.g. the Meteorite Landings data linked above) and store it as a dictionary as follows:

```
import xmltodict
with open('Meteorite_Landings.xml', 'r') as f:
    data = xmltodict.parse(f.read())
```

Then to access the data within that dictionary, remember to include an extra key for the root-level, which we added in to make valid XML. For example, you could call out the first meteorite in the list with the following:

```
print(data['data']['meteorite_landings'][0])
```

Note: The original Meteorite Landings data had the key mass (g). The open and close parentheses () are invalid characters when it comes to XML tags. The data linked above was modified to use the key mass_g instead. Don't be surprised when working with datasets if you have to make manual modifications to the data in order to make it valid in a particular format.

2.3.3 Write XML to File

As mentioned above, a dictionary must have exactly one "root" element in order to write valid XML. The following example below assembles a dictionary with multiple keys at the root level ("class", "title", "subjects"). In fact the following code will yield an error:

```
import xmltodict

data = {}

data['class'] = 'COE332'

data['title'] = 'Software Engineering and Design'

data['subjects'] = []

data['subjects'].append( {'unit': 1, 'topic': ['linux', 'python3', 'git']} )

data['subjects'].append( {'unit': 2, 'topic': ['json', 'csv', 'xml', 'yaml']} )

(continues on next page)
```

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```
with open('class.xml', 'w') as o:
    o.write(xmltodict.unparse(data, pretty=True))
```

Error:

```
ValueError: Document must have exactly one root.
```

To get this to work, you need to modify the above script to create a new dictionary, e.g. "root", with exactly one key, e.g. "data", whose value is the entire data dictionary:

Output:

```
<data>
     <class>COE332</class>
     <title>Software Engineering and Design</title>
     <subjects>
             <unit>1</unit>
             <topic>linux</topic>
             <topic>python3</topic>
             <topic>git</topic>
     </subjects>
     <subjects>
             <unit>2</unit>
             <topic>json</topic>
             <topic>csv</topic>
             <topic>xml</topic>
             <topic>yaml</topic>
     </subjects>
</data>
```

2.3.4 Additional Resources

- The xmltodict Library
- XML Linter

2.4 YAML Reference

This reference guide is designed to introduce you to YAML syntax. YAML (YAML Ain't Markup Language) is basically JSON with a couple extra features, and meant to be a little more human readable. We will be using YAML formatted configuration files in the Docker compose and Kubernetes sections, so it is important to become familiar with the syntax.

2.4.1 YAML Basics

YAML syntax is similar to Python dictionaries, and we will usually see them as key:value pairs. Values can include strings, numbers, booleans, null, lists, and other dictionaries.

Previously, we saw a simple JSON object in dictionary form like:

```
{
    "key1": "value1",
    "key2": "value2"
}
```

That same object in YAML looks like:

```
key1: value1
key2: value2
```

Notice that YAML documents all start with three hyphens on the top line (---), and end with an optional three dots (...) on the last line. Key:value pairs are separated by colons, but consecutive key:value pairs are NOT separated by commas.

We also mentioned that JSON supports list-like structures. YAML does too. So the following valid JSON block:

```
[ "thing1", "thing2", "thing3" ]
```

Appears like this in YAML:

```
---
- thing1
- thing2
- thing3
```

Elements of the same list all appear with a hyphen - at the same indent level.

We previously saw this complex data structure in JSON:

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```
"department": "COE",
   "number": 332,
   "name": "Software Engineering and Design",
   "inperson": true,
   "finalgroups": null,
   "instructors": ["Joe", "Charlie", "Joe"],
   "prerequisites": [
        {"course": "COE 322", "instructor": "Victor"},
        {"course": "SDS 322", "instructor": "Victor"}
]
```

The same structure in YAML is:

The whole thing can be considered a dictionary. The key instructors contains a value that is a list of names, and the key prerequisites contains a value that is a list of dictionaries. Booleans appear as false and true (lowercase only). Null / empty values appear as null or ~. And, as you can see above, YAML also supports comments starting with a #.

One glaring thing that is missing from the YAML file is quotation marks. In general, you don't have to use quotes in YAML. You may use quotes to force a number to be interpreted as a string (e.g. 10 will automatically be interpreted as an integer, but "10" will be interpreted as a string).

Note: Check out the list of meteorite landing sites we worked with in the JSON section, but now in YAML format here.

There is a lot more to YAML, most of which we will not use in this course. Just know that YAML files can contain:

- Comments
- Multi-line strings / text blocks
- · Multi-word keys
- · Complex objects
- · Special characters

- Explicitly declared types
- A mechanism to duplicate / inherit values across a document ("anchors")

If we encounter a need for any of these, we can refer to the official YAML syntax

2.4.2 Read YAML from File

```
Warning: There is no YAML interpreter in the Python 3.6 standard libary, so we need to install one with pip3:

[student-login]$ pip3 install --user pyyaml
```

Given the meteorite landing site data in YAML format, which you can download from this link, load it into a Python3 dictionary object using the following:

```
import yaml

data = {}

with open('Meteorite_Landings.yaml', 'r') as f:
    data = yaml.load(f, Loader=yaml.SafeLoader)
```

Very similar to the JSON module, it only requires a few simple lines then you have a dictionary object to work with. The Loader=yaml.SafeLoader parameter makes it so no arbitrary Python code is executed when loading in the data - this is typically a good choice for data from untrusted sources.

2.4.3 Write YAML to File

In a new script create a dictionary object that we can write to a new YAML file.

```
import yaml

data = {}

data['class'] = 'COE332'

data['title'] = 'Software Engineering and Design'

data['subjects'] = []

data['subjects'].append( {'unit': 1, 'topic': ['linux', 'python3', 'git']} )

data['subjects'].append( {'unit': 2, 'topic': ['json', 'csv', 'xml', 'yaml']} )

with open('class.json', 'w') as o:
 yaml.dump(data, o)
```

Notice that most of the code in the script above was simply assembling a normal Python3 dictionary. The json.dump() method only requires two arguments - the object that should be written to file, and the filehandle.

Inspect the output file and paste the contents into an online YAML validator.

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2.4.4 Additional Resources

- YAML Spec
- YAML Validator
- JSON / YAML Converter
- PyYAML Docs

UNIT 3: BEST PRACTICES IN PYTHON

In this unit, we will work on improving our Python3 code-writing habits to make our code easier to read, easier to debug, and easier to test. A little extra effort towards writing good code now will pay off down the line when it comes to developing and testing new features or re-using old code blocks in new applications. Specifically, we will learn and practice topics in code organization, documentation, logging, unit testing, and exception handling.

3.1 Code Organization

Following standard Python3 code organization practices will make our code easier to read by other developers, and by our future selves who are looking back to see what we did. After going through this module, students should be able to:

- Organize code into main() functions
- Import functions into other scripts without executing the main() block
- Write functions in a generalizable way so they are reusable
- Use a shebang in their Python3 scripts to make them executable

3.1.1 Main Function

In many Python programs, you will find the developer has organized their code into a main() function. Then, they will only call the main() function if the variable __name__ is equal to the string '__main__'. For example:

```
def main():
    # the meat of the main function goes here

if __name__ == '__main__':
    main()
```

If this script is executed on the command line directly, then the internal variable __name__ will be set to the string '__main__'. The conditional evaluates as True and the main() function is called.

If this script is instead **imported into another script**, say, to reuse some of the functions defined within, then the internal variable __name__ will instead be set to the name of the script. Thus, the main() function is not called, but other functions defined in this script would be available.

Consider the script we wrote in the previous unit for analyzing the Meteorite Landings JSON file (called ml_data_analysis.py):

```
import json
   def compute_average_mass(a_list_of_dicts, a_key_string):
       total_mass = 0.
       for item in a_list_of_dicts:
           total_mass += float(item[a_key_string])
       return(total_mass / len(a_list_of_dicts) )
   def check_hemisphere(latitude, longitude):
       location = 'Northern' if (latitude > 0) else 'Southern'
10
       location = f'{location} & Eastern' if (longitude > 0) else f'{location} & Western'
       return(location)
12
   with open('Meteorite_Landings.json', 'r') as f:
14
       ml_data = json.load(f)
16
   print(compute_average_mass(ml_data['meteorite_landings'] ,'mass (g)' ))
18
   for row in ml_data['meteorite_landings']:
19
       print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
20
```

To reorganize this code, we would put the file read operation and the two function calls into a main function:

```
import json
2
   def compute_average_mass(a_list_of_dicts, a_key_string):
       total_mass = 0.
4
       for item in a_list_of_dicts:
           total_mass += float(item[a_key_string])
6
       return(total_mass / len(a_list_of_dicts) )
   def check_hemisphere(latitude, longitude):
       location = 'Northern' if (latitude > 0) else 'Southern'
10
       location = f'{location} & Eastern' if (longitude > 0) else f'{location} & Western'
11
       return(location)
12
13
                          # notice the below lines are now indented
   def main():
14
       with open('Meteorite_Landings.json', 'r') as f:
15
           ml_data = json.load(f)
17
       print(compute_average_mass(ml_data['meteorite_landings'] , 'mass (g)' ))
19
       for row in ml_data['meteorite_landings']:
           print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
21
   if __name__ == '__main__':
23
       main()
24
```

If this code is imported into another Python3 script, that other script will have access to the compute_average_mass() and check_hemisphere() functions, but it will not execute the code in the main() function.

EXERCISE

Write a new script to import the above code, assuming that above code is saved in a file called ml_data_analysis.py:

Try executing this new script with and without protecting the imported code in a main() function. How do the outputs differ?

Tip: The main function does not have to be called literally main(). But, if someone else is reading your code, calling it main() will certainly help orient the reader.

3.1.2 Generalizing Functions

A good habit to get into while writing functions is to write them in a *generalizable* way. This means writing them in such a way that they can be used for multiple purposes or in multiple applications. The trick is to try to think ahead about how else you might use the function, think about what form the input data takes, and try not to hardcode indices or variable names.

compute_average_mass

In our compute_average_mass function, we knew we needed to send it *something*, and we knew it needed to return an average mass. The main question was what form should the input take?

```
def compute_average_mass( xyz ):
    # do some computation
    return(average_mass)
```

We could have just sent the function the entire dictionary data structure, then have it parse the data to get masses out. But if we did that, we would also need to hardcode the name of the main key 'meteorite_landings' as well as the name of the key referring to the masses 'mass (g)'.

```
# BAD
def compute_average_mass( a_dictionary ):
    total_mass = 0.
    for item in a_dictionary['meteorite_landings']:
        total_mass += float(item['mass (g)'])
    return(total_mass / len(a_dictionary['meteorite_landings']) )

print(compute_average_mass(ml_data))
```

Since we will be working with lists of dictionaries most frequently in this class, it makes more sense to send it a list of dictionaries data structure and the name of the key to extract.

```
# GOOD
def compute_average_mass(a_list_of_dicts, a_key_string):
    total_mass = 0.
    (continues on next page)
```

```
for item in a_list_of_dicts:
    total_mass += float(item[a_key_string])
    return(total_mass / len(a_list_of_dicts) )

print(compute_average_mass(ml_data['meteorite_landings'] ,'mass (g)' ))
```

check_hemisphere

The check_hemisphere function is very similar - we send it something and it returns (or prints) a string.

```
def check_hemisphere( xyz )
    # run through some conditionals
    return(location)
```

Here we could have also sent a list of dictionaries along with the names of two keys representing the latitude and longitude. That would have been ok, and would have worked for most of the data structures we use in this class.

However, to make it even more generalizable, we could abstract one layer further and just send it two floats: latitude and longitude. That would make the function useful for our list of dictionaries data structure, and for one-off checks given just a pair of floats:

```
# BETTER
def check_hemisphere(latitude, longitude):
    location = 'Northern' if (latitude > 0) else 'Southern'
    location = f'{location} & Eastern' if (longitude > 0) else f'{location} & Western'
    return(location)

for row in ml_data['meteorite_landings']:
    print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
```

EXERCISE

Write a new function to count how many of each 'class' of meteorite there is in the list. The output should look something like:

```
type, number
H, 1
H4, 2
L6, 6
...etc
```

Consider carefully what inputs you are sending to the function. How can you write it in a generalizable way?

3.1.3 Shebang

A "shebang" is a line at the top of your script that defines what interpreter should be used to run the script when treated as a standalone executable. You will often see these used in Python, Perl, Bash, C shell, and a number of other scripting languages. In our case, we want to use the following shebang, which should appear on the first line of our Python3 scripts:

```
#!/usr/bin/env python3
```

The env command simply figures out which version of python3 appears first in your path, and uses that to execute the script. We usually use that form instead of, e.g., #!/usr/bin/python3.8 because the location of the Python3 executable may differ from machine to machine, whereas the location of env will not.

Next, you also need to make the script executable using the Linux command chmod:

```
[student-login]$ chmod u+x ml_data_analysis.py
```

That enables you to call the Python3 code within as a standalone executable without invoking the interpreter on the command line:

```
[student-login]$ ./ml_data_analysis.py
```

This is helpful to lock in a Python version (e.g. Python3) for a script that may be executed on multiple different machines or in various environments.

3.1.4 Other Tips

As our Python3 scripts become longer and more complex, we should put more thought into how the different contents of the script are ordered. As a rule of thumb, try to organize the different sections of your Python3 code into this order:

```
# Shebang
# Imports
# Global variables / constants
# Class definitions
# Function definitions
# Main function definition
# Call to main function
```

Other general tips for writing code that is easy to read can be found in the PEP 8 Style Guide, including:

- Use four spaces per indentation level (no tabs)
- Limit lines to 80 characters, wrap and indent where needed
- Avoid extraneous whitespace unless it improves readability
- · Be consistent with naming variables and functions

- Classes are usually CapitalWords
- Constants are usually ALL_CAPS
- Functions and variables are usually lowercase_with_underscores
- Consistency is the key
- Use functions to improve organization and reduce redundancy
- · Document and comment your code

Note: Beyond individual Python3 scripts, there is a lot more to learn about organizing *projects* which may consist of many files. We will get into this later in the semester.

3.1.5 Additional Resources

• PEP 8 Style Guide

3.2 Documentation

As we have probably all heard before, good documentation is almost as important (if not equally as important) as good code itself. You may have written some elegant and powerful code to solve your problems today, but weeks or months from now, that code may become functionally useless if you forget what it does or how to call it. Python3 users have a special built-in tool at their disposal called *docstrings* that make documenting functions easy. After going through this module, students should be able to:

- Write well-crafted docstrings for all functions
- Add type hints to function definitions
- Write effective READMEs for a project

3.2.1 Docstrings

Docstrings are special strings that appear immediately following function definitions in our code. They should be surrounded by three double-quotation marks on each side, and they may span multiple lines. For example:

```
def a_function():
    """
    This is a docstring.
    """
    # code goes here
    return
```

The above is a valid docstring, but it is not a very helpful docstring. When you write docstrings, at a minimum try to include the following sections:

- 1. A short description of the purpose of the function
- 2. A list of arguments, including type
- 3. A list of returned values, including type

A better template for a docstring (based on the Google Style Guide) might look like:

```
def a_function(arg1, arg2):
    """
    This function does XYZ.

Args:
    arg1 (type): Define what is expected for arg1.
    arg2 (type): Define what is expected for arg2.

Returns:
    result (type): Define what is expected for result.
    """
# code goes here
return(result)
```

The description should be succinct, yet complete. Arguments should be listed by name and the expected type (e.g., bool, float, str, etc) should be stated. And the return result(s) should be listed along with the expected type(s).

Let's look at one more example using a real function:

```
def add_and_square(num1, num2):
    """
    Given two numbers, this function will first add them together, then square the sum
    and return the result.

Args:
    num1 (float): The first number.
    num2 (float): The second number.

Returns:
    result (float): The square of the sum of input arguments.

"""
result = (num1+num2)**2
    return(result)
```

Note: Notice above we are using more-or-less complete sentences with proper grammar.

Next, let's add docstrings to our ml_data_analysis.py code we have been working on:

```
#!/usr/bin/env python3
   import json
   def compute_average_mass(a_list_of_dicts, a_key_string):
5
       Iterates through a list of dictionaries, pulling out values associated with
6
       a given key. Returns the average of those values.
       Args:
           a_list_of_dicts (list): A list of dictionaries, each dict should have the
10
                                    same set of keys.
11
           a_key_string (string): A key that appears in each dictionary associated
12
                                   with the desired value (will enforce float type).
13
14
```

(continues on next page)

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```
Returns:
15
           result (float): Average value.
17
       total_mass = 0.
       for item in a_list_of_dicts:
19
            total_mass += float(item[a_key_string])
20
       return(total_mass / len(a_list_of_dicts) )
21
22
   def check_hemisphere(latitude, longitude):
23
24
       Given latitude and longitude in decimal notation, returns which hemispheres
25
       those coordinates land in.
26
       Args:
28
            latitude (float): Latitude in decimal notation.
            longitude (float): Longitude in decimal notation.
30
31
       Returns:
32
           location (string): Short string listing two hemispheres.
33
34
       location = 'Northern' if (latitude > 0) else 'Southern'
35
       location = f'{location} & Eastern' if (longitude > 0) else f'{location} & Western'
36
       return(location)
37
38
   def count_classes(a_list_of_dicts, a_key_string):
39
40
       ???
41
42
       classes_observed = {}
43
       for item in a_list_of_dicts:
44
            if item[a_key_string] in classes_observed:
45
                classes_observed[item[a_key_string]] += 1
            else:
47
                classes_observed[item[a_key_string]] = 1
       return(classes_observed)
49
   def main():
51
       with open('Meteorite_Landings.json', 'r') as f:
52
           ml_data = json.load(f)
53
       print(compute_average_mass(ml_data['meteorite_landings'], 'mass (g)'))
55
56
       for row in ml_data['meteorite_landings']:
57
            print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
58
59
       print(count_classes(ml_data['meteorite_landings'], 'recclass'))
60
      __name__ == '__main__':
   if
62
       main()
```

In general, your main() function usually does not need a docstring. It is good habit to write the main() function simply and clearly enough that it is self explanatory, with perhaps a few comments to help. If you do add a docstring to the main() function, you may write a few short summary sentences but omit the Args and Returns sections.

EXERCISE

Write the missing docstring for the count_classes() function above.

EXERCISE

Open up the Python3 interactive interpreter. Import your ml_data_analysis.py methods. Use the commands dir() and help() to find and read the docstrings that you wrote.

3.2.2 Type Hints

Type hints in function definitions indicate what types are expected as input and output of a function. No checking actually happens at runtime, so if you send the wrong type of data as an argument, the type hint itself won't cause it to return an error. Think of type hints simply as documentation or annotations to help the reader understand how to use a function.

Warning: In the code blocks below, we omit docstrings for brevity only. Please keep including docstrings in your code.

Type hints should take form:

```
def a_function(arg_name: arg_type) -> return_type:
    # code goes here
    return(result)
```

In the above example, we are providing a single argument called arg_name that should be of type arg_type. The expected return value should be return_type. Let's look at an example using a real function:

```
def add_and_square(num1: float, num2: float) -> float:
   result = (num1+num2)**2
   return(result)
```

Next, add type hints to the function definitions of the ml_data_analysis.py script (only showing snippets below):

```
from typing import List
def compute_average_mass(a_list_of_dicts: List[dict], a_key_string: str) -> float:
```

```
def check_hemisphere(latitude: float, longitude: float) -> str:
```

```
def count_classes(a_list_of_dicts, a_key_string): # what about this one?
```

In the first example above we need to include the line from typing import List to get access to a special object called List (capital L). We use that to object to not only hint that a_list_of_dicts should be a list, but it also includes information about what type of list we expect - in this case it is a list of dictionaries. In Python3.8 you cannot do this with the normal list (lowercase l) object.

Although Python3 does not check or enforce types at run time, there are other tools that make use of type hints to check types at the time of development. For example, some IDEs (including PyCharm) will evaluate type hints as you write code and provide an alert if you call a function in a way other than what the type hint suggests. In addition, there are Python3 libraries like *mypy* that can wrap your Python3 programs and check / evaluate type hints as you go, provided errors where types don't match.

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Warning: Be aware that there is some redundancy in the information contained in type hints and in the docstrings. Be careful not to let them get out of sync as your code evolves.

3.2.3 README

A README file should be included at the top level of every coding project you work on. Websites like GitHub will automatically look for README files and render them directly in the web interface. Markdown is probably the most common syntax people use to write READMEs. It is very easy to create headers, code blocks, tables, text emphases, and other fancy renderings to make the README pleasant and easy to read.

Note: In this class we ask you to include READMEs in each of your homework folders on GitHub. Each homework is essentially a standalone project, so a dedicated README for each is warranted.

At a minimum, plan to include the following sections in all of your READMEs:

- Title: a descriptive, self-explanatory title for the project.
- Description: a high-level description of the project that informs the reader what the code does, why it exists, what problem it solves, etc.
- Installation: As we advance into the semester our code bases will become more complex with more moving
 parts. Eventually we will need to start providing detailed instructions about getting the project working plus any
 requirements.
- Usage: The key here is **examples**! Show code blocks of what it looks like to execute the code from start to finish. Describe what output is expected and how it should be interpreted.

Other general advice includes:

- Use proper grammar and more-or-less complete sentences.
- Use headers, code blocks, and text emphases (e.g. bold, italics) to make the document readable. There are plenty
 of tools to preview Markdown before committing to GitHub, so plan to go through several cycles of editing ->
 previewing to make your README look nice.
- Be prepared to include other information about authors, acknowledgements, and licenses in the READMEs as appropriate
- Spend some time browsing GitHub and look for READMEs of other popular projects. There are many correct ways to write a README.

Remember, the README is your chance to document for yourself and explain to others why the project is important, what the code is, and how to use it / interpret the outputs. The advice above is general advice, but it is not one-size-fits-all. Every project is different and ultimately your README may include other sections or organization schemes that are unique to your project.

3.2.4 Additional Resources

- Google Style Guide for docstrings
- Type hints spec
- · Mypy project
- · Markdown syntax
- Tips on writing a good README

3.3 Logging

As your Python3 applications grow in complexity, so too does your need to be able to track what is going on in the code during run time. *Logging* can be used to track arbitrary events as the code runs. As we will see, logging will be useful to keep track of the progression of your code, and it will also be useful to help us track what parts of our code are causing errors. This is especially useful when working with multiple applications across distributed systems. After going through this module, students should be able to:

- Import the logging module into their Python3 scripts
- Set log level to either DEBUG, INFO, WARNING, ERROR, or CRITICAL
- Write appropriate log messages for each log level
- Read output logs and track warnings / errors back to specific spots in their code

3.3.1 Log Levels

Many of us have probably used arbitrary print statements in our code as a means to debug errors. Yes, there is a better way! The Python3 logging module, part of the Standard Library, provides functions for reporting different types of events that occur during run time. Save print statements for printing out the normal things that the code is supposed to display, and use exceptions to interrupt the code when it encounters errors. Use logging for everything else, including:

- Printing detailed information about normal things that are supposed to occur, but should not be in the standard output
- Printing warnings about particular run time events
- Printing when an error has occurred but was suppressed by, e.g., an error handler.

Log levels are used to distinguish between the severity or importance of the different events. Using different log levels, you can always leave the log statements which print useful information in your code, but toggle them on and off depending on which level of severity you want to monitor. The standard log levels and their purposes are:

- DEBUG: Detailed information, typically of interest only when diagnosing problems
- INFO: Confirmation that things are working as expected.
- WARNING: An indication that something unexpected happened, or indicative of some problem in the near future (e.g. 'disk space low'). The software is still working as expected.
- ERROR: Due to a more serious problem, the software has not been able to perform some function.
- CRITICAL: A serious error, indicating that the program itself may be unable to continue running.

(Source: Python Docs https://docs.python.org/3/howto/logging.html)

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3.3.2 Initialize Logging

Let's work through an example. Add the following lines to a script called, e.g. log_test.py:

```
import logging
logging.basicConfig() # configs the logging instance

logging.debug('This is a DEBUG message')
logging.info('This is an INFO message')
logging.warning('This is a WARNING message')
logging.error('This is an ERROR message')
logging.critical('This is a CRITICAL message')
```

Executing that code will output the following messages:

```
[student-login]$ python3 log_test.py
WARNING:root:This is a WARNING message
ERROR:root:This is an ERROR message
CRITICAL:root:This is a CRITICAL message
```

By default, the log level is set to WARNING, and only messages that are WARNING or higher in level of severity will be printed to screen.

If you set a lower log level, e.g. to DEBUG, all levels of log messages will be printed:

```
import logging
logging.basicConfig(level='DEBUG')

logging.debug('This is a DEBUG message')
logging.info('This is an INFO message')
logging.warning('This is a WARNING message')
logging.error('This is an ERROR message')
logging.critical('This is a CRITICAL message')
```

```
[student-login]$ python3 log_test.py
DEBUG:root:This is a DEBUG message
INFO:root:This is an INFO message
WARNING:root:This is a WARNING message
ERROR:root:This is an ERROR message
CRITICAL:root:This is a CRITICAL message
```

An even better set up would be to enable the option to pass the desired log level on the command line when you execute the code. E.g.:

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```
logging.debug('This is a DEBUG message')
logging.info('This is an INFO message')
logging.warning('This is a WARNING message')
logging.error('This is an ERROR message')
logging.critical('This is a CRITICAL message')
```

Tip: Try running the above code with and without the -1 flag on the command line.

3.3.3 What to Include in a Log

As we work toward systems in which we are running multiple applications distributed over remote systems, it is important to be mindful of what sort of log information will be useful. In particular, it would be a good idea to be able to gather information about:

- Timestamp: when the error occurred, also acts as a good reference point when referring to a specific log message
- Hostname: what (virtual) machine the error occurred on, as you may have multiple instances of an application running on different machines
- Locale: what script and/or what function did the message originate from, helps to pinpoint where the message is coming from

To include some of this information in a log message, we need to specify a little more information in the basic config. We also need to import the **socket** module from the Standard Library so we can grab information about the hostname from the environment. We also will be calling a few other of the logging formatter's pre-defined macros.

```
import argparse
   import logging
   import socket
   parser = argparse.ArgumentParser()
   parser.add_argument('-1', '--loglevel', type=str, required=False, default='WARNING',
                       help='set log level to DEBUG, INFO, WARNING, ERROR, or CRITICAL')
   args = parser.parse_args()
   format_str=f'[%(asctime)s {socket.gethostname()}] %(filename)s:%(funcName)s:%(lineno)s -
   →%(levelname)s: %(message)s'
   logging.basicConfig(level=args.loglevel, format=format_str)
11
12
   logging.debug('This is a DEBUG message')
13
   logging.info('This is an INFO message')
14
   logging.warning('This is a WARNING message')
15
   logging.error('This is an ERROR message')
   logging.critical('This is a CRITICAL message')
```

```
[student-login]$ python3 log_test.py
[2024-01-27 21:13:36,258 student-login] log_test.py:<module>:15 - WARNING: This is a..

→WARNING message
[2024-01-27 21:13:36,258 student-login] log_test.py:<module>:16 - ERROR: This is an..

→ERROR message
[2024-01-27 21:13:36,258 student-login] log_test.py:<module>:17 - CRITICAL: This is a..

(continues on next page)
```

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```
□ CRITICAL message

[student-login]$ python3 log_test.py -l CRITICAL

[2024-01-27 21:13:40,265 student-login] log_test.py:<module>:17 - CRITICAL: This is a □ □ CRITICAL message
```

Later in the semester, most of the work we will do will be containerized. It is a little difficult to retrieve log *files* from inside containers, especially if they crash with an error. An easy work around is to use logging to print to standard out (as above), and those messages will end up in the container logs from which they are easily extracted.

EXERCISE

Given the Meteorite Landings analysis script we have been working on, add some logging throughout the script, focusing on DEBUG and ERROR messages.

```
#!/usr/bin/env python3
   import json
2
   from typing import List
   def compute_average_mass(a_list_of_dicts: List[dict], a_key_string: str) -> float:
6
       Iterates through a list of dictionaries, pulling out values associated with
       a given key. Returns the average of those values.
       Args:
10
           a_list_of_dicts (list): A list of dictionaries, each dict should have the
11
                                     same set of kevs.
12
            a_key_string (string): A key that appears in each dictionary associated
13
                                    with the desired value (will enforce float type).
14
15
       Returns:
16
           result (float): Average value.
17
18
       total\_mass = 0.
19
       for item in a_list_of_dicts:
20
           total_mass += float(item[a_key_string])
21
       return(total_mass / len(a_list_of_dicts) )
22
23
   def check_hemisphere(latitude: float, longitude: float) -> float:
24
25
       Given latitude and longitude in decimal notation, returns which hemispheres
26
       those coordinates land in.
27
       Aras:
29
           latitude (float): Latitude in decimal notation.
           longitude (float): Longitude in decimal notation.
31
32
       Returns:
33
           location (string): Short string listing two hemispheres.
34
35
       location = 'Northern' if (latitude > 0) else 'Southern'
36
```

(continues on next page)

```
location = f'{location} & Eastern' if (longitude > 0) else f'{location} & Western'
37
       return(location)
39
   def count_classes(a_list_of_dicts: List[dict], a_key_string: str) -> dict:
41
       Iterates through a list of dictionaries, and pulls out the value associated
       with a given key. Counts the number of times each value occurs in the list of
43
       dictionaries and returns the result.
44
45
       Args:
46
           a_list_of_dicts (list): A list of dictionaries, each dict should have the
47
                                     same set of keys.
48
           a_key_string (string): A key that appears in each dictionary associated
                                    with the desired value.
50
51
       Returns:
52
           classes_observed (dict): Dictionary of class counts.
53
54
       classes_observed = {}
55
       for item in a_list_of_dicts:
56
           if item[a_key_string] in classes_observed:
                classes_observed[item[a_key_string]] += 1
58
                classes_observed[item[a_key_string]] = 1
       return(classes_observed)
61
62
   def main():
63
       with open('Meteorite_Landings.json', 'r') as f:
64
           ml_data = json.load(f)
65
       print(compute_average_mass(ml_data['meteorite_landings'], 'mass (g)'))
67
       for row in ml_data['meteorite_landings']:
69
           print(check_hemisphere(float(row['reclat']), float(row['reclong'])))
       print(count_classes(ml_data['meteorite_landings'], 'recclass'))
72
73
   if __name__ == '__main__':
       main()
75
```

3.3.4 Additional Resources

• Python3 Logging How To Guide

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3.4 Unit Testing

As our code continues to grow, how can we be sure it is working as expected? If we make minor changes to the code, what tests can we run to make sure we didn't break anything? Are our functions written well enough to capture and correctly handle all of the edge cases we throw at them? In this module, we will use the Python pytest library to write unit tests: small tests that are designed to test specific individual components of code. After working through this module, students should be able to:

- Find the documentation for the Python pytest library
- Identify parts of code that should be tested
- · Identify appropriate assertions and exceptions to test for
- Write and run reasonable unit tests

3.4.1 Getting Started

Unit tests are designed to test small components (e.g. individual functions) of your code. They should demonstrate that things that are expected to work actually do work, and things that are expected to break raise appropriate errors. The Python pytest unit testing framework supports test automation, set up and shut down code for tests, and aggregation of tests into collections. It is not part of the Python Standard Library, so we must install it.

```
[student-login]$ pip3 install --user pytest
```

Find the documentation here.

Pull a copy of the meteorite landings data analysis script we have been working on, and a copy of the meteorite landings json file, if you don't have copies already.

3.4.2 Devise a Reasonable Test

The functions in this Python3 script are relatively simple, but how can we be sure they are working as intended? Let's begin with the compute_average_mass() function. We might choose to test it manually using the Python3 interactive interpreter:

```
>>> from ml_data_analysis import compute_average_mass
>>>
>>> data = [{'thing': 1}, {'thing': 2}]
>>>
>>> print(compute_average_mass(data, 'thing'))
1.5
```

So simple! We import our code, hand-craft a simple data structure, and send the data plus the key we are interested in to our function. We know off the top of our heads that the average of 1 and 2 is 1.5, and that is in fact the number we get back.

Instead of writing that out each time we want to test, let's instead put this into another Python3 script. When writing test scripts, it is a common convention to name them the same name as the script you are testing, but with the test_prefix added at the beginning.

```
[student-login]$ ls
Meteorite_Landings.json ml_data_analysis.py test_ml_data_analysis.py
```

Open up the script with VIM and put in our testing code from before:

```
from ml_data_analysis import compute_average_mass

data = [{'thing': 1}, {'thing': 2}]
print(compute_average_mass(data, 'thing'))
```

Next try to execute the test script on the command line:

```
[student-login]$ python3 test_ml_data_analysis.py
1.5
```

Great! We assume the test is working. But we still have to look at the output (1.5) and remember back to our hand-crafted data and make sure that is the correct result. It would be more efficient if we had a way to check that the correct answer is returned in our test script itself. To do this, we can use the assert statement.

```
from ml_data_analysis import compute_average_mass

data = [{'thing': 1}, {'thing': 2}]
assert(compute_average_mass(data, 'thing') == 1.5)
```

Now instead of printing the result, we use assert to make sure it is equal to our expected outcome. If the conditional is true, nothing will be printed. If the conditional is false, we will see an AssertionError.

EXERCISE

- Write a few more tests to convince yourself that the function is in fact returning the average of the input values.
- · Modify one of the tests so that it should fail, and execute the tests to confirm that it does fail.
- If you have multiple tests that pass and multiple tests that fail, how would you know?

3.4.3 Automate Testing with Pytest

Pytest is an excellent framework for small unit tests and for large functional tests (as we will see later in the semester). If you previously installed pytest with pip3, now would be a good time to double check that the installation worked and there is an executable called pytest in your PATH:

```
[student-login]$ pytest --version
pytest 8.0.0
```

Next, we just need to make a minor organizational change to our test code. We group all of our tests for a given function (e.g. all the tests for compute_average_mass) into their own function. By convention, we typically name that function as "test_" plus the name of the function we are testing. Pytest will automatically look in our working tree for files that start with the test_ prefix, and execute the test functions within.

```
from ml_data_analysis import compute_average_mass

def test_compute_average_mass():

(continues on next page)
```

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```
assert compute_average_mass([{'a': 1}, {'a': 2}], 'a') == 1.5
assert compute_average_mass([{'a': 1}, {'a': 2}, {'a': 3}], 'a') == 2
assert compute_average_mass([{'a': 10}, {'a': 1}, {'a': 1}], 'a') == 4
```

Call the pytest executable in your top directory, it will find your test function in your test script, run that function, and finally print some informative output:

3.4.4 What Else Should We Test?

The simple tests we wrote above seem almost trivial, but they are actually great sanity tests to tell us that our code is working. What other behaviors of our compute_average_mass() function should we test? In no particular order, we could test the following non-exhaustive list:

- If the list only contains one dictionary object, the function still behaves as expected
- The return value should be type float
- If we send it an empty list, that should raise some sort of exception
- If we send it a list of non-uniform dictionaries (e.g. the dictionaries don't all have the expected key), we should get a KeyError
- If we send it bad values (e.g. a value is a string instead of an expected float), we should get a ValueError
- If we send it a string that doesn't appear in the dictionaries, we should get a KeyError

Tip: A list of all of the built-in Python3 exceptions can be found in the Python docs.

To test some of these behaviors, let's create some additional assertions and organize them into their own functions.

```
from ml_data_analysis import compute_average_mass
import pytest

def test_compute_average_mass():
    assert compute_average_mass([{'a': 1}], 'a') == 1
    assert compute_average_mass([{'a': 1}, {'a': 2}], 'a') == 1.5
    assert compute_average_mass([{'a': 1}, {'a': 2}, {'a': 3}], 'a') == 2
    assert compute_average_mass([{'a': 10}, {'a': 1}, {'a': 1}], 'a') == 4
    assert isinstance(compute_average_mass([{'a': 1}, {'a': 2}], 'a'), float) == True

def test_compute_average_mass_exceptions():

(continues on next page)
```

```
with pytest.raises(ZeroDivisionError):
12
           compute_average_mass([], 'a')
                                                                          # send an empty list
       with pytest.raises(KeyError):
14
           compute_average_mass([{'a': 1}, {'b': 1}], 'a')
                                                                          # dictionaries not_
   →uniform
       with pytest.raises(ValueError):
16
           compute_average_mass([{'a': 1}, {'a': 'x'}], 'a')
                                                                         # value not a float
17
       with pytest.raises(KeyError):
18
           compute_average_mass([{'a': 1}, {'a': 2}], 'b')
                                                                         # key not in dicts
```

After adding the above tests, run pytest again:

Success! The tests for our first function are passing. Our test suite essentially documents our intent for the behavior of the compute_average_mass() function. And, if ever we change the code in that function, we can see if the behavior we intend still passes the test.

EXERCISE

In the same test script, but under new test function definitions:

- Write tests for the check_hemisphere() function
- Write tests for the count_classes() function

3.4.5 Capturing Standard Out

If you have a function that prints to standard out (stdout), we can write a unit test for that using the capsys utility. Imagine a function that takes an argument and prints something to screen:

```
def print_func(num):
    print(f'hello {num}')

def main():
    print_func(5)

if __name__ == '__main__':
    main()
```

Executing this code prints hello 5 to screen. To write a unit test for this, we import the function into our test script, call the function normally, then capture the response using the capsys.readouterr() method. Then we assert that the response matches our expectations. Assume the above Python code is in a script called print_hello.py.

3.4. Unit Testing 91

```
from print_hello import print_func

def test_print_func(capsys):
    print_func(1)
    captured = capsys.readouterr()
    assert captured.out == 'hello 1\n'
```

Notice that we put a newline character (\n) at the end of the expected output. This character is automatically added by the print function. See the additional resources below for more information on using capsys.

3.4.6 Additional Resources

- Pytest Documentation
- Exceptions in Python
- · Capsys Examples

3.5 Error Handling

Error handling is an important part of data science. Even syntactically-sound code can run into errors if the input data is messy. Being able to understand error messages, anticipate where errors might happen, and program defensively against errors will make your code more robust. After working through this module, students should be able to:

- · Anticipate where and what types of errors might occur in their code
- Read traceback statements and identify exceptions
- Write code blocks to catch and handle exceptions

3.5.1 Why Do We Need Error Handling?

1. Prevents program from crashing if an error occurs

• If an error occurs in a program, we don't want the program to unexpectedly crash on the user. Instead, error handling can be used to notify the user of why the error occurred and gracefully exit the process that caused the error.

2. Saves time debugging errors

- Following reason #1, having the program display an error instead of immediately crashing will save a lot of time when debugging errors.
- The logic inside the error handler can be updated to display useful information for the developer, such as the code traceback, type of error, etc.

3. Helps define requirements for the program

• If the program crashes due to bad input, the error handler could notify the user of why the error occurred and define the requirements and constraints of the program.

Source

3.5.2 Errors in Data

Imagine you have a data set of meteorite landings in a list-of-dictionaries format, and that one of the descriptors for each meteorite was mass. You might reasonable expect each mass to have a value that is a positive number.

We have been through the code in compute_average_mass many times at this point and we are pretty sure it is free of errors. But, what if the error comes from the data?

At this point we need to make a choice. If we have input data which could be 10s or 100s of thousands of lines (or more), do we want to go through it and pull out all the data points with null values for masses?

It would be better to update our code to anticipate this possible error and handle it in a way such that our code does not crash and we still get a result that makes sense.

3.5.3 Understanding Exceptions

When errors do occur, Python3 prints a **traceback** message to help you pinpoint where the specific **exception** occurred. With traceback messages, you generally want to read the bottom line first, which identifies the specific exception, and then start reading up to find out where in the code (i.e. in what function) the exception occurred. For most errors, you can probably get away with only looking at the last three or so lines of the traceback message.

At first glance, exceptions and traceback messages may seem to be undecipherable, but understanding that there are a finite number of built in exceptions and each named exception actually is a pretty useful hint to where the error occurred. Consider some of the following exceptions:

```
>>> 10 * (1/0)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ZeroDivisionError: division by zero

(continues on next page)
```

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```
>>> 4 + spam*3
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
NameError: name 'spam' is not defined

>>> '2' + 2
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
TypeError: can only concatenate str (not "int") to str
```

ZeroDivisionError, NameError, and TypeError are somewhat self explanatory when you see when they are raised. Knowing what circumstances can cause a built-in exception to occur (e.g. NameErrors are raised when a name is not found) is the first step toward identifying the cause and the solution. Some common situations that generate exceptions are:

- Trying to open a file that does not exist raises a FileNotFoundError.
- Trying to divide by zero raises a ZeroDivisionError.
- Trying to access a list at an index beyond its length raises an IndexError.
- Trying to use an object of the wrong type in a function raises a TypeError (for example, trying to call json. dumps() with an object that is not of type str).
- Trying to use an object with the wrong kind of value in a function raises a ValueError (for example, calling int('abc')).
- Trying to access a non-existent attribute on an object raises an AttributeError (a special case is accessing a null/uninitialized object, resulting in the dreaded AttributeError: 'NoneType' object has no attribute 'foo' error).

A list of all built-in exceptions that could occur can be found here.

Note: Note that syntax errors stand apart as exceptions that can't be handled at runtime:

```
>>> print 'Hello, world!'
File "<stdin>", line 1
   print 'Hello, world!'
   ^
SyntaxError: Missing parentheses in call to 'print'. Did you mean print('Hello, world!')?
```

3.5.4 Handling Exceptions

We can use a strategy called *exception handling* to prevent our program from crashing if it encounters an exception during runtime. The specific statements we use for this in Python3 are try and except. In general, it follows the format:

```
try:
    # execute some statements that could raise an exception...
    f(x, y, z)
except ExceptionType1 as e:
    # do something if the exception was of type ExceptionType1...
(continues on next page)
```

```
except ExceptionType2 as e:
    # do something if the exception was of type ExceptionType2...
# . . . additional except blocks . . .
finally:
    # do something regardless of whether an exception was raised or not.
```

A few notes:

- If a statement(s) within the try block does not raise an exception, the except blocks are skipped.
- If a statement within the try block does raise an exception, Python looks at the except blocks for the first one matching the type of the exception raised and executes that block of code.
- The finally block is optional but it executes regardless of whether an exception was raised by a statement or not.
- The as e clause puts the exception object into a variable (e) that we can use.
- The use of e was arbitrary; we could choose to use any other valid variable identifier.
- We can also leave off the as e part altogether if we don't need to reference the exception object in our code.

Consider again our meteorite landing data, and the original compute_average_mass function:

```
def compute_average_mass(a_list_of_dicts, a_key_string):
    total_mass = 0.
    for item in a_list_of_dicts:
        total_mass += float(item[a_key_string])
    return(total_mass / len(a_list_of_dicts))
```

And update it as follows:

If a TypeError is raised in the try block, (i.e. beause item[a_key_string] is not a float) then that exception is handled by executing the lines in the except block. In this case, a message is logged and the code continues to the next iteration of the for loop. If any other kind of error occurs, the program would raise the error and exit with a traceback message. Here, we are currently only handling TypeErrors.

With this modified function, we can execute our lines of code from above:

3.5. Error Handling 95

3.5.5 Exception Hierarchy

Exceptions form a class hierarchy with the base Exception class being at the root. So, for example:

- FileNotFoundError is a type of OSError as is PermissionError, which is raised in case the attempted file access is not permitted by the OS due to lack of permissions.
- ZeroDivisionError and OverflowError are instances of ArithmeticError, the latter being raised whenever the result of a calculation exceeds the limits of what can be represented (try running 2.**5000 in a Python shell).
- Every built-in Python exception is of type Exception.

Therefore, we could use any of the following to deal with a FileNotFoundError:

- except FileNotFoundError
- except OSError
- except Exception

Here are some best practices to keep in mind for handling exceptions:

- Put a minimum number of statements within a try block so that you can detect which statement caused the error.
- Similarly, put the most specific exception type in the except block that is appropriate so that you can detect exactly what went wrong. Using except Exception... should be seen as a last resort because an Exception could be any kind of error.

See the resources below for tips on building more complicated try-except statements.

3.5.6 Additional Resources

- Python 3 Error Handling
- Python 3 Exception Class

UNIT 4: SOFTWARE DESIGN CONCEPTS

In this mini-unit, we will briefly introduce the major Software Design concepts and principles that we will be practicing throughout the semester. We will also briefly cover some different types of diagrams for software design, as well as tools to create diagrams.

4.1 Introduction to Software Design

In this section, we introduce the topic of Software Design. There are many aspects and concepts related to Software Design – many more than can be covered in a single semester – and indeed, the topics we present throughout the rest of the semester will be, at least in part, aimed at tackling one or more aspects of design. Here, we simply provide a high-level overview of the Software Design landscape.

4.1.1 Software Design as a Process

On the one hand, designing software is a process involving different types of people – architects, developers, project managers, funding groups, etc. – and there are different paradigms, methodologies and frameworks for guiding this process.

Here are just a few examples:

- Waterfall Method Software tasks are organized into sets or "phases" with a linear ordering; tasks from each phase are completed before moving to the next phase. In practice, phases tended to be longer (on the order of weeks or months) for larger projects that could span years.
- Agile Method— In contrast to Waterfall, Agile advocates smaller, complete software development life cycles, where "minimal" products are released and then incrementally improved.
- Test Driven Development Developers write tests asserting what the software should do before writing any software. Initially, all the tests fail, but as the software gets closer to completion and more functionality is developed, the tests increasingly pass.

We will not focus a whole lot on Software Design as a process, and, in particular, we will not discuss any of the specific methodologies or frameworks in depth. We will, however, introduce some common phases, such as requirements gathering, architectural design, acceptance testing, etc.

4.1.2 Software Design Principles

Another way to think of Software Design is as a set of principles and associated techniques for achieving software with certain qualities. In this class, we will be mostly focusing on Software Design principles.

Throughout the course of the semester we will discuss techniques that help achieve the following Software Design principles:

#1: Modularity

Modularity involves dividing the components of software into parts. There are two principles that guide how we decompose software:

Intra-Module Cohesion

Cohesion refers to the similarity of the elements contained within a component (or "module"). When designing software, we strive to *increase* cohesion within a module. That is, we want to group similar functionality together. This can be at a low-level or at a high-level.

For example, thinking at a "low level", we want to group together Python functions, variables, etc. into modules and packages based on functionality. We've already seen examples of this from the Python standard library: the json module collects Python code related to working with JSON data.

At a higher level, as the class progresses we will be developing multiple individual programs that integrate together to form a complete system. These individual programs focus on specific tasks, providing good cohesion.

Inter-Module Coupling

Coupling refers to the degree to which two components depend on each other. There are several ways to formalize the notion of coupling and make it something one can measure. For example, given components A and B, we can ask:

- If component A changes, to what extent must component B change for component B to continue to function?
- If component A fails, to what extent can component B continue to function?
- For each piece of functionality in component A, when executing that function, how many pieces of functionality in component B execute?

According to the design principle, we want to *reduce* inter-module coupling (sometimes called "loose coupling"). Reduced coupling allows different parts of the software to be modified independently and created more robust software.

#2: Abstraction

You likely already know the concept of abstraction from math and science courses. The real world is very complicated. With abstraction, we replace an exact concept with a simplified model. For example, the Bohr model is an abstraction of the actual atom.

You have seen examples of abstractions in software also. For instance, we saw how the Python function open() returns a "file object" (cf., https://docs.python.org/3/glossary.html#term-file-object). A file object is an abstraction representing data stored in different formats. With a file object, you can do certain actions, represented by functions, e.g.,:

- Read data from the file object.
- Write data to the file object.

Note that when dealing with an actual file stored on a hard drive, the individual bytes are organized into blocks and sectors. These details and others are hidden from us when we use Python's file object abstraction, which makes it much easier to use. It also allows the file object to be used for other kinds of data storage, as we'll see in the next section.

#3: Generalization

Generalization allows the same software component to be used in different situations. It improves the reusability of software.

Generalization and Abstraction go hand and hand: using well-designed abstractions allows the same model to be used in many places. Continuing with the example above, it turns out that we can use the same file objects to handle data from a lot of different sources, including:

- · Actual files stored on the hard drive
- · Standard input and output
- · In-memory buffers
- Sockets
- · Unix pipes

And more! That illustrates the power of abstraction: by learning just a few concepts and functions (e.g., open, read, write, etc.) one is able to deal with all of these different kinds of data sources!

#4: Portability and Reproducibility

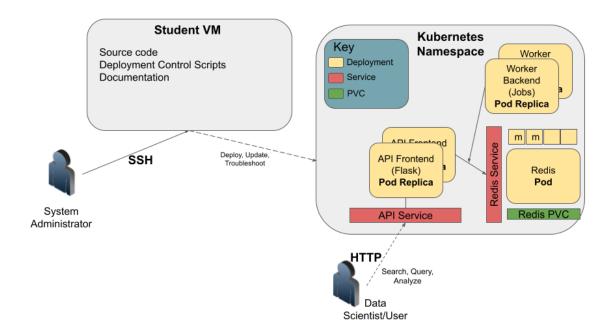
The last design principle we will mention is that of software portability and the related concept of reproducibility. Portability refers to the ability to access and execute software from different kinds of computers, while reproducibility means that the results obtained from executing the software at one time can be obtained later. We will spend a significant amount of time this semester working with techniques that improve the portability of the software we develop.

4.1.3 Software Design Goals for COE 332

During the course of the semester, you will build a large (by some measure), distributed sofware system for data analysis. Your system will comprise many components and thousands of lines of code. An example illustration of a typical final class project is shown below, to give an indication of where we are headed.

As we add components and complexity, these software design principles will become increasingly important.

Our goals for COE 332 are to illustrate these design concepts so that you can recognize them and apply them, not just towards the design of distributed systems and/or data analysis, but all kinds of different software. While in this course we'll illustrate these principles in the context of distributed systems, they are broadly applicable to all large software projects.



4.2 Diagrams for Software Design

In this module, we provide a brief introduction to diagrams for software design. By the end of this module, the student should be able to:

- Explain the basic utility of diagrams for software design
- Describe the differences between structural diagrams and behavioral diagrams.
- Create different types of structural and/or behavioral diagrams for their flask-based API system.

As a software system grows in its size and complexity, it becomes increasingly difficult to describe in written text. Diagrams help us visualize the components of a software system, allowing us to provide a more concise and holistic description. There are many tools and approaches to creating diagrams for software systems. In this short module, we provide only a brief introduction to diagrams for software design, and we include some references for further reading.

Generally speaking, a diagram can convey two types of information:

- Static relationships between components, sometimes called a structural diagram.
- Dynamic information describing how the system changes or how different components react to each other. These
 are called behavior diagrams.

4.2.1 Structural Diagrams

With a structural diagram, the goal is to represent the components of the system with different shapes, and to indicate connections between the components, usually with an arrow. Different diagrams will represent different types of components in the system at different granularity. For example, we could use boxes to represent:

- · Classes in software utilizing object oriented programming
- Modules and libraries in a large code base
- Containers or services in a distributed system utilizing a microservice architecture

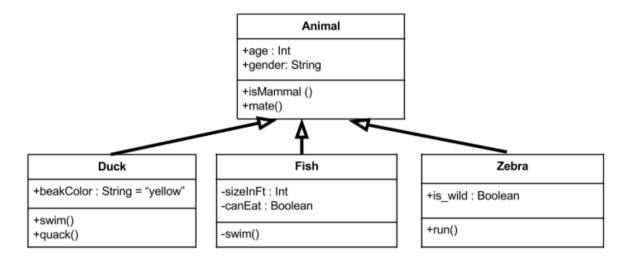


Fig. 1: An example of a class diagram

Similarly, arrows between components represent different types of connections.

- For classes in OOP, arrows represent different types of relationships between the classes, such as inheritance (when one class is a child of another class) or dependency (when one class uses methods from another class).
- For a diagram containing microservices, arrows represent the communication between services.

Kubernetes - Deployment and Container Orchestration

PVC - persistent storage (Ceph)

Service - Networking

Deployments

- API Server
- Persistence
- Async components

Jobs

- Initializations
- DB Migrations

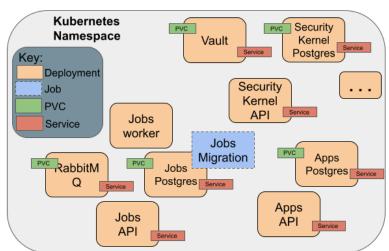


Fig. 2: An example of a microservices diagram

4.2.2 Behavioral Diagrams

By contrast to structural diagrams, behavioral diagrams capture the how components within the system respond to changes. Some common behavioral diagrams include:

Flowcharts

Flowcharts depict the step-by-step process of an algorithm or component of a program. Each box represents a different step in the process. Different shapes are used for different types of steps, such as a rhombus for collecting input, a diamond for an IF/THEN conditional, and a rectangle for a computation.

Sequence Diagrams

Sequence diagrams describe the sequence of interactions (usually, communications) between components of a system and even end users. The components represented in a sequence diagram could be web pages or URLs within a single web application, or they could be entirely different services in a microservice architecture.

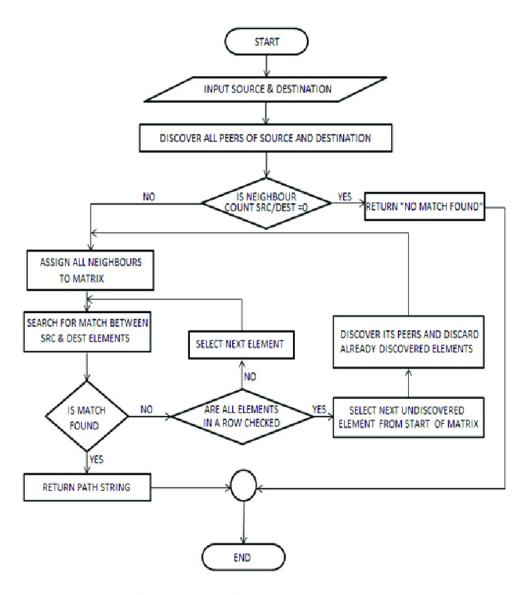


Fig. 3: A flowchart of the all-pairs-shortest-path (APSP) algorithm.

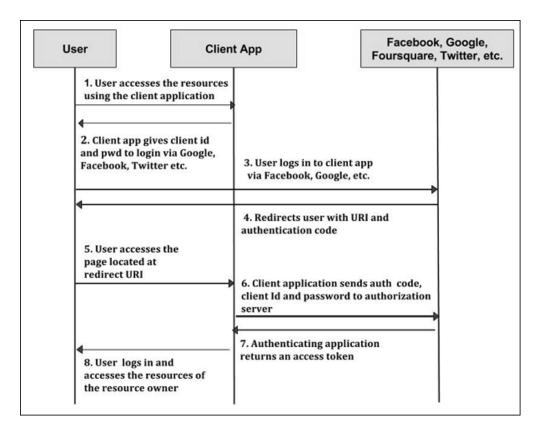


Fig. 4: A sequence diagram of the OAuth2 authorization code flow.

4.2.3 Unified Modeling Language (UML)

The Unified Modeling Language (UML) is a modeling language for describing diagrams. It was created in 1994 and became an ISO standard in 2005. There are two major versions of UML, v1 and v2. In v2, there are at least 14 different types of diagrams.

Some UML diagrams, such as the class diagram, are precise enough to be able to generate code from them. While this is a neat idea, in practice some software engineers find UML heavyweight and cumbersome. If you are interested in UML, there are a number of tutorials on the web.

Here is an example description of a C4 UML Plant diagram describing a hypothetical COE 332 final project:

```
→the task queue, and works them to completion.")
    ContainerDb(database, "Redis", "Redis Database", "Stores sun spots dataset and...
→information and jobs in the system.")
    Container(task_queue, "Task Queue", "Redis Task Queue", "Stores pending jobs in the...
→system")
}
Rel_Down(scientist, api, "Uses", "HTTP/S")

Rel_Down(task_queue, worker, "Dequeues jobs")
Rel_Down(database, worker, "Reads from and writes to")
Rel_Down(api, database, "Reads from and writes to", "python, redis")
Rel_Down(api, task_queue, "Adds new jobs to queue")

@enduml
```

This generates the following diagram:

4.2.4 Options for Creating Diagrams

There are a lot of options for creating diagrams:

- 1. Google Slides/Google Draw Both options allow you to create basic shapes and connectors, fill, arranges, etc. Free with a google account.
- 2. draw.io Similar to google slides but some find it to be more ergonomic to use. Free.
- 3. Microsoft Powerpoint Similar to the other options above; requires access to Microsoft Office.

And if you want to make diagrams from UML...

- 4. Visual Paradigm This is kind of like the others above where you click and drag boxes and arrows (I think). I got the "Community Edition" installed on Ubuntu without much trouble. It is free.
- 5. kroki.io This project is kind of fun. It provides an HTTP API for making diagrams (what could be better?) You describe your diagrams in text (for example, in UML) and make an HTTP request to the diagram endpoint and it returns to you HTML that renders your figure. You can use their community server, or you can run the whole API as a docker container on your machine. It's all free.

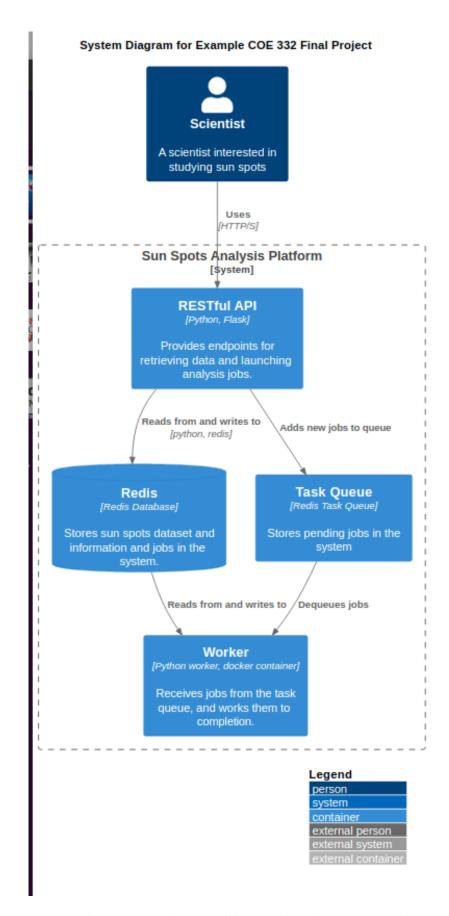


Fig. 5: A sequence diagram of the OAuth2 authorization code flow.

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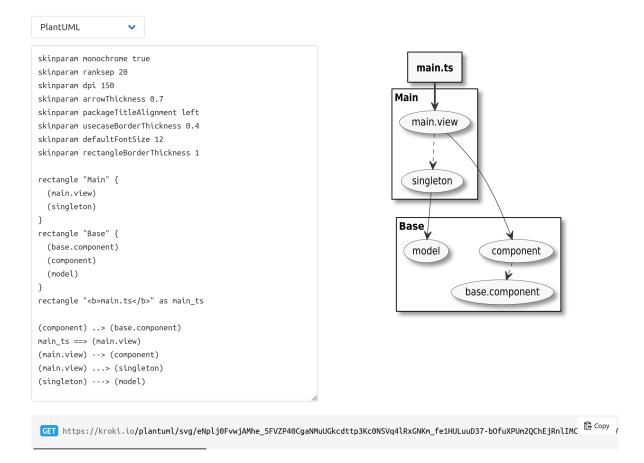


Fig. 6: From the kroki.io documentation.

CHAPTER

FIVE

UNIT 5: CONTAINERIZATION AND AUTOMATION

In this unit we begin to isolate our work from our development environment through a process called *containerization*. We will learn how to use existing containers, build our own containers, and push containers to a public container registry. We will also see how to automate some of our more tedious processes in order to speed up the development cycle.

If you don't have one already, please create an account on Docker Hub, which we will use extensively in this class. (The username does not have to be the same as your GitHub username, but it will make things less confusing later on if the usernames match).

5.1 Introduction to Containers

Containers are an important common currency for app development, web services, scientific computing, and more. Containers allow you to package an application along with all of its dependencies, isolate it from other applications and services, and deploy it consistently and reproducibly and *platform-agnostically*. In this introductory module, we will learn about containers and their uses, in particular the containerization platform **Docker**.

After going through this module, students should be able to:

- Describe what a container is
- Use essential docker commands
- · Find and pull existing containers from Docker Hub
- Run containers interactively and non-interactively
- Design Principles: Additionally, we will see how containers contribute to the portability of software projects

5.1.1 Logging in to the Jetstream VMs

We will all be running Docker on our own private VMs that are accessible through the student-login gateway. It takes two hops to log in to your VM:

Note: Below, replace username with your TACC username.

```
[local]$ ssh username@student-login.tacc.utexas.edu
(enter password)
(enter token)

[student-login]$ ssh username-COE332-vm
```

```
(no password or token required)

[user-vm]$ whoami
ubuntu
[user-vm]$ hostname -f
username-coe332-vm.js2local
```

Note: This is a new machine. Don't forget, you likely want to run git config, pip install, and possibly some other commands to set up your environment.

5.1.2 What is a Container?

- A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another.
- Containers allow a developer to package up an application with all of the parts it needs, such as libraries and other dependencies, and ship it all out as one package.
- Multiple containers can run on the same machine and share the OS kernel with other containers, each running as isolated processes in user space, hence are *lightweight* and have *low overhead*.
- Containers ensure portability and reproducibility by isolating the application from environment.

5.1.3 How is a Container Different from a VM?

Virtual machines enable application and resource isolation, run on top of a hypervisor (high overhead). Multiple VMs can run on the same physical infrastructure - from a few to dozens depending on resources. VMs take up more disk space and have long start up times (~minutes).

Containers enable application and resource isolation, run on top of the host operating system. Many containers can run on the same physical infrastructure - up to 1,000s depending on resources. Containers take up less disk space than VMs and have very short start up times (~ 100 s of ms).

5.1.4 Docker

Docker is a containerization platform that uses OS-level virtualization to package software and dependencies in deliverable units called containers. It is by far the most common containerization platform today, and most other container platforms are compatible with Docker. (E.g. Singularity and Shifter are two containerization platforms you'll find in HPC environments).

We can find existing containers at:

- 1. Docker Hub
- 2. Quay.io
- 3. BioContainers

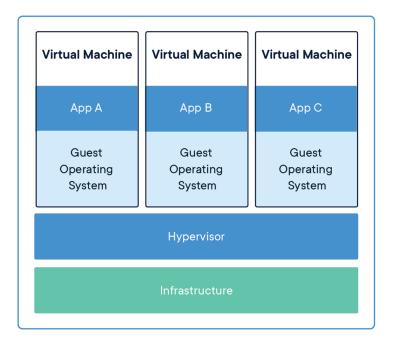


Fig. 1: Applications isolated by VMs.

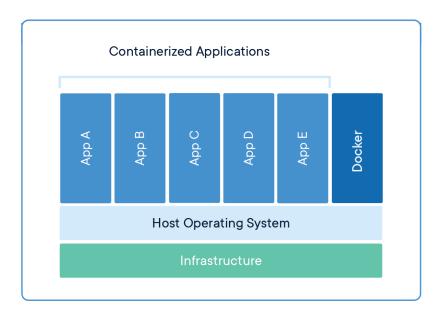


Fig. 2: Applications isolated by containers.

5.1.5 Some Quick Definitions

Container

A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another. Containers includes everything from the operating system, user-added files, metadata.

Image

A Docker image is a read-only file used to produce Docker containers. It is comprised of layers of other images, and any changes made to an image can only be saved and propagated on by adding new layers. The "base image" is the bottom-most layer that does not depend on any other layer and typically defines, e.g., the operating system for the container. Running a Docker image creates an instance of a Docker container.

Dockerfile

The Dockerfile is a recipe for creating a Docker image. They are simple, usually short plain text files that contain a sequential set of commands (*a recipe*) for installing and configuring your application and all of its dependencies. The Docker command line interface is used to "build" an image from a Dockerfile.

Image Registry

The Docker images you build can be stored in online image registries, such as Docker Hub. (It is similar to the way we store Git repositories on GitHub.) Image registries support the notion of tags on images to identify specific versions of images. It is mostly public, and many "official" images can be found.

5.1.6 Summing Up

If you are developing an app or web service, you will almost certainly want to work with containers. First you must either **build** an image from a Dockerfile, or **pull** an image from a public registry. Then, you **run** (or deploy) an instance of your image into a container. The container represents your app or web service, running in the wild, isolated from other apps and services.

5.1.7 Getting Started With Docker

Much like the git command line tools, the docker command line tools follow the syntax: docker <verb> <parameters>. Discover all the verbs available by typing docker --help, and discover help for each verb by typing docker <verb> --help. Open up your favorite terminal, log in to your own student VM, and try running the following:

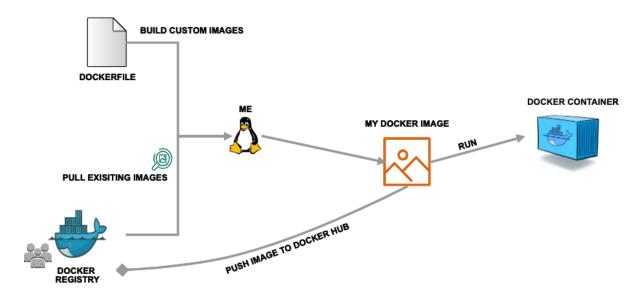


Fig. 3: Simple Docker workflow.

Context: default Server: Engine: Version: 24.0.5 API version: 1.43 (minimum version 1.12) Go version: go1.20.3 Git commit: 24.0.5-0ubuntu1~22.04.1 Built: Mon Aug 21 19:50:14 2023 linux/amd64 OS/Arch: Experimental: false containerd: Version: 1.7.2 GitCommit: runc: Version: 1.1.7-0ubuntu1~22.04.1 GitCommit: docker-init: Version: 0.19.0 GitCommit:

Warning: Please let the instructors know if you get any errors on issuing the above command.

EXERCISE

Take a few minutes to run docker --help and a few examples of docker <verb> --help to make sure you can find and read the help text.

5.1.8 Working with Images from Docker Hub

To introduce ourselves to some of the most essential Docker commands, we will go through the process of listing images that are currently available on your student server, we will pull a 'hello-world' image from Docker Hub, then we will run the 'hello-world' image to see what it says.

List images on your server with the docker images command. This peeks into the Docker daemon, to see which images are available, when they were created, and how large they are:

```
[user-vm]$ docker images
REPOSITORY
                      TAG
                                 IMAGE ID
                                                 CREATED
                                                                ST7F
quacamole/quacamole
                                 a385e28f9fd6
                                                 20 months ago
                                                                  642MB
                       <none>
guacamole/guacd-dev
                       <none>
                                 315a12ba560b
                                                 21 months ago
                                                                 228MB
```

Pull an image from Docker hub with the docker pull command. This looks through the Docker Hub registry and downloads the 'latest' version of that image:

```
[user-vm]$ docker pull hello-world
Using default tag: latest
latest: Pulling from library/hello-world
0e03bdcc26d7: Pull complete
Digest: sha256:31b9c7d48790f0d8c50ab433d9c3b7e17666d6993084c002c2ff1ca09b96391d
Status: Downloaded newer image for hello-world:latest
docker.io/library/hello-world:latest
```

Run the image we just pulled with the docker run command. In this case, running the container will execute a simple shell script inside the container that has been configured as the 'default command' when the image was built:

```
For more examples and ideas, visit: https://docs.docker.com/get-started/
```

Check to see if any containers are still running using docker ps:

```
[user-vm]$ docker ps
CONTAINER ID IMAGE COMMAND CREATED STATUS PORTS NAMES
```

EXERCISE

The command docker ps shows only currently running containers. Pull up the help text for that command and figure out how to show all containers, not just currently running containers.

5.1.9 Pull An Official Image

One powerful aspect of developing with containers and the Docker ecosystem is the large collection of container images freely available. There are 100s of thousands of images on Docker Hub alone (10s of millions if you count the tags), but beware: using an image that you don't know anything about comes with the same risks involved with running any software.

Warning: Be careful running container images that you are not familiar with. Some could contain security vulnerabilities or, even worse, malicious code like viruses or ransomware.

To combat this, Docker Hub provides "Official Images", a well-maintained set of container images providing high-quality installations of operating systems, programming language environments and more.

We can search through the official images on Docker Hub here.

Scroll down to find the Python official image called python, then click on that image.

We see a lot of information about how to use the image, including information about the different "tags" available. We see tags such as 3.13-rc, 3.12.1, 3.12, 3, etc. We'll discuss tags in detail later, but for now, does anyone have a guess as to what the Python tags refer to?

We can pull the official Python image using command, then check to make sure it is available locally:

```
[user-vm]$ docker pull python
...
[user-vm]$ docker images
...
[user-vm]$ docker inspect python
...
```

Tip: Use docker inspect to find some metadata available for each image.

5.1.10 Start an Interactive Shell Inside a Container

Using an interactive shell is a great way to poke around inside a container and see what is in there. Imagine you are ssh-ing to a different Linux server, have root access, and can see what files, commands, environment, etc., is available.

Before starting an interactive shell inside the container, execute the following commands on your private VM (we will see why in a minute):

```
[user-vm] $ whoami
ubuntu
[user-vm] $ pwd
/home/ubuntu
[user-vm]$ cat /etc/os-release
PRETTY_NAME="Ubuntu 22.04.3 LTS"
NAME="Ubuntu"
VERSION_ID="22.04"
VERSION="22.04.3 LTS (Jammy Jellyfish)"
VERSION_CODENAME=jammy
ID=ubuntu
ID_LIKE=debian
HOME_URL="https://www.ubuntu.com/"
SUPPORT_URL="https://help.ubuntu.com/"
BUG_REPORT_URL="https://bugs.launchpad.net/ubuntu/"
PRIVACY_POLICY_URL="https://www.ubuntu.com/legal/terms-and-policies/privacy-policy"
UBUNTU_CODENAME=jammy
```

Now start the interactive shell inside a Python container:

```
[user-vm]$ docker run --rm -it python /bin/bash
root@fc5b620c5a88:/#
```

Here is an explanation of the command options:

```
docker run  # run a container
--rm  # remove the container when we exit
-it  # interactively attach terminal to inside of container
python  # use the official python image
/bin/bash  # execute the bash shell program inside container
```

Try the following commands - the same commands you did above before starting the interactive shell in the container - and note what has changed:

```
root@fc5b620c5a88:/# whoami
root
root@fc5b620c5a88:/# pwd
/
root@fc5b620c5a88:/# cat /etc/os-release
PRETTY_NAME="Debian GNU/Linux 12 (bookworm)"
NAME="Debian GNU/Linux"
VERSION_ID="12"
VERSION="12 (bookworm)"
VERSION_CODENAME=bookworm
ID=debian
HOME_URL="https://www.debian.org/"
```

```
SUPPORT_URL="https://www.debian.org/support"
BUG_REPORT_URL="https://bugs.debian.org/"
```

Now you are the root user on a different operating system inside a running Linux container! You can type exit to escape the container.

EXERCISE

Before you exit the container, try running the command python. What happens? Compare that with running the command python directly on your student VM.

5.1.11 Run a Command Inside a Container

Back out on your student VM, we now know we have a container image called python that has a particular version of Python (3.12.1) that is otherwise not available on your student server. The 3.12.1 Python interpreter, it's standard library, and all of the dependencies of those are included in the container image and are *isolated* from everything else. This image (python) is portable and will run the exact same way on any OS that Docker supports.

In practice, though, we don't want to start interactive shells each time we need to use a software application inside an image. Docker allows you to spin up an *ad hoc* container to run applications from outside. For example, try:

```
[user-vm] docker run --rm python whoami
root
[user-vm] $ docker run --rm python pwd
[user-vm]$ docker run --rm python cat /etc/os-release
PRETTY_NAME="Debian GNU/Linux 12 (bookworm)"
NAME="Debian GNU/Linux"
VERSION_ID="12"
VERSION="12 (bookworm)"
VERSION_CODENAME=bookworm
ID=debian
HOME_URL="https://www.debian.org/"
SUPPORT_URL="https://www.debian.org/support"
BUG_REPORT_URL="https://bugs.debian.org/"
[user-vm] $ docker run -it --rm python
Python 3.12.1 (main, Feb 1 2024, 04:22:19) [GCC 12.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
```

In the first three commands above, we omitted the -it flags because they did not require an interactive terminal to run. On each of these commands, Docker finds the image the command refers to, spins up a new container based on that image, executes the given command inside, prints the result, and exits and removes the container.

The last command, which did not specify a command to run inside the container, uses the container's default command. We don't know ahead of time what (if any) default command is provided for any given image, but what default command was provided for the python image?

Yes, it was the python command itself, and that requires an interactivity to use, so we provide the -it flags.

5.1.12 Essential Docker Command Summary

Command	Usage
docker login	Authenticate to Docker Hub using username and password
docker images	List images on the local machine
docker ps	List containers on the local machine
docker pull	Download an image from Docker Hub
docker run	Run an instance of an image (a container)
docker exec	Execute a command in a running container
docker inspect	Provide detailed information on Docker objects
docker rmi	Delete an image
docker rm	Delete a container
docker stop	Stop a container
docker build	Build a docker image from a Dockerfile in the current working directory
docker tag	Add a new tag to an image
docker push	Upload an image to Docker Hub

If all else fails, display the help text:

```
[user-vm]$ docker --help
shows all docker options and summaries
```

```
[user-vm]$ docker COMMAND --help
shows options and summaries for a particular command
```

5.1.13 Additional Resources

- · Docker Docs
- Best practices for writing Dockerfiles
- Docker Hub
- Docker for Beginners
- Play with Docker

5.2 Advanced Containers

In the first part, we pulled and ran existing container images from Docker Hub. In this section, we will build an image from scratch for running some of our own Python3 code. Then, we will push that image back up to Docker Hub so others may find and use it. After going through this module, students should be able to:

- Install and test code in a container interactively
- Write a Dockerfile from scratch
- Build a Docker image from a Dockerfile
- · Push a Docker image to Docker Hub
- · Volume mount external data inside a Docker container

5.2.1 Getting Set Up

Scenario: You are a developer who has written some code for reading and parsing meteorite landing data in JSON format. You now want to distribute that code for others to use in what you know to be a stable production environment (including OS and dependency versions). End users may want to use this application on their local workstations, in the cloud, or on an HPC cluster.

The first step in a typical container development workflow entails installing and testing an application interactively within a running Docker container.

Note: We recommend doing this on your Jetstream VMs. But, one of the most important features of Docker is that it is platform agnostic. These steps could be done anywhere Docker is installed.

To begin, make a new folder for this work and prepare to gather some important files.

```
[user-vm]$ mkdir -p coe-332/docker-exercise/
[user-vm]$ cd coe-332/docker-exercise/
[user-vm]$ pwd
/home/ubuntu/coe-332/docker-exercise
```

Specifically, you need your ml_data_analysis.py script and the input data file called Meteorite_Landings.json. You can make copies of your own, our download sample copies from the links below. You also need a Dockerfile, and we can just make an empty one with no contents for now.

Warning: It is important to carefully consider what files and folders are in the same PATH as a Dockerfile (known as the 'build context'). The docker build process will index and send all files and folders in the same directory as the Dockerfile to the Docker daemon, so take care not to docker build at a root level.

5.2.2 Containerize Code Interactively

There are several questions you must ask yourself when preparing to containerize code for the first time:

- 1. What is an appropriate base image?
- 2. What dependencies are required for my program?
- 3. What is the installation process for my program?
- 4. What environment variables may be important?

We can work through these questions by performing an **interactive installation** of our Python script. Our development environment (e.g. the student-login server) is a Linux server running Ubuntu 20.04. We know our code works there, so that is how we will containerize it. Use **docker** run to interactively attach to a fresh Ubuntu 20.04 container.

```
[user-vm]$ docker run --rm -it -v $PWD:/code ubuntu:20.04 /bin/bash
[root@7ad568453e0b /]#
```

Here is an explanation of the options:

```
docker run  # run a container
--rm  # remove the container on exit
-it  # interactively attach terminal to inside of container
-v $PWD:/code  # mount the current directory to /code
ubuntu:20.04  # image and tag from Docker Hub
/bin/bash  # shell to start inside container
```

The command prompt will change, signaling you are now 'inside' the container. And, new to this example, we are using the -v flag which mounts the contents of our current directory (\$PWD) inside the container in a folder in the root directory called (/code).

Update and Upgrade

The first thing we will typically do is use the Ubuntu package manager apt to update the list of available packages and install newer versions of the packages we have installed. We can do this with:

```
[root@7ad568453e0b /]# apt-get update
[root@7ad568453e0b /]# apt-get upgrade
...
```

Note: You may need to press 'y' followed by 'Enter' to download and install updates

Install Required Packages

For our Python scripts to work, we need to install a few dependencies: Python3, pip, and the 'pytest' package (more on the 'pytest' package later, let's just assume for now we need it).

```
[root@7ad568453e0b /]# apt-get install python3
...
[root@7ad568453e0b /]# apt-get install python3-pip
...
[root@7ad568453e0b /]# python3 --version
Python 3.8.10
[root@7ad568453e0b /]# pip3 install pytest==8.0.0
Collecting pytest==8.0.0
...
Installing collected packages: exceptiongroup, iniconfig, packaging, tomli, pluggy, pytest
Successfully installed exceptiongroup-1.2.0 iniconfig-2.0.0 packaging-23.2 pluggy-1.4.0 pytest-8.0.0 tomli-2.0.1
```

Warning: An important question to ask is: Does the versions of Python and other dependencies match the versions you are developing with in your local environment? If not, make sure to install the correct version of Python.

Install and Test Your Code

At this time, we should make a small edit to the code that will make it a little more flexible and more amenable to running in a container. (Note: You may need to apt-get install ... your favorite text editor). Instead of hard coding the filename 'Meteorite_Landings.json' in the script, let's make a slight modification so we can pass the filename on the command line. In the script, add this line near the top:

Tip: If you've already done this with something like argparse, that works too.

```
import sys
```

And change the with open... statements to these, as appropriate:

```
with open(sys.argv[1], 'r') as f:
    ml_data = json.load(f)
```

Since we are using a simple Python script, there is not a difficult install process. However, we can make it executable and add it to the user's *PATH*.

```
[root@7ad568453e0b /]# cd /code
[root@7ad568453e0b /]# chmod +rx ml_data_analysis.py
[root@7ad568453e0b /]# export PATH=/code:$PATH
```

Now test with the following:

```
[root@7ad568453e0b /]# cd /home
[root@7ad568453e0b /]# cp /code/Meteorite_Landings.json .
[root@7ad568453e0b /]# ml_data_analysis.py Meteorite_Landings.json
83857.3
Northern & Eastern
...etc
```

We now have functional versions of our script 'installed' in this container. Now would be a good time to execute the *history* command to see a record of the build process. When you are ready, type *exit* to exit the container and we can start writing these build steps into a Dockerfile.

5.2.3 Assemble a Dockerfile

After going through the build process interactively, we can translate our build steps into a Dockerfile using the directives described below. Open up your copy of Dockerfile with a text editor and enter the following:

The FROM Instruction

We can use the FROM instruction to start our new image from a known base image. This should be the first line of our Dockerfile. In our scenario, we want to match our development environment with Ubuntu 20.04. We know our code works in that environment, so that is how we will containerize it for others to use:

```
FROM ubuntu: 20.04
```

Base images typically take the form *os:version*. Avoid using the '*latest*' version; it is hard to track where it came from and the identity of '*latest*' can change.

Tip: Browse Docker Hub to discover other potentially useful base images. Keep an eye out for the 'Official Image' badge.

The RUN Instruction

We can install updates, install new software, or download code to our image by running commands with the RUN instruction. In our case, our only dependencies were Python3 and the "pytest" library. So, we will use a few RUN instructions to install them. Keep in mind that the the docker build process cannot handle interactive prompts, so we use the -y flag with yum and pip3.

```
RUN apt-get update
RUN apt-get upgrade -y
RUN apt-get install -y python3
RUN apt-get install -y python3-pip
RUN pip3 install pytest==8.0.0
```

Each RUN instruction creates an intermediate image (called a 'layer'). Too many layers makes the Docker image less performant, and makes building less efficient. We can minimize the number of layers by combining RUN instructions. Dependencies that are more likely to change over time (e.g. Python3 libraries) still might be better off in in their own RUN instruction in order to save time building later on:

```
RUN apt-get update && \
    apt-get upgrade -y && \
    apt-get install -y python3 && \
    apt-get install -y python3-pip
RUN pip3 install pytest==8.0.0
```

Tip: In the above code block, the character at the end of the lines causes the newline character to be ignored. This can make very long run-on lines with many commands separated by && easier to read.

The COPY Instruction

There are a couple different ways to get your source code inside the image. One way is to use a RUN instruction with wget to pull your code from the web. When you are developing, however, it is usually more practical to copy code in from the Docker build context using the COPY instruction. For example, we can copy our script to the root-level /code directory with the following instructions:

```
COPY ml_data_analysis.py /code/ml_data_analysis.py
```

And, don't forget to perform another RUN instruction to make the script executable:

```
RUN chmod +rx /code/ml_data_analysis.py
```

The ENV Instruction

Another useful instruction is the ENV instruction. This allows the image developer to set environment variables inside the container runtime. In our interactive build, we added the /code folder to the PATH. We can do this with ENV instructions as follows:

```
ENV PATH="/code: $PATH"
```

Putting It All Together

The contents of the final Dockerfile should look like:

```
FROM ubuntu:20.04

RUN apt-get update && \
apt-get upgrade -y && \
apt-get install -y python3 && \
apt-get install -y python3-pip

RUN pip3 install pytest==8.0.0

COPY ml_data_analysis.py /code/ml_data_analysis.py

RUN chmod +rx /code/ml_data_analysis.py

ENV PATH="/code:$PATH"
```

5.2.4 Build the Image

Once the Dockerfile is written and we are satisfied that we have minimized the number of layers, the next step is to build an image. Building a Docker image generally takes the form:

```
[user-vm]$ docker build -t <dockerhubusername>/<code>:<version> .
```

The -t flag is used to name or 'tag' the image with a descriptive name and version. Optionally, you can preface the tag with your **Docker Hub username**. Adding that namespace allows you to push your image to a public registry and share it with others. The trailing dot '.' in the line above simply indicates the location of the Dockerfile (a single '.' means 'the current directory').

To build the image, use:

```
[user-vm]$ docker build -t username/ml_data_analysis:1.0 .
```

Note: Don't forget to replace 'username' with your Docker Hub username.

Use docker images to ensure you see a copy of your image has been built. You can also use *docker inspect* to find out more information about the image.

```
[user-vm]$ docker images
REPOSITORY TAG IMAGE ID CREATED SIZE
(continues on next page)
```

```
username/ml_data_analysis 1.0
                                      2883079fad18
                                                     About a minute ago
                                                                           446MB
```

```
[user-vm]$ docker inspect username/ml_data_analysis:1.0
```

If you need to rename your image, you can either re-tag it with docker tag, or you can remove it with docker rmi and build it again. Issue each of the commands on an empty command line to find out usage information.

5.2.5 Test the Image

We can test a newly-built image two ways: interactively and non-interactively. In interactive testing, we will use docker run to start a shell inside the image, just like we did when we were building it interactively. The difference this time is that we are NOT mounting the code inside with the -v flag, because the code is already in the container:

```
[user-vm]$ docker run --rm -it username/ml_data_analysis:1.0 /bin/bash
[root@c5cf05edddcd /]# ls /code
ml_data_analysis.py
[root@c5cf05edddcd /]# cd /home
[root@c5cf05edddcd home]# pwd
/home
[root@c5cf05edddcd home]# ml_data_analysis.py Meteorite_Landings.json
Traceback (most recent call last):
  File "/code/ml_data_analysis.py", line 96, in <module>
   main()
  File "/code/ml_data_analysis.py", line 82, in main
    with open(sys.argv[1], 'r') as f:
FileNotFoundError: [Errno 2] No such file or directory: 'Meteorite_Landings.json'
```

Here is an explanation of the options:

```
docker run
                # run a container
                # remove the container when we exit
--rm
                # interactively attach terminal to inside of container
-it
                # image and tag on local machine
username/...
/bin/bash
                # shell to start inside container
```

Uh oh! We forgot about Meteorite_Landings. json! We get a FileNotFoundError in Python3. This is because we did not (1) copy the JSON file into the container at build time, nor did we (2) copy the JSON file into the container at run time.

We should pause at this moment to think about how we want to distribute this application. Should the data be encapsulated within? Or should we expect potential users to be bring their own data for analysis?

Let's try again, but this time mount the data inside the container so we can access it. If we mount the current folder as, e.g., /data, then everything in the current folder will be available. In addition, if we write any new files inside the container to /data, those will be preserved and persist outside the container once it stops.

```
[user-vm] $ docker run --rm -it -v $PWD/Meteorite_Landings.json:/data/Meteorite_Landings.
→json username/ml_data_analysis:1.0 /bin/bash
### Same command as above, but easier to read:
```

Everything looks like it works now! Next, exit the container and test the code non-interactively. Notice we are calling the container again with docker run, but instead of specifying an interactive (-it) run, we just issue the command as we want to call it on the command line. Also, notice the return of the -v flag, because we need to create a volume mount so that our data (Meteorite_Landings.json) is available inside the container.

Much simpler and cleaner! Our only local dependencies are the Docker runtime and some input data that we provide. Then we pull and run the image, mounting our data inside the container and executing the embedded Python3 script. Anyone with their own data could follow our same steps to replicate our work in their own environments.

5.2.6 Share Your Docker Image

Now that you have containerized, tested, and tagged your code in a Docker image, the next step is to disseminate it so others can use it.

Docker Hub is the *de facto* place to share an image you built. Remember, the image must be name-spaced with either your Docker Hub username or a Docker Hub organization where you have write privileges in order to push it:

```
[user-vm]$ docker login
...
[user-vm]$ docker push username/ml_data_analysis:1.0
```

You and others will now be able to pull a copy of your container with:

```
[user-vm]$ docker pull username/ml_data_analysis:1.0
```

As a matter of best practice, it is highly recommended that you store your Dockerfiles somewhere safe. A great place to do this is alongside the code in, e.g., GitHub. GitHub also has integrations to automatically update your image in the public container registry every time you commit new code. (More on this later in the semester).

For example, see: Publishing Docker Images

5.2.7 Additional Resources

- Docker for Beginners
- · Play with Docker

5.3 Docker Compose

Up to this point, we have been looking at single-container applications - small units of code that are containerized, executed *ad hoc* to generate or read a JSON file, then exit on completion. But what if we want to do something more complex? For example, what if our goal is to orchestrate a multi-container application consisting of, e.g., a Flask app, a database, a message queue, an authentication service, and more.

Docker compose is a tool for managing multi-container applications. A YAML file is used to define all of the application service, and a few simple commands can be used to spin up or tear down all of the services.

In this module, we will get a first look at Docker compose. Later in this course we will do a deeper dive into advanced container orchestration. After going through this module, students should be able to:

- Translate Docker run commands into YAML files for Docker compose
- Run commands inside ad hoc containers using Docker compose
- · Manage small software systems composed of more than one script, and more than one container
- · Copy data into and out of containers as needed

5.3.1 Another Script, Another Container

We have been working a lot with a script for reading in and analyzing a JSON file of meteorite landing data. Let's quickly write a new script to generate that data, then we will package it into its own container. Consider the following script for **generating** sample Meteorite Landing data like we have been working with:

```
#!/usr/bin/env python3
   import json
   import random
   import sys
   import names
   NUM = 10
   CLASSES = ['CI1', 'CR2-an', 'CV3', 'EH4', 'H4', 'H5', 'H6', 'L5', 'L6', 'LL3-6', 'LL5']
   def main():
10
11
       data = {'meteorite_landings': [{} for _ in range (NUM)]}
12
13
       for i in range(NUM):
14
           rand_lat = '{:.4f}'.format(random.uniform(-90.0000, 90.0000))
           rand_lon = '\{:.4f\}'.format(random.uniform(-90.0000, 90.0000))
16
           data['meteorite_landings'][i]['name'] = names.get_first_name()
           data['meteorite_landings'][i]['id'] = str(10000 + 1 + i)
18
           data['meteorite_landings'][i]['recclass'] = random.choice(CLASSES)
           data['meteorite_landings'][i]['mass (g)'] = str(random.randrange(1, 10000))
20
           data['meteorite_landings'][i]['reclat'] = rand_lat
```

Copy that into a file called gen_ml_data.py, save it, make it executable, and test it. You'll find that this script requires a **command line argument**. Meaning we have to invoke it AND pass some information on the command line in order to get it to work. In this case, it is expecting the name of the output file.

```
# copy contents into file called ``gen_ml_data.py`` and save
[user-vm]$ chmod +rx gen_ml_data.py
[user-vm]$ ./gen_ml_data.py
Traceback (most recent call last):
  File "./gen_ml_data.py", line 29, in <module>
   main()
  File "./gen_ml_data.py", line 25, in main
   with open(sys.argv[1], 'w') as o:
IndexError: list index out of range
# need to provide output filename on command line
[user-vm]$ ./gen_ml_data.py data.json
Data written to data.json!
[user-vm]$ ls
data.json Dockerfile gen_ml_data.py Meteorite_Landings.json ml_data_analysis.py
[user-vm] $ head -n11 data.json
{
  "meteorite_landings": [
      "name": "Sandra",
      "id": "10001",
      "recclass": "EH4"
      "mass (g)": "4119",
      "reclat": "73.8716".
      "reclong": "14.8207",
      "GeoLocation": "(73.8716, 14.8207)"
   },
```

Containerizing this script should be easy enough - we already worked through containerizing another very similar script. Let's say for this new script we do not need the pytest dependency, because there is not really anything interesting to test. But, we do need a different dependency: the Python3 names library.

To make things a little more clear, rename the existing Dockerfile as Dockerfile-analysis, and make a copy of it called Dockerfile-gen.

```
gen_ml_data.py Meteorite_Landings.json ml_data_analysis.py
```

Edit Dockerfile-gen as follows:

```
FROM ubuntu:20.04

RUN apt-get update && \
apt-get upgrade -y && \
apt-get install -y python3 && \
apt-get install -y python3-pip

RUN pip3 install names==0.3.0

COPY gen_ml_data.py /code/gen_ml_data.py

RUN chmod +rx /code/gen_ml_data.py

ENV PATH="/code:$PATH"
```

Now that we have a Dockerfile named something other than the default name, we need to modify our command line a little bit to build it:

```
[user-vm]$ docker build -t username/gen_ml_data:1.0 -f Dockerfile-gen .
```

After the image is successfully built, change directories to a new folder just to be sure you are not running the local scripts or looking at the local data. Then, test the container as follows:

```
[user-vm]$ mkdir test
[user-vm]$ cd test
[user-vm]$ ls
[user-vm]$ docker run --rm username/gen_ml_data:1.0 gen_ml_data.py ml.json
Data written to ml.json!
```

If you list your local files, can you find ml.json? No! This is because whatever data generated inside the container is lost when the container completes its task. What we need to do is use the -v flag to mount a directory somewhere inside the container, write data into that directory, then the data will be captured after the container exists. For example:

Note: To reiterate, because we mounted our current location as a folder called "/data" (-v \$PWD:/data), and we made sure to write the output file to that location in the container (gen_ml_data.py /data/ml.json), then we get to keep the file after the container exits, and it shows up in our current location (\$PWD).

Alas, there is one more issue to address. The new file is owned by root, simply because it is root who created the file inside the container. This is one minor Docker annoyance that we run in to from time to time. The simplest fix is to use one more docker run flag (-id)to specify the user and group ID namespace that should be used inside the container.

EXERCISE

Spend a few minutes testing both containers. Be sure you can generate data with one container, then read in and analyze the same data with the other. Data needs to persist outside the containers in order to do this.

5.3.2 Write a Compose File

Docker compose works by interpreting rules declared in a YAML file (typically called docker-compose.yml). The rules we will write will replace the docker run commands we have been using, and which have been growing quite complex. For example, the commands we used to run our JSON parsing scripts in a container looked like the following:

The above docker run commands can be loosely translated into a YAML file. Navigate to the folder that contains your Python scripts and Dockerfiles, then create a new empty file called docker-compose.yml:

Next, open up docker-compose.yml with your favorite text editor and type / paste in the following text:

```
build:
15
                context: ./
                dockerfile: ./Dockerfile-analysis
17
            depends_on:
                - gen-data
19
            image: username/ml_data_analysis:1.0
20
            volumes:
21
                - ./test:/data
22
            command: ml_data_analysis.py /data/ml.json
23
24
```

Warning: The highlighted lines above may need to be edited with your username / userid / groupid in order for this to work. See instructions below.

The version key must be included and simply denotes that we are using version 3 of Docker compose.

The services section defines the configuration of individual container instances that we want to orchestrate. In our case, we define two called gen-data for the gen_ml_data functionality, and analyze-data for the ml_data_analysis functionality.

Each of those services is configured with its own Docker image, a mounted volume (equivalent to the -v option for docker run), a user namespace (equivalent to the -u option for docker run), and a default command to run.

Please note that the image name above should be changed to use your image. Also, the user ID / group ID are specific to ubuntu - to find your user and group ID, execute the Linux commands id -u and id -g.

Note: The top-level services keyword shown above is just one important part of Docker compose. Later in this course we will look at named volumes and networks which can be configured and created with Docker compose.

5.3.3 Running Docker Compose

The Docker compose command line tool follows the same syntax as other Docker commands:

```
docker-compose <verb> <parameters>
```

Just like Docker, you can pass the --help flag to docker-compose or to any of the verbs to get additional usage information. To get started on the command line tools, try issuing the following two commands:

```
[user-vm]$ docker-compose version
[user-vm]$ docker-compose config
```

The first command prints the version of Docker compose installed, and the second searches your current directory for docker-compose.yml and checks that it contains only valid syntax.

To run one of these services, use the docker-compose run verb, and pass the name of the service as defined in your YAML file:

```
[user-vm]$ ls test/ # currently empty
[user-vm]$ docker-compose run gen-data
Data written to /data/ml.json!
[user-vm]$ ls test/
(continues on next page)
```

```
ml.json # new file!
[user-vm]$ docker-compose run analyze-data
6004.5
Southern & Eastern
... etc.
```

Now we have an easy way to run our *ad hoc* services consistently and reproducibly. Not only does docker-compose. yml make it easier to run our services, it also represents a record of how we intend to interact with this container.

5.3.4 Essential Docker Compose Command Summary

Command	Usage
docker-compose version	Print version information
docker-compose config	Validate docker-compose.yml syntax
docker-compose up	Spin up all services
docker-compose down	Tear down all services
docker-compose build	Build the images listed in the YAML file
docker-compose run	Run a container as defined in the YAML file

5.3.5 Additional Resources

• Docker Compose Docs

UNIT 6: APIS AND FLASK

In this unit, we will be introduced to Application Programming Interfaces (APIs). This introduction will form the foundation of our ultimate goal to create large, complex, Python-based applications that are accessible through the web. The particular Python web framework we will be working with most is called Flask.

6.1 Introduction to APIs

In this section, we will discuss Application Programming Interfaces (APIs) focusing on Web APIs, and in particular REST APIs. We will learn how to interact with APIs using Python scripts. After going through this module, students should be able to:

- Identify and describe Web APIs (including REST APIs).
- List the four most important HTTP verbs and define how they are used in REST APIs.
- Describe how URLs are used to represent objects in a REST API.
- Explore API endpoints provided by various websites, e.g., GitHub.
- Install the Python requests library, and use it to interact with a web API in a Python script, including making requests and parsing responses.
- **Design Principles**: Additionally, we will see how designing software with APIs contributes to the *modularity*, *portability*, *abstraction* and *generalization* of software (all four major design principles).

6.1.1 What are APIs?

An Application Programming Interface (API) establishes the protocols and methods for one piece of a program to communicate with another. APIs are useful for allowing large software systems to be built from smaller components, allowing the same components to be used by different systems, and insulating consumers from changes to the implementation.

Some examples of where you might see APIs implemented:

- In OOP languages, abstract classes provide the interface for all concrete classes to implement.
- Software libraries provide an external interface for consuming programs.
- Web APIs (or "web services") provide interfaces for computer programs to communicate over the internet.

While a User Interface connects humans to computer programs, an API is an interface that connects one piece of software to another. Specifically, APIs:

• Provide functionality to external software in the form of a contract that specifies the inputs that the consuming software must provide and the outputs that the API will produce from the inputs.

- Conceal the implementation of this functionality from the consuming software so that changes can be made to the implementation without impacting consumers.
- Provide errors when the consuming software doesn't fulfill the contract of the API or when unexpected circumstances are encountered.

We have already been working with APIs. For example, the Python json library presents us with an API for working with JSON data. Try opening up the Python3 interactive interpreter:

```
[user-vm]$ python3
Python 3.10.12 (main, Nov 20 2023, 15:14:05) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

And enter the following:

We use json.dumps() to convert Python objects to JSON (string) data and we use json.loads() to convert JSON strings to Python objects.

```
>>> json.dumps({'a': 1})
'{"a": 1}'
>>> type(_)
<class 'str'>
>>> json.loads('{"a": 1}')
{'a': 1}
>>> type(_)
<class 'dict'>
```

We say that dumps and loads are part of the Python json API. In terms of the contract, we might say something like:

- json.loads() This function accepts a single input (string, bytes or bytes array) representing a valid JSON document and returns the equivalent Python object.
 - It will raise a JSONDecodeError if the input is not a valid JSON document.
- json.dumps() This function accepts a single input (a Python object) and serializes it to a string. The Python object must be JSON serializable.
 - It will raise a TypeError if the input is not JSON serializable.

Design Principles. Can you see how the existence of the API provided by the json module increases modularity of the Python software ecosystem?

6.1.2 Web APIs / HTTP

In this course, we will be building Web APIs or HTTP APIs. These are interfaces that are exposed over HTTP, allowing them to be consumed by software running on different machines.

There are a number of advantages to Web-based APIs that we will use in this class:

- A Web API can be made accessible to any computer or application that can access the public internet. Alternatively, a Web API can be restricted to a private network.
- No software installation is required on the client's side to consume a Web API.
- Web APIs can change their implementation without clients knowing (or caring).
- Virtually every modern programming language provides one or more libraries for interacting with a Web API; thus, Web APIs are "programming language agnostic".

HTTP (Hyper Text Transfer Protocol) is one way for two computers on the internet to communicate with each other. It was designed to enable the exchange of data (specifically, "hypertext"). In particular, our web browsers use HTTP when communicating with web servers running web applications. HTTP uses a message-based, **client-server model**: clients make requests to servers by sending a message, and servers respond by sending a message back to the client.

HTTP is an "application layer" protocol in the language of the Internet Protocols; it assumes a lower level transport layer protocol. While this can swapped, in practice it is almost always TCP (Transmission Control Protocol). The basics of the protocol are:

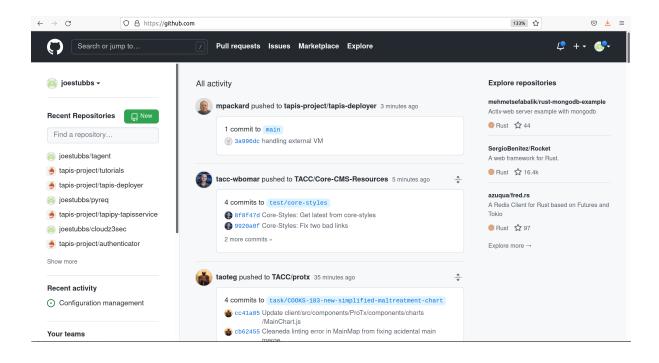
- Web resources are identified with URLs (Uniform Resource Locators). Originally, **resources** were just files/directories on a server, but today resources refer to more general objects.
- HTTP verbs represent actions to take on the resource. The most common verbs are GET, POST, PUT, and DELETE.
- A request is made up of a URL, an HTTP verb, and a message
- A **response** consists of a status code (numerical between 100-599) and a message. The first digit of the status code specifies the kind of response:
 - 1xx informational
 - 2xx success
 - 3xx redirection
 - 4xx error in the request (client)
 - 5xx error fulfilling a valid request (server)

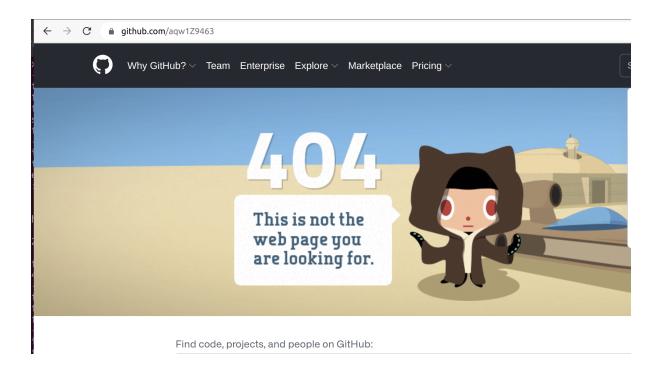
6.1.3 Web Page Examples

Open a browser window, type https://github.com into the address bar and hit go. We see the GitHub home page which looks something like this:

In fact, a multi-step process just occurred; here is a slightly simplified version of what happened:

- (1) Your browser made an HTTP GET request to https://github.com.
- (2) A GitHub server received the request from your browser, formulated a response message containing the data (in HTML format) of your home page, with a 200 response code to indicate success.
- (3) Your browser received the response message from the GitHub server, and determined that the request was successful, due to the 200 response code.
- (4) It then drew the HTML message in the browser window.

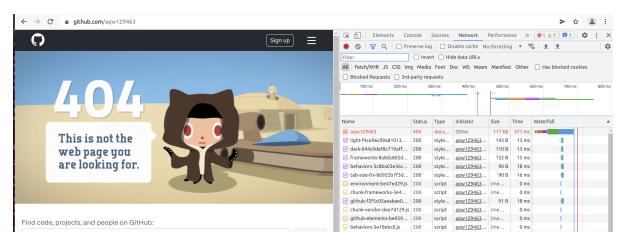




If we enter a URL that GitHub doesn't recognize, we get a page that looks like this:

Most browsers have tools for determining what requests and responses were made. For example, in Chrome, we can use "More Tools -> Developer Tools" from the Customize and Control menu (the three dots in the top-right corner), to open up a panel for introspecting the requests being made.

If we click the "Network" tab and try our request again, we will see something like this:



The top row in red represents the request to https://github.com/aqw1Z9463 and it shows the status code of the response was 404.

6.1.4 REST APIs - Overview

REST (Representational State Transfer) is a way of building APIs for computer programs on the internet leveraging HTTP. In other words, a program on computer 1 interacts with a program on computer 2 by making an HTTP request to it and receiving HTTP responses.

The basic idea with REST is to associate objects in the application domain with URLs, and to use HTTP verbs to represent the actions we want to take on the objects. A REST API has a **base URL** from which all other URLs in that API are formed. For example, the base URL for the GitHub REST API which we will look at in more detail momentarily is https://api.github.com/.

The other URLs in the API are then "collections", typically represented by a plural noun, following the base URL; e.g.:

Or they are specific items in a collection, represented by an identifier following the collection name, e.g.:

```
<base_url>/users/12345
<base_url>/files/test.txt
<base_url>/programs/myapplication
```

Or subcollections or items in subcollections, e.g.:

```
<base_url>/companies/<company_id>/employees
<base_url>/companies/<company_id>/employees/<employee_id>
```

As mentioned, the HTTP verbs represent "operations" or actions that can be taken on the resources:

• GET - list items in a collection or retrieve a specific item in the collection

- POST create a new item in the collection based on the description in the message
- PUT replace an item in a collection with the description in the message
- DELETE delete an item in a collection

Thus,

- GET <base_url>/users would list all users.
- POST <base_url>/users would create a new user.
- PUT <base_url>/users/12345 would update user 12345.
- DELETE <base_url>/users/98765 would delete user 98765.

The combination of an HTTP verb and URL (path) is called an **endpoint** in an API. A REST API is typically comprised of many endpoints. Note that not all HTTP verbs make sense for all URLs. For example, an API would probably not include a PUT

base_url>/users endpoint, because semantically, that would mean updating the entire list of users.

Note: Response messages often make use of some data serialization format standard such as JSON, CSV or XML.

Design Principles. Note that the architecture of REST, combining URL paths that represent *resources* with HTTP verbs that represent *actions* to take on resources, constitutes *abstraction* and *generalization* as a large number of applications can be described in this way.

6.1.5 REST APIs - Additional Simple Examples

Virtually every application domain can be mapped into a REST API architecture. Some examples may include:

Articles in a collection (e.g., on a blog or wiki) with author attributes:

```
<base_url>/articles
<base_url>/articles/<id>
<base_url>/articles/<id>/authors
```

Properties in a real estate database with associated purchase history:

```
<base_url>/properties
<base_url>/properties/<id>
<base_url>/properties/<id>/purchases
```

A catalog of countries, cities and neighborhoods:

```
<base_url>/countries
<base_url>/countries/<country_id>/cities
<base_url>/countries/<country_id>/cities/<city_id>/neighborhoods
```

6.1.6 REST APIs - A Real Example

We have been using GitHub to host our class code repositories. It turns out GitHub provides an HTTP API that is architected using REST (for the most part). We're going to explore the GitHub API.

To begin, open a web browser and navigate to https://api.github.com

You will see something like this:

```
{
 "current_user_url": "https://api.github.com/user",
 "current_user_authorizations_html_url": "https://github.com/settings/connections/
→applications{/client_id}",
 "authorizations_url": "https://api.github.com/authorizations",
 "code_search_url": "https://api.github.com/search/code?q={query}{&page,per_page,sort,
→order}",
 "commit_search_url": "https://api.github.com/search/commits?q={query}{&page,per_page,
⇒sort,order}",
 "emails_url": "https://api.github.com/user/emails",
 "emojis_url": "https://api.github.com/emojis",
 "events_url": "https://api.github.com/events",
 "feeds_url": "https://api.github.com/feeds",
 "followers_url": "https://api.github.com/user/followers",
 "following_url": "https://api.github.com/user/following{/target}",
 "gists_url": "https://api.github.com/gists{/gist_id}",
 "hub_url": "https://api.github.com/hub",
 "issue_search_url": "https://api.github.com/search/issues?q={query}{&page,per_page,
→sort,order}",
 "issues_url": "https://api.github.com/issues",
 "keys_url": "https://api.github.com/user/keys",
 "label_search_url": "https://api.github.com/search/labels?q={query}&repository_id=
→{repository_id}{&page,per_page}",
 "notifications_url": "https://api.github.com/notifications",
 "organization_url": "https://api.github.com/orgs/{org}",
 "organization_repositories_url": "https://api.github.com/orgs/{org}/repos{?type,page,
→per_page,sort}",
 "organization_teams_url": "https://api.github.com/orgs/{org}/teams",
 "public_gists_url": "https://api.github.com/gists/public",
 "rate_limit_url": "https://api.github.com/rate_limit",
 "repository_url": "https://api.github.com/repos/{owner}/{repo}",
 "repository_search_url": "https://api.github.com/search/repositories?q={query}{&page,
→per_page,sort,order}",
  "current_user_repositories_url": "https://api.github.com/user/repos{?type,page,per_
→page,sort}",
 "starred_url": "https://api.github.com/user/starred{/owner}{/repo}",
 "starred_gists_url": "https://api.github.com/gists/starred",
 "topic_search_url": "https://api.github.com/search/topics?q={query}{&page,per_page}",
 "user_url": "https://api.github.com/users/{user}",
 "user_organizations_url": "https://api.github.com/user/orgs",
 "user_repositories_url": "https://api.github.com/users/{user}/repos{?type,page,per_
→page.sort}".
 "user_search_url": "https://api.github.com/search/users?q={query}{&page,per_page,sort,
⊶order}"
}
```

This should look familiar – it's a JSON document, and it describes various collections of endpoints in the GitHub API. For example, we see:

- "events_url": "https://api.github.com/events", Work with GitHub events
- "organization_url": "https://api.github.com/orgs/{org}", Work with GitHub orgs
- "repository_url": "https://api.github.com/repos/{owner}/{repo}", Work with GitHub repos

Many of the endpoints within the GitHub API require *authentication*, i.e., that the requesting application prove its identity – we'll ignore this topic for now and just work with the endpoints that do not require authentication.

Let's discover what the GitHub API can tell us about TACC's GitHub organization, which is just called tacc.

EXERCISE

Based on the information above, how would we retrieve information about the TACC GitHub organization from the API? What HTTP verb and URL would we use?

SOLUTION

We see that the "organization_url" is defined to be "https://api.github.com/orgs/{org}". The use of the {org} notation is common in API documentation – it indicates a variable to be substituted with a value. In this case, we should substitute tacc for {org}, as that is the organization we are interested in.

Since we want to retrieve (or list) information about the TACC organization, the HTTP verb we want to use is GET.

We can use the browser to make this request, as before. If we enter https://api.github.com/orgs/tacc into the URL bar, we should see:

```
"login": "TACC",
"id": 840408,
"node_id": "MDEyOk9yZ2FuaXphdGlvbjg0MDQwOA==",
"url": "https://api.github.com/orgs/TACC",
"repos_url": "https://api.github.com/orgs/TACC/repos",
"events_url": "https://api.github.com/orgs/TACC/events",
"hooks_url": "https://api.github.com/orgs/TACC/hooks",
"issues_url": "https://api.github.com/orgs/TACC/issues",
"members_url": "https://api.github.com/orgs/TACC/members{/member}",
"public_members_url": "https://api.github.com/orgs/TACC/public_members{/member}",
"avatar_url": "https://avatars.githubusercontent.com/u/840408?v=4",
"description": "",
"name": "Texas Advanced Computing Center",
"company": null,
"blog": "http://www.tacc.utexas.edu",
"location": "Austin, TX",
"email": null,
"twitter_username": null,
"is_verified": false,
"has_organization_projects": true,
"has_repository_projects": true,
"public_repos": 152,
"public_gists": 0,
```

(continued from previous page)

```
"followers": 0,
   "following": 0,
   "html_url": "https://github.com/TACC",
   "created_at": "2011-06-09T16:47:08Z",
   "updated_at": "2021-04-07T17:34:55Z",
   "type": "Organization"
}
```

6.1.7 Using Python to Interact with Web APIs

Viewing API response messages in a web browser provides limited utility. We can interact with Web APIs in a much more powerful and programmatic way using the Python requests library.

First install the requests library in your local site-packages on the ISP server using pip3:

```
[user-vm]$ pip3 install --user requests
...
Successfully installed requests-2.25.1
```

You might test that the install was successful by trying to import the library in the interactive Python interpreter:

```
[user-vm]$ python3
Python 3.10.12 (main, Nov 20 2023, 15:14:05) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import requests
>>>
```

The basic usage of the requests library is as follows:

```
>>> # make a request: typical format
>>> # response = requests.<method>(url=some_url, data=some_message, <other options>)
>>>
>>> # e.g. try:
>>> response = requests.get(url='https://api.github.com/orgs/tacc')
>>>
>>> # return the status code:
>>> response.status_code
>>>
>>> # return the raw content
>>> response.content
>>> # return a Python list or dictionary from the response message
>>> response.json()
```

EXERCISE

Let's use requests to explore the GitHub API. Write functions to return the following:

- Given a GitHub organization id, retrieve all information about the organization. Return the information as a Python dictionary.
- Given a GitHub organization id, retrieve a list of all of the members of the organization. Return the list of members as a Python list of strings, where each string contains the member's login (i.e., GitHub username) attribute.
- Given a GitHub organization id, return a list of repositories controlled by the organization. Return the list f repositories as a Python list of strings, where each string contains the repository full_name attribute.

Design Principles. We will use the concept of web APIs in a critical way for developing portable software. As web APIs are accessible to any software running in an environment with a stable internet connection, we can build software components distributed across different computers (and even the entire internet) that work together. The precise locations of the software components won't matter and, when combined with other techniques, we will be able to freely move those components around and still have a fully functioning system.

6.2 Introduction to Flask

In this section, we will get a brief introduction into Flask, the Python web framework, including how to set up a REST API with multiple routes (URLs). After going through this module, students should be able to:

- Install the Python Flask library and import it into a Python program.
- Define and implement various "routes" or API endpoints in a Flask Python program.
- Run a local Flask development server.
- Use curl to test routes defined in their Flask program when the local Flask development server is running.
- **Design Principles**: Additionally, we will see how using Flask contributes to the *modularity*, *abstraction*, and *generalization* of software.

Flask is a Python library and framework for building web servers. Some of the defining characteristics of Flask make it a good fit for this course:

- Flask is small and lightweight relatively easy to use and get setup initially
- Flask is robust a great fit for REST APIs and microservices
- Flask is performant when used correctly, it can handle the traffic of sites with 100Ks of users

6.2.1 What is a Microservice?

Microservices - also known as the microservice architecture - is an architectural style that structures an application as a collection of services that are:

- Highly maintainable and testable
- · Loosely coupled
- · Independently deployable
- Organized around business capabilities

The microservice architecture enables the continuous delivery/deployment of large, complex applications. It also enables an organization to evolve its technology stack. Many heavily-used, well-known sites use microservices including Netflix, Amazon, and eBay.

There is a great article on DevTeam.Space about microservices.

6.2.2 Setup and Installation

The Flask library is not part of the Python standard library but can be installed with standard tools like pip3. In addition to making Flask available to import into a Python program, it will also expose some new command line tools. On your Jetstream VM, perform the following:

```
[user-vm] pip3 install --user flask
Successfully installed flask-3.0.2
[user-vm]$ flask --help
Usage: flask [OPTIONS] COMMAND [ARGS]...
  A general utility script for Flask applications.
  An application to load must be given with the '--app' option, 'FLASK_APP'
  environment variable, or with a 'wsgi.py' or 'app.py' file in the current
  directory.
Options:
                       Load environment variables from this file. python-
  -e, --env-file FILE
                        dotenv must be installed.
                        The Flask application or factory function to load, in
  -A, --app IMPORT
                        the form 'module:name'. Module can be a dotted import
                        or file path. Name is not required if it is 'app',
                        'application', 'create_app', or 'make_app', and can be
                        'name(args)' to pass arguments.
  --debug / --no-debug Set debug mode.
  --version
                        Show the Flask version.
  --help
                        Show this message and exit.
Commands:
  routes Show the routes for the app.
  run
         Run a development server.
  shell
         Run a shell in the app context.
```

Tip: If you aren't already using a virtual environment to help manage your Python libraries, now is a good time to start!

6.2.3 A Hello World Flask App

In a new directory on the class server, create a file called app.py and open it for editing. Enter the following lines of code:

```
from flask import Flask
app = Flask(__name__)

# the next statement should usually appear at the bottom of a flask app
if __name__ == '__main__':
    app.run(debug=True, host='0.0.0.0')
```

On the first line, we are importing the Flask class.

On the third line, we create an instance of the Flask class (called app). This so-called "Flask application" object holds the primary configuration and behaviors of the web server.

Finally, the app.run() method launches the development server. The debug=True option tells Flask to print verbose debug statements while the server is running. The host=0.0.0.0 option instructs the server to listen on all network interfaces; basically this means you can reach the server from inside and outside the host VM.

6.2.4 Run the Flask App

There are a few options when starting the Flask app. For now, we recommend you start your Flask application using the flask run command, specifying the name of the Python file (in our case app.py) using the --app option, and running in debug mode using the --debug flag.

That's it! We now have a server up and running. Some notes on what is happening:

- Note that the program took over our shell; we could put it in the background, but for now we want to leave it in the foreground. (Multiple PIDs are started for the Flask app when started in daemon mode; to get them, find all processes listening on the port 5000 socket with lsof -i:5000).
- If we make changes to our Flask app while the server is running in development mode, the server will detect those changes automatically and "reload"; you will see a log to the effect of Detected change in <file>.
- We can stop the program with Ctrl+C just like any other (Python) program.
- If we stop our Flask programs, the server will no longer be listening and our requests will fail.

Note: The order of the arguments and command is important. Be sure the --app and --debug parameters appear **before** run.

Next we can try to talk to the server using curl. Note this line:

```
* Running on http://127.0.0.1:5000/ (Press CTRL+C to quit)
```

That tells us our server is listening on the localhost - 127.0.0.1, and on the default Flask port, port 5000.

Ports Basics

Ports are a concept from networking that allows multiple services or programs to be running at the same time, listening for messages over the internet, on the same computer.

- For us, ports will always be associated with a specific IP address. In general, we specify a port by combining it with an IP separated by a colon (:) character. For example, 129.114.97.16:5000.
- One and only one program can be listening on a given port at a time.
- Some ports are designated for specific activities; Port 80 is reserved for HTTP, port 443 for HTTPS (encrypted HTTP), but other ports can be used for HTTP/HTTPS traffic.

Note: Only one application can be associated with a given port. If you try to run a second Flask application on the same default port (5000) on the same machine, you will hit errors. You can specify the port you want Flask to listen on using the -p (or --port) option to the flask run command; e.g., flask --app app --debug run -p 5001

curl Basics

You can think of curl as a command-line version of a web browser: it is just an HTTP client.

- The basic syntax is curl <some_base_url>:<some_port>/<some_url_path>. This will make a GET request to the URL and port print the message response.
- Curl will default to using port 80 for HTTP and port 443 for HTTPS.
- You can specify the HTTP verb to use with the -X flag; e.g., curl -X GET <some_url> (though -X GET is redundant because that is the default verb).
- You can set "verbose mode" with the -v flag, which will then show additional information such as the headers passed back and forth (more on this later).

Try the following, for example:

```
[user-vm]$ curl https://api.github.com
```

6.2.5 Make a Request

Because the terminal window running your Flask app is currently locked to that process, the simplest thing to do is open up a new terminal and SSH into the class server again.

To make a request to your Flask app, type the following in the new terminal:

```
[user-vm]$ curl 127.0.0.1:5000
- or -
[user-vm]$ curl localhost:5000
```

You should see something like the following response:

```
<!doctype html>
<html lang=en>
<title>404 Not Found</title>
<h1>Not Found</h1>
The requested URL was not found on the server. If you entered the URL manually please check your spelling and try again.
```

Our server is sending us HTML! It's sending a 404 that it could not find the resource we requested. Although it appears to be an error (and technically it is), this is evidence that the Flask server is running successfully. It's time to add some routes.

6.2.6 Routes in Flask

In a Flask app, you define the URLs in your application using the @app.route decorator. Specifications of the @app.route decorator include:

- Must be placed on the line before the declaration of a Python function.
- Requires a string argument which is the path of the URL (not including the base URL)
- Takes an argument methods which should be a list of strings containing the names of valid HTTP methods (e.g. GET, POST, PUT, DELETE)

When the URL + HTTP method combination is requested, Flask will call the decorated function.

Tangent: What is a Python Decorator?

A decorator is a function that takes another function as an input and extends its behavior in some way. The decorator function itself must return a function which includes a call to the original function plus the extended behavior. The typical structure of a decorator is as follows:

```
def my_decorator(some_func):

    def func_to_return():

    # extend the behavior of some_func by doing some processing
    # before it is called (optional)
    do_something_before()

# call the original function
    some_func(*args, **kwargs)

# extend the behavior of some_func by doing some processing
    # after it is called (optional)
    do_something_after()

return func_to_return
```

As an example, consider this test program:

```
def print_decorator(f):
    def func_to_return(*args, **kwargs):
        print(f'args: {args}; kwargs: {kwargs}')
        (continues on next page)
```

(continues on next page)

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Our @print_decorator decorator gets executed automatically when we call foo(2). Without the decorator, the final output would be:

```
Got the result: 3
```

By using the decorator, however, the final output is instead:

```
args: (2,); kwargs: {}
return: 3
Got the result: 3
```

6.2.7 Define the Hello World Route

The original Flask app we wrote above (in app.py) did not define any routes. Let's define a "hello world" route for the base URL. Meaning if someone were to curl against the base URL (/) of our server, we would want to return the message "Hello, world!". To do so, add the following lines to your app.py script:

```
from flask import Flask

app = Flask(__name__)

def proute('/', methods=['GET'])
def hello_world():
    return 'Hello, world!\n'

# the next statement should usually appear at the bottom of a flask app
if __name__ == '__main__':
    app.run(debug=True, host='0.0.0.0')
```

The @app.route decorator on line 5 is expecting GET requests at the base URL /. When it receives such a request, it will execute the hello_world() function below it.

In your active SSH terminal, execute the curl command again (you may need to restart the Flask app); you should see:

```
[user-vm]$ curl localhost:5000/
Hello, world!
```

6.2.8 Routes with URL Parameters

Flask makes it easy to create routes (or URLs) with variables in the URL. The variable name simply must appear in angled brackets (<>) within the @app.route() decorator statement. Then, specify the variable as a parameter to the actual function.

For example, the following would grant the function below it access to a variable called year:

```
@app.route('/<year>', methods=[...])
def f(year):
    # function implementation...
```

In the next example, we extend our app.py Flask app by adding a route with a variable (<name>):

```
from flask import Flask
   app = Flask(__name__)
   @app.route('/', methods=['GET'])
   def hello_world():
6
       return 'Hello, world!\n'
   @app.route('/<name>', methods=['GET'])
   def hello_name(name):
10
       return f'Hello, {name}!\n'
12
   # the next statement should usually appear at the bottom of a flask app
13
   if __name__ == '__main__':
14
       app.run(debug=True, host='0.0.0.0')
```

Now, the Flask app supports multiple routes with different functionalities:

```
[user-vm]$ curl localhost:5000/
Hello, world!
[user-vm]$ curl localhost:5000/joe
Hello, joe!
[user-vm]$ curl localhost:5000/jane
Hello, jane!
```

EXERCISE

Let's use the sample Meteorite Landing data (see here) to define some more interesting routes. We will create a route that allows a user to download the entire dataset over HTTP. Consider the following:

- What should the name of our function be?
- What URL path should it respond to?
- What HTTP verb(s) should it handle?

Once those questions are answered, we'll need to actually implement the new route function. What will we need to do to implement the function? The implementation will require two steps:

- 1) Read the data into Python from the JSON file. (What Python library will you use for this step?)
- 2) Return the result of step 1)

Once implemented, test the function using curl.

Next, write one more route to access the information of a specific meteorite. In REST API parlance, assume the whole data set is a "collection", and the data from one meteorite is an "item" of that collection.

6.2.9 Additional Resources

· Flask Docs

6.3 Advanced Flask

We continue using Flask in this module with a look at more complex endpoints and data retrieval functions for our REST API. After going through this module, students should be able to:

- · Identify valid and invalid Flask route return types
- Convert unsupported types (e.g. int) to valid Flask route return types
- Extract Content-Type and other headers from Flask route responses
- · Add query parameters to GET requests, and extract their values inside Flask routes
- Deal with errors from user-supplied input to an API and handle Python exceptions
- Handle multiple request methods to support CRUD operations

Note: We will continue to work on the the individual student VMs. Like last time, it will be helpful for you to have two SSH terminals open to your VM at the same time so you can run your Flask application in one terminal and test it in the other.

6.3.1 Defining the URLs of Our API

One of our first goals for our API will be to provide an interface to a dataset. Since the URLs in a REST API are defined by the "nouns" or collections of the application domain, we can use a noun that represents our data.

For example, suppose we have the following dataset that represents the number of students earning an undergraduate degree for a given year:

In this case, one collection described by the data is "degrees". So, let's define a route, /degrees, that by default returns all of the data points.

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EXERCISE 1

Create a new file, degrees_api.py to hold a Flask application then do the following:

- 1) Import the Flask class and instantiate a Flask application object.
- 2) Add code so that the Flask server is started when this file is executed directly by the Python interpreter.
- 3) Copy the get_data() method above into the application script.
- 4) Add a route (/degrees) which responds to the HTTP GET request and returns the complete list of data returned by get_data().

In a separate Terminal use curl to test out your new route. Does it work as expected?

Tip: Refer back to the Intro to Flask material if you need help remembering the boiler-plate code.

EXERCISE 2

Back inside the degrees_api.py file, let's add a second route, /degrees/<id> that returns the data associated with a single dictionary. There are often design questions one should consider when writing new code. In this case, we have:

- What method(s) should it accept?
- What type will the incoming id field be from the user?
- How will you find the corresponding dictionary?
- What should happen if the user enters an id that doesn't exist?

Discussion

By default, Flask uses String for the types of path variables. If we use a route declaration like this,

```
@app.route('/degrees/<id>', methods=['GET'])
def degrees_for_id(id):
    # implementation...
```

Then GET any request with a URL path that starts with /degrees/ and ends with any string will match. That is,

- /degress/0 -> id holds the value "0" as a Python String.
- /degrees/A -> id holds the value "A" as a Python String.
- /degrees/one -> id holds the value "one" as a Python String.

will all match the degrees_for_id route and the variable, id will hold a str value. In this case, we'll have to deal with the str type in our function, converting it to int, etc.

6.3.2 Typed URL Parameters

We can specify the types of the URL parameters we are expecting using the syntax <type:variable_name>. For example, we could change our degrees_for_id route declaration as follows, to indicate we required the id variable to be an integer:

```
@app.route('/degrees/<int:id>', methods=['GET'])
def degrees_for_id(id):
    # implementation...
```

With the above definition, a request like GET /degrees/A will no longer match our degrees_for_id route while a request like GET /degrees/2 will call degrees_for_id with an integer type for the id variable.

Here is a summary of the types supported in Flask; see the docs for more details.

Table 1: Type Support in Flask URL Path Parameters

Туре	Support
string	(default) accepts any text without a slash
int	accepts positive integers
float	accepts positive floating point values
path	like string but also accepts slashes
uuid	accepts UUID strings

Warning: The numeric types, int and float do not accept negative values!

EXERCISE 3

Modify your degrees_for_id route to specify an integer path parameter.

6.3.3 Responses in Flask

Suppose we wanted to add a third route that just returns a single value, the number of degrees associated with a a particular dictionary. We might proceed as follows:

- For the URL path, use /degrees/<int:id>/degrees
- Iterate through the list looking for the dictionary with the same id as the input.
- If we find a dictionary, d, with the same id, return d['degrees'].

Let's try that and see what happens.

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EXERCISE 4

Implement a new route for the /degrees/<int:id>/degrees endpoint. Does it work as you expect?

If you tried to return the integer object, d['degrees'] directly in your route function definition, you got an error when you tried to request it with curl. A long stack trace is returned, but at the end you will see:

TypeError: The view function did not return a valid response. The return type must be a string, dict, list, tuple with headers or status, Response instance, or WSGI callable, but it was a int.

Flask allows you four options for creating responses:

- 1) Return a string (str) object
- 2) Return a dictionary (dict) or list list object
- 3) Return a tuple (tuple) object in particular form we'll return to this later.
- 4) Return a flask. Response object

Some notes:

- Option 1 is good for text or html such as when returning a web page or text file.
- Option 2 is good for returning rich information in JSON format.
- Option 3 is good for returning additional information including headers and status code.
- Option 4 gives you the most flexibility, as it allows you to customize the headers and other aspects of the response.

For our REST API, we will want to return JSON-formatted data. Flask will handle all of this for us, so long as we return a list or dictionary.

Tip: Refer back to the Working with JSON material for a primer on the JSON format and relevant JSON-handling methods.

6.3.4 Returning JSON (and Other Kinds of Data)

You probably are thinking at this point we can fix our solution to Exercise 4 by changing the return type. Instead of returning a raw integer, we can return a type that Flask recognized. What type should we return?

EXERCISE 5

Update your code from Exercise 4 to return a Python type that Flask accepts. Then, with your API server running in one window, open a Python interactive session in another window and:

- Make a GET request to your /degrees URL and capture the response in a variable, say r
- Verify that r.status_code is what you expect (what do you expect it to be?)
- Verify that r.content is what you expect.
- Use r.json() to decode the response and compare the type to that of r.content.

Then, repeat the above with the /degrees/<id>/degrees endpoint.

6.3.5 HTTP Content Type Headers

Requests and responses have headers which describe additional metadata about them. Headers are key:value pairs (much like dictionary entries). The key is called the header name and the value is the header value.

There are many pre-defined headers for common metadata such as specifying the size of the message (Content-Length), the domain the server is listening on (Host), and the type of content included in the message (Content-Type).

We can use curl or the Python requests library to see all of the headers returned on a response from our Flask server. Let's try it.

EXERCISE 6

- 1) Use curl to make a GET request to your /degrees endpoint and pass the -v (for "verbose") option. This will show you additional information, including the headers. Note that with -v, curl shows headers on both the request and the response. Request headers are lines that start with a > while response headers are lines that start with a <.
- 2) Use curl again to make the same request, but this time pass the --head option instead of the -v; this will show you **only** the headers being returned in the response.
- 3) Inside a Python shell, use requests to make the same GET request to your /degrees endpoint, and capture the result in a variable, r. Inspect the r.headers attribute. What is the type of r.headers?

```
[user-vm] curl localhost:5000/degrees -v
* Trying 127.0.0.1:5000...
* TCP_NODELAY set
* Connected to localhost (127.0.0.1) port 5000 (#0)
> GET /degrees HTTP/1.1
> Host: localhost:5000
> User-Agent: curl/7.68.0
> Accept: */*
* Mark bundle as not supporting multiuse
< HTTP/1.1 200 OK
< Server: Werkzeug/2.2.2 Pvthon/3.8.10
< Date: Sun, 12 Feb 2023 16:42:55 GMT
< Content-Type: application/json
< Content-Length: 303
< Connection: close
<
```

```
>>> import requests
>>>
>>> response = requests.get('http://127.0.0.1:5000/degrees')
>>>
>>> response.headers
{'Server': 'Werkzeug/2.2.2 Python/3.8.10', 'Date': 'Sun, 12 Feb 2023 16:41:23 GMT',
'Content-Type': 'application/json', 'Content-Length': '49', 'Connection': 'close'}
```

We see that we are sending a Content-Type of 'application/json', which is what we want. That is how the Python requests library is able to provide the r.json() function to automatically convert to a Python list or dictionary.

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Media Type (or Mime Type)

The allowed values for the Content-Type header are the defined **media types** (formerly, **mime types**). The main thing you want to know about media types are that they:

- Consist of a type and subtype
- The most common types are application, text, audio, image, and multipart
- The most common values (type and subtype) are application/json, application/xml, text/html, audio/mpeg, image/png, and multipart/form-data

6.3.6 Query Parameters

The HTTP specification allows for parameters to be added to the URL in form of key=value pairs. Query parameters come after a ? character and are separated by & characters; for example, the following request to a hypothetical API:

```
GET https://api.example.com/degrees?limit=3&offset=2
```

passes two query parameters: limit=3 and offset=2. Note that the URL path in the example above is still /degrees; that is, the ? character terminates the URL path, and any characters that follow create the query parameter set for the request.

In REST architectures, query parameters are often used to allow clients to provide additional, optional arguments to the request.

Common uses of query parameters in RESTful APIs include:

- Pagination: specifying a specific page of results from a collection
- Search terms: filtering the objects within a collection by additional search attributes
- Other parameters that might apply to most if not all collections such as an ordering attribute (ascending vs descending)

Extracting Query Parameters in Flask

Flask makes the query parameters available on the request.args object, which is a "dictionary-like" object. To work with the query parameters supplied on a request, you must import the Flask request object, and use the args.get method to extract the passed query parameter into a variable.

Note: The flask.request object is different from the Python requests library we used to make http requests. the flask.request object represents the incoming request that our flask application server has received from the client.

For example, consider the following line of Python code:

```
start = request.args.get('start')
```

In this case, the start variable will be the value of the start parameter if one is passed, or it will be None otherwise.

Note: request.args.get() will always return a string, regardless of the type of data being passed in.

EXERCISE 7

Implement the start query parameter on your GET /degrees endpoint and check the behavior by issuing some curl requests in another window, e.g.,

```
[user-vm]$ curl http://api.example.com/degrees?start=1993
```

Let's use this idea to update our degrees_api to only return the years starting from the start query parameter year, if that parameter is provided.

Solution

To implement a start query parameter on the GET /degrees endpoint that only returns data for years on or after the start year, we first might write something like the following:

```
@app.route('/degrees', methods=['GET'])
def degrees():
    start = request.args.get('start')
    data = get_data()
    # iterate through data and check if years are >= start...
```

However, there are a couple of issues here:

- 1. The user may not provide a start query parameter, in which case our start variable will be None.
- 2. If the user does provide a start query parameter, it will be a string type, which cannot be compared to an integer year.

Here is a first approach to fixing it:

```
from flask import Flask, request

@app.route('/degrees', methods=['GET'])

def degrees():
    # provide a default value that is less than all the years and
    start = int(request.args.get('start', 0))

data = get_data()
    result = []

for d in data:
    if d['year'] >= start:
        result.append(d)
    return result
```

6.3.7 Error Handling

However, there is one more problem with our solution above: What happens if the user enters a non-numeric value for the start parameter? Try it and see what happens:

```
[user-vm]$ curl http://127.0.0.1:5000/degrees?start=abc
```

Yikes! If we try this we get a long traceback that ends like this:

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```
File "/home/ubuntu/test/degrees_api.py", line 26, in degrees2
  start = int(request.args.get('start', 0))
ValueError: invalid literal for int() with base 10: 'abc'
```

Checking User Input

If we get a request like this, in the best case, the user didn't understand what kind of data to put in the start query parameter; in the worst case, they were intentionally trying to send our program bad data to break it. We should always be very careful with user-supplied data and make sure it contains the kind of data we expect.

So, what is it we expect from the start query parameter? At a minimum, it needs to be some kind of integer data, because we are casting it to the int type. Therefore, at a minimum, we should check if it is an integer.

We can use the Python isnumeric() method on a Python string to test whether a string contains non-negative integer data

Let's try some examples in the Python shell:

```
>>> '123'.isnumeric()
True
>>> 'abc'.isnumeric()
False
>>> '1.23'.isnumeric()
False
>>> '-1'.isnumeric()
False
```

Now, let's fix our route function; we can check if it is numeric before casting to an int. If it is not numeric, we can return an error message to the user.

```
def degrees():
    start = request.args.get('start', 0)
    if not start.isnumeric():
        return "Error: start must be an integer\n"
    start = int(start)
    data = get_data()
    result = []
    for d in data:
        if d['year'] >= start:
            result.append(d)
    return result
```

Exceptions

Using the <code>isnumeric()</code> function allowed us to check for invalid user input in the specific case above, but Python provides a far more general and powerful error handling capability, called Exceptions. Refer back to the unit on Error Handling for reference.

Here's how we could deal with an invalid start parameter provided by the user using exceptions:

```
try:
    start = int(start)
except ValueError:
    # return some kind of error message...

# at this point in the code, we know the int(start) "worked" and so we are safe
# to use it as an integer..
```

Here is the full code for our route function with exception handling.

```
@app.route('/degrees', methods=['GET'])
   def degrees():
2
       start = request.args.get('start', 0)
       try:
4
           start = int(start)
       except ValueError:
6
           return "Invalid start parameter; start must be an integer."
       data = get_data()
       result = []
       for d in data:
10
           if d['year'] >= start:
               result.append(d)
12
       return result
```

Warning: When curling a URL with multiple query parameters separated by an & symbol, make sure to put the URL in quotes, e.g.:

```
curl 'http://127.0.0.1:5000/degrees?start=1990&limit=2'
```

EXERCISE 8

Add support for a limit parameter to the code you wrote for Exercise 7. The limit parameter should be optional. When passed with an integer value, the API should return no more than limit data points.

6.3.8 CRUD Operations

To this point, we have looked at only the GET method. There are three other methods that are important to learn when working with REST APIs - PUT, POST, and DELETE. Collectively, these four methods perform **CRUD** operations on our data:

- Create: POST add a new item to a collection
- Read: GET get an item from a collection
- Update: PUT edit an existing item in a collection

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• Delete: DELETE - delete an item from a collection

To implement one of these methods into a Flask route, the method first must be listed in the decorator. Then, the function below the decorator must contain some logic to act according to the method and request. The Flask request library again comes in handy here. Suppose we want to add a DELETE method to our /degrees route. Consider the following reduced code:

```
from flask import Flask, request
2
   app = Flask(__name___)
   data = [ {'id': 0, 'year': 1990, 'degrees': 5818},
             {'id': 1, 'year': 1991, 'degrees': 5725},
             {'id': 2, 'year': 1992, 'degrees': 6005},
6
             {'id': 3, 'year': 1993, 'degrees': 6123},
             {'id': 4, 'year': 1994, 'degrees': 6096} ]
   @app.route('/degrees', methods=['GET', 'DELETE'])
10
   def degrees():
11
       global data
12
       if request.method == 'GET':
           return(data)
14
       elif request.method == 'DELETE':
15
           content = request.get_json()
16
           new_data = []
           for item in data:
18
                if item['id'] != content['id']:
19
                    new_data.append(item)
20
           data = new_data
21
           return(data)
22
23
   if __name__ == '__main__':
24
       app.run(debug=True, host='0.0.0.0')
25
```

Note that data is now declared at the beginning of the script rather than returned via a function call. And, on line 12 we use the global keyword to indicate that references to data within the degrees() function (including changes) should be made to the variable which belongs to the global scope.

Curling this route with a GET request returns the entire list of degrees:

```
[user-vm]$ curl http://127.0.0.1:5000/degrees
-or-
[user-vm]$ curl -X GET http://127.0.0.1:5000/degrees
```

But now we are able to make a DELETE request to this route, where it is expecting to receive a JSON data packet containing the id of the item to delete:

The important changes here are that we are now specifying a delete request (-X DELETE) instead of the default get request, the header (-H) flag is used to indicate that we are sending some data in JSON format ('Content-Type: application/json'), and finally the data packet that we send is just plain JSON (-d '{"id": 4}').

After invoking this delete request, perform another GET request on the /degrees URL to see what has changed.

EXERCISE 9

Add support for the PUT and POST methods to your /degrees route. What information should be sent in the JSON data packet? What exception handling should be performed in the route?

6.3.9 Additional Resources

- Flask JSON support
- Flask query parameter support

6.4 Containerizing Flask

As we have discussed previously, Docker containers are critical to packaging an application along with all of its dependencies, isolating it from other applications and services, and deploying it in a consistent and reproducible way across different platforms.

Here, we will walk through the process of containerizing a Flask application with Docker, and then using curl to interact with it as a containerized microservice. After going through this module, students should be able to:

- · Assemble the different components needed for a containerized microservice into on directory.
- Establish and document requirements (e.g. dependencies, Python packages) for the project.
- Build and run in the background a containerized Flask microservice.
- Map ports on the Jetstream VM to ports inside a container, and use curl with the the correct ports to make requests to and generate responses from the microservice.
- Deploy the microservice with docker-compose
- **Design Principles:** By combining Flask and Docker, we will see how both contribute to the *modularity*, *portability*, *abstraction*, and *generalization* of software (all four major design principles).

6.4.1 Organize Your App Directory

First, create a new directory for this exercise, and change directories to it:

```
[user-vm]$ mkdir flask-container && cd flask-container
[user-vm]$ pwd
/home/ubuntu/flask-container
```

Then, create a new app.py (or copy an existing one) into this folder. It should have the following contents:

```
from flask import Flask

app = Flask(__name__)

@app.route('/', methods = ['GET'])
def hello_world():
    return 'Hello, world!\n'

@app.route('/<name>', methods = ['GET'])
def hello_name(name):
```

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```
return f'Hello, {name}!\n'

if __name__ == '__main__':
    app.run(debug=True, host='0.0.0.0')
```

6.4.2 Specify Requirements

The Python package manager pip can utilize a text file for managing package dependencies of your application. It is standard practice to to capture the required libraries and packages for a project in a file called requirements.txt. For our example here, create a file called requirements.txt and add the following line:

```
Flask==3.0.2
```

This indicates that our project requires the Flask package, version number 3.0.2. You can specify your requirements in more lenient ways – for example, we could have put Flask>=3.0.2 to indicate that any version greater than or equal to 3.0.2 would work, or we could have even put Flask with no version indicating we don't care what version of Flask is installed.

Note:

- Specifying a package, such as Flask as a dependency instructs pip to install Flask *and all of its dependencies*. Those dependencies could in turn have dependencies, etc., and pip will take care of installing all of those.
- Specifying the exact version improves the odds that your application will work correctly because the packages that get installed will be the versions you specified. Therefore, it is usually best to specify the exact version of the library your application requires.

6.4.3 Build a Docker Image

As we saw in a previous section, we write up the recipe for our application installation process in a Dockerfile. Create a file called Dockerfile for our Flask microservice and add the following lines:

```
FROM python:3.9

RUN mkdir /app

WORKDIR /app

COPY requirements.txt /app/requirements.txt

RUN pip install -r /app/requirements.txt

COPY app.py /app/app.py

ENTRYPOINT ["python"]

CMD ["app.py"]
```

Here we see usage of the Docker ENTRYPOINT and RUN instructions, which essentially specify a default command (python app.py) that should be run when an instance of this image is instantiated.

Note also that we copied the requirements.txt file before copying the full current working directory. Why did we do that?

The answer has to do with how Docker caches image layers. We could have written the following instead:

```
FROM python:3.9

RUN mkdir /app
WORKDIR /app
COPY . /app
RUN pip install -r /app/requirements.txt

ENTRYPOINT ["python"]
CMD ["app.py"]
```

The above is actually shorter; i.e., fewer lines of code in the Dockerfile.

However, with the above approach, Docker is going to re-run the command pip install -r /app/requirements. txt every time there is any change to the contents of the current working directory (i.e., any time we change our app code or any other files). This is not a big deal with a small requirements.txt file and only a few packages to install, but as the requirements.txt file gets bigger, the time to install all the packages can be significant.

As a general rule of thumb, put more expensive (in term of time) operations whose are less likely to change at the beginning of your Dockerfile to maximize the value of the Docker image layer cache.

Save the file and build the image with the following command:

```
[user-vm]$ docker build -t username/flask-helloworld:1.0 .
```

6.4.4 Run a Docker Container

To create an instance of your image (a "container"), use the following command:

The -d flag detaches your terminal from the running container - i.e. it runs the container in the background. The -p flag maps a port on the Jetstream VM (5000, in the above case) to a port inside the container (again 5000, in the above case). In the above example, the Flask app was set up to use the default port inside the container (5000), and we can access that through our specified port on Jetstream (5000). This explicit mapping is convenient if you have multiple services running on the same VM and you want to avoid port collisions.

Check to see that things are up and running with:

```
[user-vm]$ docker ps -a
```

The list should have a container with the name you gave it, an UP status, and the port mapping that you specified.

If the above is not found in the list of running containers, try to debug with the following:

```
[user-vm]$ docker logs "your-container-name"
-or-
[user-vm]$ docker logs "your-container-ID"
```

6.4.5 Access Your Microservice

Now for the payoff - you can use curl to interact with your Flask microservice by specifying the correct port on the ISP server. Following the example above, which was using port 5000:

```
[user-vm]$ curl localhost:5000/
Hello, world!
[user-vm]$ curl localhost:5000/Joe
Hello, Joe!
```

6.4.6 Clean Up

Finally, don't forget to stop your running container and remove it.

```
CONTAINER ID
               IMAGE
                                               COMMAND
                                                                                  STATUS _
                                                                  CREATED
         PORTS
                                                      NAMES
                                               "python app.py"
a785237628d6
              username/flask-helloworld:1.0
                                                                  4 minutes ago
                                                                                  Up 4
minutes 0.0.0.0:5000->5000/tcp, :::5000->5000/tcp flask-helloworld-app
[user-vm] $ docker stop a785237628d6
a785237628d6
[user-vm] $ docker rm a785237628d6
a785237628d6
```

EXERCISE

Containerize your Flask degrees app from last week:

- 1. Create a Dockerfile for your app
- 2. Build the image from the Dockerfile
- 3. Run the server locally and test the endpoints using curl

6.4.7 Docker Compose, Revisited

Using the docker run command to start containers is OK for simple commands, but as we started to see in the previous material, the commands can get long pretty quickly. It can be hard to remember all of the flags and options that we want to use when starting our containers.

Moreover, so far we have been looking at single-container applications. But what if we want to do something more complex involving multiple containers? In this course, our goal is to ultimately develop and orchestrate a multi-container application consisting of, e.g., a Flask app, a database, a message queue, an authentication service, and more.

6.4.8 Write a Compose File

Docker compose works by interpreting rules declared in a YAML file (typically called docker-compose.yml). The rules we will write will replace the docker run commands we have been using, and which have been growing quite complex. Recall from the past exercise that the command we were using to start our Flask application container looked like the following:

The above docker run command can be translated into a YAML file. Navigate to the folder that contains your Python scripts and Dockerfiles, then create a new empty file called docker-compose.yml:

```
[user-vm]$ pwd
/home/ubuntu/flask-contaienr
[user-vm]$ touch docker-compose.yml
[user-vm]$ ls
Dockerfile app.py docker-compose.yaml requirements.txt
```

Next, open up docker-compose.yml with your favorite text editor and type / paste in the following text:

```
version: "3"

services:
flask-app:
build:
context: ./
dockerfile: ./Dockerfile

image: username/flask-helloworld:1.0
container_name: flask-helloworld-app
ports:
- "5000:5000"
```

Note: Be sure to update the highlighted line above with your username.

The version key must be included and simply denotes that we are using version 3 of Docker compose.

The services section defines the configuration of individual container instances that we want to orchestrate. In our case, we define just one container called flask-app. We can use any allowable name for the services we defined, but each name should be unique within the docker-compose.yml file.

The flask-app service is configured with its own Docker image, including a reference to a Dockerfile to be used to build the image, a recognizable name for the running container, and a port mapping for the Flask service. Recall from the previous unit that other speicifications can be defined in this file including a list of mounted volumes, user IDs for running the service, default commands, and many others. The choice of which options to use entirely depends on the app and the context.

Note: The top-level services keyword shown above is just one important part of Docker compose. Later in this course we will look at named volumes and networks which can be configured and created with Docker compose.

6.4.9 Running Docker Compose

To run our Flask application container, we simply use the docker-compose up verb, which will start up all containers defined in the file. Alternatively, we could use docker-compose run and pass the name of a service to run, in this case, flask-app:

```
[user-vm]$ docker-compose up
Creating network "flask-container_default" with the default driver
Creating flask-helloworld-app ... done
Attaching to flask-helloworld-app
flask-helloworld-app | * Serving Flask app 'app'
flask-helloworld-app | * Debug mode: on
flask-helloworld-app | WARNING: This is a development server. Do not use it in a_____production deployment. Use a production WSGI server instead.
flask-helloworld-app | * Running on all addresses (0.0.0.0)
flask-helloworld-app | * Running on http://127.0.0.1:5000
flask-helloworld-app | * Running on http://172.23.0.2:5000
flask-helloworld-app | * Restarting with stat
flask-helloworld-app | * Debugger is active!
flask-helloworld-app | * Debugger PIN: 109-459-387
```

Note that docker-compose starts the container in the foreground and takes over our terminal. If we use Ctrl+C we will stop the container. We can see confirm that the container is stopped using the docker ps -a command:

```
[user-vm] docker ps -a

CONTAINER ID IMAGE COMMAND CREATED STATUS.

→ PORTS NAMES

289ea2d0fed6 username/flask-helloworld:1.0 "python app.py" 32 seconds ago Exited.

→ (0) 4 seconds ago flask-helloworld-app
```

To start the service in the background, use the -d flag:

```
[user-vm]$ docker-compose up -d
```

Once the service is running, perform some curl commands to test the running Flask app before stopping the service with:

```
[user-vm]$ docker-compose down
```

6.4.10 Essential Docker Compose Command Summary

Command	Usage
docker-compose version	Print version information
docker-compose config	Validate docker-compose.yml syntax
docker-compose up	Spin up all services
docker-compose down	Tear down all services
docker-compose build	Build the images listed in the YAML file
docker-compose run	Run a container as defined in the YAML file

6.4.11 Additional Resources

Docker Compose Docs

6.5 Flask Special Topics

6.5.1 Writing Unit Tests for Flask

There are several different approaches for writing *unit tests* for Flask apps, some of which are included in the Flask documentation. The approach I like the best, and which is most congruent with the topics we already covered in this class, is to instead write *integration tests*.

For these tests, the key thing is that you have to have an actual copy of your Flask server running. Then, the tests will perform requests.get() to the various routes and you can evaluate the output. Be careful to make sure that your tests are independent of the data, which may change over time. The job of these unit tests is not to check / validate that the right data is being returned; rather, the goal is to make sure the routes work and return the right kind of response.

If your code also has standalone functions separate from the functions decorated as Flask routes, (e.g., in the case of the ISS data you may have written standalone functions for finding the time closest to now or computing average speed that are called from other functions), then you would still want to import those and test them as normal in your unit test file.

Consider the following pytest snippet that tests the /epochs and /epochs/epoch> routes for the ISS tracker:

```
import pytest
import requests

response1 = requests.get('http://127.0.0.1:5000/epochs')
a_representative_epoch = response1.json()[0]
response2 = requests.get('http://127.0.0.1:5000/epochs/'+a_representative_epoch)

def test_epochs_route():
    assert response1.status_code == 200
    assert isinstance(response1.json(), list) == True

def test_specific_epoch_route():
    assert response2.status_code == 200
    assert isinstance(response2.json(), dict) == True
```

These lines may need to be modified depending on the format of data returned by your API. And, as mentioned above, it assumes these tests are performed when your API is already running.

6.5.2 Reverse Proxy with ngrok

Up to now, our Flask apps have been isolated to their host hardware. What if we want to access our Flask apps from outside our host hardware? A utility called ngrok can be used to provide a reverse proxy on the fly.

Note: To do this, you need an ngrok account and access token, which can be obtained here

First, install ngrok:

Confirm ngrok is working and add your access token:

```
[user-vm]$ ngrok --help
NAME:
  ngrok - tunnel local ports to public URLs and inspect traffic
...
[user-vm]$ ngrok config add-authtoken <TOKEN>
Authtoken saved to configuration file: /home/ubuntu/.config/ngrok/ngrok.yml
```

Assuming you have a Flask app running on localhost and port 5000, then do the following:

```
[user-vm]$ ngrok http http://localhost:5000
```

This will lock your terminal into an interface that looks like the following:

```
ngrok
K8s Gateway API https://ngrok.com/early-access/kubernetes-gateway-api
Session Status
                               online
Account
                               username (Plan: Free)
Version
                               3.8.0
Region
                               United States (us)
Latency
                               37ms
Web Interface
                               http://127.0.0.1:4040
Forwarding
                               https://9750-129-141-63-209.ngrok-free.app -> http://
→localhost:5000
Connections
                               ttl
                                       opn
                                               rt1
                                                       rt5
                                                                p50
                                                                        p90
```

Navigate to or curl the link provided to access your Flask app from outside the Jetstream VM. Press Ctrl+C to quit forwarding.

6.5.3 Flask and HTML

Flask has the ability to render HTML templates that contain a mix of static data and variables (for run-time dynamic data). The route you write will take the template from a predefined location, inject any variables, and render it into a final HTML document to return to the client.

In your Flask project directory, create a folder called templates and add the following HTML document as example. html. It uses Jinja syntax for injecting dynamic data ({{name}}):

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```
</head>
<body>
     <h1>Hello, {{name}}!</h1>
     This file should be stored in the "templates" folder as "example.html"
</body>
</html>
```

Then, adapt the /<name> Flask route to return that HTML document using Flask's render_template() method. The old version of the route which returns a plain string is also provided as reference.

```
from flask import Flask, render_template
2
   app = Flask(__name__)
   @app.route('/<name>', methods=['GET'])
   def hello_name(name):
       return render_template('example.html', name=name)
   ### For reference, this is the /<name> route without render_template
   # @app.route('/<name>', methods=['GET'])
10
   # def hello_name(name):
11
         return f'Hello, {name}!\n'
12
13
   if __name__ == '__main__':
14
       app.run(debug=True, host='0.0.0.0')
15
```

6.5.4 Additional Resources

- Ngrok
- Flask Templates

UNIT 7: DATABASES, PERSISTENCE, AND REDIS

In this unit, we will implement a Redis database to store our data sets such that they persist beyond the lifetime of our application containers. We will also learn how to query our data from within a Python script, and connect our containerized Flask API with a containerized Redis database.

7.1 Introduction to Databases and Persistence

Application data that lives inside a container is ephemeral - it only persists for the lifetime of the container. We can use databases to extend the life of our application (or user) data, and even access it from outside the container.

After going through this module, students should be able to:

- Explain the differences between SQL and NoSQL databases
- Choose the appropriate type of database for a given application / data set
- Start and find the correct port for a Redis server
- · Install and import the Redis Python library
- · Add data to and retrieve data from a Redis database from a Python script
- **Design Principles:** Separating the database service from the application container is a great example illustrating the *modularity* design principle.

7.1.1 What Is Our Motivation?

In this unit, we will begin the work to extend our Flask API to enable users to query and analyze data in our data sets. We want to expose this functionality through our Flask API, but there is an issue: the analysis to be performed may take "a long time" to compute, longer than the acceptable time window for an HTTP request/response cycle. We need a way to coordinate the work of computing the analysis in a separate Python program from our Flask API. The database will play a central role.

Our basic approach will be:

- 1. Our dataset will be stored in a database.
- 2. The user submits a request to a Flask endpoint describing some sort of analysis they wish to perform on the data.
- 3. We will create a separate Python program to perform the analysis. This program will retrieve the desired data from the database and store the final results in the database.
- 4. The Flask API will determine the status of the analysis by querying the database, and it will retrieve the final results of the analysis from the database to serve to the user when they are ready.

There are a lot of details to fill in over the course of the rest of the semester, but for now we are going to focus on getting data into and out of a database.

7.1.2 Intro to Databases

What is a database?

- A database is an organized collection of structured information, or data, typically stored electronically in a computer system.
- Databases provide a **query language** a small, domain-specific language for interacting with the data. The query language is not like a typical programming language such as Python or C++; you cannot create large, complex programs with it. Instead, it is intended to allow for easy, efficient access to the data.

Why use a database?

- Our data needs permanence and we want to be able to stop and start our Flask API without losing data.
- We want multiple Python processes to be able to access the data at the same time, including Python processes that may be running on different computers.

Why not use a file?

- It is not easy to make a file accessible to Python processes on different computers / VMs.
- When multiple processes are reading from and writing to a file, race conditions can occur.
- With files, our Flask API would have to implement all the structure in the data.

Databases sometimes get classified into two broad categories: SQL databases (also called relational databases) and NoSQL databases.

7.1.3 SQL Databases

Structured Query Language (SQL) is a language for managing structured or relational data, where certain objects in the dataset are related to other objects in a formally or mathematically precise way. SQL is the language used when working with a relational database. You will often see SQL database technologies referred to as Relational Database Management Systems (RDBMS).

The SQL language is governed by an ISO standard, and relational databases are among the most popular databases in use today. SQL was originally based on a strong, theoretical framework called the Relational Model (and related concepts). However, today's SQL has departed significantly from that formal framework.

Popular open-source RBDMS include:

- MySQL
- Postgres
- Sqlite

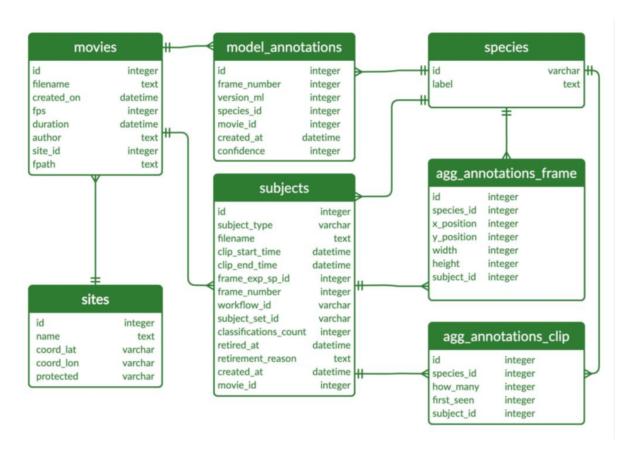


Fig. 1: Example of a relational database. Source1

7.1.4 NoSQL Databases

As the name implies, a NoSQL database is simply a database that does not use SQL. There are many different types of NoSQL databases, including:

- · Time series databases
- Document stores
- · Graph databases
- Simple key-value stores (like the one we will use in this class)

In some ways, it is easier to say what a NoSQL database isn't than what it is; some of the key attributes include:

- NoSQL databases do NOT use tables (data structured using rows and columns) connected through relations
- NoSQL databases store data in "collections", "logical databases", or similar containers
- NoSQL databases often allow for missing or different attributes on objects in the same collection
- Objects in one collection do not relate or link to objects in another collection
- For example, the objects themselves could be JSON objects without a pre-defined schema

Phone directory

Key	Value
Paul	(091) 9786453778
Greg	(091) 9686154559
Marco	(091) 9868564334

MAC table

Key	Value
10.94.214.172	3c:22:fb:86:c1:b1
10.94.214.173	00:0a:95:9d:68:16
10.94.214.174	3c:1b:fb:45:c4:b1

Fig. 2: Example of a key-value database. Source2

SQL vs NoSQL

Comparing SQL and NoSQL is an apples to oranges comparison.

- Both SQL and NoSQL databases have advantages and disadvantages.
- The *primary* deciding factor should be the *shape* of the data and the requirements on the integrity of the data. In practice, many other considerations could come into play, such as what expertise the project team has.
- Also consider how the data may change over time, and how important is the relationship between the different types of data being stored.
- SQL databases "enforce" relationships between data types, including one-to-one, one-to-many, and many-to-many. When the integrity of the data is important, SQL databases are a good choice.
- In many NoSQL databases, the relationship enforcement must be programmed into the application. This can be error-prone and can increase the development effort needed to build the application. On the other hand, this can allow the database to be used for use cases where relationship enforcement is not possible.
- SQL databases historically cannot scale to the "largest" quantities of data because of the ACID (Atomicity, Consistency, Isolation, Durability) guarantees they make (though this is an active area of research).
- NoSQL databases trade ACID guarantees for weaker properties (e.g., "eventual consistency") and greater scalability. It would be difficult to scale a relational database to contain the HTML of all websites on the internet or even all tweets ever published.

For the projects in this class, we are going to use Redis, a simple (NoSQL) "data structure" store. There are a few reasons for this choice:

- We need a flexible data model, as the structure of the data we will store in the database will be changing significantly over the course of the semester.
- We need a tool that is quick to learn and simple to use. This is not a databases course, and learning the SQL language would take significantly more time than we can afford.
- Redis can also easily be used as a task queue, which we will make use of in the asynchronous programming unit.

7.1.5 Redis

Redis is a very popular NoSQL database and "data structure store" with lots of advanced features including:

Note: Before going any further, let's play around with Redis a little bit in a browser: https://try.redis.io/ Try the commands SET, GET, HSET, HGET, KEYS, HKEYS

Key-Value Store

Redis provides key-value store functionality:

- The items stored in a Redis database are structured as key:value objects.
- The primary requirement is that the key be unique across the database.
- A single Redis server can support multiple databases, indexed by an integer.
- The data itself can be stored as JSON.

Notes about Keys

Redis keys have the following properties/requirements:

- Keys are often strings, but they can be any "binary sequence".
- Long keys can lead to performance issues.
- A format such as <object_type>:<object_id> is a good practice.

Notes on Values

- Values are typed; some of the primary types include:
 - Binary-safe strings
 - Lists (sorted collections of strings)
 - Sets (unsorted, unique collections of strings)
 - Hashes (maps of fields with associated values; both field and value are type string)
- There is no native "JSON" type; to store JSON, one can use an encoding and store the data as a binary-safe string, or one can use a hash and convert the object into and out of JSON.
- The basic string type is a "binary-safe" string, meaning it must include an encoding.
 - In Python terms, the string is stored and returned as type bytes.

- By default, the string will be encoded with UTF-8, but we can specify the encoding when storing the string.
- Since bytes are returned, it will be our responsibility to decode using the same encoding.

Hash Maps

- · Hashes provide another way of storing dictionary-like data in Redis
- The values of the keys are type string

7.1.6 Running Redis

To use Redis on your Jetstream VMs, we must have an instance of the Redis server running. We will use a containerized version of Redis that we each need to pull from Docker Hub:

```
# start the Redis server on the command line:

[user-vm]$ docker run -p 6379:6379 redis:7

1:C 27 Feb 2024 03:53:38.154 * o000000000000 Redis is starting o00000000000

1:C 27 Feb 2024 03:53:38.154 * Redis version=7.2.4, bits=64, commit=00000000, modified=0, pid=1, just started

1:C 27 Feb 2024 03:53:38.154 # Warning: no config file specified, using the default. config. In order to specify a config file use redis-server /path/to/redis.conf

1:M 27 Feb 2024 03:53:38.154 * monotonic clock: POSIX clock_gettime

1:M 27 Feb 2024 03:53:38.155 * Running mode=standalone, port=6379.

1:M 27 Feb 2024 03:53:38.156 * Server initialized

1:M 27 Feb 2024 03:53:38.156 * Ready to accept connections tcp
```

The Redis server is up and available on port **6379**. Although we could use the Redis CLI to interact with the server directly, in this class we will focus on the Redis Python library so we can interact with the server from our Python scripts.

Warning: Pause for a minute to think about why we are running redis:7. In the terminal output, it looks like the actual version of Redis is version=7.2.4. What do you need to know about semantic versioning in order to future-proof your code?

To interact with this Redis server, open up another terminal and install the Redis Python library:

```
[user-vm]$ pip3 install --user redis
```

Then open up an interactive Python interpreter to connect to the server:

```
[user-vm]$ python3
Python 3.10.12 (main, Nov 20 2023, 15:14:05) [GCC 11.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

```
>>> import redis
>>>
>>> rd=redis.Redis(host='127.0.0.1', port=6379, db=<some integer>)
>>>
>>> type(rd)
<class 'redis.client.Redis'>
```

You've just created a Python client object to the Redis server called rd. This object has methods for adding, modifying, deleting, and analyzing data in the database instance, among other things.

Some quick notes:

- We are using the IP of the gateway (127.0.0.1) on our localhost and the default Redis port (6379).
- Redis organizes collections into "databases" identified by an integer index. Here, we are specifying db=<some integer>; if that database does not exist it will be created for us.

7.1.7 Working with Redis

We can create new entries in the database using the .set() method. Remember, entries in a Redis database take the form of a key:value pair. For example:

```
>>> rd.set('my_key', 'my_value')
True
```

This operation saved a key in the Redis server (db=0) called my_key and with value my_value. Note the method returned True, indicating that the request was successful.

We can retrieve it using the .get() method:

```
>>> rd.get('my_key')
b'my_value'
```

Note that b'my_value' was returned; in particular, Redis returned binary data (i.e., type bytes). The string was encoded for us (in this case, using Unicode). We could have been explicit and set the encoding ourselves. The bytes class has a .decode() method that can convert this back to a normal string, e.g.:

```
>>> rd.get('my_key')
b'my_value'
>>> type(rd.get('my_key'))
<class 'bytes'>
>>>
>>> rd.get('my_key').decode('utf-8')
'my_value'
>>> type( rd.get('my_key').decode('utf-8') )
<class 'str'>
```

7.1.8 Redis and JSON

A lot of the information we exchange comes in JSON or Python dictionary format. To store pure JSON as a binary-safe string value in a Redis database, we need to be sure to dump it as a string (json.dumps()):

```
>>> import json
>>> d = {'a': 1, 'b': 2, 'c': 3}
>>> rd.set('k1', json.dumps(d))
True
```

Retrieve the data again and get it back into JSON / Python dictionary format using the json.loads() method:

```
>>> rd.get('k1')
b'{"a": 1, "b": 2, "c": 3}'
>>> type(rd.get('k1'))
<class 'bytes'>
>>>
>>> json.loads(rd.get('k1'))
{'a': 1, 'b': 2, 'c': 3}
>>> type(json.loads(rd.get('k1')))
<class 'dict'>
```

Note: In some versions of Python, you may need to specify the encoding as we did earlier, e.g.:

```
>>> json.loads(rd.get('k1').decode('utf-8'))
{'a': 1, 'b': 2, 'c': 3}
```

Hashes

Hashes provide another way of storing dictionary-like data in Redis.

- Hashes are useful when different fields are encoded in different ways; for example, a mix of binary and unicode data.
- Each field in a hash can be treated with a separate decoding scheme, or not decoded at all.
- Use hset() to set a single field value in a hash or to set multiple fields at once.
- Use hget() to get a single field within a hash or to get all of the fields.

```
# set multiple fields on a hash
>>> rd.hset('k2', mapping={'name': 'Joe', 'email': 'wallen@tacc.utexas.edu'})

# set a single field on a hash
>>> rd.hset('k2', 'type', 'instructor')

# get one field
>>> rd.hget('k2', 'name')
b'Joe'

# get all the fields in the hash
>>> rd.hgetall('k2')
{b'name': b'Joe', b'email': b'wallen@tacc.utexas.edu', b'type': b'instructor'}
```

Tip: You can use rd.keys() to return all keys from a database, and rd.hkeys(key) to return the list of keys within hash 'key', e.g.:

```
>>> rd.hkeys('k2')
[b'name', b'email', b'type']
```

EXERCISE 1

Save the Meteorite Landings data (i.e., the Meteorite_Landings.json file from Unit 2/3) into Redis. Each landing data point should be stored as a single Redis object. Think about what data type you want to use in Redis for storing the data.

If needed, you can download the JSON file with the following command:

\$ wget https://raw.githubusercontent.com/TACC/coe-332-sp24/main/docs/unit02/sample-data/

→Meteorite_Landings.json

EXERCISE 2

Check that you stored the data correctly:

- Check the total number of keys in your Redis database against the total number of objects in the JSON file.
- Read all of the landing objects out of Redis and check that each object has the correct fields.

EXERCISE 3

- Exit the Python interactive interpreter or kill the Python script that is running your Redis client. In a new Python session, re-establish the Redis client. What is in the database?
- Now kill the Redis container. Start the Redis container again. What is in the database?

7.1.9 Additional Resources

- Redis Docs
- · Redis Python Library
- Try Redis in a Browser
- Semantic Versioning

7.2 Redis and Flask

Now that we have gained some experience with starting a containerized Redis service and interacting with that service from a simple Python script, it is time to integrate it into a larger software project. We will next learn how to mount a host volume inside the Redis container in order to persist the database, incorporate the Redis service into our Docker compose files, and interact with the Redis service from our Flask apps. After going through this module, students should be able to:

- Mount a host volume inside a Redis container to save data between restarts of Redis itself.
- Pass an argument into the Redis container to influence the saving behavior.
- Connect to a Redis container from within a Flask application.
- Incorporate a Redis service into a Docker compose file.
- **Design Principles:** Separating the database service from the application container is a great example illustrating the *modularity* design principle.

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7.2.1 Recap: Start a Redis Container

Recall from last time when we started a Redis container and mapped port 6379 inside the container to port 6379 on the host. This allows us to interact with the Redis server on that port.

```
# start the Redis server on the command line:

[user-vm]$ docker rum -p 6379:6379 redis:7

1:C 27 Feb 2024 03:53:38.154 * o000000000000 Redis is starting o00000000000

1:C 27 Feb 2024 03:53:38.154 * Redis version=7.2.4, bits=64, commit=00000000, modified=0, pid=1, just started

1:C 27 Feb 2024 03:53:38.154 # Warning: no config file specified, using the default. config. In order to specify a config file use redis-server /path/to/redis.conf

1:M 27 Feb 2024 03:53:38.154 * monotonic clock: POSIX clock_gettime

1:M 27 Feb 2024 03:53:38.155 * Running mode=standalone, port=6379.

1:M 27 Feb 2024 03:53:38.156 * Server initialized

1:M 27 Feb 2024 03:53:38.156 * Ready to accept connections tcp
```

The above command will start the Redis container in the foreground which can be helpful for debugging, seeing logs, etc. However, it may also be useful to start it in the background (detached or daemon mode). You can do that by adding the -d flag:

```
[user-vm]$ docker run -d -p 6379:6379 redis:7
3a28cb265d5e09747c64a87f904f8184bd8105270b8a765e1e82f0fe0db82a9e
```

At this point, Redis is running and available from your host. Double check this is true by executing docker ps -a. Let's explore the persistence of the data in Redis.

We can open a Python shell, connect to our Redis container, and add some data:

```
>>> import redis
>>> rd = redis.Redis(host='127.0.0.1', port=6379, db=0)

# create some data
>>> rd.set('k', 'v')
True

# check that we can read the data
>>> rd.get('k')
```

If we exit our Python shell and then go into a new Python shell and connect to Redis, what do we see?

```
>>> import redis
>>> rd = redis.Redis(host='127.0.0.1', port=6379, db=0)
# previous data is still there
>>> rd.get('k')
b'v'
```

Great! Redis has persisted our data across Python sessions. That was one of our goals. But what happens if we shut down the Redis container itself? Let's find out by killing our Redis container and starting a new one.

```
# start a new redis container
[user-vm]$ docker run -d -p 6379:6379 redis:7
```

Now go back into the Python shell and connect to Redis:

```
>>> import redis
>>> rd = redis.Redis(host='127.0.0.1', port=6379, db=0)

# previous data is gone!
>>> rd.get('k')

# no keys at all!
>>> rd.keys()
[]
```

All the data that was in Redis is gone. The problem is we are not permanently persisting the Redis data across different Redis containers. But wasn't that the whole point of using a database? Are we just back to where we started?

Actually, we only need a few small changes to the way we are running the Redis container to make the Redis data persist across container executions.

7.2.2 Modifications Required to Support Data Persistence

Container Bind Mounts

A container bind mount (or just "mount" for short) is a way of replacing a file or directory in a container image with a file or directory on the host file system in a running container.

Bind mounts are specified with the -v flag to the docker run statement. The full syntax is

where:

- <host_path> and <container_path> are absolute paths in the host and container file systems, and
- <mode> can take the value of ro for a read-only mount and rw for a read-write mount.

Note: Note that mode is optional and defaults to read-write.

It is important to keep the following in mind when using bind mounts:

- If the container image originally contained a file or directory at the <container_path> these will be replaced entirely by the contents of <host_path>.
- If the container image did not contain contents at <container_path> the mount will still succeed and simply create a new file/directory at the path.
- If the <mode> is read-write (the default), any changes made by the running container will be reflected on the host file system. Note that the process running in the container still must have permission to write to the path.
- If <host_path> does not exist on the host, Docker will create a **directory** at the path and mount it into the container. **This may or may not be what you want.**

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Save Data to File Periodically

We can use bind mounts to persist Redis data across container executions: the key point is that Redis can be started in a mode such that it periodically writes all of its data to the host.

From the Redis documentation, we see that we need to set the --save flag when starting Redis so that it writes its dataset to the file system periodically. The full syntax is:

```
--save <frequency> <number_of_backups>
```

where <frequency> is an integer, in seconds. We'll instruct Redis to write its data to the file system every second, and we'll keep just one backup.

Entrypoints and Commands in Docker Containers

Let's take a moment to revisit the difference between an entrypoint and a command in a Docker container image. When executing a container from an image, Docker uses both an entrypoint and an (optional) command to start the container. It combines the two using concatenation, with entrypoint first, followed by command.

When we use docker run to create and start a container from an existing image, we can choose to override either the command or the entrypoint that may have been specified in the image. Any string <string> passed after the <image> in the statement:

```
[user-vm]$ docker run <options> <image> <string>
```

will override the command specified in the image, but the original entrypoint set for the image will still be used.

A common pattern when building Docker images is to set the entrypoint to the primary program, and set the command to a default set of options or parameters to the program.

Consider the following simple example of a Dockerfile:

```
FROM ubuntu
ENTRYPOINT ["ls"]
CMD ["-1"]
```

If we build and tag this image as test/ls, then:

```
# run with the default command, equivalent to "ls -1"
[user-vm]$ docker run --rm -it test/ls
total 48
lrwxrwxrwx 1 root root
                           7 Jan 5 16:47 bin -> usr/bin
drwxr-xr-x 2 root root 4096 Apr 15 2020 boot
drwxr-xr-x 5 root root 360 Mar 23 18:37 dev
drwxr-xr-x 1 root root 4096 Mar 23 18:37 etc
drwxr-xr-x 2 root root 4096 Apr 15 2020 home
# override the command, but keep the entrypoint; equivalent to running "ls -a" (note the
\rightarrow lack of "-1")
[user-vm]$ docker run --rm -it test/ls -a
    .dockerenv
                    boot etc lib
                                       lib64
                                               media opt
                                                            root sbin sys
                                                                            usr
                     dev home lib32 libx32 mnt
   bin
                                                      proc run
                                                                  srv
                                                                        tmp
                                                                             var
```

(continues on next page)

```
# override the command, specifying a different directory
[user-vm]$ docker run --rm -it test/ls -la /root
total 16
drwx----- 2 root root 4096 Jan 5 16:50 .
drwxr-xr-x 1 root root 4096 Mar 23 18:38 ..
-rw-r--r- 1 root root 3106 Dec 5 2019 .bashrc
-rw-r--r- 1 root root 161 Dec 5 2019 .profile
```

Modifying the Command in the Redis Container

The official redis container image provides an entrypoint which starts the redis server (check out the Dockerfile if you are interested.).

Since the save option is a parameter, we can set it when running the redis server container by simply appending it to the end of the docker run command; that is,

```
[user-vm]$ docker run <options> redis:7 --save <options>
```

7.2.3 Bring it All Together for a Complete Solution

With save, we can instruct Redis to write the data to the file system, but we still need to save the files across container executions. That's where the bind mount comes in. But how do we know which directory to mount into Redis? Fortunately, the Redis documentation tells us what we need to know: Redis writes data to the /data directory in the container.

Putting all of this together, we can update the way we run our Redis container as follows:

```
[user-vm]$ docker run -d -p 6379:6379 -v </path/on/host>:/data redis:7 --save 1 1
```

Tip: You can use the \$PWD shortcut for the present working directory.

For example, I might use:

```
[user-vm]$ docker run -d -p 6379:6379 -v $PWD/data:/data:rw redis:7 --save 1 1
```

Now, Redis should be periodically writing all of its state to the data directory. You should see a file called dump.rdb in the directory because we are using the default persistence mechanism for Redis. This will suffice for our purposes, but Redis has other options for persistence which you can read about here if interested.

EXERCISE 1

Test out persistence of your Redis data across Redis container restarts by starting a new Redis container using the method above, saving some data to it in a Python shell, shutting down the Redis container and starting a new one, and verifying back in the Python shell that the original data is still there.

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7.2.4 Using Redis in Flask

Using Redis in our Flask apps is identical to using it in the Python shells that we have been using to explore with. We simply create a Python Redis client object using the redis.Redis() constructor. Since we might want to use Redis from different parts of the code, we'll create a function for generating the client:

```
def get_redis_client():
    return redis.Redis(host='127.0.0.1', port=6379, db=0)

rd = get_redis_client()
```

Then, within the function definitions for your routes, use the rd client to set or get data as appropriate, e.g.:

```
@app.route('/get-keys', methods=['GET'])
def get_keys():
    return rd.keys()
```

EXERCISE 2

In the last module, we wrote some code to put the Meteorite Landings data (i.e., the Meteorite_Landings.json file from Unit 2/3) into Redis. In this exercise, let's turn this function into a Flask API with one route that handles POST, GET, and DELETE requests.

- Use /data as the URL path for the one route.
- A POST request to /data should load the Meteorite Landings data into Redis.
- A GET request to /data should read the data out of Redis and return it as a JSON list.
- A DELETE request to /data should delete the Meteorite Landings data from Redis.

Access the Meteorite Landings data at this link1

A sample template for the Flask app can be found at this link2

7.2.5 Docker Compose

We now have two services to consider: Flask and Redis. We need to launch one container for Flask, and a separate container for Redis. Each service requires a long list of options to the docker run command, and it would be convenient to launch them as a unit. This is where the concept of container orchestration really starts to become useful.

Consider the following update to your Docker compose file from Unit 5:

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```
flask-app:
    build:
        context: ./
        dockerfile: ./Dockerfile

depends_on:
        - redis-db
    image: username/ml_flask_app:1.0
    ports:
        - 5000:5000
```

One thing to note is a new specification under the flask-app service called 'depends_on'. This ensures that the redis-db service is up before starting the flask-app service. Why might this be important?

Another question to ask yourself is why does the redis-db service omit the build specification? Should we provide a context and Dockerfile for Redis?

One slight modification to the Flask app is required to enable container-to-container communication over the Docker bridge network. Instead of using an IP address like '127.0.0.1' or an alias like 'localhost', use the docker-compose alias for the Redis service, redis-db. Specifically, in your containerized Flask app, establish a Redis client like:

```
rd = redis.Redis(host='redis-db', port=6379, db=0)
```

Given the above, try launching both services using the following command:

```
[user-vm] $ docker-compose up -d
Creating network "redis_default" with the default driver
Creating redis_flask-app_1 ... done
Creating redis_redis-db_1 ... done
[user-vm] $ docker ps -a
CONTAINER ID
              IMAGE
                                           COMMAND
                                                                     CREATED
→ STATUS
                 PORTS
                                                             NAMES
                                           "docker-entrypoint.s..."
d266fbd99e4c
             redis:7
                                                                      3 seconds ago
                                                                                       Up_
              0.0.0.0:6379->6379/tcp, :::6379->6379/tcp
                                                          redis_redis-db_1
→2 seconds
                                           "python3 /ml_flask_a..."
193f057687a8
              username/ml_flask_app:1.0
                                                                      3 seconds ago
                                                                                       Up_
                                                          redis_flask-app_1
→2 seconds
              0.0.0.0:5000->5000/tcp, :::5000->5000/tcp
```

You should see the containers running. When you are ready to kill the services:

```
[user-vm]$ docker-compose down
Stopping redis_redis-db_1 ... done
Stopping redis_flask-app_1 ... done
Removing redis_redis-db_1 ... done
Removing redis_flask-app_1 ... done
Removing network redis_default
[user-vm]$ docker ps -a
```

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EXERCISE 3

- Launch both services using Docker compose
- Query the appropriate route to POST the ML data, and ensure that it is in the database
- Take all services back down and ensure both containers have stopped running
- Launch both services again using Docker compose
- Query the appropriate route to see if the data is still in the database

Redis Python API Cheat Sheet

Command	Effect
import redis	Import Redis library
rd = redis.Redis()	Create a redis client, defaults to (host=localhost, port=6379, db=0)
rd.set('k', 'v')	Set key k to value v
rd.get('k')	Get value associated with k
rd.hset('k1', 'k2', 'v')	Set key k1 to hash value k2:v
<pre>rd.hset('k1', mapping=d)</pre>	Set key k1 to hash value d, where d is a Python dictionary
rd.hget('k1', 'k2')	Get value associated with k2 in hash stored at k1
rd.hgetall('k1')	Get all key / value pairs in hash stored at k1
rd.keys()	Return list of keys
rd.delete('k')	Delete key / value pair associated with key k

7.2.6 Additional Resources

- Redis Docs
- Redis Python Library
- Try Redis in a Browser
- Semantic Versioning

UNIT 8: ASYNCHRONOUS PROGRAMMING

In this unit, we will discuss *Asynchronous Programming*, a method for computer programs (like our web apps) to handle multiple tasks simultaneously. We will introduce the concepts of concurrency, queues, and messaging systems to achieve our goal of adding a "long running" job functionality to our Flask API projects. We will also write a series of functions (the "Jobs API") to help us create, manage, and process tasks submitted by users.

8.1 Concurrency and Queues

We begin with an introduction to the concept of concurrency and a basic treatment of the queue data structure. By the end of this module, students should be able to:

- Describe concurrency and some basic examples of concurrent and nonconcurrent algorithms.
- Explain at a high level how concurrency will be used to implement a long-running task in our flask-based API system.
- Utilize Python in-memory queues as well as the hotqueue library to work with queues in Redis.
- **Design Principles.** The integration of a queue into our APIs will demonstrate the principle of abstraction (removing the laborious and time consuming functionality of our code from our API interface).

8.1.1 Motivation

Our Flask API is useful because it can return information about objects in our database, and in general, looking up or storing objects in the database is a very "fast" operation, on the order of a few 10s of milliseconds. However, many interesting and useful operations are not nearly as quick to perform. They are many examples from both research computing and industrial computing where the computations take much longer; for example, on the order of minutes, hours, days or even longer.

Examples include:

- Executing a large mathematical model simulating a major weather event such as a hurricane, or an astronomical process such as galaxy formation
- Aligning a set of genomic sequence fragments to a reference genome
- Running the payroll program at the end of the month to send checks to all employees of a large enterprise.
- Sending a "welcome back" email to every student enrolled at the university at the start of the semester.

We want to be able to add functionality like this to our API system. We'd like to provide a new API endpoint where a user could describe some kind of long-running computation to be performed and have our system perform it for them. But there are a few issues:

- The HTTP protocol was not built for long-running tasks, and most programs utilizing HTTP expect responses "soon", on the order of a few seconds. Many programs have hard timeouts around 30 or 60 seconds.
- The networks on which HTTP connections are built can be interrupted (even just briefly) over long periods of time. If a connection is severed, even for a few milliseconds, what happens to the long-running computation?
- Long-running tasks like the ones above can be computationally intensive and require a lot of computing resources. If our system becomes popular (even with a single, enthusiastic user), we may not be able to keep up with demand. We need to be able to throttle the number of computations we do.

To address these challenges, we will implement a "Jobs API" as an *asynchronous* endpoint. Over the next few lectures, we will spell out precisely what this means, but for now, we'll give a quick high-level overview as motivation. Don't worry about understanding all the details here.

8.1.2 Jobs API – An Introduction

The basic idea is that we will have a new endpoint in our API at a path /jobs (or something similar). A user wanting to have our system perform a long-running task will create a new job. We will use RESTful semantics, so the user will create a new job by making an HTTP POST request to /jobs, describing the job in the POST message body (in JSON).

However, instead of performing the actual computation, the Jobs API will simply record that the user has requested such a computation. It will store that in Redis and immediately respond to the user. So, the response will not include the result of the job itself but instead it will indicate that the request has been received and it will be worked on in due time. Also, and critically, it will provide an id for the job that the user can use to check the status later and, eventually, get the actual result.

So, in summary:

- 1. User makes an HTTP POST to /jobs to create a job.
- 2. Jobs API validates that the job is a valid job, creates an id for it, and stores the job description with the id in Redis.
- 3. Jobs API responds to the user immediately with the id of the job it generated.
- 4. In the background, *some other Python program* we write (referred to as a "worker") will, at some point in the future, actually start the job and monitor it to completion.

This illustrates the *asynchronous* and *concurrent* nature of our Jobs API, terms we will define precisely in the sequel. Intuitively, you can probably already imagine what we mean here – multiple jobs can be worked on at the same time by different instances of our program (i.e., different workers), and the computation happens asynchronously from the original user's request.

8.1.3 Concurrency and Queues

A computer system is said to be *concurrent* if multiple agents or components of the system can be in progress at the same time without impacting the correctness of the system.

While components of the system are in progress at the same time, the individual operations themselves may happen sequentially. In general, a system being concurrent means that the different components can be executed at the same time or in different orders without impacting the overall correctness of the system.

There are many techniques for making programs concurrent; we will primarily focus on a technique that leverages the *queue* data structure. But first, an example.

A First Example

Suppose we want to build a system for maintaining the balance of a bank account where multiple agents are acting on the account (withdrawing and/or depositing funds) at the same time. We will consider two different approaches.

Approach 1. Whenever an agent receives an order to make a deposit or withdraw, the agent does the following steps:

- 1. Makes a query to determine the current balance.
- 2. Computes the new balance based on the deposit or withdraw amount.
- 3. Makes a query to update the balance to the computed amount.

This approach is not concurrent because the individual operations of different agents cannot be reordered.

For example, suppose we have:

- Two agents, agent A and agent B, and a starting balance of \$50.
- Agent A gets an order to deposit \$25 at the same time that agent B gets an order to withdraw \$10.

In this case, the final balance should be \$65 (=\$50 + \$25 - \$10).

The system will arrive at this answer as long as steps 1, 2 and 3 for one agent are done before any steps for the other agent are started; for ex, A1, A2, A3, B1, B2, B3.

However, if the steps of the two agents are mixed then the system will not arrive at the correct answer.

For example, suppose the steps of the two agents were performed in this order: A1, A2, B1, B2, A3, B3. What would the final result be? The listing below shows what each agents sees at each step.

- A1. Agent A determines the current balance to be \$50.
- A2. Agent A computes a new balance of \$50 + \$25 = \$75.
- B1. Agent B determines the current balance to be \$50.
- B2. Agent B computes a new balance of \$50 \$10 = \$40.
- A3. Agent A updates the balance to be \$75.
- B3. Agent B updates the balance to be \$40.

In this case, the system will compute the final balance to be \$40! Hopefully this is not your account! We will explore an alternative approach that is concurrent, but to do that we first need to introduce the concept of a queue.

Queues

A queue is data structure that maintains an ordered collection of items. The queue typically supports just two operations:

- Enqueue (aka "put") add a new item to the queue.
- Dequeue (aka "get") remove an item from the queue.

Items are removed from a queue in First-In-First-Out (FIFO) fashion: that is, the item removed from the first dequeue operation will be the first item added to the queue, the item removed from the second dequeue operation will be the second item added to the queue, and so on.

Sometimes queues are referred to as "FIFO Queues" for emphasis.

Basic Queue Example

Consider the set of (abstract) operations on a Queue object.

Enqueue 5
 Enqueue 7
 Enqueue A
 Dequeue 5
 Enqueue 4
 Dequeue 8
 Dequeue 8

The order of items returned is:

```
5, 7, A
```

And the contents of the Queue after Step 8 is

```
\begin{bmatrix} 1, & 4 \end{bmatrix}
```

In-memory Python Queues

The Python standard library provides an in-memory queue data structure via its queue module. To get started, import the queue module and instantiate a queue.Queue object:

```
>>> import queue
>>> q = queue.Queue()
```

The Python Queue object has the following features:

- The q object supports .put() and .get() to put a new item on the queue, and get an item off the queue, respectively
- q.put() can take an arbitrary Python object and q.get() returns a Python object from the queue.

Let's perform the operations above using the q object.

EXERCISE 1

Use a series of q.put() and q.get() calls to perform Steps 1-8 above. Verify the the order of items returned.

EXERCISE 2

Verify that arbitrary Python objects can by put onto and retrieved from the queue by inserting a list and a dictionary. Queues are a fundamental ingredient in concurrent programming, a topic we will turn to next.

A Concurrent Approach to our Example

Approach 2. Whenever an agent receives an order to make a withdraw or deposit, the agent simply writes the order to a queue; a positive number indicates a deposit while a negative number indicates a withdraw. The account system keeps a running "balancer" agent whose only job is to read items off the queue and update the balance.

This approach is concurrent because the order of the agents' steps can be mixed without impacting the overall result. This fact essentially comes down to the commutativity of addition and subtraction operations: i.e., 50 + 25 - 10 = 50 - 10 + 25.

Note that the queue of orders could be generalized to a "queue of tasks" (transfer some amount from account A to account B, close account C, etc.).

8.1.4 Queues in Redis

The Python in-memory queues are very useful for a single Python program, but we ultimately want to share queues across multiple Python programs/containers.

The Redis DB we have been using can also be used to provide a queue data structure for clients running in different containers. The basic idea is:

- Use a Redis list data structure to hold the items in the queue.
- Use the Redis list operations rpush, 1pop, 11en, etc. to create a queue data structure.

For example:

- rpush will add an element to the end of the list.
- 1pop will return an element from the front of the list, and return nothing if the list is empty.
- 11en will return the number of elements in the list.

Fortunately, we don't have to implement the queue ourselves, but know that if we needed to we could without too much effort.

Using the HotQueue Library

We will leverage a small, open source Python library called hotqueue which has already implemented a version of the queue data structure in Redis using the approach outlined above. Besides not having to write it ourselves, the use of hotqueue will afford us a few additional features which we will look at later.

Here are the basics of the hotqueue library:

- Hotqueue is not part of the Python standard library; you can install it with pip install hotqueue
- Creating a new queue data structure or connecting to an existing queue data structure is accomplished by creating a HotQueue object.
- Constructing a HotQueue object takes very similar parameters to that of the Redis but also takes a name attribute. The HotQueue object ultimately provides a connection to the Redis server.
- Once constructed, a HotQueue object has .put() and .get() methods that act just like the corresponding methods of an in-memory Python queue.

A HotQueue Example

We will work this example using containers on the Jetstream VMs. You will just need a Redis container running that is exposing port 6379. You will either need to do this in the background (-d), or you will need to open up a second terminal.

Start a Python interactive shell and create the hotQueue.Queue object. What value should you put in for the Redis IP address?

```
>>> from hotqueue import HotQueue
>>> q = HotQueue("queue", host="<Redis_IP>", port=6379, db=1)
```

Note how similar the HotQueue() instantiation is to the Redis instantiation. In the example above we named the queue queue (not too creative), but it could have been anything.

Note: In the definition above, we have set db=1 to ensure we don't interfering with the main data of your Flask app.

Now we can add elements to the queue using the .put(); just like with in-memory Python queues, we can put any Python object into the queue:

```
>>> q.put(1)
>>> q.put('abc')
>>> q.put(['1', 2, {'key': 'value'}, True])
```

We can check the number of items in queue at any time using the len built in:

```
>>> len(q)
3
```

And we can remove an item with the .get() method; remember - the queue follows a FIFO principle:

```
>>> q.get()
1
>>> len(q)
2
>>> q.get()
'abc'
>>> len(q)
1
```

Under the hood, the hotqueue. Queue is just a Redis object, which we can verify using a redis client:

```
>>> import redis
>>> rd = redis.Redis(host="<Redis IP>", port=6379, db=1)
>>> rd.keys()
[b'hotqueue:queue']
```

Note that the queue is just a single key in the Redis server (db=1).

And just like with other Redis data structures, we can connect to our queue from additional Python clients and see the same data.

EXERCISE 3

In a second terminal, start a second Python interactive session. In that session, import hotqueue, and establish a connection to the same Redis container. Prove to yourself that you can add items to the queue in one terminal and retrieve items from the queue in the other terminal. This represents a form of "communication" between two Python programs.

8.1.5 Additional Resources

• HotQueue

8.2 Messaging Systems

The Queue is a powerful data structure which forms the foundation of many concurrent design patterns. Often these design patterns center around passing messages between agents within the concurrent system. We will explore one of the simplest and most useful of these message-based patterns - the so-called "Task Queue". By the end of this module, students should be able to:

- Describe the components of a task queue system, and explain how it will be utilized within our Flask-based API system architecture.
- Create task queues in Redis using the hotqueue library, and work with the put() and consume() methods to queue and receive messages across two Python programs.
- Use the @q.worker decorator in hotqueue to create a simple Python consumer program.
- Explain the general approach to organizing Python code into different modules and describe how to do this for the flask-based API system we are building.
- Implement good code organization practices including denoting objects as public or private.

8.2.1 Task Queues

In a task queue system,

- Agents called "producers" write messages to a queue that describe work to be done.
- A separate set of agents called "consumers" receive the messages and do the work. While work is being done, no new messages are received by the consumer.
- Each message is delivered exactly once to a single consumer to ensure no work is "duplicated".
- Multiple consumers can be processing "work" messages at once, and similarly, 0 consumers can be processing messages at a given time (in which case, messages will simply queue up).

The Task Queue pattern is a good fit for our jobs service.

- Our Flask API will play the role of producer.
- One or more "worker" programs will play the role of consumer.
- Workers will receive messages about new jobs to execute and performing the analysis steps.

8.2.2 Task Queues in Redis

The HotQueue class provides two methods for creating a task queue consumer; the first is the .consume() method and the second is the @q.worker decorator.

The Consume Method

With a q object defined like $q = HotQueue('queue', host='<Redis_IP>', port=6379, db=1)$, the consume method works as follows:

- The q.consume() method returns an iterator which can be looped over using a for loop (much like a list).
- Each object returned by the iterator is a message received from the task queue.
- The q.consume() method blocks (i.e., waits indefinitely) when there are no additional messages in the queue arbitrarily named queue.

The basic syntax of the consume method is this:

```
for item in q.consume():
    # do something with item
```

In this case, the item object is the message that was retrieved from the task queue.

EXERCISE 1

Complete the following on your JetStream VM.

- 1. Start a Redis container in the background and expose port 6379.
- 2. Open two separate terminals, each logged in to the user VM and running an interactive Python shell.
- 3. In each terminal, create a HotQueue object pointing to the same Redis queue.
- 4. In the first terminal, add three or four Python strings to the queue; check the length of the queue.
- 5. In the second terminal, use a for loop and the .consume() method to print objects in the queue to the screen.
- 6. Observe that the strings are printed out in the second terminal.
- 7. Back in the first terminal, check the length of the queue; add some more objects to the queue.
- 8. Confirm the newly added objects are "instantaneously" printed to the screen back in the second terminal.

EXERCISE 2

Repeat the above steps, but this time orchestrate three containers together using docker-compose: a Redis container and two other Python containers which may simulate, for example, a Flask app and a worker.

```
version: "3"
services:
    redis-db:
        image: redis:7
        volumes:
            - ./data:/data
        ports:
            - 6379:6379
        user: "1000:1000"
        command: ["--save", "1", "1"]
    python1:
        image: python:3.10
        command: ["sleep", "9999999"]
    python2:
        image: python:3.10
        command: ["sleep", "9999999"]
```

Use the above docker-compose.yml file (make sure you understand what each part is doing), and execute the command:

```
[user-vm]$ docker-compose up -d
Creating network "messaging_default" with the default driver
Creating messaging_redis-db_1 ... done
Creating messaging_python2_1 ... done
Creating messaging_python1_1 ... done
```

Once the containers are running, use docker ps -a to find the names of the container, and docker exec to create two new shells inside the running containers:

```
# From terminal 1
[user-vm]$ docker exec -it messaging_python1_1 /bin/bash
root@ba734c20dfe3:/#
```

```
# From terminal 2
[user-vm]$ docker exec -it messaging_python2_1 /bin/bash
root@22ca40c5cf18:/#
```

Note: Once inside the running containers, what IP / alias do you use to refer to the Redis container? What libraries might you have to pip install?

When finished with the exercise, clean up your running containers by doing:

```
[user-vm]$ docker-compose down
Stopping messaging_python2_1 ... done
Stopping messaging_python1_1 ... done
(continues on next page)
```

```
Stopping messaging_redis-db_1 ... done
Removing messaging_python2_1 ... done
Removing messaging_python1_1 ... done
Removing messaging_redis-db_1 ... done
Removing network messaging_default
```

The @q.worker Decorator

Given a HotQueue queue object, q, the @q.worker decorator is a convenience utility to turn a function into a consumer without having to write a for loop. The basic syntax is:

```
>>> @q.worker
>>> def do_work(item):
>>> # do something with item
```

In the example above, item will be populated with the item dequeued.

Then, to start consuming messages, simply call the function:

```
>>> do_work()
# ... blocks until new messages arrive
```

Note: The @q.worker decorator replaces the for loop. Once you call a function decorated with @q.worker, the code never returns unless there is an unhandled exception.

EXERCISE 3

Write a function, echo(item), to print an item to the screen, and use the @q.worker decorator to turn it into a consumer. Call your echo function in one terminal and in a separate terminal, send messages to the Redis queue. Verify that the message items are printed to the screen in the first terminal.

In practice, we will use the @q.worker in a Python source file like so -

```
# A simple example of Python source file, worker.py
q = HotQueue('queue', host='<Redis_IP>', port=6379, db=1)

@q.worker
def do_work(item):
    # do something with item...

do_work()
```

Assuming the file above was saved as worker.py, calling python worker.py from the shell would result in a non-terminating program that "processed" the items in the "queue" queue using the do_work(item) function. The only thing that would cause our worker to stop is an unhandled exception.

8.2.3 Additional Resources

• HotQueue

8.3 The Jobs API

We have been introduced to the concept of *concurrency*: a method for managing resources such that multiple agents or components of the system can be in progress at the same time without impacting the correctness of the system. We have also discussed the utility of *asynchronicity*: an approach in concurrency wherein we can schedule a task, receive an immediate response, and continue on to other tasks while the previous task works in the background. The tools we will use to achieve this in the software systems we are building include worker containers, a messaging system, a task queue, and now the *Jobs API*.

The basic idea is that we will have a new endpoint in our API at a path /jobs (or something similar). A user wanting to have our system perform a long-running task will create a new job by making an HTTP POST request to /jobs, describing the job in the POST message body (in JSON). Instead of performing the actual computation, the request will simply be recorded in Redis and a response will be immediately provided to the user. The response will not include the result of the job itself, but instead it will indicate that the request has been received and it will be worked on once it gets to the top of the queue. Also, critically, the response will include an id for the job so that the user can check the status and, eventually, get the actual result. The Jobs API is a Python module that we will write which includes methods and tools for managing jobs in our software system.

By the end of this module, students should be able to:

- Explain the purpose and reasoning behind all variables and methods in Jobs API
- Decide which variables and methods should be private and which should be public
- · Organize code for software system into API, worker, and jobs modules
- Import the Jobs API into other modules to use for jobs functionality
- Perform appropriate curl requests to POST jobs and GET the result of jobs

8.3.1 Concurrency in the Jobs API

Recall that our big-picture goal is to add a Jobs endpoint to our Flask system that can process long-running tasks. We will implement our Jobs API with concurrency in mind. The goals will be:

The overall architecture will thus be:

- 1. Save the request in a database and respond to the user that the analysis will eventually be run.
- 2. Give the user a unique identifier with which they can check the status of their job and fetch the results when they are ready,
- 3. Queue the job to run so that a worker can pick it up and run it.
- 4. Build the worker to actually work the job.

Parts 1-3 are the tasks of the Flask API, while part 4 will be a worker, running as a separate container, that is waiting for new items in the Redis queue.

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8.3.2 Code Organization

As software systems get larger, it is very important to keep code organized so that finding the functions, classes, etc. responsible for different behaviors is as easy as possible. To some extent, this is technology-specific, as different languages, frameworks, etc., have different rules and conventions about code organization. We'll focus on Python, since that is what we are using.

The basic unit of code organization in Python is called a "module". This is just a Python source file (ends in a .py extension) with variables, functions, classes, etc., defined in it. We've already used a number of modules, including modules that are part of the Python standard library (e.g. json) and modules that are part of third-party libraries (e.g., redis).

The following should be kept in mind when designing the modules of a larger system:

- Modules should be focused, with specific tasks or functionality in mind, and their names (preferably, short) should match their focus.
- Modules are also the most typical entry-point for the Python interpreter itself, (e.g., python some_module.py).
- Accessing code from external modules is accomplished through the import statement.
- Circular imports will cause errors if module A imports an object from module B, module B cannot import from
 module A.

8.3.3 Module Design

The Python standard library is a good source of examples of module design. You can browse the standard library for Python 3.10 here.

- We see the Python standard library has modules focused on a variety of computing tasks; for example, for working with different data types, such as the datetime module and the array module. The descriptions are succinct:
 - The datetime module supplies classes for manipulating dates and times.
 - This module defines an object type which can compactly represent an array of basic values: characters, integers, floating point numbers
- For working with various file formats: e.g., csv, configparser
- For working with concurrency: threading, multiprocessing, etc.

With this in mind, a first approach might be to break up our system into two modules:

- api.py this module contains the Flask web server.
- worker.py this module contains the code to execute jobs.

However, both the API server and the workers will need to interact with the database and the queue:

- The API will create new jobs in the database, put new jobs onto the queue, and retrieve the status of jobs (and probably the output products of the job).
- The worker will pull jobs off the queue, retrieve jobs from the database, and update them.

This suggests a different structure:

- api.py this module contains the Flask web server.
- worker.py this module contains the code to execute jobs.
- jobs.py this module contains core functionality for working with jobs in Redis (and on the queue).

Common code for working with redis/hotqueue can go in the jobs.py module and be imported in both api.py and worker.py.

Note: High-quality modular design is a crucial aspect of building good software. It requires significant thought and experience to do correctly, and when done poorly it can have dire consequences. In the best case, poor module design can make the software difficult to maintain/upgrade; in the worst case, it can prevent it from running correctly at all.

We can sketch out our module design by making a list of the functionality that will be available in each module. This is only an initial pass at listing the functionality needed – we will refine it over time – but making an initial list is important for thinking through the problem.

api.py: This file will contain all the functionality related to the Flask web server, and will include functions related to each of the API endpoints in our application.

- POST /data Load the data into the application. Will write to Redis.
- GET /data?search=... List all of the data in the system, optionally filtering with a search query parameter. Will read from Redis.
- GET /data/<id> Get a specific object from the dataset using its id. Will read from Redis.
- POST /jobs Create a new job. This function will save the job description to Redis and add a new task on the queue for the job. Will write to Redis and the queue.
- GET /jobs List all the jobs. Will read from Redis.
- GET /jobs/<id> Get the status of a specific job by id. Will read from Redis.
- GET/jobs/<id>/results Return the outputs (results) of a completed job. Will read from Redis.

worker.py: This file will contain all of the functionality needed to get jobs from the task queue and execute the jobs.

- Get a new job Hotqueue consumer to get an item off the queue. Will get from the queue and write to Redis to update the status of the job.
- Perform analysis -
- Finalize job Saves the results of the analysis and updates the job status to complete. Will write to Redis.

jobs.py: This file will contain all functionality needed for working with jobs in the Redis database and the Hotqueue queue.

- Save a new job Will need to write to Redis.
- Retrieve an existing job Will need to read from Redis.
- Update an existing jobs Will need to read and write to Redis.

8.3.4 Private vs Public Objects

As software projects grow, the notion of public and private access points (functions, variables, etc.) becomes an increasingly important part of code organization.

- Private objects should only be used within the module they are defined. If a developer needs to change the implementation of a private object, she only needs to make sure the changes work within the existing module.
- Public objects can be used by external modules. Changes to public objects need more careful analysis to understand the impact across the system.

Like the layout of code itself, this topic is technology-specific. In this class, we will take a simplified approach based on our use of Python. Remember, this is a simplification to illustrate the basic concepts - in practice, more advanced/robust approaches are used.

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- We will name private objects starting with a single underscore (_) character.
- If an object does not start with an underscore, it should be considered public.

We can see public and private objects in use within the standard library as well. If we open up the source code for the datetime module, which can be found on GitHub we see a mix of public and private objects and methods.

- Private objects are listed first.
- Public objects start on line 442 with the timedelta class.

EXERCISE 1

Create three files, api.py, worker.py, and jobs.py in your local directory. You may wish to start from the files you prepared for Homework 06. You should also have a Dockerfile, docker-compose.yml, and requirements.txt in this directory to help with containerization and orchestration.

```
[user-vm] $ ls
Dockerfile api.py docker-compose.yaml jobs.py requirements.txt worker.py
```

Add the following function and variable definitions to jobs.py. Closely examine each line to make sure you understand the purpose. Carefully consider which are public and private, and why.

```
import ison
   import uuid
   import redis
   from hotqueue import HotQueue
   _redis_ip='redis-db'
   _redis_port='6379'
   rd = redis.Redis(host=_redis_ip, port=6379, db=0)
   q = HotQueue("queue", host=_redis_ip, port=6379, db=1)
10
   jdb = redis.Redis(host=_redis_ip, port=6379, db=2)
11
12
   def _generate_jid():
13
14
       Generate a pseudo-random identifier for a job.
15
16
       return str(uuid.uuid4())
18
   def _instantiate_job(jid, status, start, end):
19
20
       Create the job object description as a python dictionary. Requires the job id,
21
       status, start and end parameters.
22
23
       return {'id': jid,
24
                'status': status,
25
                'start': start,
26
                'end': end }
27
28
   def _save_job(jid, job_dict):
29
        """Save a job object in the Redis database."""
30
       jdb.set(jid, json.dumps(job_dict))
31
       return
```

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```
33
   def _queue_job(jid):
34
        """Add a job to the redis queue."""
35
       q.put(jid)
       return
37
   def add_job(start, end, status="submitted"):
39
        """Add a job to the redis queue."""
40
       jid = _generate_jid()
41
       job_dict = _instantiate_job(jid, status, start, end)
42
       _save_job(jid, job_dict)
43
       _queue_job(jid)
44
       return job_dict
45
46
   def get_job_by_id(jid):
47
        """Return job dictionary given jid"""
48
       return json.loads(jdb.get(jid))
50
   def update_job_status(jid, status):
51
        """Update the status of job with job id `jid` to status `status`."""
52
       job_dict = get_job_by_id(jid)
53
       if job_dict:
54
            job_dict['status'] = status
            _save_job(jid, job_dict)
56
       else:
57
           raise Exception()
```

EXERCISE 2

Write a skeleton for a Flask app in the file api.py. The Flask app should:

- 1. Import necessary modules, including some from jobs.py
- 2. Declare an instance of the Flask class
- 3. Support a route for POSTing a new job
- 4. Support a route for GETting job status

Tip: A job POST request might look like:

```
curl localhost:5000/jobs -X POST -d '{"start":1, "end":2}' -H "Content-Type: application/

→json"
```

In this example, we are sending a 'start' and 'end' index which is important for the "work". E.g. perhaps the worker is designed to plot all the values between 'start' and 'end'. In practice, the app that you develop may require different parameters.

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EXERCISE 3

Write a skeleton for a worker in the file worker.py: The worker should:

- 1. Import necessary modules, including some from jobs.py
- 2. Pull items (job IDs) off the queue
- 3. When it starts working on a new job, update the job status to 'in progress'
- 4. Do work (e.g. sleep for 15 seconds)
- 5. When it finishes working on a new job, update the job status to 'complete'

EXERCISE 4

Fill out the contents of the Dockerfile, docker-compose.yml, and requirements.txt in order to help with containerization and orchestration. Pay careful attention to how you set up and build the containers. Should we be using one Docker image or two? What should the entrypoint be?

EXERCISE 5

Modify the definition of the rd, q, and jdb objects to not use a hard-coded IP address, but to instead read the IP address from an environment variable, REDIS_IP. Determine how to set the value of REDIS_IP in the Dockerfile and / or docker-compose.yml file.

UNIT 9: CONTAINER ORCHESTRATION

In this unit, we begin our study of container orchestration with the Kubernetes ("k8s") system. We have already built a small HTTP application in the REST architecture using the Flask framework. This HTTP application makes use of a database to persist state. We have recently added a third component - a worker container. This set up is very typical of a modern distributed system. As the number of components grows, the work required to deploy and maintain this system increases. Container orchestration systems such as k8s aid us in this deployment and management effort by allowing us to run our applications across a cluster of machines and use APIs to make changes to the application deployment over time.

9.1 Orchestration Overview

In this module, we introduce the basic notion of container orchestration. After going through this module, the student should be able to:

- Explain the challenges associated with deploying and managing distributed systems that container orchestration systems are designed to help with.
- Describe at a high level a few of the most common container orchestration systems.

A typical distributed system is comprised of multiple components. You have already developed a simple HTTP application that includes a Python program (using the Flask library) and a database. In the subsequent weeks, we will add additional components.

Container orchestration involves deploying and managing containerized applications on one or more computers. There are a number of challenges involved in deploying and managing a distributed application, including:

- Container execution and lifecycle management To run our application, we must not only start the containers initially but also manage the entire lifecycle of the container, including handling situations where containers are stopped and/or crash. We need to ensure the correct container image is used each time.
- *Configuration* Most nontrivial applications involve some configuration. We must be able to provide configuration to our application's components.
- *Networking* The components in our distributed application will need to communicate with each other, and that communication will take place over a network.
- *Storage* Some components, such as databases, will require access to persistent storage to save data to disc so that they can be restarted without information loss.

The above list is just an initial set of concerns when deploying distributed, containerized applications. As the size and number of components grows, some systems may encounter additional challenges, such as:

• *Scaling* – We may need to start up additional containers for one or more components to handle spikes in load on the system, and shut down these additional containers to save resources when the usage spike subsides.

- *CPU and Memory management* The computers we run on have a fixed amount of CPU and memory, and in some cases, it can be important to ensure that no one container uses too many resources.
- Software version updates How do we go from version 1 to version 2 of our software? We may have to update several components (or all of them) at once. What if there are multiple containers running for a given component? As we are performing the upgrade, is the system offline or can users still use it?

9.1.1 Orchestration Systems

Orchestration systems are built to help with one or more of the above challenges. Below we briefly cover some of the more popular, open-source container orchestration systems. This is by no means an exhaustive list.

Docker Compose

You have already seen a basic container orchestration system – Docker Compose. The Docker Compose system allows users to describe their application in a docker-compose.yml file, including the services, networks, volumes and other aspects of the deployment. Docker Compose:

- Runs Docker containers on a single computer, the machine where docker-compose is installed and run.
- Utilizes the Docker daemon to start and stop containers defined in the docker-compose.yml file.
- Also capable of creating volumes, networks, port bindings, and other objects available in the Docker API.

Docker compose is a great utility for single-machine deployments and, in particular, is a great system for "local development environments" where a developer has code running on her or his laptop.

Docker Swarm

Docker Swarm provides a container orchestration system to deploy applications across multiple machines running the Docker daemon. Docker Swarm works by creating a cluster (also known as a "swarm") of computers and coordinating the starting and stopping of containers across the cluster. Docker Swarm:

- Runs Docker containers across a cluster of machines (a "swarm"), each running Docker.
- Coordinates container execution across the cluster.
- Similar API to Docker Compose: capable of creating networks spanning multiple computers as well as port-bindings, volumes, etc.

Mesos

Apache Mesos is a general-purpose cluster management system for deploying both containerized and non-containerized applications across multiple computers. Mesos by itself is quite low-level and requires the use of *frameworks* to deploy actual applications. For example, Marathon is a popular Mesos framework for deploying containerized applications, while the Mesos Hydra framework can be used for deploying MPI-powered applications, such as those used in traditional HPC applications.

Nomad

Nomad by HasiCorp is an orchestration system that can handle both containerized and non-containerized workloads. Nomad has been gaining popularity recently as an alternative to Kubernetes. Compared with Kubernete, Nomad offers a significantly simpler usage model but requires more work by the user to achieve some functionalities available in Kubernetes.

Kubernetes

Kubernetes (often abbreviated as "k8s") is a container orchestration system supporting Docker as well other container runtimes that conform to the Container Runtime Interface (CRI) such as containerd and cri-o. While Kubernetes focuses entirely on containerized applications (unlike Mesos) and is not as similar to Docker Compose as Docker Swarm is, it provides a number of powerful features for modern, distributed systems management. Additionally, Kubernetes is available as a service on a large number of commercial cloud providers, including Amazon, Digital Ocean, Google, IBM, Microsoft, and many more, and TACC provides multiple Kubernetes clusters in support of various research projects.

- Supports running containerized applications across a cluster of machines for container runtimes conforming to the Container Runtime Interface (CRI), including Docker.
- Provides powerful features for managing distributed applications.
- Available as a service from TACC and a number of commercial cloud providers.

9.1.2 Additional Resources

- Docker Compose Reference
- · Docker Swarm
- Apache Mesos Documentation
- Marathon
- · Mesos Hydra
- · Hashicorp Nomad
- Kubernetes Documentation

9.2 Introduction to Kubernetes

In this section we give an overview of the Kubernetes (**k8s**) system and test to see whether the **kubectl** CLI is configured correctly to allow us to interact with the cluster

After going through this module, students should be able to:

- Issue basic commands using kubect1
- · Connect to the class Kubernetes cluster and
- **Design Principles**. Kubernetes improves our software portability, particularly for large distributed applications that need to run across multiple machines

9.2.1 Kubernetes Overview

Kubernetes (k8s) is itself a distributed system of software components that run a cluster of one or more machines (physical computers or virtual machines). Each machine in a k8s cluster is either a "manager" or a "worker" node.

Users communicate with k8s by making requests to its API. The following steps outline how Kubernetes works at a high level:

- 1) Requests to k8s API describe the user's *desired state* on the cluster; for example, the desire that 3 containers of a certain image are running.
- 2) The k8s API schedules new containers to run on one or more worker nodes.
- 3) After the containers are started, the Kubernetes deployment controller, installed on each worker node, monitors the containers on the node.
- 4) The k8s components, including the API and the deployment controllers, maintain both the *desired state* and the *actual state* in a distributed database. The components continuously coordinate together to make the actual state converge to the desired state.

Developer or Administrator Deployment Controller Distributed database User's application containers

Note: It is important to note that most of the time, the k8s API as well as the worker nodes are running on separate machines from the machine we use to interact with k8s (i.e., make API requests to it). The machine we use to interact with k8s only needs to have the k8s client tools installed, and in fact, as the k8s API is available over HTTP, we don't strictly speaking require the tools – we could use curl or some other http client – but the tools make interacting with the API much easier.

9.2.2 Connecting to the TACC Kubernetes Instance

In this class, we will use a Kubernetes cluster running at TACC that we have created for use in this class for deploying our applications. To simplify the process of accessing the Kubernetes cluster, we have enabled connectivity to it from the student-login host. Therefore, any time you want to work with k8s, simply SSH to student-login with your TACC username as you have throughout the semester and then issue your kubectl commands

```
[local] $ ssh username@student-login.tacc.utexas.edu
[student-login] $ ...do kubernetes work...
```

This machine has Kubernetes tools installed on it and has *access to the Kubernetes API* for the cluster, but you should be aware that this server is *not part of the Kubernetes cluster* itself. Note that it will require careful organization and work to keep files in sync between the student-login host and your Jetstream VM.

9.2.3 First Commands with k8s

We will use the Kubernetes Command Line Interface (CLI) referred to as "kubectl" (pronounced "Kube control") to make requests to the Kubernetes API. We could use any HTTP client, including a command-line client such as curl, but kubectl simplifies the process of formatting requests.

The kubectl software should already be installed and configured to use the Freetail K8s cluster. Let's verify that is the case by running the following:

```
[student-login]$ kubectl version -o yaml
```

You should see output similar to the following:

```
clientVersion:
 buildDate: "2023-12-19T13:42:57Z"
 compiler: gc
 gitCommit: 506050d61cf291218dfbd41ac93913945c9aa0da
 gitTreeState: clean
 gitVersion: v1.28.5
 goVersion: go1.20.12
 major: "1"
 minor: "28"
 platform: linux/amd64
kustomizeVersion: v5.0.4-0.20230601165947-6ce0bf390ce3
serverVersion:
 buildDate: "2023-12-19T13:32:53Z"
 compiler: qc
 gitCommit: 506050d61cf291218dfbd41ac93913945c9aa0da
 gitTreeState: clean
 gitVersion: v1.28.5
 goVersion: go1.20.12
 major: "1"
 minor: "28"
 platform: linux/amd64
```

This command made an API request to the TACC k8s cluster and returned information about the version of k8s running there (under serverVersion) as well as the version of the kubectl that we are running (under clientVersion).

Note: The output of the kubectl command was yaml because we used the -o yaml flag. We could have asked for

the output to be formatted in json with -o json. The -o flag is widely available on kubectl commands.

9.2.4 Authentication and Namespaces in Kubernetes

Before we can do any real work on the Kubernetes cluster, we need to understand the concept of a *namespace*. In Kubernetes, a *namespace* is a logical partition of objects defined on the cluster, and different users can have different levels of access (including no access at all) to different namespaces. In this way, Kubernetes supports launching different applications – even different applications owned by different users or organizations – on the same physical cluster in an isolated way from each other. Each different user or organization would be assigned a different namespace where their k8s objects would live, and users wouldn't have access to any other namespace.

That is how the class Kubernetes cluster has been set up. Each of you has been assigned your own namespace in the Kubernetes cluster where you have administrative access. Inside that namespace, you can create and manage the Kubernetes objects for your application. And while all of the Kubernetes objects for every student is running on the same cluster, you won't see or have access to the objects in different namespaces.

We haven't introduced pods yet – we will shortly – but let's try a simple experiment: issue the following command

```
[student-login]$ kubectl get pods
```

You will get a response like the following:

```
No resources found in USERNAME namespace
```

Your kubectl client is configured to make requests in your private namespace, so it is only looking for pods running on the cluster within your namespace. There may be many other pods currently running on the cluster, you just do not have access to see them.

Try the following experiment. Specify a different namespace directly on the command line using the --namespace argument. Provide a namespace (e.g. wallen) that you would not expect to have access to:

```
[student-login]$ kubectl get pods --namespace=wallen
```

The response might look like:

```
Error from server (Forbidden): pods is forbidden: User

→"system:serviceaccount:USERNAME:USERNAME"

cannot list resource "pods" in API group "" in the namespace "wallen"
```

This is the output we expect because we would not have access to that user's pods.

To see more information about how k8s and the kubectl CLI is configured in your environment, inspect the file located at ~/.kube/config.

To install the k8s CLI on your Jetstream instance, log in to Jetstream and issue the following commands (replacing USERNAME with your username):

```
[user-vm]$ sudo curl -LO "https://dl.k8s.io/release/v1.28.5/bin/linux/amd64/kubectl"
[user-vm]$ sudo install -o root -g root -m 0755 kubectl /usr/local/bin/kubectl
[user-vm]$ scp -r USERNAME@student-login.tacc.utexas.edu:~/.kube ./
```

To confirm whether it worked, try the following commands:

```
[user-vm]$ kubectl version --client
Client Version: v1.28.5

(continues on next page)
```

```
Kustomize Version: v5.0.4-0.20230601165947-6ce0bf390ce3
[user-vm]$ kubectl get pods
No resources found in USERNAME namespace.
```

Additional Resources

• Kubernetes Reference

9.3 Introduction to Pods

In this section we give an overview of the first major Kubernetes abstraction, the Pod.

After going through this module, students should be able to:

- Connect to the class Kubernetes cluster and issue basic commands using kubect1
- Describe a Kubernetes pod in a yaml file and use kubectl to deploy the pod to the cluster
- · Retrieve details about the pod including status and logs
- Use labels to organize pods deployed to the Kubernetes cluster
- **Design Principles**. Kubernetes improves our software portability, particularly for large distributed applications that need to run across multiple machines

9.3.1 Introduction to Pods

Pods are a fundamental abstraction within Kubernetes and are the most basic unit of computing that can be deployed onto the cluster. A pod can be thought of as generalizing the notion of a container: a pod contains one or more containers that are tightly coupled and need to be scheduled together, on the same computer, with access to a shared file system and a shared network address.

Note: By far, the majority pods you will meet in the wild, including the ones used in this course, will only include one container. A pod with multiple containers can be thought of as an "advanced" use case.

9.3.2 Hello, Kubernetes

To begin, we will define a pod with one container. As we will do with all the resources we want to create in k8s, we will describe our pod in a yaml file.

Create a file called pod-basic.yml, open it up in an editor and paste the following code in:

```
apiVersion: v1
kind: Pod
metadata:
name: hello
spec:
containers:
name: hello
(continues on next page)
```

```
image: ubuntu:22.04
command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
```

Let's break this down. The top four attributes are common to all k8s resource descriptions:

- apiVersion describes what version of the k8s API we are working in. We are using v1.
- kind tells k8s what kind of resource we are describing, in this case a Pod.
- metadata in general, this is additional information about the resource we are describing that doesn't pertain to its operation. Here, we are giving our pod a name, hello.
- spec This is where the actual description of the resource begins. The contents of this stanza vary depending on the kind of resource you are creating. We go into more details on this in the next section.

Warning: Only one Kubernetes object of a specific kind can have a given name at a time. If you define a second pod with the same name you will overwrite the first pod. This is true of all the different types of k8s objects we will be creating.

The Pod Spec

In k8s, you describe resources you want to create or update using a spec. The required and optional parameters available depend on the kind of resource you are describing.

The pod spec we defined looked like this:

```
spec:
   containers:
        - name: hello
        image: ubuntu:22.04
        command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
```

There is just one stanza, the containers stanza, which is a list of containers (recall that pods can contain multiple containers). Here we are defining just one container. For each container, we provide:

- name (optional) this is the name of the container, similar to the name attribute in Docker.
- image (required) the image we want to use for the container, just like with Docker.
- command (optional) the command we want to run in the container. Here we are running a short BASH script.

9.3.3 Creating the Pod In K8s

We are now ready to create our pod in k8s. To do so, we use the kubectl apply command. In general, when you have a description of a resource that you want to create or update in k8s, the kubectl apply command can be used.

In this case, our description is contained in a file, so we use the -f flag. Try this now:

```
[user-vm]$ kubectl apply -f pod-basic.yml
```

If all went well and k8s accepted your request, you should see an output like this:

```
pod/hello created
```

Note: The message pod/hello created indicates that the description of the pod was valid, that k8s has saved the pod definition in its database and that it is working on starting the pod on the cluster. It does **not** mean the pod is already created/running on the cluster.

In practice, we won't be creating many Pod resources directly – we'll be creating other resources, such as deployments that are made up of pods – but it is important to understand pods and to be able to work with pods using kubectl for debugging and other management tasks.

Note: The pod we just created is running on the k8s cluster, NOT on your student VM and NOT on kube controller node. You will not be able to find it using commands like docker ps, etc.

During the lecture, we'll go to the diagram to help explain what is going on.

9.3.4 Working With Pods

We can use additional kubectl commands to get information about the pods we run on k8s.

Listing Pods

For example, we can list the pods on the cluster with kubectl get <object_type> - in this case, the object type is "pods":

The output is fairly self-explanatory. We see a line for every pod which includes its name, status, the number of times it has been restarted and its age. Our hello pod is listed above, with an age of 99s because we just started it but it is already Running.

Getting and Describing Pods

We can pass the pod name to the get command -i.e., kubectl get pods <pod_name> - to just get information on a single pod

```
[user-vm] $ kubectl get pods hello
NAME READY STATUS RESTARTS AGE
hello 1/1 Running 0 3m1s
```

The -o wide flag can be used to get more information:

```
[user-vm]$ kubectl get pods hello -o wide
NAME
        READY
                STATUS
                           RESTARTS
                                      AGE
                                               ΙP
                                                                NODE
→NOMINATED NODE
                    READINESS GATES
hello
        1/1
                Running
                                      4m56s
                                               10.233.97.195
                                                                coe332-kubernetes-4
                                                                                       <none>
             <none>
```

Finally, the kubectl describe <resource_type> <resource_name> command gives additional information, including the k8s events at the bottom. While we won't go into the details now, this information can be helpful when troubleshooting a pod that has failed:

```
[user-vm]$ kubectl describe pods hello
Name:
                                           hello
Namespace:
                                           USERNAME
Priority:
Service Account: default
Node:
                                           coe332-kubernetes-4/129.114.36.49
Start Time:
                                           Tue, 02 Apr 2024 09:10:03 -0500
Labels:
                                           <none>
Annotations:
                                           cni.projectcalico.org/containerID:
 -bea7a74509b2535625185701985ce4f3440a6f0e022ec9ba6a5cdee9b0886e06
                                           cni.projectcalico.org/podIP: 10.233.97.195/32
                                            cni.projectcalico.org/podIPs: 10.233.97.195/32
Status:
                                           Running
IP:
                                            10.233.97.195
TPs:
    IP: 10.233.97.195
Containers:
    hello:
         Container ID: containerd://
 -573593ae075052990c5bf12c8f0dd52c5a11ad1f1069a0b6ead84a080a08c443
                                             ubuntu:22.04
         Image:
         Image ID:
                                              docker.io/library/
  \hspace{2.5cm} \leftarrow \hspace{-.1cm} ubuntu@sha256:77906 da86b60585 ce12215807090 eb327e7386c8 fafb5402369e421f44 eff17e1215807090 eb327e7386c8 fafb5402369 e4216400 eb327e7386c8 eb327e7366 eb327e7366 eb327e7386 eb327e7366 eb327e7366 eb327e7366 eb327e736 eb327e736 eb327e7366 eb327e736 eb327e
         Port:
                                              <none>
         Host Port:
                                              <none>
         Command:
               sh
              -c
              echo "Hello, Kubernetes!" && sleep 3600
                                                Running
         State:
              Started:
                                                Tue, 02 Apr 2024 09:10:07 -0500
         Ready:
                                                True
         Restart Count:
         Environment:
                                                <none>
         Mounts:
               /var/run/secrets/kubernetes.io/serviceaccount from kube-api-access-jkcd2 (ro)
Conditions:
                                                Status
    Type
    Initialized
                                                True
    Ready
                                                True
    ContainersReady
                                                True
    PodScheduled
                                                True
Volumes:
    kube-api-access-jkcd2:
         Type:
                                                                      Projected (a volume that contains injected data from.
 →multiple sources)
         TokenExpirationSeconds: 3607
         ConfigMapName:
                                                                      kube-root-ca.crt
         ConfigMapOptional:
                                                                      <ni1>
         DownwardAPI:
                                                                       true
QoS Class:
                                                                      BestEffort
Node-Selectors:
Tolerations:
                                                                      node.kubernetes.io/not-ready:NoExecute op=Exists for 300s
                                                                                                                                                                                      (continues on next page)
```

```
node.kubernetes.io/unreachable:NoExecute op=Exists for 300s
Events: <none>
```

Getting Pod Logs

We can use kubectl logs <pod_name> command to get the logs associated with a pod:

```
[user-vm]$ kubectl logs hello
Hello, Kubernetes!
```

Note that the logs command does not include the resource name ("pods") because it only can be applied to pods. The logs command in k8s is equivalent to that in Docker; it returns the standard output (stdout) of the container.

Using Labels

In the pod above we used the metadata stanza to give our pod a name. We can use labels to add additional metadata to a pod. A label in k8s is nothing more than a name: value pair that we create to organize objects in a meaningful way. We can choose any value for name and value that we wish but they must be strings. If you want to use a number like "10" for a label name or value, be sure to enclose it in quotes (i.e., "10").

You can think of these name:value pairs as variables and values. So for example, you might create a label called shape with values circle, triangle, square, etc. A more realistic label might be component_type with values api, database, worker, etc. Or, you could imagine labeling pods as either production or development instances. Multiple pods can have the same name:value label.

Let's use the pod definition above to create a new pod with a label.

Create a file called pod-labeled.yml, open it up in an editor and paste the following code in:

```
apiVersion: v1
kind: Pod
metadata:
name: hello-labeled
labels:
version: "1.0"
spec:
containers:
- name: hello
image: ubuntu:22.04
command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
```

Let's create this pod using kubectl apply:

```
[user-vm]$ kubectl apply -f pod-labeled.yml
pod/hello-labeled created
```

Now when we list our pods, we should see it

Filtering By Labels With Selectors

Labels are useful because we can use selectors to filter our results for a given label name and value. To specify a label name and value, use the following syntax: --selector "<label_name>=<label_value>".

For instance, we can search for pods with the version 1.0 label like so:

We can also just use the label name to filter with the syntax --selector "<label_name>". This will find any pods with the label_name>, regardless of the value.

Exec into a Container inside a Pod

Just like with the Docker CLI, the kubectl CLI provides a means to attach your terminal to a shell inside a running container. This is a useful way to debug a pod or test connections between pods. Assuming you have a pod named *hello*, try:

```
[user-vm]$ kubectl exec -it hello -- /bin/bash
root@hello:/#
```

From there, type logout or press Ctrl+D to return to the command line.

Delete a Pod

Finally, we can delete a running pod using kubectl delete pods <pod_name>:

```
[user-vm]$ kubectl delete pods hello
pod "hello" deleted
```

The pod (and the container running inside the pod) has been removed from the k8s cluster. Another safe way to delete a pod is to pass kubectl delete the YAML file describing the pod. In this case, you do not in include the resource name ("pods") because that is inferred from the contents of the YAML file.

```
[user-vm]$ kubectl delete -f pod-labeled.yml
pod "hello-labeled" deleted
```

We should now be able to see that our pods have all been deleted. It is important to periodically clean up and remove old resources to save ourselves resources (e.g. AWS credits) or in this case, it is good to clean up the k8s cluster because it is a shared resource among the whole class.

```
[user-vm]$ kubectl get pods
No resources found in USERNAME namespace.
```

EXERCISE

Launch a new pod running Python v3.10.

Launch another pod running the API container from your latest homework.

Additional Resources

• k8s Pod Reference

9.4 Desired State with Deployments

In this module, we discuss the Kubernetes abstraction called "deployments". After working through this module, students should be able to:

- Explain the types of workloads that should be scheduled using the deployment abstraction in Kubernetes
- Describe a deployment in a yaml file and schedule the deployment on a Kubernetes cluster using kubect1
- Scale the pods associated with a deployment
- Define an image naming and tagging scheme to manage the development and deployment lifecycle of an application

9.4.1 Introduction to Deployments

Deployments are an abstraction and resource type in Kubernetes that can be used to represent long-running application components, such as databases, REST APIs, web servers, or asynchronous worker programs. The key idea with deployments is that they should *always be running*.

Imagine a program that runs a web server for a blog site. The blog website should always be available, 24 hours a day, 7 days a week. If the blog web server program crashes, it would ideally be restarted immediately so that the blog site becomes available again. This is the main idea behind deployments.

Deployments are defined with a pod definition and a replication strategy, such as, "run 3 instances of this pod across the cluster" or "run an instance of this pod on every worker node in the k8s cluster."

For this class, we will define deployments for our Flask application and its associated components, as deployments come with a number of advantages over defining "raw" pods. Deployments:

- Can be used to run multiple instances of a pod, to allow for more computing to meet demands put on a system.
- Are actively monitored by k8s for health if a pod in a deployment crashes or is otherwise deemed unhealthy, k8s will try to start a new one automatically.

9.4.2 Creating a Basic Deployment

We will use yaml to describe a deployment just like we did in the case of pods. Copy and paste the following into a file called deployment-basic.yml

```
apiVersion: apps/v1
kind: Deployment
metadata:
```

(continues on next page)

```
name: hello-deployment
     labels:
       app: hello-app
7
   spec:
     replicas: 1
Q
     selector:
10
       matchLabels:
11
          app: hello-app
12
     template:
13
       metadata:
14
          labels:
15
            app: hello-app
16
       spec:
          containers:
18
            - name: hellos
              image: ubuntu:22.04
20
              command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
```

Let's break this down. Recall that the top four attributes are common to all k8s resource descriptions, however it is worth noting:

- apiVersion We need to use version apps/v1 here. In k8s, different functionalities are packaged into different APIs. Deployments are part of the apps/v1 API, so we must specify that here.
- metadata The metadata.name gives our deployment object a name. This part is similar to when we defined pods. We are also using labels. Recall that k8s uses labels to allow objects to refer to other objects in a decoupled way. A label in k8s is nothing more than a name: value pair that users create to organize objects and add information meaningful to the user. In this case, app is the name and hello-app is the value. Conceptually, you can think of label names like variables and labels values as the value for the variable. In some other deployment, we may choose to use label app: profiles to indicate that the deployment is for the "profiles" app.

Let's look at the spec stanza for the deployment above.

- replicas Defines how many pods we want running at a time for this deployment, in this case, we are asking that just 1 pod be running at a time.
- selector This is how we tell k8s where to find the pods to manage for the deployment. Note we are using labels again here, the app: hello-app label in particular.
- template Deployments match one or more pod descriptions defined in the template. Note that in the metadata of the template, we provide the same label (app: hello-app) as we did in the matchLabels stanza of the selector. This tells k8s that this spec is part of the deployment.
- template.spec This is a pod spec, just like we worked with last time.

Note: If the labels, selectors and matchLables seems confusing and complicated, that's understandable. These semantics allow for complex deployments that dynamically match different pods, but for the deployments in this class, you will not need this extra complexity. As long as you ensure the label in the template is the same as the label in the selector.matchLables your deployments will work. It's worth pointing out that the first use of the app: hello-app label for the deployment itself (lines 5 and 6 of the yaml) could be removed without impacting the end result.

We create a deployment in k8s using the apply command, just like when creating a pod:

```
[user-vm]$ kubectl apply -f deployment-basic.yml
```

If all went well, k8s response should look like:

```
deployment.apps/hello-deployment created
```

We can list deployments, just like we listed pods:

```
    [user-vm]$ kubectl get deployments

    NAME
    READY
    UP-TO-DATE
    AVAILABLE
    AGE

    hello-deployment
    1/1
    1
    1m
```

We can also list pods, and here we see that k8s has created a pod for our deployment for us:

[user-vm]\$ kubectl get pods				
NAME	READY	STATUS	RESTARTS	AGE
hello	1/1	Running	0	10m
hello-deployment-55c5b77fc-hqjwx	1/1	Running	0	5 0 s
hello-label	1/1	Running	0	4m54s

Note that we see our "hello" and "hello-label" pods from earlier as well as a new pod, "hello-deployment-9794b4889-kms7p", that k8s created for our deployment. We can use all the kubectl commands associated with pods, including listing, describing and getting the logs. In particular, the logs for our "hello-deployment-9794b4889-kms7p" pod prints the same "Hello, Kubernetes!" message, just as was the case with our first pod.

9.4.3 Deleting Pods

However, there is a fundamental difference between the "hello" pod we created before and our "hello" deployment which we have alluded to. This difference can be seen when we delete pods.

To delete a pod, we use the kubectl delete pods <pod_name> command. Let's first delete our hello deployment pod:

```
[user-vm]$ kubectl delete pods hello-deployment-55c5b77fc-hqjwx
```

It might take a little while for the response to come back, but when it does you should see:

```
pod "hello-deployment-55c5b77fc-hqjwx" deleted
```

If we then immediately list the pods, we see something interesting:

```
[user-vm]$ kubectl get pods
NAME
                                     READY
                                              STATUS
                                                        RESTARTS
                                                                    AGE
hello
                                     1/1
                                              Running
                                                        0
                                                                    13m
hello-deployment-55c5b77fc-76lzz
                                     1/1
                                              Running
                                                                    39s
hello-label
                                     1/1
                                              Running
                                                                    7m25s
```

We see a new pod (in this case, "hello-deployment-55c5b77fc-76lzz") was created and started by k8s for our hello deployment automatically! k8s did this because we instructed it that we wanted 1 replica pod to be running in the deployment's spec – this was the *desired* state – and when that didn't match the actual state (0 pods) k8s worked to change it. Remember, deployments are for programs that should *always be running*.

What do you expect to happen if we delete the original "hello" pod? Will k8s start a new one? Let's try it

```
[user-vm] $ kubectl delete pods hello
pod "hello" deleted
[user-vm]$ kubectl get pods
                                             STATUS
                                                        RESTARTS
NAME
                                     READY
                                                                   AGE
hello-deployment-55c5b77fc-76lzz
                                     1/1
                                             Running
                                                        0
                                                                   19m
hello-label
                                     1/1
                                             Running
                                                        0
                                                                   26m
```

k8s did not start a new one. This "automatic self-healing" is one of the major difference between deployments and pods.

9.4.4 Scaling a Deployment

If we want to change the number of pods k8s runs for our deployment, we simply update the replicas attribute in our deployment file and apply the changes. Let's modify our "hello" deployment to run 4 pods. Modify deployment-basic.yml as follows:

```
apiVersion: apps/v1
   kind: Deployment
3
   metadata:
4
     name: hello-deployment
     labels:
6
       app: hello-app
   spec:
     replicas: 4
     selector:
10
       matchLabels:
11
          app: hello-app
12
     template:
13
       metadata:
14
         labels:
            app: hello-app
16
       spec:
          containers:
18
            - name: hellos
19
              image: ubuntu:22.04
20
              command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
21
```

Apply the changes with:

```
[user-vm]$ kubectl apply -f deployment-basic.yml
deployment.apps/hello-deployment configured
```

When we list pods, we see k8s has quickly implemented our requested change:

```
[user-vm]$ kubectl get pods
                                            STATUS
NAME
                                    READY
                                                       RESTARTS
                                                                  AGE
hello-deployment-55c5b77fc-76lzz
                                    1/1
                                            Running
                                                                  22m
hello-deployment-55c5b77fc-nsx6w
                                    1/1
                                            Running
                                                       0
                                                                  95
hello-deployment-55c5b77fc-wt4fz
                                    1/1
                                            Running
                                                       0
                                                                  9s
hello-deployment-55c5b77fc-xtfb9
                                            Running
                                    1/1
                                                       0
                                                                  9s
hello-label
                                            Running
                                    1/1
                                                                  29m
```

EXERCISE

- 1) Delete several of the hello deployment pods and see what happens.
- 2) Scale the number of pods associated with the hello deployment back down to 1.

9.4.5 Updating Deployments with New Images

When we have made changes to the software or other aspects of a container image and we are ready to deploy the new version to k8s, we have to update the pods making up the corresponding deployment. We will use two different strategies, one for our "test" environment and one for "production".

Test Environments

A standard practice in software engineering is to maintain one or more "pre-production" environments, often times called "test" or "quality assurance" environments. These environments look similar to the "real" production environment where actual users will interact with the software, but few if any real users have access to them. The idea is that software developers can deploy new changes to a test environment and see if they work without the risk of potentially breaking the software for real users if they encounter unexpected issues.

Test environments are essential to maintaining quality software, and every major software project the Cloud and Interactive Computing group at TACC develops makes use of multiple test environments. We will have you create separate test and production environments as part of building the final project in this class.

It is also common practice to deploy changes to the test environment often, as soon as code is ready and tests are passing on a developer's laptop. We deploy changes to our test environments dozens of times a day while a large enterprise like Google may deploy many thousands of times a day. We will learn more about test environments and automated deployment strategies in the Continuous Integration section.

Image Management and Tagging

As you have seen, the tag associated with a Docker image is the string after the: in the name. For example, ubuntu:22.04 has a tag of 22.04 representing the version of Ubuntu packaged in the image, while username/hello-flask:dev has a tag of dev, in this case indicating that the image was built from the dev branch of the corresponding git repository. Use of tags should be deliberate and is an important detail in a well designed software development release cycle.

Once you have created a deployment for a pod with a given image, there are two basic approaches to deploying an updated version of the container images to k8s:

- 1. Use a new image tag or
- 2. Use the same image tag and instruct k8s to download the image again.

Using new tags is useful and important whenever you may want to be able to recover or revert back to the previous image easily, but on the other hand, it can be tedious to update the tag every time there is a minor change to a software image.

Therefore, we suggest the following guidelines for image tagging:

1. During development when rapidly iterating and making frequent deployments, use a tag such as dev to indicate the image represents a development version of the software (and is not suitable for production) and simply overwrite the image tag with new changes. Instruct k8s to always try to download a new version of this tag whenever it creates a pod for the given deployment (see next section).

- 2. Once the primary development has completed and the code is ready for end-to-end testing and evaluation, begin to use new tags for each change. These are sometimes called "release candidates" and therefore, a tagging scheme such as rc1, rc2, rc3, etc., can be used for tagging each release candidate.
- 3. Once testing has completed and the software is ready to be deployed to production, tag the image with the version of the software. There are a number of different schemes for versioning software, such as Semantic Versioning (https://semver.org/), which has been mentioned previously.

ImagePullPolicy

When defining a deployment, we can specify an ImagePullPolicy which instructs k8s about when and how to download the image associated with the pod definition. For our test environments, we will instruct k8s to always try and download a new version of the image whenever it creates a new pod. We do this by specifying imagePullPolicy: Always in our deployment.

For example, we can add imagePullPolicy: Always to our hello-deployment as follows:

```
apiVersion: apps/v1
   kind: Deployment
   metadata:
     name: hello-deployment
     labels:
6
       app: hello-app
   spec:
     replicas: 1
     selector:
10
       matchLabels:
11
          app: hello-app
12
     template:
13
       metadata:
14
          labels:
15
            app: hello-app
        spec:
17
          containers:
            - name: hellos
19
              imagePullPolicy: Always
20
              image: ubuntu:22.04
21
              command: ['sh', '-c', 'echo "Hello, Kubernetes!" && sleep 3600']
22
```

Now k8s will always try to download the latest version of ubuntu:22.04 from Docker Hub every time it creates a new pod for this deployment. As discussed above, using imagePullPolicy: Always is nice during active development because you ensure k8s is always deploying the latest version of your code. Other possible values include IfNotPresent (the current default) which instructs k8s to only pull the image if it doesn't already exist on the worker node. This is the proper setting for a production deployment in most cases.

Deleting Pods to Update the Deployment

Note that if we have an update to our :dev image and we have set imagePullPolicy: Always on our deployment, all we have to do is delete the existing pods in the deployment to get the updated version deployed: as soon as we delete the pods, k8s will determine that an insufficient number of pods are running and try to start new ones. The imagePullPolicy instructs k8s to first try and download a newer version of the image.

Note: Consult the software diagram to understand the flow of source code changes => updated container running on the k8s cluster.

9.4.6 Additional Resources

• Kubernetes Deployments Documentation

9.5 Mounts, Volumes, and Persistent Volume Claims

In this module, we discuss the Kubernetes abstraction called "persistent volume claims", or "pvc"s for short. After working through this module, students should be able to:

- Describe a pvc in a yaml file and create the pvc on a Kubernetes cluster using kubect1
- · Exec into a pod that is part of a deployment
- Utilize Kubernetes mounts, volumes and persistent volume claims to persist application data across pod/container restarts

9.5.1 Persistent Storage on the Kubernetes Cluster

Some applications such as databases need access to storage where they can save data that will persist across container starts and stops. We saw how to solve this with Docker using a host bind mount. With k8s, the pods (containers) get started automatically for us on different nodes in the clusters, so a mount from a host won't work. Which host would we use to store the files to be persisted?

The solution in k8s involves a combination of what are called volume mounts, volumes, and persistent volume claims. The basic idea is similar to that of a Docker host bind mount – we'll be replacing some location in the container image with some data stored outside of the container. But in order to handle the fact that the application container could get started on different compute nodes, we'll utilize a backend "storage resource" which provides block storage over a network.

Create a new file, deployment-pvc.yml, with the following contents, replacing "<username>" with your username:

```
apiVersion: apps/v1
kind: Deployment
metadata:
name: hello-pvc-deployment
labels:
app: hello-pvc-app
spec:
replicas: 1
selector:
```

(continues on next page)

```
matchLabels:
11
          app: hello-pvc-app
12
     template:
13
       metadata:
         labels:
15
            app: hello-pvc-app
16
       spec:
17
          containers:
18
            - name: hellos
19
              image: ubuntu:22.04
20
              command: ['sh', '-c', 'echo "Hello, Kubernetes!" >> /data/out.txt && sleep 3600
21
   ']
              volumeMounts:
22
              - name: hello-<username>-data
23
                mountPath: "/data"
24
          volumes:
25
          - name: hello-<username>-data
            persistentVolumeClaim:
27
              claimName: hello-<username>-data
```

Note: Be sure to replace **<username>** with your actual username in the YAML above.

We have added a volumeMounts stanza to spec.containers and we added a volumes stanza to the spec. These have the following effects:

- The volumeMounts include a mountPath attribute whose value should be the path in the container that is to be provided by a volume instead of what might possibly be contained in the image at that path. Whatever is provided by the volume will overwrite anything in the image at that location.
- The volumes stanza states that a volume with a given name should be fulfilled with a specific persistentVolume-Claim. Since the volume name (hello-<username>-data) matches the name in the volumeMounts stanza, this volume will be used for the volumeMount.
- In k8s, a persistent volume claim makes a request for some storage from a storage resource configured by the k8s administrator in advance. While complex, this system supports a variety of storage systems without requiring the application engineer to know details about the storage implementation.

Note also that we have changed the command to redirect the output of the echo command to the file /data/out.txt. This means that we should not expect to see the output in the logs for pod but instead in the file inside the container.

However, if we create this new deployment and then list pods we see something curious:

```
[user-vm]$ kubectl apply -f deployment-pvc.yml
[user-vm]$ kubectl get pods
                                          READY
                                                  STATUS
                                                             RESTARTS
                                                                        AGE
hello-deployment-6949f8ddbc-d6rqb
                                          1/1
                                                  Running
                                                             0
                                                                        3m13s
hello-label
                                          1/1
                                                  Running
                                                             0
                                                                        39m
hello-pvc-deployment-7c5f879cd8-zpgq5
                                          0/1
                                                  Pending
                                                             0
                                                                        5s
```

Our "hello-deployment" pods are still running fine but our new "hello-pvc-deployment" pod is still in "Pending" status. It appears to be stuck. What could be wrong?

We can ask k8s to describe that pod to get more details:

```
[user-vm] $ kubectl describe pods hello-pvc-deployment-7c5f879cd8-zpgq5
Name:
                hello-pvc-deployment-7c5f879cd8-zpgq5
Namespace:
                USERNAME
Priority:
Node:
                <none>
Labels:
                app=hello-pvc-app
                pod-template-hash=7c5f879cd8
Annotations:
                <none>
<... some output omitted ...>
Tolerations:
                node.kubernetes.io/not-ready:NoExecute op=Exists for 300s
                 node.kubernetes.io/unreachable:NoExecute op=Exists for 300s
Events:
Type
         Reason
                           Age
                                 From
                                                    Message
                                ____
Warning FailedScheduling 61s default-scheduler 0/3 nodes are available: 3.
→persistentvolumeclaim "hello-USERNAME-data" not found. preemption: 0/3 nodes are...
→available: 3 Preemption is not helpful for scheduling.
```

At the bottom we see the "Events" section contains a clue: persistent/volumeclaim "hello-USERNAME-data" not found.

This is our problem. We told k8s to fill a volume with a persistent volume claim named "hello-USERNAME-data" but we never created that persistent volume claim. Let's do that now!

Open up a file called pvc-basic.yml and copy the following contents, being sure to replace <username> with your TACC username:

```
apiVersion: v1
kind: PersistentVolumeClaim
metadata:
name: hello-<username>-data
spec:
accessModes:
- ReadWriteOnce
storageClassName: cinder-csi
resources:
requests:
storage: 1Gi
```

Note: Again, be sure to replace **<username>** with your actual username in the YAML above.

We will use this file to create a persistent volume claim against the storage that has been set up in the TACC k8s cluster. In order to use this storage, you do need to know the storage class (in this case, "cinder-csi", which is the storage class for utilizing the Cinder storage system), and how much you want to request (in this case, just 1 Gig), but you don't need to know how the storage was implemented.

Note: Different k8s clusters may offer persistent storage that utilize different storage classes. Within TACC, we also have k8s clusters that utilize the **rbd** and **nfs** storage classes, for example. Be sure to check with the k8s administrators to see what storage class(es) might be available.

We create this pvc object with the usual kubectl apply command:

```
[user-vm]$ kubectl apply -f hello-pvc.yml
persistentvolumeclaim/hello-USERNAME-data created
```

Great, with the pvc created, let's check back on our pods:

```
[user-vm]$ kubectl get pods
NAME
                                          READY
                                                   STATUS
                                                                 RESTARTS
                                                                             AGE
hello-deployment-9794b4889-mk6qw
                                          1/1
                                                   Running
                                                                 46
                                                                             46h
hello-deployment-9794b4889-sx6jc
                                                                             46h
                                          1/1
                                                   Running
                                                                 46
hello-deployment-9794b4889-v2mb9
                                          1/1
                                                   Running
                                                                 46
                                                                             46h
hello-deployment-9794b4889-vp6mp
                                          1/1
                                                   Running
                                                                 46
                                                                             46h
hello-pvc-deployment-ff5759b64-sc7dk
                                                   Running
                                          1/1
                                                                             45s
```

Like magic, our "hello-pvc-deployment" now has a running pod without us making any additional API calls to k8s! This is the power of the declarative aspect of k8s. When we created the hello-pvc-deployment, we told k8s to always keep one pod with the properties specified running at all times, if possible, and k8s continues to try and implement our wishes until we instruct it to do otherwise.

Note: You cannot scale a pod with a volume filled by a persistent volume claim.

9.5.2 Exec Commands in a Running Pod

Because the command running within the "hello-pvc-deployment" pod redirected the echo statement to a file, the hello-pvc-deployment-ff5759b64-sc7dk will have no logs. (You can confirm this is the case for yourself using the logs command as an exercise).

In cases like these, it can be helpful to run additional commands in a running pod to explore what is going on. In particular, it is often useful to run shell in the pod container.

In general, one can run a command in a pod using the following:

```
[user-vm]$ kubectl exec <options> <pod_name> -- <command>
```

To run a shell, we will use:

```
[user-vm]$ kubectl exec -it <pod_name> -- /bin/bash
```

The -it flags might look familiar from Docker – they allow us to "attach" our standard input and output to the command we run in the container. The command we want to run is /bin/bash for a shell.

Let's exec a shell in our "hello-pvc-deployment-ff5759b64-sc7dk" pod and look around:

```
[user-vm]$ kubectl exec -it hello-pvc-deployment-5b7d9775cb-xspn7 -- /bin/bash
root@hello-pvc-deployment-5b7d9775cb-xspn7:/#
```

Notice how the shell prompt changes after we issue the exec command – we are now "inside" the container, and our prompt has changed to "root@hello-pvc-deployment-5b7d9775cb-xspn" to indicate we are the root user within the container.

Let's issue some commands to look around:

```
[container] $ pwd / (continues on next page)
```

```
# exec put us at the root of the container's file system
[container]$ ls -l
total 8
drwxr-xr-x 2 root root 4096 Jan 18 21:03 bin
drwxr-xr-x 2 root root 6 Apr 24 2018 boot
drwxr-xr-x 3 root root 4096 Mar 4 01:06 data
drwxr-xr-x 5 root root 360 Mar 4 01:12 dev
drwxr-xr-x 1 root root 66 Mar 4 01:12 etc
drwxr-xr-x 2 root root
                       6 Apr 24 2018 home
drwxr-xr-x 8 root root 96 May 23 2017 lib
drwxr-xr-x 2 root root 34 Jan 18 21:03 lib64
drwxr-xr-x 2 root root 6 Jan 18 21:02 media
drwxr-xr-x 2 root root 6 Jan 18 21:02 mnt
drwxr-xr-x 2 root root 6 Jan 18 21:02 opt
dr-xr-xr-x 887 root root 0 Mar 4 01:12 proc
drwx----- 2 root root 37 Jan 18 21:03 root
drwxr-xr-x 1 root root 21 Mar 4 01:12 run
drwxr-xr-x 1 root root 21 Jan 21 03:38 sbin
drwxr-xr-x 2 root root 6 Jan 18 21:02 srv
dr-xr-xr-x 13 root root 0 May 5 2020 sys
drwxrwxrwt 2 root root 6 Jan 18 21:03 tmp
drwxr-xr-x 1 root root 18 Jan 18 21:02 usr
drwxr-xr-x 1 root root 17 Jan 18 21:03 var
# as expected, a vanilla linux file system.
# we see the /data directory we mounted from the volume...
[container]$ ls -l data/out.txt
-rw-r--r-- 1 root root 19 Mar 4 01:12 data/out.txt
# and there is out.txt, as expected
[container]$ cat data/out.txt
Hello, Kubernetes!
# and our hello message!
[container]$ exit
# we're ready to leave the pod container
```

Note: To exit a pod from within a shell (i.e., /bin/bash) type "exit" at the command prompt.

Note: The exec command can only be used to execute commands in *running* pods.

9.5.3 Persistent Volumes Are... Persistent

The point of persistent volumes is that they live beyond the length of one pod. Let's see this in action. Do the following:

- 1. Delete the "hello-pvc" pod. What command do you use?
- 2. After the pod is deleted, list the pods again. What do you notice?
- 3. What contents do you expect to find in the /data/out.txt file? Confirm your suspicions.

Solution:

```
[user-vm] kubectl delete pods hello-pvc-deployment-5b7d9775cb-xspn7
pod "hello-pvc-deployment-5b7d9775cb-xspn7" deleted
[user-vm]$ kubectl get pods
NAME
                                        READY
                                                 STATUS
                                                                     RESTARTS
                                                                                AGE
hello-deployment-9794b4889-mk6qw
                                                 Running
                                                                                47h
                                        1/1
                                                                     47
hello-deployment-9794b4889-sx6jc
                                        1/1
                                                 Running
                                                                                47h
                                                                     47
hello-deployment-9794b4889-v2mb9
                                        1/1
                                                 Running
                                                                     47
                                                                                47h
hello-deployment-9794b4889-vp6mp
                                        1/1
                                                 Running
                                                                                47h
hello-pvc-deployment-5b7d9775cb-7nfhv
                                        0/1
                                                 ContainerCreating
                                                                     0
                                                                                46s
# wild -- a new hello-pvc-deployment pod is getting created automatically!
# let's exec into the new pod and check it out!
[user-vm] kubectl exec -it hello-pvc-deployment-5b7d9775cb-7nfhv -- /bin/bash
[container] $ cat /data/out.txt
Hello, Kubernetes!
Hello, Kubernetes!
```

Warning: Deleting a persistent volume claim deletes all data contained in all volumes filled by the PVC permanently! This cannot be undone and the data cannot be recovered!

9.5.4 Additional Resources

- Persistent Volumes
- Storage Classes in k8s

9.6 Services and Ingress

Services are the k8s resource one uses to expose HTTP APIs, databases and other components that communicate on a network to other k8s pods and, ultimately, to the outside world. After working through this module, students should be able to:

- · Set up port forwarding from pods on a Kubernetes cluster
- Use a debug deployment to test access
- · Create and attach a service to a deployment
- Use a NodePort service to expose a Flask API on the public internet
- Use an Ingress object to map a NodePort port to a subdomain on the host

9.6.1 k8s Networking Overview

To understand services we need to first discuss how networking works in k8s.

Note: We will be covering just the basics of k8s networking, enough for you to become proficient with the main concepts involved in deploying your application. Many details and advanced concepts will be omitted.

k8s creates internal networks and attaches pod containers to them to facilitate communication between pods. For a number of reasons, including security, these networks are not reachable from outside k8s.

Recall that we can learn the private network IP address for a specific pod with the following command:

```
[user-vm]$ kubectl get pods <pod_name> -o wide
```

For example:

```
[user-vm] kubectl get pods hello-deployment-9794b4889-mk6qw -o wide
                                                               RESTARTS
                                         READY
                                                 STATUS
                                                                               AGE
                                                                                     IP
                            NOMINATED NODE
            NODE
                                              READINESS GATES
hello-deployment-6949f8ddbc-znx75
                                         1/1
                                                 Running
                                                               21 (31m ago)
                                                                               21h
                                                                                     10.
→233.116.45
               kube-worker-1
                               <none>
                                                 <none>
```

This tells us k8s assigned an IP address of 10.233.116.45 to our hello-deployment pod. IP addresses starting with 10. are private IP addresses which are part of a private network, isolated to this k8s cluster. k8s assigns every pod on this private network an IP address. Pods that are on the same network can communicate with other pods using their IP address.

9.6.2 Ports

To communicate with a program running on a network, we use ports. We saw how our Flask program used port 5000 to communicate HTTP requests from clients. We can expose ports in our k8s deployments by defining a ports stanza in our template.spec.containers object. Let's try that now.

Create a file called deployment-hello-flask.yml and copy the following contents

```
apiVersion: apps/v1
2
   kind: Deployment
   metadata:
     name: hello-flask
     labels:
       app: hello-flask
   spec:
     replicas: 1
     selector:
10
       matchLabels:
11
          app: hello-flask
12
     template:
13
       metadata:
          labels:
15
            app: hello-flask
       spec:
17
          containers:
```

(continues on next page)

```
- name: hello-flask
imagePullPolicy: Always
image: wjallen/hello-flask:1.0
ports:
- name: http
containerPort: 5000
```

Much of this will look familiar. We are creating a deployment that matches the pod description given in the template. spec stanza. The pod description uses an image, wjallen/hello-flask:1.0. This image runs a very simple flask server that responds with simple text message at the / endpoint.

The ports attribute is a list of k8s port descriptions. Each port in the list includes:

- name the name of the port, in this case, http. This could be anything we want really.
- containerPort the port inside the container to expose, in this case 5000. This needs to match the port that the containerized program (in this case, flask server) is binding to.

Next create the hello-flask deployment using kubectl apply

```
[user-vm]$ kubectl apply -f deployment-hello-flask.yml
deployment.apps/deployment-hello-flask configured
```

With our deployment created, we should see a new pod.

EXERCISE

Determine the IP address of the new pod for the deployment-hello-flask.

SOLUTION

```
[user-vm]$ kubectl get pods
NAME
                                                        RESTARTS
                                                                       AGE
                                      READY
                                              STATUS
                                                        21 (36m ago)
hello-deployment-6949f8ddbc-znx75
                                                                        2.1h
                                      1/1
                                              Running
hello-label
                                      1/1
                                              Running
                                                        21 (57m ago)
                                                                        21h
hello-label2
                                                                       21h
                                      1/1
                                              Running
                                                        21
hello-flask-7bf64cc577-17f52
                                      1/1
                                              Running
                                                                        2m34s
 [user-vm] kubectl get pods helloflask-86d4c7d8db-2rkg5 -o wide
NAME
                               READY
                                       STATUS
                                                  RESTARTS AGE
                                                                     ΙP
                                                                                      NODE_
             NOMINATED NODE
                              READINESS GATES
hello-flask-7bf64cc577-17f52 1/1
                                        Running
                                                             3m46s
                                                                     10.233.116.59
                                                                                      kube-
⊶worker-1
             <none>
                              <none>
# Therefore, the IP address is 10.233.116.59
```

We found the IP address for our Flask container, but if we try to communicate with it from our Jetstream VMs, we will either find that it hangs indefinitely or possible gives an error:

```
[user-vm]$ curl 10.233.116.59:5000/
curl: (7) Failed connect to 10.233.116.59:5000; Network is unreachable
```

This is because the 10.233.*.* private k8s network is not available from the outside. However, it *is* available from other pods in the namespace.

9.6.3 A Debug Deployment

For exploring and debugging k8s deployments, it can be helpful to have a basic container on the network. We can create a deployment for this purpose.

For example, let's create a deployment using the official Python 3.10 image. We can run a sleep command inside the container as the primary command, and then, once the container pod is running, we can use **exec** to launch a shell inside the container.

EXERCISE

Create a new "debug" deployment using the following definition:

```
apiVersion: apps/v1
2
   kind: Deployment
   metadata:
     name: py-debug
     labels:
       app: py-debug
   spec:
     replicas: 1
     selector:
10
       matchLabels:
11
          app: py-debug
12
     template:
13
       metadata:
14
          labels:
            app: py-debug
16
17
       spec:
          containers:
18
            - name: py-debug
              image: python:3.10
20
              command: ['sleep', '999999999']
```

Once it is ready, exec into the running pod for this deployment. Once we have a shell running inside our debug deployment pod, we can try to access our Flask server. Recall that the IP and port for the Flask server were determined above to be 10.244.7.95:5000 (yours will be different).

If we try to access it using curl from within the debug container, we get:

```
root@py-debug-deployment-5cc8cdd65f-xzhzq: $ curl 10.233.116.59:5000
Hello, world!
```

Great! k8s networking from within the private network is working as expected!

9.6.4 Services

We saw above how pods can use the IP address of other pods to communicate. However, that is not a great solution because we know the pods making up a deployment come and go. Each time a pod is destroyed and a new one created it gets a new IP address. Moreover, we can scale the number of replica pods for a deployment up and down to handle more or less load.

How would an application that needs to communicate with a pod know which IP address to use? If there are 3 pods comprising a deployment, which one should it use? This problem is referred to as the *service discovery problem* in distributed systems, and k8s has a solution for it.. the Service abstraction.

A k8s service provides an abstract way of exposing an application running as a collection of pods on a single IP address and port. Let's define a service for our hello-flask deployment.

Copy and paste the following code into a file called service-hello-flask.yml:

```
apiVersion: v1
2
   kind: Service
   metadata:
     name: hello-flask-service
   spec:
6
     type: ClusterIP
7
     selector:
       app: hello-flask
     ports:
10
     - name: hello-flask
11
       port: 5000
12
       targetPort: 5000
13
```

Let's look at the spec description for this service.

- type There are different types of k8s services. Here we are creating a ClusterIP service. This creates an IP address on the private k8s network for the service. We may see other types of k8s services later.
- selector This tells k8s what pod containers to match for the service. Here we are using a label, app: hello-flask, which means k8s will link all pods with this label to our service. Note that it is important that this label match the label applied to our pods in the deployment, so that k8s links the service up to the correct pods.
- ports This is a list of ports to expose in the service.
- ports.port This is the port to expose on the service's IP. This is the port clients will use when communicating via the service's IP address.
- ports.targetPort This is the port on the pods to target. This needs to match the port specified in the pod description (and the port the containerized program is binding to).

We create this service using the kubectl apply command, as usual:

```
[user-vm]$ kubectl apply -f hello-flask-service.yml
service/hello-service configured
```

We can list the services:

We see k8s created a new service with IP 10.233.12.76. We should be able to use this IP address (and port 5000) to communicate with our Flask server. Let's try it. Remember that we have to be on the k8s private network, so we need to exec into our debug deployment pod first.

```
[user-vm] $ kubectl exec -it py-debug-deployment-5cc8cdd65f-xzhzq -- /bin/bash

# from inside the container ---
root@py-debug-deployment-5cc8cdd65f-xzhzq:/ $ curl 10.233.12.76:5000/
Hello, world!
```

It worked! Now, if we remove our hello-flask pod, k8s will start a new one with a new IP address, but our service will automatically route requests to the new pod. Let's try it.

```
# remove the pod ---
[user-vm] $ kubectl delete pods hello-flask-86d4c7d8db-2rkg5
pod "helloflask-86d4c7d8db-2rkg5" deleted
# see that a new one was created ---
[user-vm] $ kubectl get pods
NAME
                                         READY
                                                 STATUS
                                                           RESTARTS
                                                                       AGE
                                                                       175m
hello-deployment-9794b4889-w4jlq
                                         1/1
                                                 Running
                                                           2
hello-pvc-deployment-6dbbfdc4b4-sxk78
                                                 Running
                                                           233
                                                                       9d
                                         1/1
hello-flask-86d4c7d8db-vbn4g
                                          1/1
                                                  Running
                                                            0
                                                                        62s
# it has a new IP ---
[user-vm] kubectl get pods helloflask-86d4c7d8db-vbn4g -o wide
NAME
                                       STATUS
                                                 RESTARTS
                                                                                  NODE
                              READY
                                                            AGE
                                                                    ΙP
→NOMINATED NODE
                   READINESS GATES
                                                  0
                                                             112s
                                                                                    c05
hello-flask-86d4c7d8db-vbn4g
                               1/1
                                        Running
                                                                     10.233.12.96
<none>
                   <none>
# Yep, 10.233.12.96 -- that's different; the first pod had IP 10.233.116.59
# but back in the debug deployment pod, check that we can still use the service IP --
root@py-debug-deployment-5cc8cdd65f-xzhzq:/ $ curl 10.233.12.76:5000/
Hello, world!
```

Note that k8s is doing something non-trivial here. Each pod could be running on one of any number of worker computers in the TACC k8s cluster. When the first pod was deleted and k8s created the second one, it is quite possible it started it on a different machine. So k8s had to take care of rerouting requests from the service to the new machine.

k8s can be configured to do this "networking magic" in different ways. While the details are beyond the scope of this course, keep in mind that the virtual networking that k8s uses does come at a small cost. For most applications, including long-running web APIs and databases, this cost is negligible and isn't a concern. But for high-performance applications, and in particular, applications whose performance is bounded by the performance of the underlying network, the overhead can be significant.

EXERCISE

Now, you have enough tools in your k8s toolbox to deploy your entire web app on the k8s cluster. Follow the steps below to try to launch your web app. In each step, you will be creating a new k8s resource described by its own k8s yaml file. We recommend carefully naming the files following a pattern like <name>-<env>-<resource>-<item>.yml. In this case <name> is the name of your app, <env> is the environment - test or prod, <resource> is the k8s resource used - e.g. deployment or service or pvc, and <item> is the identity of the service - e.g. flask or redis or worker. For example, imagine you are creating a deployment for the Flask front end for the test copy of an web app for analyzing the HGNC data. You might name this yaml file HGNC-test-deployment-flask.yml. Other naming schemes for these files are perfectly valid as long as there is *consistency* among them.

- **Step 1:** Create a PVC for Redis to write dump files
- Step 2: Create a deployment for your Redis database which binds the PVC from Step 1
- Step 3: Create a service for your Redis deployment so you have a persistent IP address to use to communicate with Redis
- Step 4: Create a deployment for your Flask API
- Step 5: Create a service for your Flask API so you have a persistent IP address to use to communicate with Flask
- Step 6: Create a deployment for your Worker which is scaled to three replicas

As you apply files, be sure to check your work in between each step. Make sure deployments and pods are ready and available, make sure PVCs are bound, make sure services are correctly associated with deployments, etc. Use a debug deployment to test things as much as possible along the way.

9.6.5 Public Access to Your Deployment

The final objective is to make your Flask API available on the public internet. This process assumes you have already created a deployment and a service (of type ClusterIP) for your Flask API. There are two new k8s objects required:

- 1. A second Service object of type NodePort which selects your deployment using the deployment label and exposes your Flask API on a public port.
- 2. An Ingress object which specifies a subdomain to make your Flask API available on and maps this domain to the public port created in Step 1.

9.6.6 Create a NodePort Service

The first step is to create a NodePort Service object pointing at your Flask deployment. Copy the following code into a new file called service-nodeport-hello-flask.yml or something similar:

```
kind: Service
apiVersion: v1
metadata:
name: hello-flask-nodeport-service
spec:
type: NodePort
selector:
app: hello-flask
ports:
- port: 5000
targetPort: 5000
```

Update the highlighted lines:

- 1. The name of the Service object can be anything you want, so long as it is unique among the Services you have defined in your namespace. In particular, it needs to be a different name from your ClusterIP service defined previously.
- 2. The value of app in the selector stanza needs to match the app label in your deployment. This should be exactly the same as what you did in the ClusterIP service created previously. As mentioned before, be sure the selector targets the **label** in your Flask deployment, **not the deployment name**.

As usual, create the NodePort using kubect1:

```
[user-vm]$ kubectl apply -f service-nodeport-hello-flask.yml
service/hello-flask-nodeport-service created
```

Change the command to reference the file name you used. Check that the service was created successfully and determine the port that was created for it:

```
[user-vm]$ kubectl get services
NAME
                                 TYPE
                                              CLUSTER-IP
                                                               EXTERNAL-IP
                                                                              PORT(S)
-AGE
hello-flask-nodeport-service
                                 NodePort
                                               10.233.1.87
                                                               <none>
                                                                              5000:32627/TCP
<u></u>
-24s
hello-flask-service
                                 ClusterIP
                                               10.233.58.60
                                                                              5000/TCP
                                                               <none>
-4d10h
```

Here we see that port 32627 was created for this service. Your port will be different.

You can test that the NodePort service is working by using the special domain coe332.tacc.cloud to exercise your Flask API from the kube-access VM:

```
[user-vm]$ curl coe332.tacc.cloud:32627/
Hello, world!
```

Change the port (32627) to the port associated with your nodeport service, and the URL path (/) to a path your Flask API recognizes.

Note: The curl above only works on the public internet - in the next section, we will map the port to a subdomain of the host.

9.6.7 Create an Ingress

Next we will create an Ingress object which will map the NodePort port defined previously (in the above example, 32627) to a specific domain on the public internet.

Copy the following code into a new file called ingress-hello-flask.yml or similar:

```
kind: Ingress
apiVersion: networking.k8s.io/v1
metadata:
name: hello-flask-ingress
annotations:
nginx.ingress.kubernetes.io/ssl-redirect: "false"

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```

```
spec:
     ingressClassName: nginx
10
      - host: "username-flask.coe332.tacc.cloud"
       http:
12
            paths:
13
            - pathType: Prefix
14
              path: "/"
15
              backend:
                service:
                  name: hello-flask-nodeport-service
19
                       number: 5000
```

Be sure to update the highlighted lines:

- 1. Specify a meaningful name for the ingress. Keep in mind it should be unique among all Ingress obejcts within your namespace.
- 2. Update the host value to include your username in the subdomain, i.e., use the format host: "<username>.coe332.tacc.cloud".

Create the Ingress object:

Double check that the object was successfully created:

```
[user-vm]$ kubectl get ingressNAMECLASSHOSTSADDRESSPORTSAGEhello-flask-ingress<none>username-flask.coe332.tacc.cloud80102s
```

At this point our Flask API should be available on the public internet from the domain we specified in the host field. We can test by running the following curl command from anywhere, including our laptops.

```
[local]$ curl username-flask.coe332.tacc.cloud/
Hello, world!
```

9.6.8 Additional Resources

· Services in k8s

9.7 k8s Cheat Sheet

This all-in-one k8s cheat sheet can be used for quick reference.

9.7.1 k8s Resource Types

Here are the primary k8s resource types we have covered in this class:

- Pods Pods are the simplest unit of compute in k8s and represent a generalization of the Docker container. Pods can contain more than one container, and every container within a pod is scheduled together, on the same machine, with a single IP address and shared file system. Pod definitions include a name, a (Docker) image, a command to run, as well as an ImagePullPolicy, volumeMounts and a set of ports to expose. Pods can be thought of as disposable and temporary.
- Deployments Deployments are the k8s resource type to use for deploying *long-running* application components, such as APIs, databases, and long-running worker programs. Deployments are made up of one or more matching pods, and the matching is done using labels and labelSelectors.
- PersistentVolumeClaims (PVCs) PVCs create a named storage request against a storage class available on the k8s cluster. PVCs are used to fill volumes with permenant storage so that data can be saved across different pod executions for the same stateful application (e.g., a database).
- Services Services are used to expose an entire application component to other pods. Services get their own IP address which persists beyond the life of the individual pods making up the application.
- Ingresses Map services running on specific ports to subdomains on the host. These are useful if you want to give your web app a unique and descriptive domain name.

9.7.2 kubectl Commands

Here we collect some of the most commonly used kubectl commands for quick reference.

Command	Description	Example
kubectl get <resource_type></resource_type>	List all objects of a given resource type.	kubectl get pods
kubectl get <type> <name></name></type>	Get one object of a given type by name.	kubectl get pods hello-pod
kubectl get <type> <name> -o wide</name></type>	Show additional details of an object	kubectl get pods hello-pod -o wide
kubectl describe <type></type>	Get full details of an object by name.	kubectl describe pods hello-pod
kubectl logs <name></name>	Get the logs of a running pod by name.	kubectl logs hello-pod
kubectl logs -f <name></name>	Tail the logs of a running pod by name.	kubectl logs -f hello-pod
kubectl logs -since <time></time>	Get the logs of a running pod since a given	kubectl logs -since 1m -f hello-
<name></name>	time.	pod
kubectl exec -it <name> <cmd></cmd></name>	Run a command, <cmd>, in a running pod.</cmd>	kubectl exec -it hello-pod/bin/bash
kubectl apply -f <file></file>	Create or update an object description using a file.	kubectl apply -f hello-pod.yml
kubectl delete <type> <name></name></type>	Delete an object of a given type by name.	kubectl delete pods hello-pod
kubectl delete -f <file></file>	Delete an object using a file.	kubectl delete -f hello-pod.yml

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CHAPTER

TEN

UNIT 10: SPECIAL TOPICS

Up to this point, we have worked on all of the different tools, technologies, and components that will go into the software systems we will build for our final projects. In this unit, we will further discuss how we will approach building our software systems between our development environment (Jetstream) and the deployment environment (Kubernetes). We will also learn some new techniques to help speed up the development cycle and catch errors as we go - namely integration testing and continuous integration.

10.1 Development Environment

Development of the software systems for our final projects should be performed on the Jetstream VMs. The containers built and run on individual user VMs will be ephemeral - only lasting long enough to test and debug new features. They should never be seen by end users. After going through this module, students should be able to:

- Set up the files and folders necessary to work on the final project
- Describe each component and why they are important to the overall system
- Describe the general development cycle from a new idea all the way to production
- Write targets for the major steps into a Makefile

10.1.1 File Organization

Our final software systems should have three main components:

- 1. A Flask API front end for accessing data and jobs functionality
- 2. A Redis database for storing job and queue information
- 3. A Worker back end which runs the analysis job

An example file organization scheme for developing this API may look like:

```
my-api/
— data
— .gitcanary
— docker-compose.yml
— Dockerfile
— requirements.txt
— src
— flask_api.py
— jobs.py
— worker.py
```

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In this example, the data/ subfolder is mounted inside a Redis container. All the data is captured in regular intervals in dump.rdb for testing purposes only (real end users will not see this copy of the data). It is common practice to put an empty file like .gitcanary in a folder so that you can commit it to a Git repo.

The Dockerfile, in this case, containerizes all source code and tests scripts along with each of their dependencies. Alternative entrypoint commands allow us to reuse the same container image for multiple functions (Flask API and Worker). We don't need a Dockerfile for the Redis container because we will use the stock redis:7 image.

The src/ folder contains the source Python scripts that are injected into the API and worker containers. This is where the majority of the development will occur.

The test/ folder contains our unit and integration tests, compatible with pytest. It is safe to assume that one should expect the service to be deployed in order to test, and that the tests should be run inside of a container. In fact, the simplest way to organize the tests is to copy all test scripts and source code into the same directory within the container and execute tests from there.

Tip: Make sure to put your folders under version control and commit regularly as you work. Don't save it all until the end.

QUESTIONS

- Is the data set I'm working with part of this repository? Why or why not?
- Should we commit dump.rdb to GitHub? Why or why not?
- I am not using a requirements.txt file above. Should I?
- I am using two Dockerfiles one for the worker and one for the API. Should I be doing this or should I just have one Dockerfile?

10.1.2 Docker

We previously talked at great length about why it is a good idea to containerize an app / service that you develop. One of the main reasons was for portability to other machines. All the development / testing done in this development environment will directly translate to our deployment environment (Kubernetes), as we will see in the next module.

The development cycle for each of the three containerized components generally follows the form:

- 1. Edit some source code (e.g. add a new Flask route)
- 2. Delete any running container with the old source code
- 3. Re-build the image
- 4. Start up a new container
- 5. Test the new code / functionality
- 6. Repeat

This 6-step cycle is great for iterating on the API and Worker containers independently, or at the same time. However, watch out for potential error sources. For example if you take down the Redis container, a worker container that is in the middle of watching the queue may also go down and will need to be restarted (once a new Redis container is up).

10.1.3 Makefile

Makefiles are a useful automation tool for building, running, testing, and pushing your services. Now that our development cycle is becoming longer and more complicated, it is worth investing some time in Makefiles to speed up the development process. Here, we will set up a Makefile to help with the 6-step cycle above. Using certain keywords (called "targets") we will create shortcuts to cleaning up running containers, re-building docker images, and running new containers.

Targets are listed in a file called Makefile in this format:

```
target: prerequisite(s)
    recipe
```

Targets are short keywords, and recipes are shell commands. For example, a simple target might look like:

```
ps-me:
docker ps -a | grep username
```

Put this text in a file called Makefile in your current directory, (replacing "username" with your username, and then you simply need to type:

And that will list all the Docker containers with the username "username" either in the image name or the container name. Makefiles can be further abstracted with variables to make them a little bit more flexible. Consider the following Makefile:

Here we have added a variable NAME at the top so we can easily customize the targets below. We have also added two new targets: im-me which lists images, and all which does not contain any recipes, but does contain two prerequisites - the other two targets. So these two are equivalent:

```
# make all targets
[user-vm]$ make all

# or make them one-by-one
[user-vm]$ make ps-me
[user-vm]$ make im-me

# Try this out:
[user-vm]$ NAME="redis" make all
```

EXERCISE

Write a Makefile that, at a minimum:

- 1. Builds all necessary images for your app from Dockerfile(s)
- 2. Starts up new containers / services
- 3. Removes running containers in your namespace (be careful!)
- 4. Runs your unit tests
- 5. Cycles through steps 2-5 listed above in one command

Note: Docker-compose automates much of the build and run process for us. But it is limited in scope. Makefiles can be used to automate any arbitrary command that is part of your development cycle.

10.2 Deployment Environment

Our deployment environment for this API will be the class Kubernetes cluster. It could just as easily be AWS, or Azure, or Google Cloud, or another Kubernetes cluster. Remember if you containerize everything, it becomes extremely portable. In contrast to our development environment, the Kubernetes deployment is meant to be long-lasting, highly available, and consumable by the public. We will have test and prod deployments, so that new changes can be seen by developers in the test deployment environment (sometimes also called "staging") before finally making their way to the prod (production) deployment environment. After going through this module, students should be able to:

- · Name and organize YAML files for test and prod deployments of a software system
- Sync files between two remote copies of a Git repository
- · Version code following semantic versioning specification
- · Attach a NodePort service to an API deployment
- Deploy production and test copies of software system in Kubernetes

10.2.1 File Organization

To support the deployment environment (prod and test), our file tree may grow to something similar to the following:

```
my-api/
— data
— .gitcanary
— docker-compose.yml
— Dockerfile
— kubernetes
— prod
— app-prod-deployment-flask.yml
— app-prod-deployment-redis.yml
— app-prod-deployment-worker.yml
— app-prod-ingress-flask.yml
— app-prod-pvc-redis.yml
— app-prod-service-flask.yml
— app-prod-service-nodeport-flask.yml
```

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```
app-prod-service-redis.yml
     test
        app-test-deployment-flask.yml
         app-test-deployment-redis.yml
         app-test-deployment-worker.yml
         app-test-ingress-flask.yml
         app-test-pvc-redis.yml
         app-test-service-flask.yml
         app-test-service-nodeport-flask.yml
        app-test-service-redis.yml
requirements.txt
 src
    flask_api.py
    jobs.py
    worker.py
 test
   - test_flask_api.py
    test_jobs.py
    test_worker.py
```

In this example, you will find 16 new YAML files with somewhat descriptive names. Eight are organized into a 'test' directory, and eight are organized into a 'prod' directory, although there are other acceptable ways to organize these files.

These YAML files closely follow the naming convention and content we have seen in previous lectures. There are three deployments - one each for the API, database, and worker. There are two services - one each for the API and database. And, there is a persistent volume claim (PVC) for the database. Without looking into the contents of the files, it is clear what function each serves, and it is clear that there is one-to-one correspondence between the test and prod deployments.

10.2.2 Test Deployment

The purpose of this testing / staging environment is to see the entire API exactly as it appears in production before actually putting new code changes into production.

Generally the process to get code into testing follows these steps:

- 1. Develop / test code in the development environment (Jetstream) as described in the previous module
- 2. Push code to GitHub and tag it with an appropriate version number (avoid using "latest" see Versioning section below)
- 3. Push images to Docker Hub Kubernetes needs to pull from here. Make sure the Docker image tag matches the GitHub tag so you always know what exact version of code is running.
- 4. Edit the appropriate testing deployment(s) with the new tags and apply the changes. Pods running within a deployment under the old tag number should be automatically terminated.

The yaml files above can be applied one by one, or the entire directory at a time like the following:

```
[user-vm]$ kubectl apply -f kubernetes/test/
```

Kubernetes will apply all the files found in the test folder. Be careful, however, about the order in which things are applied. For example, the Redis DB deployment needs the PVC to exist in order to deploy successfully. But, Kubernetes is usually pretty smart about this kind of thing, so it should keep retrying all deployments, services, and PVCs until everything is happy and connected.

Once deployed, you should rigorously test all services using the Python debug pod and, if applicable, the NodePort Service connection to the outside world. We will see more on automating integration tests later in this unit.

10.2.3 Syncing Git Repos

A challenge you might encounter while working in a shared repo with other team members has to do with keeping your repos in sync. If Student A develops some code that they commit and push to GitHub, Student B will need to pull those changes in to their local copy of the repo before they can push anything to GitHub. A sample workflow may resemble:

1) Imagine the repository on GitHub is newly cloned by both Student A and Student B to their respective Jetstream VMs. We would say each student is in sync with the upstream repo. Then, Student A edits some files, commits changes, and pushes to GitHub:

```
# ...edit some file(s)
[student-A-vm]$ git add .
[student-A-vm]$ git commit -m "message"
[student-A-vm]$ git push
```

2) Now we would say Student A is in sync with the upstream repo, but Student B's remote repository on their Jetstream VM is one commit behind. Student B will need to pull those changes into their repository:

```
[student-B-vm]$ git remote update
[student-B-vm]$ git pull
```

3) Everything is back in sync again. Next, Student B edits some files on their Jetstream VM, commits changes, and pushes to GitHub:

```
# ...edit some file(s)
[student-B-vm]$ git add .
[student-B-vm]$ git commit -m "message"
[student-B-vm]$ git push
```

4) Now we would say GitHub is one commit ahead of the report repository in Student A's Jetstream VM. Student A needs to pull in the changes:

```
[student-A-vm]$ git remote update
[student-A-vm]$ git pull
```

Finally the origin (GitHub) and both remote copies of the repository are in sync again. This strategy works not only for collaborating with others on a repository, but it also works for keeping copies of your own repository in sync between multiple machines. (Although there are better ways to collaborate).

10.2.4 Versioning

We have not spent much time discussing versioning in this class other than to see do not use the tag 'latest' when versioning your repos or Docker images. There is a well-accepted standard for versioning called 'Semantic Versioning'. It follows the specification:

Given a version number MAJOR.MINOR.PATCH, increment the:

- MAJOR version when you make incompatible API changes,
- MINOR version when you add functionality in a backwards compatible manner, and
- PATCH version when you make backwards compatible bug fixes.

You can assign a tag to the current state of a repository on the command line by doing:

```
[user-vm]$ git tag -a 0.1.0 -m "first release"
[user-vm]$ git push origin 0.1.0
```

Tip: Do you have a new software system that just kind of works and has a little bit of functionality, but you don't know what version tag to assign it? A good place to start is version 0.1.0.

10.2.5 Production Deployment

If everything with the test / staging deployment looks good and passes tests, follow the same steps for your production environment. Kubernetes is fast at stopping / starting containers, and the services should provide pretty seamless access to the underlying API. If larger-scale changes are needed and significant downtime is anticipated, it would be a good idea to post an outage notice to users.

10.2.6 Additional Resources

- Collaborate on Git Repos
- Semantic Versioning

10.3 Integration Testing

Unlike unit tests, integration tests exercise multiple components, functions, or units of a software system at once. Some properties of integration tests include:

- Each test targets a higher-level capability, requirement or behavior of the system, and exercises multiple components of the system working together.
- Broader scope means fewer tests are required to cover the entire application/system.
- A given test failure provides more limited information as to the root cause.

It's worth pointing out that our definition of integration test leaves some ambiguity. You will also see the term "functional tests" used for tests that exercise entire aspects of a software system. After going through this module, students should be able to:

- Identify Python frameworks for integration testing
- Identify aspects of a software system that should be tested with integration testing
- Use the Python requests library to interact with the API of your software system
- Write and execute useful integration tests using pytest and assert statements

10.3.1 Challenges When Writing Integration Tests

Integration tests against large, distributed systems with lots of components that interact face some challenges.

- We want to keep tests independent so that a single test can be run without its result depending on other tests.
- Most interesting applications change "state" in some way over time; e.g., files are saved/updated, database records are written, queue systems updated. In order to properly test the system, specific state must be established before and after a test (for example, inserting a record into a database before testing the "update" function).
- Some components have external interactions, such as an email server, a component that makes an update in an external system (e.g. GitHub) etc. A decision has to be made about whether or not this functionality will be validated in the test and if so, how.

10.3.2 Initial Integration Tests for Our Flask API

For our first set of integration tests, we'll use the following strategy:

- Start the Flask API, Redis DB, and Worker services
- Use the requests library in our test scripts to make requests directly to the running API server
- Check various aspects of the response; each check can be done with a simple assert statement, just like for unit tests

Note: In large software projects you may see unit tests and integration tests separated into different tests scripts. The projects in this class are small enough and the tests will run quickly enough that it is generally fine to just keep everything together.

Organizing Test Files

As we have seen before, test scripts should be named strategically and organized into a subdirectory similar to:

```
my-api/
   data
     gitcanary
    docker-compose.yml
   Dockerfile
   kubernetes
       . . .
   requirements.txt
   src
      flask_api.py
      - jobs.py
      — worker.py
   test
      — test_flask_api.py
      - test_jobs.py
       - test_worker.py
```

The simplest way to import target methods into your test scripts is to containerize the test scripts in the same directory as your src files. For example, a few lines of your Dockerfile could resemble:

```
WORKDIR /app
COPY src/* ./
COPY test/* ./
...
```

Then, your test scripts could import directly from your src files without needing to account for relative path For unit tests, you will need to import the target method. For integration tests, you likely can get away without importing the target method and instead just using the requests library.

A Simple pytest Example

Assume you have a simple Flask app in the file flask_api.py with a 'Hello, world!' route like:

```
@app.route('/hello', methods=['GET'])
def hello():
    return 'Hello, world!\n'
```

You could approach this function from a unit test point of view and write a simple check to make sure it returns the correct string. In test_hello_flask.py you would have lines of code similar to:

```
from flask_api import hello

def test_hello():
   assert (hello()) == 'Hello, world!\n'
```

However, to test the Flask app as it is integrated into the overall software system, it would be useful to approach this test from a different angle:

```
import requests

def test_integration_hello():
    response = requests.get('http://localhost:5000/hello')
    assert response.status_code == 200
```

Notice this time we do not need to import the hello() method directly. This small test just checks to make sure curling the route (with the Python requests library) returns a successful status code, 200. In practice, it may be useful to keep both tests.

Running Containerized Tests

To run the tests in a container, first ensure that the test scripts are containerized along side the src code. Before running the tests, however, it is important to understand more about Docker networks. When you perform docker-compose up, Docker creates a bridge network such that different services that are part of the same docker-compose.yml file can communicate with each other using service names as host aliases. This is what allows us to use, e.g. redis-db as the IP address for the Redis container, so long as the database service is named redis-db in the docker-compose.yml file.

To run containerized tests, we need to (1) ensure that the container running the tests is on the same bridge network as the services and (2) inject a hostname alias for the Flask API into the test file.

First perform docker-compose up and identify the name of the bridge network:

```
[user-vm]$ docker-compose up --build -d
...
[user-vm]$ docker network ls
...
eea9458e6e9f demo_default bridge local
...
```

There are typically several networks. Look for one with the same name as the folder your files are in. You can also use docker inspect on a running container to see what network it is on. Once you identify the network, you need to launch the test container on the same network using a flag:

Remember, the tests will become a little more flexible if you create a way to dynamically set the Flask API hostname. (We did something similar for the Redis IP address in a previous lesson). Imaging updating the test script(s) to include something similar to the following:

```
import requests
import os
from flask_api import hello

flask_ip=os.environ.get('FLASK_IP')

def test_hello():
    assert (hello()) == 'Hello, world!\n'

def test_integration_hello():
    response = requests.get(f'http://{_flask_ip}:5000/hello')
    assert response.status_code == 200
```

QUESTIONS

- How do we set the value of FLASK_IP in the environment?
- What should the value be set to?

EXERCISE

Continue working in the test file, test_api.py, and write a new functional test that use the requests library to make a GET request to the /jobs endpoint and check the response for, e.g.:

- The response returns a 200 status code
- The response returns a valid JSON string
- The response can be decoded to a Python dictionary

Remember, your services should be running and as much as possible, functional tests should be testing the end-to-end functionality of your entire app.

10.4 Continuous Integration

In a multi-developer environment, typically no one person has complete knowledge of the entire system, and multiple changes can be happening at the same time. Even if the changes are made in different components, it is possible for something to break when they are integrated. The primary goal of Continuous Integration (CI) is to enable multiple developers to work on the same code base while ensuring the quality of the final product. After going through this module, students should be able to:

- Identify the importance of CI to a large software system
- Choose a CI service that meets the needs of their software system
- · Perform a integration testing CI workflow with GitHub Actions
- Perform a docker build / docker push CI workflow with GitHub Actions

10.4.1 An Example CI Workflow

An "integration server" (or "build server") is a dedicated server (or VM) that prepares software for release. The server automates common tasks, including:

- Building software binaries from source code (for compiled languages)
- · Running tests
- · Creating images, installers, or other artifacts
- Deploying/installing the software

We are ultimately aiming for the following "Continuous Integration" work flow or process; this mirrors the process used by a number of teams working on "large" software systems, both in academia and industry:

- Developers (i.e., you) check out code onto a machine where they will do their work. This could be a VM somewhere or their local laptop.
- They make changes to the code to add a feature or fix a bug.
- Once their work is done they add any additional tests as needed and then run all unit tests "locally" (i.e., on the same machine).
- Assuming the tests pass, the developer commits their changes and pushes to the origin (in this case, GitHub).
- · A pre-established build server gets a message from the origin that a new commit was pushed.
- The build server:
 - Checks out the latest version

- Executes any build steps to create the software
- Runs unit tests
- Starts an instance of the system
- Runs integration tests
- Deploys the software to a staging environment

If any one of the steps above fails, the process stops. In such a situation, the code defect should be addressed as soon as possible.

10.4.2 Popular Automated CI Services

Jenkins is one of the most popular free open-source CI services. It is server-based, and it requires a web server to operate on.

- · Local application
- · Completely free
- · Deep workflow customization
- · Intuitive web interface management
- Can be distributed across multiple machines / VMs
- · Rich in features and plugins
- Easy installation thanks to the pre-installed OS X, Unix and Windows packages
- A well-established product with an excellent reputation

TravisCI is another CI service with limited features in the free tier, and a comprehensive paid tier. It is a cloud-hosted service, so there is no need for you to host your own server.

- · Quick setup
- · Live build views
- Pull request support
- · Multiple languages and platforms support
- · Pre-installed database services
- Auto deployments on passing builds
- Parallel testing (paid tier)
- Scaling capacity on demand (paid tier)
- · Clean VMs for every build
- Mac, Linux, and iOS support
- · Connect with Github, Bitbucket and more

GitHub Actions is a relatively new CI service used to automate, customize, and execute software development workflows right in your GitHub repository.

- One interface for both your source code repositories and your CI/CD pipelines
- Catalog of available Actions you can utilize without reinventing the wheel
- Hosted services are subject to usage limits, although the free-tier limits are fairly generous (for now)

- Simple YAML descriptions of workflows, many templates and examples available
- It is a newer platform, so not as many features as some of the others, but it is quickly gaining steam

10.4.3 What Will We Do With CI?

Two obvious and useful forms of CI we can incorporate into the development of our final projects with GitHub Actions include:

- 1) Automatically run our integration tests (with pytest) each time new code is pushed to GitHub
- 2) Automatically build a Docker image and push it to Docker Hub each time our code is tagged with a new release

10.4.4 Integration Testing with GitHub Actions

To set up GitHub Actions in an existing repository, create a new folder as follows:

```
[user-vm] * mkdir -p .github/workflows/
```

Within that folder we will put YAML files describing when, how, and what workflows should be triggered. For instance, create a new YAML file (.github/workflows/integration-test.yml) to perform our integration testing with the following contents:

```
name: Integration tests with pytest
on: [push]
jobs:
  integration-tests-with-pytest:
   runs-on: ubuntu-latest
   steps:
    - name: Check out repo
     uses: actions/checkout@v3
    - name: Create docker bridge network
      run: docker network create API-DB-WRK
    - name: Set up a database
     run:
       mkdir ./data/
        docker run --name redis-db --network API-DB-WRK -p 6379:6379 -d -v ${PWD}/data:/
⇔data redis:7 --save 1 1
    - name: Build and run the API and worker
      run:
       docker build -f Dockerfile -t image:test .
       docker run --name api-test --network API-DB-WRK -p 5000:5000 -d --env REDIS_IP=$
→{RIP} image:test python3 api.py
       docker run --name wrk-test --network API-DB-WRK -d --env REDIS_IP=${RIP}_
→image:test python3 worker.py
     env:
       RIP: redis-db
```

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```
    name: Run pytest
        run: docker run --network API-DB-WRK -d --env REDIS_IP=${RIP} image:test pytest
    name: Stop images
        run: |
            docker stop wrk-test && docker rm -f wrk-test
            docker stop api-test && docker rm -f api-test
            docker stop redis-db && docker rm -f redis-db
            docker network rm API-DB-WRK
```

The workflow above runs our integration tests, and it is triggered on every push (on: [push]). This particular workflow will run in an ubuntu-latest VM, and it has 10 total steps.

Some steps contain a uses keyword, which utilizes a pre-canned action from the catalog of GitHub Actions. For example, the pre-canned actions might be used to clone your whole repository or install Python3. The other stops contain a run keyword which are the commands to run on the VM. In the above example, commands are run to stage the data, set up containers, and run pytest.

QUESTION

In the above example, Python v3.9 and external libraries (pytest, requests) are installed in different steps. Can this be done in one step? Is there a better way to do it?

Trigger the Integration

To trigger this integration, simply edit some source code, commit the changes, and push to GitHub.

```
[user-vm]$ git add *
[user-vm]$ git commit -m "added a new route to do something"
[user-vm]$ git push
```

Then navigate to the repo on GitHub and click the 'Actions' tab to watch the progress of the Action. You can click on your saved workflows to narrow the view, or click on a specific instance of a workflow (a "run") to see the logs.

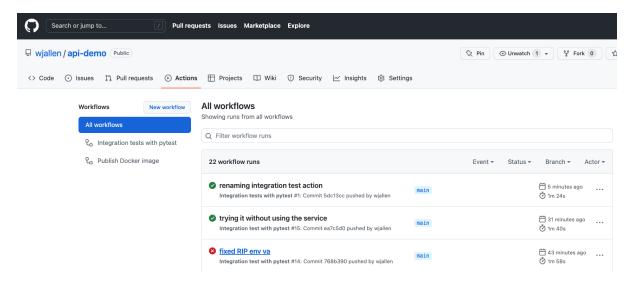


Fig. 1: History of all workflow runs.

By looking through the history of recent workflow runs, you can see that each is assigned to a specific commit and commit message. That way, you know who to credit or blame for successful or errant runs.

10.4.5 Docker Hub Integration with GitHub Actions

Rather than commit to GitHub AND push to Docker Hub each time you want to release a new version of code, you can set up an integration between the two services that automates it. The key benefit is you only have to commit to one place (GitHub), and you can be sure the image on Docker Hub will always be in sync.

Consider the following workflow, located in .github/workflows/push-to-registry.yml:

```
name: Publish Docker image
   on:
     push:
       tags:
         _ 1 & 1
6
   jobs:
     push-to-registry:
       name: Push Docker image to Docker Hub
10
       runs-on: ubuntu-latest
12
       steps:
         - name: Check out the repo
14
          uses: actions/checkout@v3
15
16
        - name: Log in to Docker Hub
17
          uses: docker/login-action@f054a8b539a109f9f41c372932f1ae047eff08c9
           with:
19
             username: ${{ secrets.DOCKERHUB_USERNAME }}
20
             password: ${{ secrets.DOCKERHUB_PASSWORD }}
21
22
         - name: Set up Docker Buildx
23
          uses: docker/setup-buildx-action@v1
24
25
        - name: Extract metadata (tags, labels) for Docker
           id: meta-api
27
          uses: docker/metadata-action@98669ae865ea3cffbcbaa878cf57c20bbf1c6c38
           with:
29
             images: wjallen/mldata-api
31
        - name: Build and push Docker image
32
          uses: docker/build-push-action@ad44023a93711e3deb337508980b4b5e9bcdc5dc
           with:
34
             context: .
35
             push: true
             file: ./docker/Dockerfile.api
             tags: ${{ steps.meta-api.outputs.tags }}
38
             labels: ${{ steps.meta-api.outputs.labels }}
        - name: Extract metadata (tags, labels) for Docker
41
           id: meta-wrk
42
```

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(continued from previous page) uses: docker/metadata-action@98669ae865ea3cffbcbaa878cf57c20bbf1c6c38 43 with: images: wjallen/mldata-wrk 45 - name: Build and push Docker image 47 uses: docker/build-push-action@ad44023a93711e3deb337508980b4b5e9bcdc5dc with: 49 context: . 50 push: true 51 file: ./docker/Dockerfile.wrk 52 tags: \${{ steps.meta-wrk.outputs.tags }} 53 labels: \${{ steps.meta-wrk.outputs.labels }}

This workflow waits is triggered when a new tag is pushed (tag: - '*'). As in the previous action, this one checks out the code and stages the sample data. Then, it uses the docker/login-action to log in to Docker Hub on the command line. The username and password can be set by navigating to Settings => Secrets => New Repository Secret within the project repository.

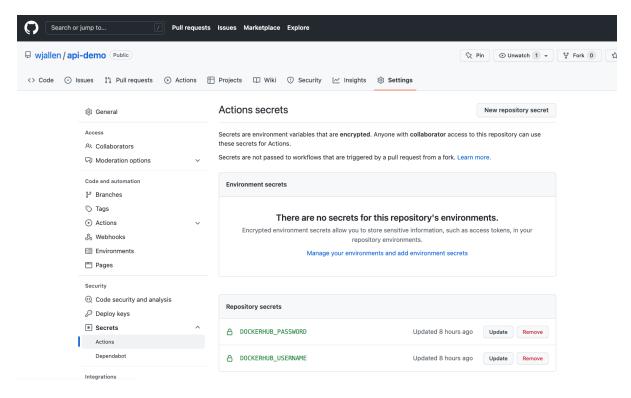


Fig. 2: Secrets are tied to specific repos.

Finally, this workflow extracts the tag from the environment and builds / pushes the API container, then builds / pushes the worker container both using actions from the GitHub Actions catalogue.

Tip: Don't re-invent the wheel when performing GitHub Actions. There is likely an existing action that already does what you're trying to do.

Trigger the Integration

To trigger the build in a real-world scenario, make some changes to your source code, push your modified code to GitHub and tag the release as X.Y.Z (whatever new tag is appropriate) to trigger another automated build:

```
[user-vm]$ git add *
[user-vm]$ git commit -m "added a new route to do something"
[user-vm]$ git push
[user-vm]$ git tag -a 0.1.1 -m "release version 0.1.1"
[user-vm]$ git push origin 0.1.1
```

By default, the git push command does not transfer tags, so we are explicitly telling git to push the tag we created (0.1.1) to the remote (origin).

Now, check the online GitHub repo to make sure your change / tag is there, and check the Docker Hub repo to see if your new tag has been pushed.

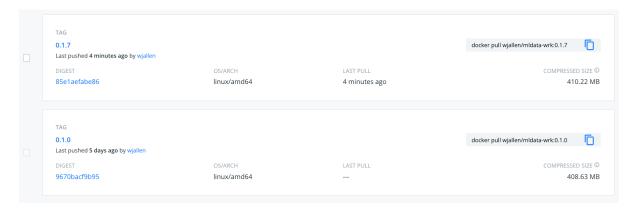


Fig. 3: New tag automatically pushed.

10.4.6 Deploy to Kubernetes

The final step in our example is to update the image tag in our deployment YAML files in both test and prod, and apply them all. Apply to test (staging) first as one final check that things are working as expected. Then, deploy to prod. Because the old containers are Running right up until the moment the new containers are deployed, there is virtually no disruption in service.

Note: Some CI / CD services can even handle the deployment to Kubernetes following Docker image builds and passing tests.

10.4.7 Additional Resources

- · GitHub Actions Docs
- · Demo Repository

10.5 Plotting with Matplotlib

Matplotlib a graphing library for Python. It has a nice collection of tools that you can use to create anything from simple graphs, to scatter plots, to 3D graphs. It is used heavily in the scientific Python community for data visualization.

10.5.1 Using Matplotlib

Tip: An easy place to test the examples below is in a browser-based Jupyter notebook

First install matplotlib with pip, or add it to your requirments.txt file. Installing matplot lib will install some other dependencies as well, including numpy which is a library with support for arrays and high-level mathematical functions.

```
[user-vm]$ pip install matplotlib
```

If you generate plots on a Linux VM (e.g. Jetstream), you typically won't be able to view them on that VM unless you enable X-forwarding. It takes a bit of setting up, but the alternative is to copy images to your laptop where you can open them directly.

10.5.2 Simple Plots

Plot a simple sin wave:

```
import matplotlib.pyplot as plt
import numpy as np

x = np.linspace(0, 2*np.pi, 50)
plt.plot(x, np.sin(x))
plt.savefig('my_sinwave.png') # writes a file you can download
plt.show() # displays the file if in graphics-supporting environment
```

Continuing from the same file, plot two graphs on the same axis:

```
plt.plot(x, np.sin(x), x, np.sin(2*x))
plt.savefig('my_sinwavex2.png')
plt.show()
```

Change the colors and add markers:

```
plt.plot(x, np.sin(x), 'r-o', x, np.sin(2*x), 'g--')
plt.savefig('my_sinwavex2a.png')
plt.show()
```

Matplot lib supports some built-in colors, and others can be accessed using HTML hex strings (e.g. '#eeefff'):

• Blue - 'b'

- Green 'g'
- Red 'r'
- Cyan 'c'
- Magenta 'm'
- Yellow 'y'
- · Black 'k'
- White 'w'

Built-in line and marker options:

- Solid Line '-'
- · Dashed '-'
- Dotted '.'
- Dash-dotted '-:'
- Point '.'
- Pixel ','
- · Circle 'o'
- Square 's'
- Triangle '^'

10.5.3 Subplots

Using the subplot() function, we can plot two graphs at the same time within the same "canvas". Think of the subplots as "tables", each subplot is set with the number of rows, the number of columns, and the active area, the active areas are numbered left to right, then up to down.

```
plt.subplot(2, 1, 1) # (row, column, active area)
plt.plot(x, np.sin(x))
plt.subplot(2, 1, 2) # switch the active area
plt.plot(x, np.sin(2*x))
plt.savefig('my_sinwavex2b.png')
plt.show()
```

10.5.4 Scatter plots

A simple scatter plot based on the sine function:

```
y = np.sin(x)
plt.scatter(x,y)
plt.savefig('my_scattersin.png')
plt.show()
```

Use random numbers and add a colormap to a scatter plot:

```
x = np.random.rand(1000)
y = np.random.rand(1000)
size = np.random.rand(1000) * 50
color = np.random.rand(1000)
plt.scatter(x, y, size, color)
plt.colorbar()
plt.savefig('my_scatterrandom.png')
plt.show()
```

We brought in two new parameters, size and color, which will vary the diameter and the color of our points. Then adding the colorbar() gives us a nice color legend to the side.

10.5.5 Histograms

A histogram is one of the simplest types of graphs to plot in Matplotlib. All you need to do is pass the hist() function an array of data. The second argument specifies the amount of bins to use. Bins are intervals of values that our data will fall into. The more bins, the more bars.

```
plt.hist(x, 50)
plt.savefig('my_histrandom.png')
plt.show()
```

10.5.6 Adding Labels and Legends

Plots look much more finished and professional with appropriate labels and legends added. This is highly recommended for the final project.

```
x = np.linspace(0, 2 * np.pi, 50)
plt.plot(x, np.sin(x), 'r-x', label='Sin(x)')
plt.plot(x, np.cos(x), 'g-^', label='Cos(x)')
plt.legend() # Display the legend.
plt.xlabel('Rads') # Add a label to the x-axis.
plt.ylabel('Amplitude') # Add a label to the y-axis.
plt.title('Sin and Cos Waves') # Add a graph title.
plt.savefig('my_labels_legends.png')
plt.show()
```

EXERCISE

For this exercise, take your existing Worker app and implement some of the matplotlib code above to illustrate the results of a job.

10.5.7 Additional Resources

- Try Jupyter in a Browser
- Set up X-Forwarding
- Post Images to Imgur

10.6 Storing Images in Redis

As part of the final project, your Worker must create an image or a plot. If it is created inside the Kubernetes worker pod, you'll need a convenient way to retrieve that image back out of the worker container and into whatever container you curled from.

The easiest way to retrieve the image is for the worker to add the image back to the Redis db, and for the user to query the database with a flask route and retrieve the image. This would be the general workflow:

- 1. The user submits a curl request from, e.g., the py-debug pod to the Flask API
- 2. The Flask API creates a new job entry in the appropriate Redis db, and adds the UUID to the queue
- 3. The Worker picks up the UUID from the queue, and pulls the job parameters of the Redis db
- 4. The Worker performs the job task and generates an image or plot
- 5. The Worker saves the plot in the Redis db, associated with the UUID
- 6. The user curls a new route to download the image from the db

10.6.1 Initiate a Job

Imagine that when a user submits a job, an entry is created in the jobs db of the following form:

```
[user-vm]$ curl localhost:5000/jobs
[
   "161207aa-9fe7-4caa-95b8-27f5bcbb16e7"
]
```

```
[user-vm]$ curl localhost:5000/jobs/161207aa-9fe7-4caa-95b8-27f5bcbb16e7
{
   "jobID": "161207aa-9fe7-4caa-95b8-27f5bcbb16e7",
   "status": "submitted",
   "start": "2001",
   "end": "2021"
}
```

10.6.2 Add an Image to a Redis DB

The Worker picks up the job, performs the analysis based on the 'start' and 'end' dates, and generates a plot. An example of using matplotlib to write and save a plot to file might look like:

```
import matplotlib.pyplot as plt

x_values_to_plot = []
y_values_to_plot = []

for key in raw_data.keys():  # 'raw_data' is a client to the raw data stored in redis
   if (int(start) <= key['date'] <= int(end)):
        x_values_to_plot.append(key['interesting_property_1'])
        y_values_to_plot.append(key['interesting_property_2'])

plt.scatter(x_values_to_plot, y_values_to_plot)
plt.savefig('/output_image.png')</pre>
```

Warning: The code above should be considered pseudo code and not copy/pasted directly. Depending on how your databases are set up, client names will probably be different, you may need to decode values, and you may need to cast type on values.

Warning: Also not shown above is the @q decorator. The above lines of code should probably be put in their own function, which would be called from the decorated function.

Now that an image has been generated, consider the following code that will open up the image and add it to the Redis db:

```
with open('/output_image.png', 'rb') as f:
   img = f.read()
results.hset(jobid, 'image', img) # 'results' is a client to the results db
```

10.6.3 Retrieve the Image with a Flask Route

Now that the image has been added back to the database, you can expect this type of data structure to exist:

```
{
    "161207aa-9fe7-4caa-95b8-27f5bcbb16e7": {
        "image": <binary image data>
      }
}
```

It would not be a good idea to show that binary image data with the rest of the text output when querying a /jobs route - it would look like a bunch of random characters. Rather, write a new route to download just the image given the job ID:

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```
@app.route('/download/<jobid>', methods=['GET'])
def download(jobid):
    path = f'/app/{jobid}.png'
    with open(path, 'wb') as f:
        f.write(results.hget(jobid, 'image')) # 'results' is a client to the results db
    return send_file(path, mimetype='image/png', as_attachment=True)
```

Flask has a method called 'send_file' which can return a local file, in this case meaning a file that is saved inside the Flask container. So first, open a file handle to save the image file inside the Flask container, then return the image as mimetype='image/png'.

The setup above will print the binary code to the console, so the user should redirect the output to file like:

ELEVEN

HOMEWORK 01

Due Date: Tuesday, Jan 30, by 11:00am central time

11.1 Bottle Repository

Your task is to set up a new Git repository that will be used to turn in your homework assignments for the semester.

Here are the overall requirements for the repository:

- Must contain a top level README.md with a simple description of what the repository is for
- Must contain a directory called homework01
- Must be pushed to GitHub, must be private, and must be shared with GitHub user wjallen / wallen@tacc.utexas.edu

Here are the requirements for the homework01 directory:

- The directory homework01 must contain four Python scripts:
 - ml_csv_reader.py: reads Meteorite_Landings.csv and prints summary statistics
 - ml_json_reader.py: reads Meteorite_Landings.json and prints summary statistics
 - ml_xml_reader.py: reads Meteorite_Landings.xml and prints summary statistics
 - ml_yaml_reader.py: reads Meteorite_Landings.yaml and prints summary statistics
- The definition of "summary statistics" is open to interpretation
- You may hard-code the raw data file names into the Python scripts, but using a utility like argparse to accept the file name as an argument on the command line would be preferred
- The directory homework01 must also contain a README.md file with a descriptive title and short descriptions of each of the four Python scripts, including instructions on how to run the scripts and interpret the output

A sample Git repository should contain the following files after completing homework 01:

Note: Do not include the raw Meteorite Landing data in your repository! Stick to only the files above.

11.2 What to Turn In

Send an email to wallen@tacc.utexas.edu with the link to your GitHub repository and include "Homework 01" in the subject line. We will clone all of your repos at the due date / time for evaluation.

11.3 Additional Resources

- Meteorite Landing Data
- Please find us in the class Slack channel if you have any questions!

TWELVE

HOMEWORK 02

Due Date: Tuesday, Feb 6, by 11:00am central time

12.1 Rushmeteorite

Our in-class examples so far have used a modified and abridged Meteorite Landings data set. For this homework, we will work with the real Meteorite Landings data set from NASA while exercising our Python3 best practices.

12.1.1 PART 1

Write two Python3 scripts for reading and summarizing the Meteorite Landings data from NASA. The requirements are as follows:

- Scripts are organized following guidelines in Unit 03
- Primary script reads in CSV-formatted Meteorite Landings data
- Primary script contains at least three functions for parsing the data and printing some summary statistics to screen. These cannot be the same functions shown in the class readthedocs (i.e. not compute_average_mass, check_hemisphere, or count_classes)
- At least one function must make use of the great-circle distance algorithm to calculate the distance between landing sites
- The great-circle distance algorithm must be provided as a standalone script / function that is imported into your primary script
- All functions must contain appropriate doc strings and type hints
- All functions must contain corresponding unit tests in an appropriately-named files. Unit tests must be compatible with pytest
- Scripts must support logging, and include a mix of log statements (focus on DEBUG, WARNING, and ERROR where appropriate)
- Scripts must use appropriate error handling if, e.g., a null value is present in the input data

Note: Edit Feb 1: In addition to printing "summary statistics to screen", plotting data and storing as an image is acceptable.

12.1.2 PART 2

Your homework 02 files must be within a new subdirectory called homework02 in your COE 332 homeworks repository on GitHub. The directory should contain your primary Python3 script, the secondary script containing the great-circle distance function, two unit test scripts, and a README.md file. The README should be descriptive, use proper grammar, and contain enough instructions so anyone else could clone the repository and figure out what the scripts do and how to run them. General guidelines to follow for the README for homework 02 are:

- · Descriptive title
- High-level description of the folder contents / project objective. I.e. why does this exist and why is it important? (2-3 sentences)
- Specific description of the individual Python3 scripts (1-2 sentences each)
- Instructions to obtain any necessary data and where to copy it to
- Instructions to run the code from start to finish, plus how to interpret the results (2-3 sentences)
- Use markdown styles to your advantage, give the sections headers, use code blocks where appropriate, etc.

Remember, the README is your chance to document for yourself and explain to others why the project is important, what the code is, and how to use it / interpret the outputs / etc. This is a *software engineering and design* class, so we are not just checking to see if your code works. We are also evaluating the design of the overall submission, including how well the project is described in the README.

12.2 What to Turn In

A sample Git repository may contain the following new files after completing homework 02:

```
my-coe332-hws/
— homework01
— README.md
— ml_csv_reader.py
— ml_json_reader.py
— ml_yaml_reader.py
— homework02
— README.md
— gcd_algorithm.py # your file names may vary
— ml_data_analysis.py
— test_gcd_algorithm.py
— test_ml_data_analysis.py
— README.md
```

There is no need to email the link to your homework repo again, as we should have it on file from the first homework. We will re-clone the same repo as before at the due date / time for evaluation.

12.3 Additional Resources

- Meteorite Landings Data
- JSON guide
- Latitude and Longitude as decimals
- Great-circle distance formula
- Markdown syntax
- Tips on writing a good README
- Please find us in the class Slack channel if you have any questions!

THIRTEEN

HOMEWORK 03

Due Date: Tuesday, Feb 13, by 11:00am central time

13.1 The Royal Containers

The goal this week is to take your code from last week (all Python3 scripts including unit test scripts), containerize them, and come up with a reasonable software diagram to describe the whole project.

13.1.1 PART 1

First copy your Python3 scripts (including unit tests) from homework02 into a new homework03 folder. If you find that there are any errors or problems with any of your scripts from homework02, now would be a good time to fix them.

Next, write a Dockerfile to containerize all of the scripts and unit tests that you copied over. The Dockerfile should not pull the Meteorite Landing data into the container - instead you should plan to volume mount the data inside the container at run time. The Dockerfile needs to install all dependencies as well (e.g. pytest).

13.1.2 PART 2

Include a software diagram in your repository. The diagram should capture as many components of your system / project as possible (e.g. the user, the VM, the container, the scripts, the functions, the unit tests, the input data, the output results, etc.). There is really no wrong answer here - we just want to take a first pass at a rough diagram that we can iterate on later.

13.1.3 PART 3

The README file can be copied from homework02, but will need modifications. The README should describe how a user who has just cloned your repository can run your tool in a container from start to finish. Take special care to describe how to:

- Build the image from a Dockerfile
- Get the input data from the web (data should be cited)
- Mount the data inside the container at run time
- Run the containerized code
- Run the containerized unit tests

Please also use the appropriate markdown tags in your README to display your image as part of your README file. Include a brief 2-3 sentence description of what your image illustrates.

13.2 What to Turn In

A sample Git repository may contain the following new files after completing homework03:

```
my-coe332-hws/
— homework01
— ...
— homework02
— ...
— homework03
— Dockerfile
— README.md
— diagram.png
— gcd_algorithm.py
— ml_data_analysis.py
— test_gcd_algorithm.py
— test_ml_data_analysis.py
— README.md
```

13.3 Additional Resources

- Meteorite Landings Data
- Markdown Syntax
- Tips on Writing a Good README
- Software Diagram Tools
- Best Practices for Writing Dockerfiles
- Please find us in the class Slack channel if you have any questions!

FOURTEEN

HOMEWORK 04

Due Date: Tuesday, Feb 20, by 11:00am central time

14.1 The ISS Aquatic

Scenario: You have found an abundance of interesting positional and velocity data for the International Space Station (ISS). It is a challenge, however, to sift through the data manually to find what you are looking for. Your long-term objective is to build a web app for querying and returning interesting information from the ISS data set. For this assignment, we will just start to assemble necessary functions and containerize the tool.

14.1.1 PART 1

First, navigate to the ISS Trajectory Data website.

There are two downloads available, and they contain the same data. It is the 'Orbital Ephemeris Message (OEM)' data in either plain text or XML format. Download and examine both files to get a feel for what they contain. Please closely read the ~3 paragraphs of accompanying text on the website as well.

The most important thing to understand is that the data contains ISS state vectors over a 15 day period. The range of days may change depending on when you download the data set. 'State vectors' are the Cartesian vectors for both position {X, Y, Z} and velocity {X_DOT, Y_DOT, Z_DOT} that, along with a time stamp (EPOCH), describe the complete state of the system (the ISS). The frame of reference for these vectors is Earth, based on something called the J2000 reference frame.

Tip: The XML data is probably a little bit easier than the raw text data to ingest into dictionary format inside a python script. See the Unit on XML for tips.

14.1.2 PART 2

Write a (containerized) Python3 script that does the following:

- 1) Ingests the ISS data using the requests library, and stores it in something similar to a list-of-dictionaries format
- 2) Prints a statement about the range of data using timestamps from the first and last epochs
- 3) Prints the full epoch (time stamp, state vectors, and velocities) closest to "now" or the time when the program is executed. This will change based on when the program is run
- 4) Calculates and prints the average speed over the whole data set, as well as the instantaneous speed closest to "now".

All of the normal Python3 script best practices apply:

- · Write appropriately formatted doc strings for your routes
- Use type annotations where appropriate
- Organize your code in the same way as the other scripts we have written
- Write unit tests for all non main() functions
- Implement selective logging and error handling where appropriate

Tip: For the speed function, you will need an equation to calculate speed from Cartesian velocity vectors: $\mathbf{speed} = \mathbf{sqrt}(\mathbf{x}_{-}\mathbf{dot}^2 + \mathbf{y}_{-}\mathbf{dot}^2 + \mathbf{z}_{-}\mathbf{dot}^2)$

14.1.3 PART 3

The homework must also include a README file. The README should be descriptive, use proper grammar, and contain enough instructions so anyone else could clone the repository and figure out how to run your app and interact with it. Guidelines to follow for the README are:

- Descriptive title
- High-level description of the folder contents / project objective. I.e. why does this exist and why is it important? (2-3 sentences)
- Instructions on how to access and description of the data set from the original source (do not include the data itself in this repository!)
- Instructions on how to build a container for your code
- Instructions to run the containerized Python3 script and unit tests
- List of what to expect for output and how to interpret them
- Try to use markdown styles to your advantage, give the sections headers, use code blocks where appropriate, etc.

Remember, the README is your chance to document for yourself and explain to others why the project is important, what the code is, and how to use it / interpret the outputs / etc. This is a *software engineering and design* class, so we are not just checking to see if your code works. We are also evaluating the design of the overall submission, including how well the project is described in the README.

14.2 What to Turn In

A sample Git repository may contain the following new files after completing homework03:



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```
iss_tracker.py
test_iss_tracker.py
README.md
```

14.3 Additional Resources

- NASA Data Set
- Info on State Vectors
- Info on Reference Frame
- Unit on XML
- Please find us in the class Slack channel if you have any questions!

FIFTEEN

HOMEWORK 05

Due Date: Tuesday, Feb 27, by 11:00am central time

15.1 The Darjeeling Flask

This homework is an extension of your previous homework - homework 04. The goal this week is to transform your simple Python3 script into a full Flask web application. Please first copy all of the homework04 files into a new folder called homework05.

15.1.1 PART 1

Your Flask application will contain the same (or similar) functionality as in homework 04, but in this homework each functionality should be accessible by a Flask route. The following routes are required:

Route	Method	What it should do
/epochs	GET	Return entire data set
<pre>/epochs? limit=int&offset=int</pre>	GET	Return modified list of Epochs given query parameters
/epochs/ <epoch></epoch>	GET	Return state vectors for a specific Epoch from the data set
/epochs/ <epoch>/speed</epoch>	GET	Return instantaneous speed for a specific Epoch in the data set (math required!)
/now	GET	Return state vectors and instantaneous speed for the Epoch that is nearest in time

All of the normal Python3 script best practices apply:

- Write appropriately formatted doc strings for your functions
- Use type annotations where appropriate
- Organize your code in the same way as the other scripts we have written
- Write unit tests for all functions except the main() function special consideration may be required to write unit tests for Flask routes
- Implement selective logging and error handling where appropriate

Tip: For the speed function, you will need an equation to calculate speed from Cartesian velocity vectors: $\mathbf{speed} = \mathbf{sqrt}(\mathbf{x}_{-}\mathbf{dot}^2 + \mathbf{y}_{-}\mathbf{dot}^2 + \mathbf{z}_{-}\mathbf{dot}^2)$

15.1.2 PART 2

Include a software diagram in your repository. The diagram should capture as many components of your system / project as possible (e.g. the user, the VM, the container, the scripts, the functions, the unit tests, the input data, the output results, etc.). There is really no wrong answer here - we just want to take a first pass at a rough diagram that we can iterate on later.

Note: After collecting Homework 05, we will share some model diagrams from the class (with permission). This will give you a chance to reflect on your own diagram and update it if necessary for inclusion in the Midterm.

15.1.3 PART 3

The homework must also include a README file. The README should be descriptive, use proper grammar, and contain enough instructions so anyone else could clone the repository and figure out how to run your app and interact with it. Guidelines to follow for the README are:

- · Descriptive title
- High-level description of the folder contents / project objective. I.e. why does this exist and why is it important?
 (2-3 sentences)
- Instructions on how to access and description of the data set from the original source (do not include the data itself in this repository!)
- Instructions on how to build a container for your code
- Instructions to deploy your containerized code as a Flask app
- Instructions including specific curl commands for accessing the routes in your app
- Descriptions of what the output from each route shows / means
- Try to use markdown styles to your advantage, give the sections headers, use code blocks where appropriate, etc.

Remember, the README is your chance to document for yourself and explain to others why the project is important, what the code is, and how to use it / interpret the outputs / etc. This is a *software engineering and design* class, so we are not just checking to see if your code works. We are also evaluating the design of the overall submission, including how well the project is described in the README.

15.2 What to Turn In

A sample Git repository may contain the following new files after completing homework05:



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15.3 Additional Resources

- NASA Data Set
- Info on State Vectors
- Info on Reference Frame
- Unit on XML
- Please find us in the class Slack channel if you have any questions!

MIDTERM PROJECT

Due Date 1: Friday, Mar 8, by 11:59 pm central time

Due Date 2: Monday, Mar 18, by 11:59 pm central time

Projects turned in by due date 1 will receive +10% on midterm (+2% toward final grade). Projects will not be accepted after due date 2.

16.1 Fantastic Mr. ISS

In Homework 05, we turned our ISS tracker into a proper Flask app. Now, we will finish off this project by adding a few final routes, automate deployment with Docker Compose, and write up a short document describing the project.

16.1.1 PART 1

For the Midterm Project, start a brand new git repository. Copy over the files that you have been working on from Homework 05. Your current iteration of iss_tracker.py should have seven functional Flask routes as described in Homework 05. For this project, keep the existing routes and add the following new routes:

- A /comment route that returns the 'comment' list object from the ISS data
- A /header route that returns the 'header' dictionary object from the ISS data
- A /metadata route that returns the 'metadata' dictionary object from the ISS data
- A /epochs/<epoch>/location route that returns latitude, longitude, altitude, and geoposition for a given <epoch>. Math required! See slack for hints on this. We will also be using the Python GeoPy library for determining geoposition given a latitude and longitude.
- A /now route that returns the same information as the 'location' route above, but for the up-to-date, real time
 position of the ISS. You will need to iterate over all Epochs in the data set and figure out which one is closest
 to the current time, then return location information for that Epoch. You can confirm whether it is working by
 comparing it to the longitude and latitude of the ISS in real time using an online tracker.

After completing the above, your app should have eight total routes, one of which supports query parameters:

Route	Metho	What it should do	
/comment	GET	Return 'comment' list object from ISS data	
/header	GET	Return 'header' dict object from ISS data	
/metadata	GET	Return 'metadata' dict object from ISS data	
/epochs	GET	Return entire data set	
/epochs?	GET	Return modified list of Epochs given query parameters	
limit=int&offset=int			
/epochs/ <epoch></epoch>	GET	Return state vectors for a specific Epoch from the data set	
/epochs/ <epoch>/</epoch>	GET	Return instantaneous speed for a specific Epoch in the data set (math re-	
speed		quired!)	
/epochs/ <epoch>/</epoch>	GET	Return latitude, longitude, altitude, and geoposition for a specific Epoch in	
location		the data set (math required!)	
/now	GET	Return instantaneous speed, latitude, longitude, altitude, and geoposition for	
		the Epoch that is nearest in time	

Please use defensive programming strategies for your routes. Assume we will try to break your routes by sending bad information to your URL and query parameters Your routes should use exception handling to catch and handle these bad requests. In addition:

- Write appropriately formatted doc strings for your routes
- Use type annotations where appropriate
- Organize your code in the same way as the other Flask apps we have made
- Write appropriate unit tests to test each function

16.1.2 PART 2

requirements.txt: Our Python libraries are growing in number and complexity. Write a requirements.txt file that lists all the non-standard Python libraries that must be installed for this project.

Dockerfile: Write a Dockerfile to containerize your iss_tracker.py script. Make sure it installs any Python libraries required from requirements.txt. The default command should launch the Flask app in a standard way.

docker-compose.yml: Write a compose file to automate the deployment of your app. The compose file should be configured to build the image, and to bind the appropriate port inside the container to the appropriate port on the host.

16.1.3 PART 3

README. Standard README guidelines apply. The README should have a descriptive title (not "Midterm Project"), a short summary / description of the project, short descriptions of any very important files that the reader should know about. We will specifically be looking for:

- · A citation of the ISS data
- Instructions to deploy the app with docker compose
- Instructions to curl all routes, plus what the outputs meaning
- · Instructions to run the containerized unit tests

Be succinct, use Markdown styles, and show example commands / expected output.

Diagram.png: Include a software diagram that illustrates what you deem to be the most important parts of your project. We will share sample diagrams in class to show what would be reasonable.

Write Up. You must also turn in a written document (as a PDF) describing the project. While the README is typically more succinct and targeted towards developers / users of the application, the written document should be more verbose and targeted towards a non-user, but technically savvy layperson. For example, in the README you might instruct a user: "Run the application by performing xyz". In the Write Up, you would instead describe what users do: "Users of the application can run it by performing xyz". In other words, write this document as if you are describing to your fellow engineering students what you did in this class for your Midterm project.

In the Write Up, include some narrative about the motivation of the project and why it is an interesting or important application to have. You must also include a short section on "Ethical and Professional Responsibilities in Engineering Situations". As a suggestion, you may consider describing the importance of citing data or the importance of verifying the quality and accuracy of data that goes into applications such as these. We strongly encourage you to come up with other Ethical and Professional Responsibilities that might apply here.

Please make sure to appropriately cite the data source in both the README and the written document.

16.2 What to Turn In

This Midterm project should be pushed into a standalone repo with a descriptive name (not "coe332-midterm"). It should not be put into your existing homework repo. A sample Git repository should contain the following after completing the Midterm:

Send an email to wallen@tacc.utexas.edu with the written PDF summary of the project attached plus a link to your new GitHub repository. Please include "Midterm Project" in the subject line. We will clone all of your repos at the due date / time for evaluation.

Note: Do not include the raw data as part of your repo.

16.3 Additional Resources

- · NASA Data Set
- · Real Time ISS Position
- API for Real Time ISS Position
- Python GeoPy Docs
- Please find us in the class Slack channel if you have any questions!

16.2. What to Turn In

SEVENTEEN

HOMEWORK 06

Due Date: Tuesday, Mar 26, by 11:00am central time

17.1 Moonrise Genes

Scenario: We are going to turn our attention to a brand new dataset. The Human Genome Organization (HUGO) is a non-profit which oversees the HUGO Gene Nomenclature Committee (HGNC). The HGNC "approves a unique and meaningful name for every gene". For this homework, we will download the complete set of HGNC data and inject it into a Redis database through a Flask interface.

This homework will essentially be a re-hash of the exercises from the last Redis section.

Note: If you want to do this homework with a different data set, e.g. the data set you want to work on for your final project, just get it approved with the instructors first.

17.1.1 PART 1

You can find the HGNC data on this page: https://www.genenames.org/download/archive/

Scroll to the bottom and look for the link that says "Current tab separated hgnc_complete_set file" or "Current JSON format hgnc_complete_set file". Please spend some time reading this page to help you understand the data. I recommend opening up the tsv file in a spreadsheet tool (like Excel) to get a better feel for what it contains. Notice there are a lot more fields than we are used to (54), but it is the same *list-of-dictionaries* format that we see over and over again in this class. Another thing to notice is that this dataset is *sparse*, meaning not every cell has data in it.

17.1.2 PART 2

Start a new directory for this homework (called homework06). Write a Flask app that has a /data route and a /gene route. The routes should do the following:

- A POST request to /data should load the HGNC data to a Redis database. Use the Python requests library to get the data directly from the web.
- A GET request to /data should read all data out of Redis and return it as a JSON list.
- A DELETE request to /data should delete all data from Redis.
- The /genes route should return a json-formatted list of all hgnc_id fields. (This is the first field in the data set, and a unique identifier for each gene).

• The /genes/<hgnc_id> route should return all data associated with a given <hgnc_id>. Be careful to handle the case where something other than a valid gene ID is provided by the user, and be careful to handle the sparesely populated data it returns. An example query to this route might look like:

```
[user-vm]$ curl localhost:5000/genes/HGNC:5
{
"hgnc_id": "HGNC:5",
"symbol": "A1BG",
"name": "alpha-1-B glycoprotein",
"locus_group": "protein-coding gene",
"locus_type": "gene with protein product",
"status": "Approved",
"location": "19q13.43",
"location_sortable": "19q13.43",
"alias_symbol": "",
"alias_name": "",
"prev_symbol": "",
"prev_name": "",
"gene_group": "Immunoglobulin like domain containing",
"gene_group_id": 594,
"date_approved_reserved": "6/30/89",
"date_symbol_changed": "",
"date_name_changed": "",
"date_modified": "1/20/23",
"entrez_id": 1,
"ensembl_gene_id": "ENSG00000121410",
"vega_id": "OTTHUMG00000183507",
"ucsc_id": "uc002qsd.5",
"ena": "",
"refseq_accession": "NM_130786",
"ccds_id": "CCDS12976",
"uniprot_ids": "P04217",
"pubmed_id": 2591067,
"mgd_id": "MGI:2152878",
"rgd_id": "RGD:69417",
"lsdb": "",
"cosmic": ""
"omim_id": 138670,
"mirbase": "",
"homeodb": ""
"snornabase": "",
"bioparadigms_slc": "",
"orphanet": "",
"pseudogene.org": "",
"horde_id": "",
"merops": "I43.950",
"imgt": "",
"iuphar": "",
"kznf_gene_catalog": "",
"mamit-trnadb": "",
"cd": "",
"lncrnadb": "",
"enzyme_id": "",
```

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```
"intermediate_filament_db": "",
    "rna_central_ids": "",
    "lncipedia": "",
    "gtrnadb": "",
    "agr": "HGNC:5",
    "mane_select": "ENST00000263100.8|NM_130786.4",
    "gencc": ""
}
```

After completing the above, your app should have the following routes:

Route	Method	What it should do
/data	POST	Put data into Redis
/data	GET	Return all data from Redis
/data	DELETE	Delete data in Redis
/genes	GET	Return json-formatted list of all hgnc_ids
/genes/ <hgnc_id></hgnc_id>	GET	Return all data associated with <hgnc_id></hgnc_id>

Please use defensive programming strategies for your routes with exception handling, and use doc strings / type annotations as appropriate.

17.1.3 PART 3

The application should be containerized and orchestrated along side a Redis container. Write a Dockerfile for containerizing your Flask app, and write a Docker-compose yaml file for orchestrating the services together. Read very closely the Docker Compose section of Unit 07 for detailed instructions on how to do this part.

17.1.4 PART 4

Write a README with the standard sections from previous homeworks: there should be a descriptive title, there should be a high level description of the project, there should be concise descriptions of the main files within, and you should be using Markdown styles and formatting to your advantage. We will specifically be looking for:

- · Instructions to build a new image from your Dockerfile
- Instructions to launch the containerized app and Redis using docker-compose
- Give example API query commands and expected outputs in code blocks

Finally, your README should also have a section to describe the data itself. Please give enough information for others to understand what data they are seeing and what it means (not every field must be described, just a general overview). Please cite the data appropriately as well.

17.1. Moonrise Genes 281

17.2 What to Turn In

A sample Git repository may contain the following new files after completing homework 06:

```
my-coe332-hws/
— homework01
— ...
— homework05
— ...
— homework06
— Dockerfile
— docker-compose.yaml
— gene_api.py
— README.md

README.md
```

17.3 Additional Resources

- HGNC Data Set
- Unit on Docker Compose
- Please find us in the class Slack channel if you have any questions!

EIGHTEEN

HOMEWORK 07

Due Date: Thursday, Apr 4, by 11:00am central time

18.1 The Grand Budapest Job

Scenario: Continuing from the previous homework, we will add a jobs functionality into our web apps. Please start from the files developed in Homework 06, and continue to use the HGNC data.

At this point we assume you can orchestrate your Flask and Redis services together using docker-compose in the **development environment** (Jetstream cluster, [user-vm]\$).

Note: If you want to do this homework with a different data set, e.g. the data set you want to work on for your final project, just get it approved with the instructors first.

18.1.1 PART 1

Create two new routes in your Flask app, /jobs and /jobs/<jobid>. These should be in addition to the existing routes. The routes should satisfy the following requirements:

- A POST request to /jobs should create a new job with a unique identifier (uuid)
 - The POST request must include a data packet in JSON format which is stored along with the job information (see below)
- A GET request to /jobs should list all existing job IDs
- A GET request to /jobs/<jobid> should return job information for a given job ID

Following the example in Unit 08, job IDs should be put into a queue, and job information (e.g. ID, status, user-provided parameters) should be stored in a separate database in Redis. I highly recommend using the Jobs API code from Unit 08 for this.

The POST request to /jobs should look similar to:

```
$ curl localhost:5000/jobs -X POST -d '{"start":1, "end":2}' -H "Content-Type:

→application/json"
```

However, start and end don't really make sense in the context of the HGNC data, and probably don't make sense in the context of your final project data set. Look through the data you are using for this project and decide on at least two new parameters that would make sense for a user to pass to the jobs route. **Provide instructions in your README** on what parameters we should pass to your jobs route. If the user does not provide the right parameters, the route should not submit a job; instead it should return a message to the user describing what the problem is.

18.1.2 PART 2

Following the example in Unit 08, write a Worker Python script that satisfies the following requirements:

- The Worker should pull methods and clients from the Jobs API
- It should use the HotQueue @q.worker decorator to watch the queue and pull off Job IDs as they arrive
- When it pulls a Job ID off the queue, it should find the corresponding job information in the jobs database, update the status to "in progress", wait a bit, then update the status to "complete"

The Worker needs to be running in a separate container runtime from the Flask app. It can use the same container image as the Flask app (except with a different entrypoint command) if desired.

18.1.3 PART 3

In addition to the Python scripts described above, you will need several other files to support this software system:

requirements.txt: Should list all non-standard Python library dependencies

Dockerfile: Should install Python dependencies from requirements.txt, and should copy in Python scripts. I recommend using one Dockerfile to build one Docker image with all Python scripts inside, then using two different entrypoint commands to either deploy a Flask app or Worker container runtime.

docker-compose.yml: Should orchestrate three services together: Redis database, Flask app, Worker. The Redis container needs to be able to write snapshots to a local folder (you may have to provide some extra instructions here to solve folder permission issues).

Finally, following Exercise 5 from Unit 08, you must use an **environment variable** to dynamically set the Redis host IP. Environment variables are variables that get set in the shell and are available for programs. In Python, the os.environ.get() method will be helpful. In your docker-compose.yml file, the environment: attribute will be required.

18.1.4 PART 4

Write a README with the standard sections from previous homeworks: there should be a descriptive title, there should be a high level description of the project, there should be concise descriptions of the main files within, and you should be using Markdown styles and formatting to your advantage. We will specifically be looking for:

- Instructions to use the /jobs and /jobs/<jobid> routes
- · Instructions to launch the containerized web app
- Give example API query commands and expected outputs in code blocks

Finally, your README should also have a section to describe the data itself. Please give enough information for others to understand what data they are seeing and what it means (not every field must be described, just a general overview). Please cite the data appropriately as well.

18.2 What to Turn In

A sample Git repository may contain the following new files after completing homework 07 (notice the evolving organization):

```
my-coe332-hws/
  - homework01/
    └ ...
    homework06/
   homework07

    Dockerfile

      README.md
       - data
        ___ .gitcanary
       docker-compose.yml
       requirements.txt
       - src
          — api.py
           jobs.py
          — worker.py
    README.md
```

18.3 Additional Resources

- Environment Variables in Docker-compose
- Please find us in the class Slack channel if you have any questions!

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NINETEEN

HOMEWORK 08

Due Date: Tuesday, Apr 16, by 11:00am central time

19.1 Isle of Web Apps

Scenario: Continuing from the previous homework, we will add some more features to our growing web apps. Please start from the files developed in Homework 07, and continue to use the HGNC data.

At this point we assume you can orchestrate your Redis, Flask, and Worker services together using docker-compose in the **development environment** (Jetstream cluster, [user-vm]\$). We also assume there is a rudimentary **jobs** functionality that takes POST requests and uses the Jobs API to initiate the jobs cycle. (Essentially all parts of the previous homework should be working).

Note: If you want to do this homework with a different data set, e.g. the data set you want to work on for your final project, just get it approved with the instructors first.

19.1.1 PART 1

In the previous homework, we used a placeholder in the Worker script (e.g. a 15-second sleep command) instead of actually performing any interesting work. In this homework, update the Worker script to do some actual analysis guided by user input and pulling from the raw data. **For Example**: Imagine the data set for this web app is the ISS data from our midterm. A user might POST a data packet containing a 'start_epoch' and 'end_epoch' to the /jobs route. Then, the worker could pull all the raw data between those epochs and create a plot of, e.g., average speed over time. The challenge for this homework is to come up with a reasonable analysis for the HGNC data (or your final project data if pre-approved), and then define what needs to be POSTed by the user to initiate that analysis.

Create a new route in your Flask app /results/<jobid>. This should be in addition to the existing routes from previous homeworks. The new route should satisfy the following requirements:

• A GET request to /results/<jobid> should return some information (e.g. a computed outcome, a plot, etc.) from a given Job ID. If the job has not yet been finished, the result should return a message stating that.

Results should be stored in a separate database (e.g. db=3 from our in-class diagram) and accessed through a new client defined in the Jobs API module. Please use defensive programming strategies. E.g. if a user supplies an invalid Job ID, this should hopefully not crash any of your containers.

19.1.2 PART 2

Following our Python best practices, we will start to build out a few more elements of our web app. Specifically, we will be looking for:

- Appropriate logging statements throughout the Flask, Worker, and Jobs API codes.
- Provide support for an environment variable to set log level. The environment variable should be defined in the
 docker-compose file (e.g. LOG_LEVEL=WARNING) and read in to the appropriate Python scripts, similar to
 how we read in the Redis IP address variable.
- Doc strings and type hints throughout the Flask, Worker, and Jobs API code.
- Integration tests for functions that are Flask routes (see this link) and unit tests for all other appropriate functions in the Flask, Worker, and Jobs API code.

19.1.3 PART 3

Write a README with the standard sections from previous homeworks: there should be a descriptive title, there should be a high level description of the project, there should be concise descriptions of the main files within, and you should be using Markdown styles and formatting to your advantage. We will specifically be looking for:

- Instructions to POST a job with data packet to /jobs
- Instructions to GET and interpret results from the /results/<jobid> route
- · Instructions to launch the containerized web app
- Give example API query commands and expected outputs in code blocks

As always, your README should also have a section to describe the data itself. Please give enough information for others to understand what data they are seeing and what it means (not every field must be described, just a general overview). Please cite the data appropriately as well.

Finally, create a software diagram illustrating some interesting or important part(s) of your web apps. Software diagrams should be rendered in your README using markdown styles and sufficiently described.

19.2 What to Turn In

A sample Git repository may contain the following new files after completing homework 08 (notice the evolving organization):



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19.3 Additional Resources

- Environment Variables in Docker-compose
- Integration Tests in Flask
- Please find us in the class Slack channel if you have any questions!

TWENTY

FINAL PROJECT

Due Date for Part 1: Friday, Mar 29, by 5:00pm central time Due Date for Parts 2-4: Friday, May 3, by 1:00pm central time

20.1 The Final Dispatch

20.1.1 PART 1: Pitch

Form groups of two or three students to work collaboratively on the final project. You may choose your own groups, or you may ask the instructors to assign you to a group. Please let us know what groups you are in, or if you would like to be assigned to a group ASAP.

The first part of the final project is to identify an interesting data set that you want to work on. The data set should be Engineering focused, broadly defined. The data set should also be amenable to CRUD operations and some sort of analysis (e.g. plotting some values or generating summary statistics). Most data sets that are in a *list-of-dictionaries* format and contain time stamps and/or quantitative values should work. The Meteorite Landing data or ISS Positional data are good examples of this, but should not be used for the final project. There are several links at the bottom of this page to Engineering-focused data sets, but you may look elsewhere too.

Once your group has identified a potential data set to work on, write up a ~1 page summary of the proposed title of your project, list of group members, and a description of the data. Then schedule a ~5 minute meeting with one of the instructors in order to "pitch" your project. We want to know what the source is of the data, see what the data looks like, and hear what is your plan for working on the data.

20.1.2 PART 2: Code Repository

The final project involves building a REST API for interacting with an interesting Engineering data set. The API should allow users to perform basic HTTP requests - e.g. POST, GET, DELETE - to load in the data, view it in a RESTful / collections style, and delete the data. The API should also allow users to submit an analysis job, which is asynchronously handled by workers that generate images and store them in a database. The application must be hosted on the Kubernetes cluster and accessible to the outside world at a public URL.

All requirements from Homeworks 6-8 apply. Here are some specific requirements we will look for:

- The front-end REST API must have:
 - a /help endpoint describing all the routes within
 - appropriate endpoints (and methods) to post / get / delete the Engineering data set to the Redis database
 - sufficient REST-style endpoints for returning the data collections (and subsets therein) in an intuitive way
 - endpoints for submitting a job to plot data and retrieve the results

- The back-end workers must:
 - use queue functionality to watch for jobs being submitted by the user
 - generate a plot of some aspect of the data set as guided by the user's job instructions
 - contain functionality to add the resulting image back into the Redis databse so the user can download it
- The Redis database must support:
 - a 'raw data' database holding the Engineering data set in a logical format
 - a 'hot queue' for managing asynchronous tasks
 - a 'jobs' database for handling job instructions and statuses
 - a 'results' database for holding the final images / results generated by the workers
 - a scheme for backing up the database at regular intervals in a way that it can be restored

The project must also include a well-written README following all the guidelines given in previous class assignments. This README should emphasize two sections: instructions for deploying and testing the application both on local hardware (e.g. Jetstream) and on a Kubernetes cluster, and instructions for using the application both on local hardware (e.g. Jetstream) and at a public endpoint.

Other files including Kubernetes configuration files for both test and production environments, Dockerfile(s), a docker-compose.yml file, a requirements.txt file, test scripts compatible with pytest, and a software diagram illustrating some part of the project will be expected (see 'What to Turn In' below).

20.1.3 PART 3: Write Up

We are looking for a written document (maybe ~10-11 pages as a PDF) describing the project. The written document should be verbose and targeted towards a non-user, but technically savvy layperson (e.g. one of your fellow engineering students who is not taking this class). Here are some things we will be looking for:

- Title page. Contains descriptive title, students names
- Write up contains logical progression of sections with appropriate headers
- High level description with introduction to the project, describes the motivation
- Detailed but concise description of the data
- Key technologies (e.g. Flask, Docker, Kubernetes) are defined at a high level for people who might not know what they are
- · List of route endpoints is easy to read and gives a nice overall picture of the API
- · Usage section shows representative example code snippets not necessarily exhaustive, but just enough
- Ethical and Professional Responsibilities section is well thought out
- Section connecting parts of this project to key software design principles (see Unit 04)
- · Citations page at the end

20.1.4 PART 4: Video Demo

Prepare a < 10 minute video demo of the application. Use zoom to screen share and record your narration of the process. At a minimum, we want to see you describe and show the resources deployed to Kubernetes, curl various routes to display select data, describe the data that you are showing and the importance of it, curl the appropriate routes to submit a an analysis job and retrieve and display the results, and highlight anything else you think is interesting or unique about your application.

20.2 What to Turn In

This Final project should be pushed into a standalone repo with a descriptive name. It should not be part of your existing homework repo. A sample Git repository may contain something similar to the following after completing the Final (your filenames may vary):

```
repo-name/
  - data
    └─ .gitcanary
   diagram.png
   docker-compose.yml
  - Dockerfile

    kubernetes

       prod
            app-prod-deployment-flask.yml
            app-prod-deployment-redis.yml
           app-prod-deployment-worker.yml
           app-prod-ingress-flask.yml
           - app-prod-pvc-redis.yml

    app-prod-service-flask.yml

           app-prod-service-nodeport-flask.yml
           app-prod-service-redis.yml
       test
            app-test-deployment-flask.yml
           app-test-deployment-redis.yml
            app-test-deployment-worker.yml
           app-test-ingress-flask.yml
           app-test-pvc-redis.yml
           app-test-service-flask.yml
            app-test-service-nodeport-flask.yml
            app-test-service-redis.yml
   Makefile
  - README.md
   requirements.txt
  - src
       flask_api.py
       jobs.py
       worker.py
   test
      - test_flask_api.py
       test_jobs.py
       test_worker.py
```

Send an email to wallen@tacc.utexas.edu with the PDF write-up attached plus a link to your new GitHub repository

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plus a link to download the zoom recording. Please include "Final Project" in the subject line. We will clone all of your repos at the due date / time for evaluation. Only one email per group is required.

20.3 Additional Resources

Here are some example sites where you can find suitable data sets. This is not an exhaustive list

- Registry of Research Data Repositories
- Kaggle
- Data.gov
- NASA Earth Data
- Please find us in the class Slack channel if you have any questions!

TWENTYONE

ADDITIONAL RESOURCES

- Slack: https://tacc-learn.slack.com/
- Class Repo: https://coe-332-sp24.readthedocs.io/
- Canvas: https://utexas.instructure.com/courses/1380167