UC Santa Cruz GEODES Computing ‘On Ramp’

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Goals for today:

- Get a feeling for what a computer program is, how to start writing one and how to run it
- Practice putting some code together in Python and running it
- Feel comfortable knowing how to search for more information

What does a computer do?

Two basic tasks:

- Performs **calculations** – potentially billions of calculations per second (compute power)
- **Remembers** results – potentially 100s of gigabytes of storage (memory)

What kinds of calculations?

- **Built-in** to a programming language
- Those that **you define** as a programmer

Computers do what you tell them to do, or more specifically what your instructions (code) tells them to do

What is a program?

A detailed plan or procedure for solving a problem or performing a task with a computer

Specifically, it is an **ordered sequence of computational instructions** needed to achieve a solution/outcome

What do computers actually understand?

Computers understand data in the form of 0s and 1s – very basic machine language (native language)

They do simple manipulations with those 0s and 1s:

- Move values to different positions in a chain
- Add, multiply, subtract, divide these values
- Compare these values, and if one is less than the other they can follow one step rather than the other

What are programming languages?

A vocabulary and set of grammatical rules (like human language) that can be translated directly to computer language to communicate instructions for specific tasks

In other words, programming languages are a set of symbols and rules that form a bridge between human language and machine language

Types of programming languages

Programming languages can be classified as lower-level versus higher-level

➢ Lower-level languages are closer to machine language vs. higher-level are closer to human language, like English

Examples of higher-level languages: Python, Matlab, R, HTML, Javascript, C, C++, Fortran

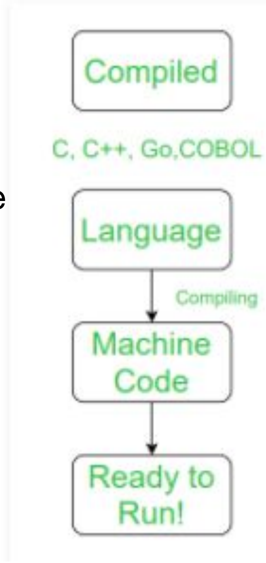
Compiled language:
Code is compiled/translated into machine language and expressed as instructions in machine language

Compilation produces an executable file that is undecipherable by humans

e.g. C, C++, Fortran

Generally faster to run
(already in machine language)

Errors may appear during compilation that prevent code from being translated



geeksforgeeks.org

Interpreted language:
Code is interpreted without compiling into machine language instructions.

Instructions are not directly executed by machine but instead read and executed by some other program

e.g. Python, Matlab, JavaScript, Perl

One step between code and execution

Interpreted programs can be modified and debugged while they are running

What is a script? How does a script differ from a program?

A **script** is a series of commands within a file that is **interpreted and controls another application**
Example: code written in any interpreted language like Python

A **program** is a set of commands that **executes independent of any other application**.
Programs are compiled before use and then one runs the executable containing machine language instructions i.e. any code written in a compiled language

1. Example python script: hello_world.py

```
# This Python script prints Hello World!
print("Hello World! \n")
```

Running Python script from Terminal

(onramp) valerelambert$ python hello_world.py
Hello World!

***The Python script is read by the Python interpreter which calls compiled programs to execute instructions in the script**

2. Example C program: hello_world.c

```
/* This C program prints Hello World! */
#include<stdio.h>
int main(void)
{
 printf("Hello World! \n");
return 0;
}
```

Compiling program from Terminal

(onramp) valerelambert$ gcc hello_world.c –o HelloWorld

Running C program from Terminal

(onramp) valerelambert$ ./Helloworld
Hello World!

What is a computing environment?

Many problems are solved by computers making use of multiple computational devices, networks and software to perform different tasks, transfer and storage information.

This **collection of software and hardware used to solve a problem** is the computing environment

What are package and environment managers?

Package managers keep track of what software is installed on your computer

- ➢ facilitate installing new software, upgrading software to newer versions and removing software

Environment managers keep track of collections of software packages used for specific projects

But why?
Imagine you have two different Python projects that use a specific software package. One requires updating the package, however if the package is updated then the other project may not function properly.

An environment manager allows on to set up two environments with different version of the package

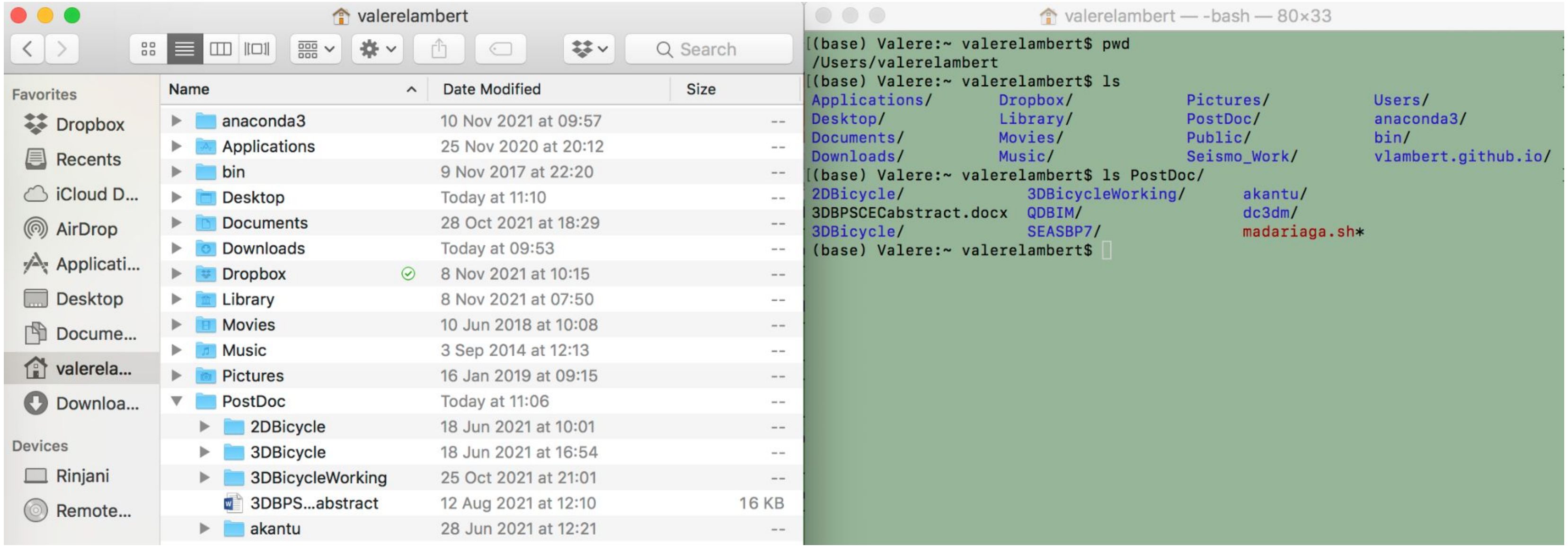
Examples: Anaconda, Homebrew, Pip
https://docs.conda.io/projects/conda/en/4.6.0/_downloads/52a95608c49671267e40c689e0bc00ca/conda-cheatsheet.pdf

Demystifying the terminal

The terminal is an application that provides text-based access to the operating system of your computer

- Provides a command-line interface compared to a graphical interface (like Finder on Mac)
- Generally faster than using graphical user interfaces (GUIs)

One can use different "shells" (e.g. bash, tcsh, zsh) which are interpreters that convert your commands in the terminal to machine instructions



Some basic terminal commands

https://www.techrepublic.com/article/16-terminal-commands-every-user-should-know/

Some basic commands:	**Examples:**
pwd : "print working directory" or current directory	pwd
ls : “List” or view the contents of a directory	ls path/to/directory
cd : “Change directory” that you are currently working in	cd path/to/directory
touch : make new empty file	touch "newfilename"
mkdir : “make a new directory”	mkdir "NewDirectoryName"
open : "open" file with default application	open "filename"
cp : “copy” a file from one location to another	cp “filename” “newfilename”
mv : “move” a file from one place or format to another	mv “filename” “newdir/newfilename”
rm : "remove" or delete one or more files or directories	rm "filename"

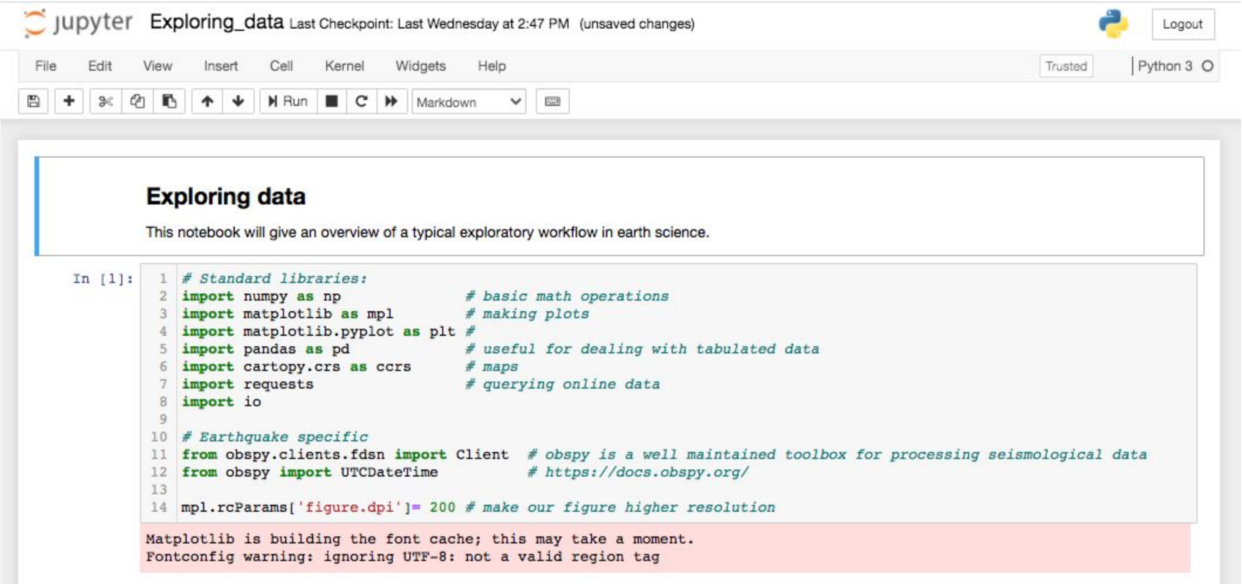
Integrated Development Environment (IDE)

IDEs are software applications that facilitate writing a computer program

- **Editing source code** – create a blank file, write some lines of code
- **Building executables** - contain necessary compilers and interpreters
- **Debugging tools**

May also have special features like syntax highlighting or autocomplete if the IDE knows language syntax

Common IDEs:
Spyder, PyCharm, Jupyterlab, Visual Studio Code, Eclipse, NetBeans, Komodo, XCode



Python versus MATLAB

Both are high-level interpreted languages that are meant to be relatively easy to use and fast to write code in

MATLAB is a proprietary, closed-source software that is aimed at technical computing

- Full package including the language, IDE to write and run code, and many different functions
- Professionally maintained, easy to develop, run and debug code
- **High-performance language optimized for matrix manipulation** and program solving based on linear algebra
  - Many additional toolboxes such as image and digital signal processing
- **Expensive**, need to pay for additional toolboxes, not everyone can afford MATLAB and thus use your code

Python is a general purpose, **open-source** language meant to be **easy to read** and simple to implement

- Useful in science and engineering, but also used for general applications (e.g. web and game development)
- Can run on all major operating systems and CPU architectures
- Free and open-source, anyone can download, look at and modify source code – anyone can contribute!
- Generally need to add packages (e.g. Numpy, Scipy, Matplotlib) and want an IDE to write/modify code

Basic differences in syntax, significance of white space, calling functions and indexing sequences
e.g. comments in python start with "#" where as in MATLAB they use "%"

Project Management Tips

https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1005510

When starting a new project is is helpful to create a new directory to contain all relevant information

You might name the directory according to the research project or course assignment:

mkdir "PathToNewDirectory/Project_name"

A common approach is then to create subfolders for different types of content:

- "Project_name/doc" = text documents (manuscripts, code documentation, papers) relevant to project
- "Project_name/src" = put code written for project
- "Project_name/bin" = compiled programs
- "Project_name/results" = generated files, intermediate data processing or simulated data, as well as final figures/tables

Writing Readable Code

1. **Give objects (variables, arrays, functions, etc) meaningful names**:

Example:

Mass = 25.0; % kg	OR	M = 25.0; % kg	RATHER THAN	Var1 = 25.0;
Velocity = 1.5; % m/s		V = 1.5; % m/s		Var2 = 1.5;

2. **Define functions for tasks that are regularly performed** and call them throughout your program
    - Make your code more compact rather than copy-pasting the same lines of code (Python example)

3. **Comment you code** – it is challenging to comment code too much!

- Define objects (variables, functions, etc.),
- Define units for objects,
- Describe methods used to solve a problem,
- Motivation for parameter values,
- Create sections of your code with different headings,
- Draw diagrams, coordinate systems, etc.

Comment code as your write it!

Makes it easier for other people (and you!) to:

- Read your code,
- Understand what you intended your code to do,
- Debug your code

Example of Commented Code in Matlab

https://github.com/vlambert/QDBIM

```
%% % % % % % % % % % % % % % % % % % % % % % % % % % % %
%                                                      %
%   2D Quasi-dynamic simulation of the evolution of    %
%   slip and stress on a fault in antiplane strain     %
%   governed by rate- and state-dependent friction     %
%                                                      %
%                    Valere Lambert, 2018              %
% % % % % % % % % % % % % % % % % % % % % % % % % % % %%
clear all;close all;

addpath('include/');
%% % % % % % % % % % % % % % % % % % % % % % % % % % % %
%                    Useful Functions                  %
% % % % % % % % % % % % % % % % % % % % % % % % % % % %%

% boxcar function
BC=@(x) (x+0.5>=0)-(x-0.5>=0);

% Heaviside function
HS=@(x) 0+x>=0;

% ramp function
Ramp=@(x) x.*BC(x-1/2)+HS(x-1);

```

```

%% % % % % % % % % % % % % % % % % % % % % % % % % % %
%                                                    %
%             Stress Interaction Functions           %
%                                                    %
% % % % % % % % % % % % % % % % % % % % % % % % % % %%
% Vertical fault in a half-space centered at x2 = 0
% 2D Antiplane problem (x2 x x3):
% Out-of-plane displacements u1 are non-zero, u2 = u3 = 0
% u1 are assumed uniform along strike, only vary in x2 x x3 plane
%
%.                              x1
%.                             /.
%.                            /.
%.                           /.
%.  Free surface (x3 = 0).  /
%.  ---------------------------------------------------->. x2
%.                         |
%.                         |
%.                         |. Vertical strike-slip
%.                         |. rate-and-state fault
%.                         |
%.                         |
%.                         |
%                          v  x3


% density (kg/m^3)
rho = 2670;

% shear wave speed (m/s)
Vs = 3464;

% shear modulus (MPa)
G = rho*Vs^2/1e6;

% Elastostatic Green's functions for displacements and stress due to
% uniform slip on a rectangular patch (Okada 1985,1992)
% For 2D antiplane we only care about Sigma_{12}
% y-coordinates represent source, x-coordinates represent receiver

% Note that these solutions take into account a free-surface using
% the method of images

% Sigma_{12}
s12h=@(x2,x3,y2,y3,W) G*( ...
    -(x3-y3)./((x2-y2).^2+(x3-y3).^2)+(x3+y3)./((x2-y2).^2+(x3+y3).^2) ...
    +(x3-y3-W)./((x2-y2).^2+(x3-y3-W).^2)-(x3+y3+W)./((x2-y2).^2+(x3+y3+W).^2) ...
    )/2/pi;

```

Version Control and Code Repositories

Platforms for code hosting, version control and collaboration
Examples: Github, Bitbucket
https://docs.github.com/en/get-started/quickstart/hello-world

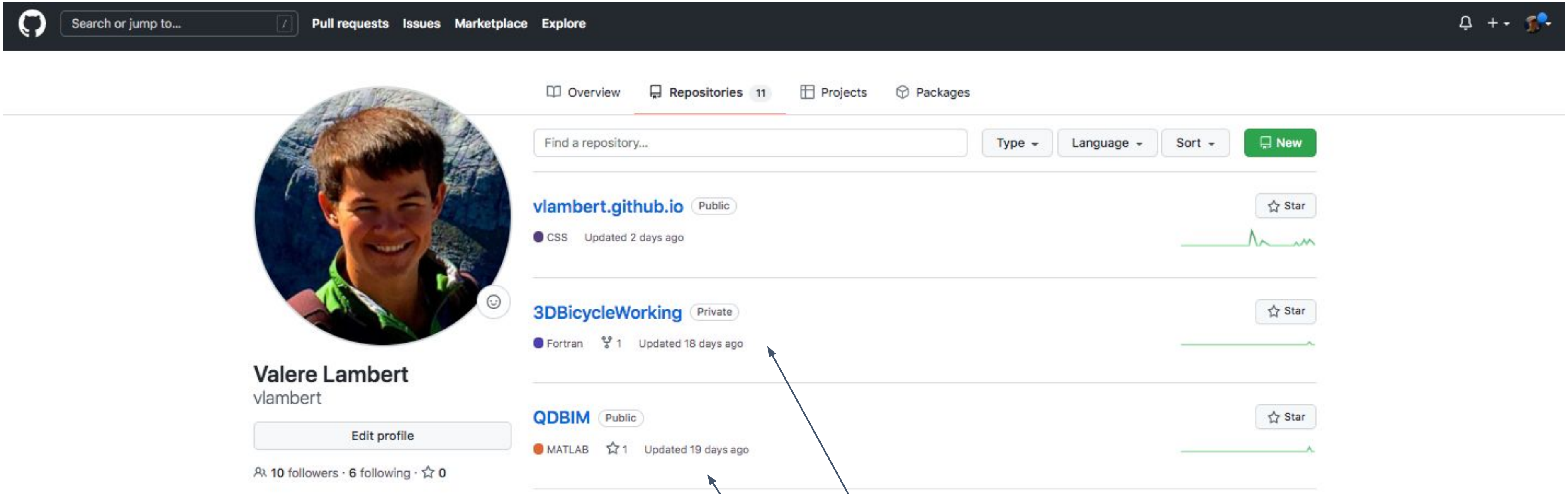
General idea:

1. Host copy of your code in the cloud (online) that may be shared with collaborators
2. "Pull" or download any updates to code that your collaborators have made to your computer
3. Make changes to "local" version of your code on your computer
4. Declare what changes you want to "push" to the cloud repository
5. Every time code is pushed to the cloud repository it creates a new "version" and the hosting service keeps a history of these versions, often showing the changes made between versions of code

Advantages:

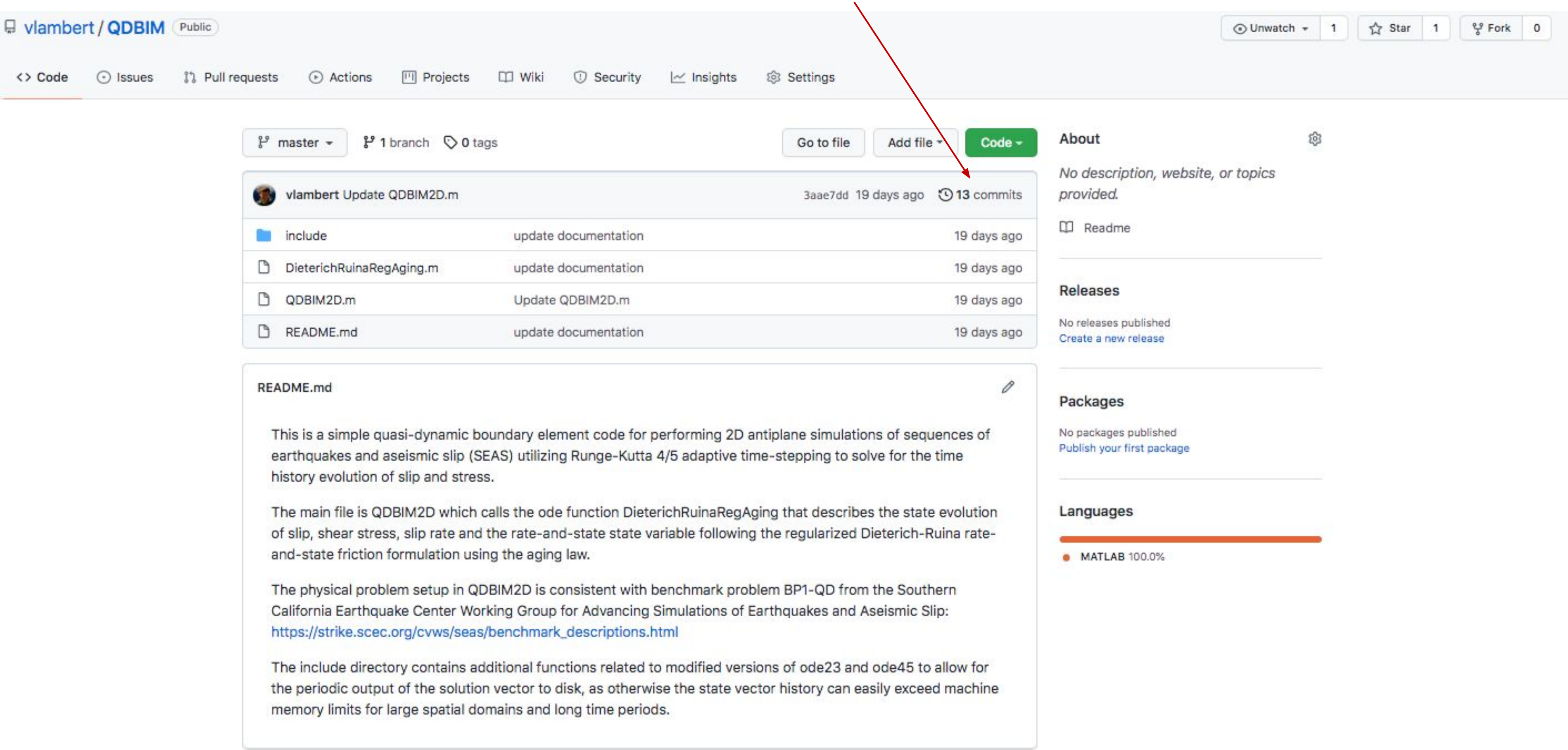
- **Code backup and version control:** Copy of your code in cloud and history of "versions" of your code and track changes over time
- **Collaboration:** Share code with public repositories or private repositories with collaborators
- Useful for **Open data and software for publications** - AGU Publications data policy

Example Git profile and list of repositories



Public and private repositories

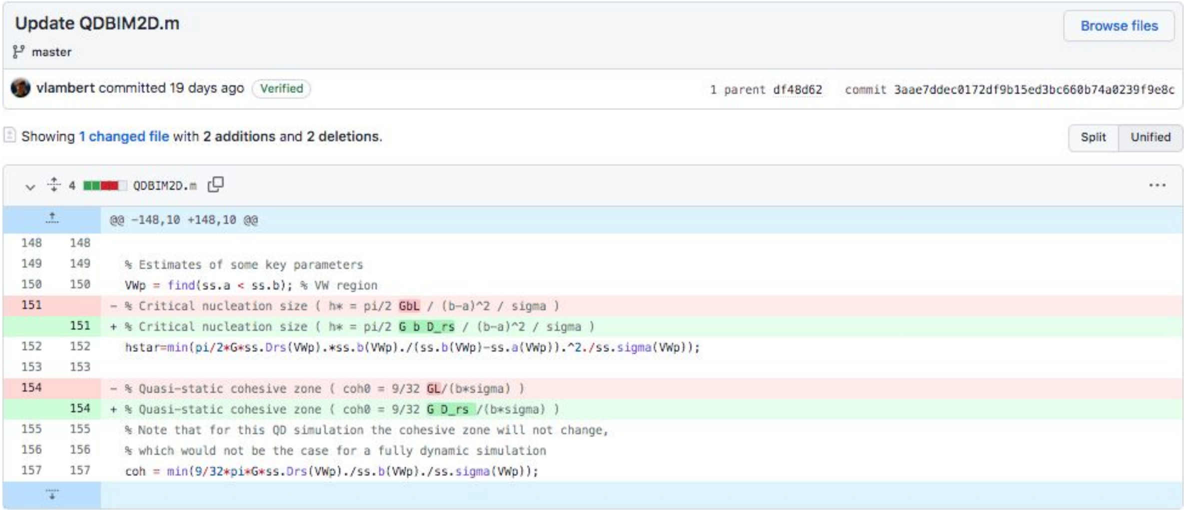
Check different times code has been committed



Different commits labelled by date and can also specify changes in "commit message"

* good to write commit messages that are more descriptive of changes than shown here

Can see what was changed between individual commits



Resources

Stack Exchange – online forums where many questions have already been asked and answered

Terminal commands
https://www.techrepublic.com/article/16-terminal-commands-every-user-should-know/

Anaconda cheat sheet
https://docs.conda.io/projects/conda/en/4.6.0/_downloads/52a95608c49671267e40c689e0bc00ca/conda-cheatsheet.pdf

Common IDEs and text editors: Spyder, PyCharm, Jupyterlab, atom, sublime, vim, emacs

Useful python packages for science:
- NumPy (fundamental scientific computing)
- SciPy (data science)
- Matplotlib (2D plotting)
- Pandas (time series analysis),
- Scikit-learn (machine learning),
- Seaborn (pretty plots),
- Cartopy (maps)