OVERVIEW OF MODERN DATA SCIENCE LANDSCAPE

ERT 474/574

Open-Source Hydro Data Analytics

August 27, 2025

University at Buffalo The State University of New York

Logistics

- Please sign up for a GitHub account and send your usernames to UBLearns (homework #1)
- Difficulties in signing up for the **GitHub Student Developer Pack**?
    - Has anyone successfully signed up?
    - If so, please show your experience in today’s lab session!

Learning objectives

- Coding languages?
  - Python? Matlab? Fortran? C++?
  - Where are different languages used in hydrologic models?
  - What is the best practice to learn the coding languages?
- GitHub

Coding languages

Python

Matlab

Fortran

C++

More language?

Coding languages

Python

- Python is the most widely used high-productivity language in Scientific Computing.

Matlab

Fortran

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More language?

Coding languages

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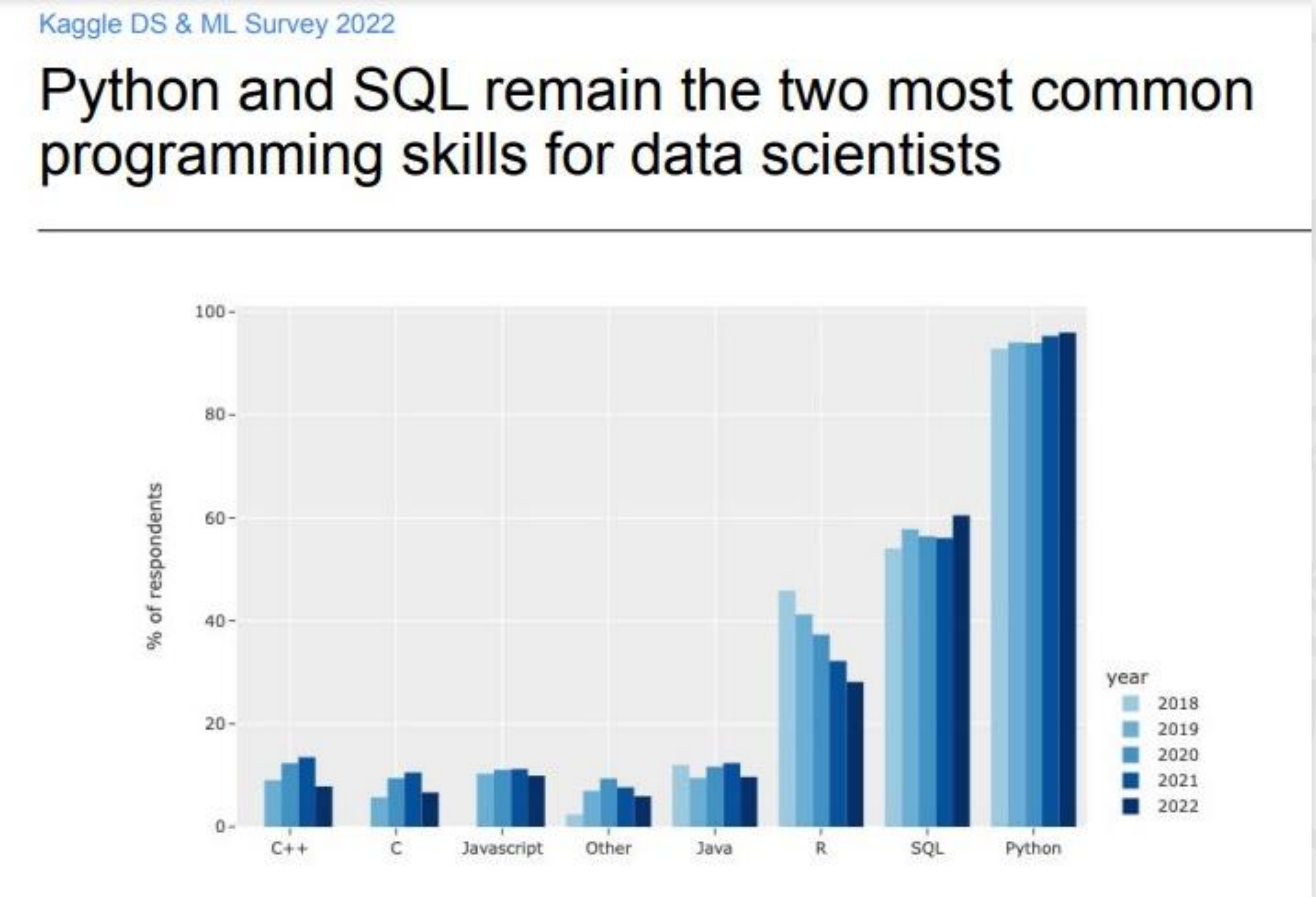

Kaggle DS & ML Survey 2022

Python and SQL remain the two most common programming skills for data scientists

Data source: Kaggle DS & ML Survey
Plot credit: https://studyopedia.com/data-science/programming-languages-for-data-science/#google_vignette

Coding languages

Python

Matlab

Fortran

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More language?

- Python is the most widely used high-productivity language in Scientific Computing.
- Its very **simple syntax** and broad library support make it ideal for quickly building scalable applications.
- The language does not natively support the type of data structures and other features needed for fast computation, so *few hydrologic models are written in Python.*
- Python is great for data analysis so we will mainly use Python in this class!

Coding languages

Python

Matlab

Fortran

C++

More language?

- Matlab is one of the oldest high-productivity languages and has been the defacto standard for fast numerical prototyping before Python.
- It is still heavily used in many numerical applications, given its excellent toolbox and huge amount of legacy code that exists.

Coding languages

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More language?

- Matlab is one of the oldest high-productivity languages and has been the defacto standard for fast numerical prototyping before Python.
- It is still heavily used in many numerical applications, given its excellent toolbox and huge amount of legacy code that exists.
- **Paywall!!!** While Matlab has quite favorable licenses for academic use, it is expensive for commercial use, and if possible Python as open-source alternative is preferable for new projects.

Coding languages

Python

Matlab

Fortran

C++

More language?

- Fortran is one of the dinosaurs of scientific computing. Fortran originated in the 1950s and its most recent incarnation is Fortran 2018.
- Fortran is still actively used for a lot of HPC code, especially when it comes to legacy applications.
- Many Global Climate Models and hydrologic models were written in Fortran!

Coding languages

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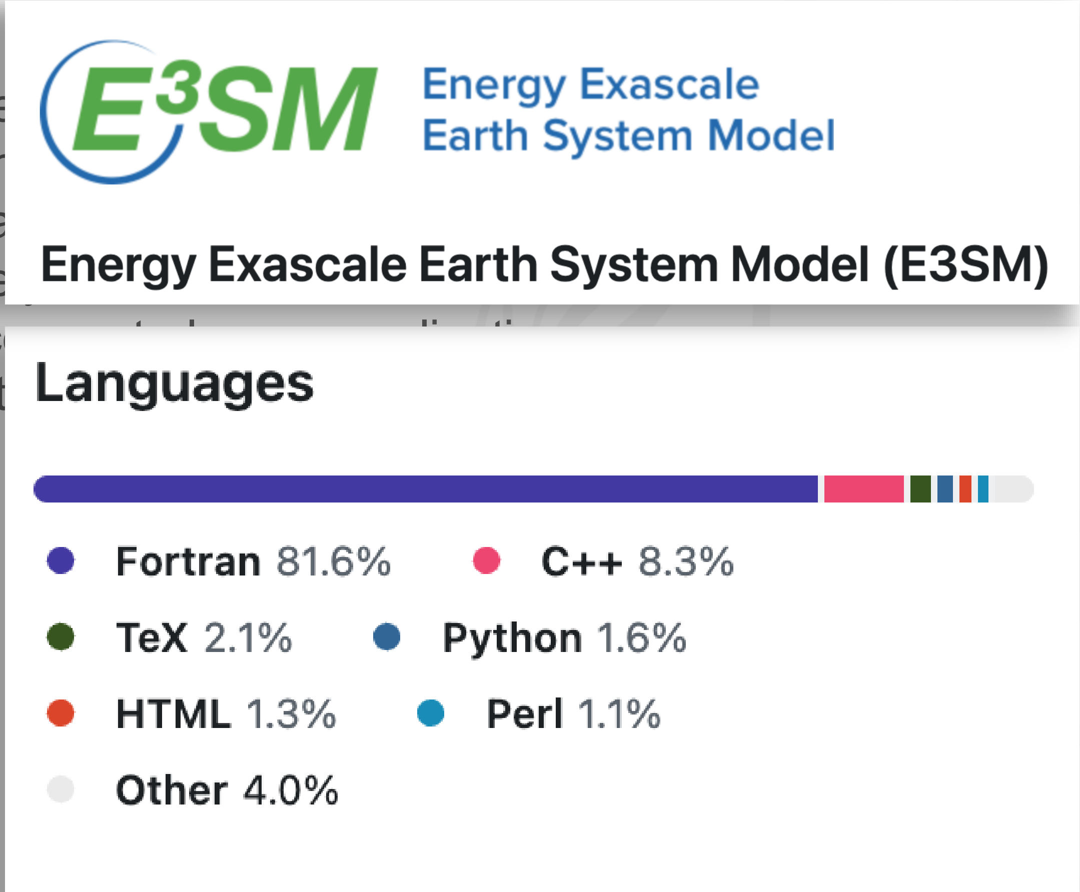


Energy Exascale Earth System Model

Energy Exascale Earth System Model (E3SM)

Languages

● **Fortran** 81.6%	● **C++** 8.3%
● **TeX** 2.1%	● **Python** 1.6%
● **HTML** 1.3%	● **Perl** 1.1%
● **Other** 4.0%	

Source: https://github.com/E3SM-Project/E3SM (accessed on Aug 26th 2024)

Coding languages

Python

Matlab

Fortran

C++

More language?

- C++ is the default language of Scientific Computing.
- It is mature, has a huge ecosystem and most modern heterogeneous compute environments (Cuda/Sycl, etc.) are developed for C++.
- Similar to Fortran, it requires compilation, and it is not as user-friendly as Python or Matlab, so it has a higher learning curves.

Examples

- Please write a function to add up two variables, **a** and **b,** **c**alculate the sum of ***a*** and ***b,*** and assign the value to the variable ***result***

How will you write this function in different languages?

Some other tools used to build this course

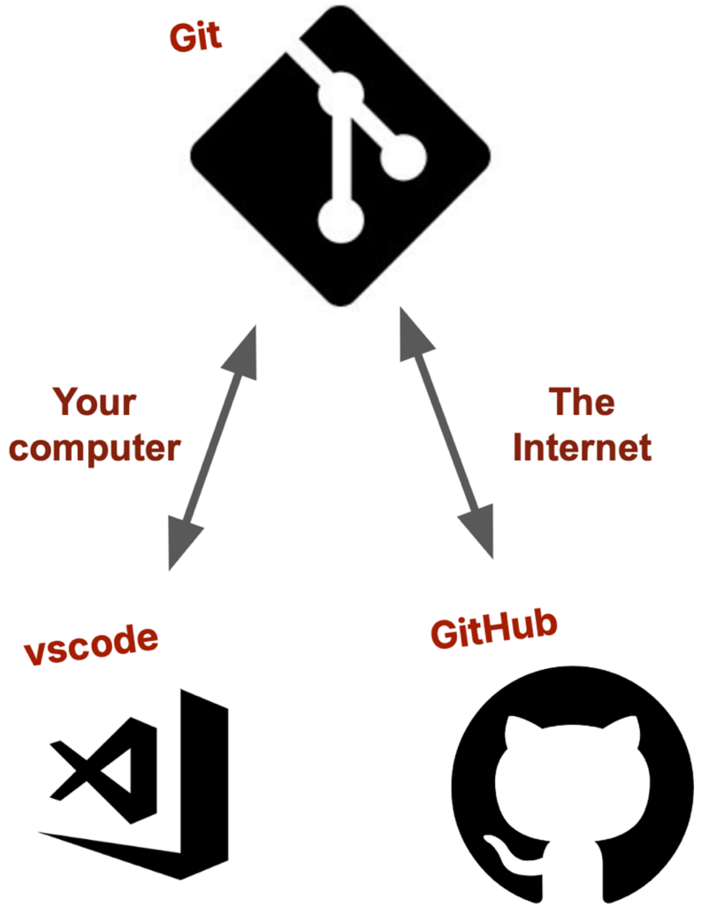
- We will be doing all of our work in **Python**
  - High-level, dynamic, and prominent programming language with massive community support
- We use **uv/pip** for environment management
  - Provides access to community-developed Python packages – more on this towards the end of the semester
- Under the hood, we use **Jupyter** as an interactive computing framework
  - Make it easy to run “snippets” of code and view their outputs. The standard framework for a lot of exploratory scientific computing
- **VSCode** will provide the user interface and code editing experience
  - A modern, extensible, and popular code editing application

GitHub

- GitHub is a web platform that enables software developers to manage and share their code
- Also has great integrations for running automation, building websites, and increasing AI integration
- We will use it for course centralization and homework management via GitHub Education.

Let’s talk about git

- Git is a version control system. It allows teams to work collaboratively on the same pieces of code (like track changes for MS Word but much more sophisticated)



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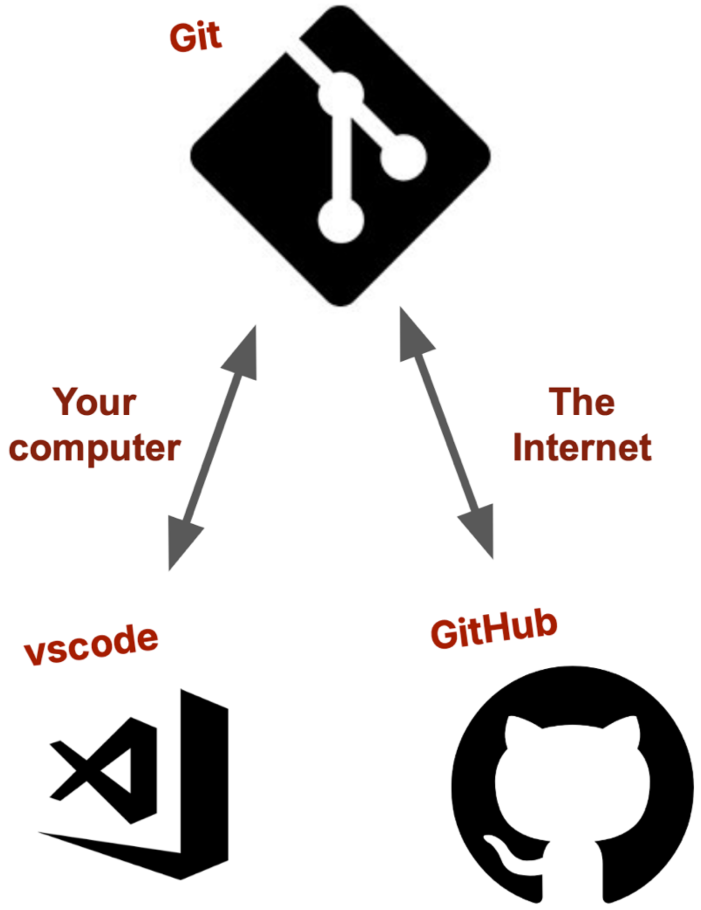
- GitHub is a website that is essentially a social platform for code, built around git as a version control system



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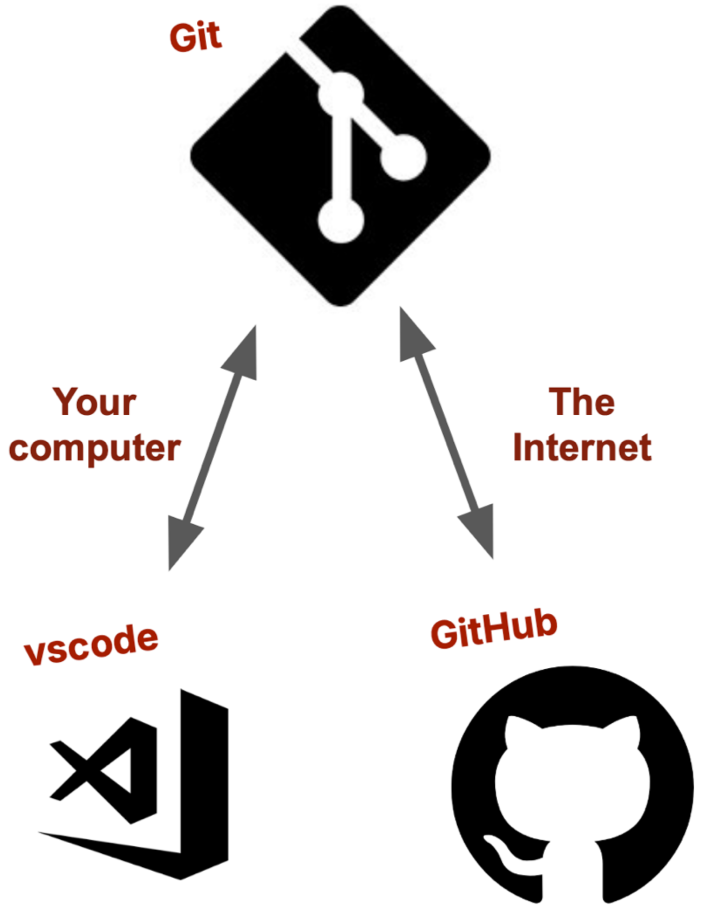
- You will mostly interact with git inside VSCode and use it to communicate with GitHub.



The first thing to know about git: Jargons

Jargons	Description
repository	The overall “container” for your work (synonym: repo) [noun]
clone	Make a copy of the repository on your local machine [verb]
commit	A snapshot in time of your work, or to save changes [noun/verb]
checkout	How to get to a particular snapshot [verb]
branch	A label to a commit, usually denoting a separate stream of work [noun]
merge	Combine changes from different branches [verb]
remote	A computer somewhere else with a repo on it (GitHub) [noun]
local	The computer you are working on (laptop) [noun]
fetch	Download information about history from a remote [verb]
pull	Do a fetch, but also update the code status with a checkout [verb]
push	Sync changes on your local to a remote [verb]
conflict	Occurs when two commits contradict each other [noun?]

Basic concepts in git: Nodes and trees

All repos start from an initial commit

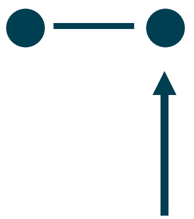
You are here

```
# Your codefile
print('hello world')
```

Basic concepts in git: Nodes and trees

All repos start from an initial commit

As you do work, you can make changes and add commits



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```
# Your codefile
name = ‘OS-Hydro’
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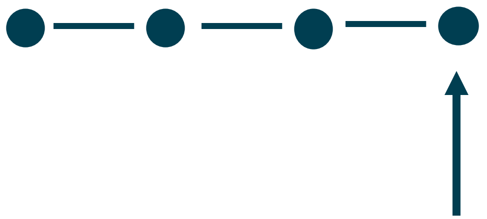


You are here

```
# Your codefile
import numpy as np
name = ‘OS-Hydro’
print(f‘hello {name}’)

x = np.arange(50)
y = np.sin(x / np.pi)

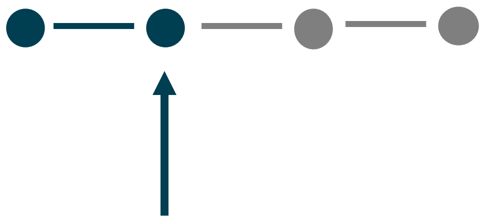
# more fun stuff here
```

Basic concepts in git: Nodes and trees

All repos start from an initial commit

As you do work, you can make changes and add commits

You can also move back and forward



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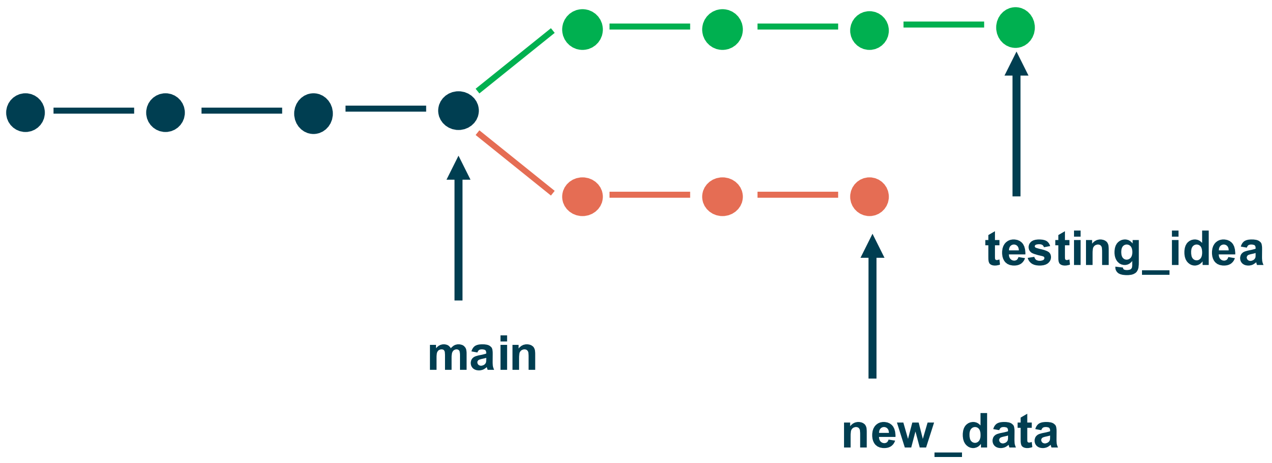
Basic concepts in git: Nodes and trees

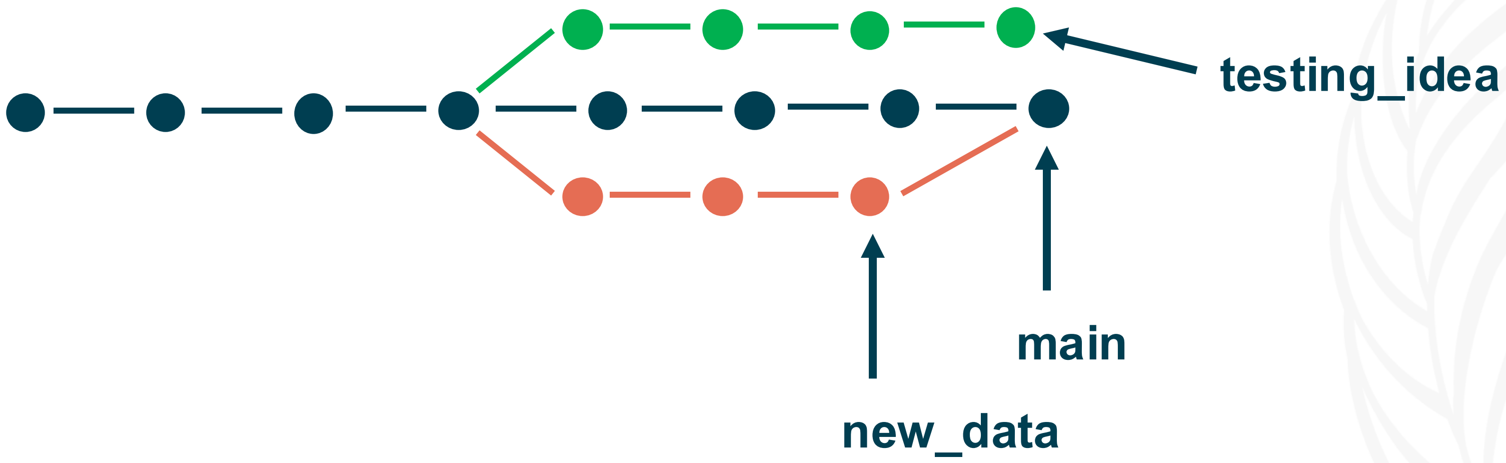
You can also start splits call branches



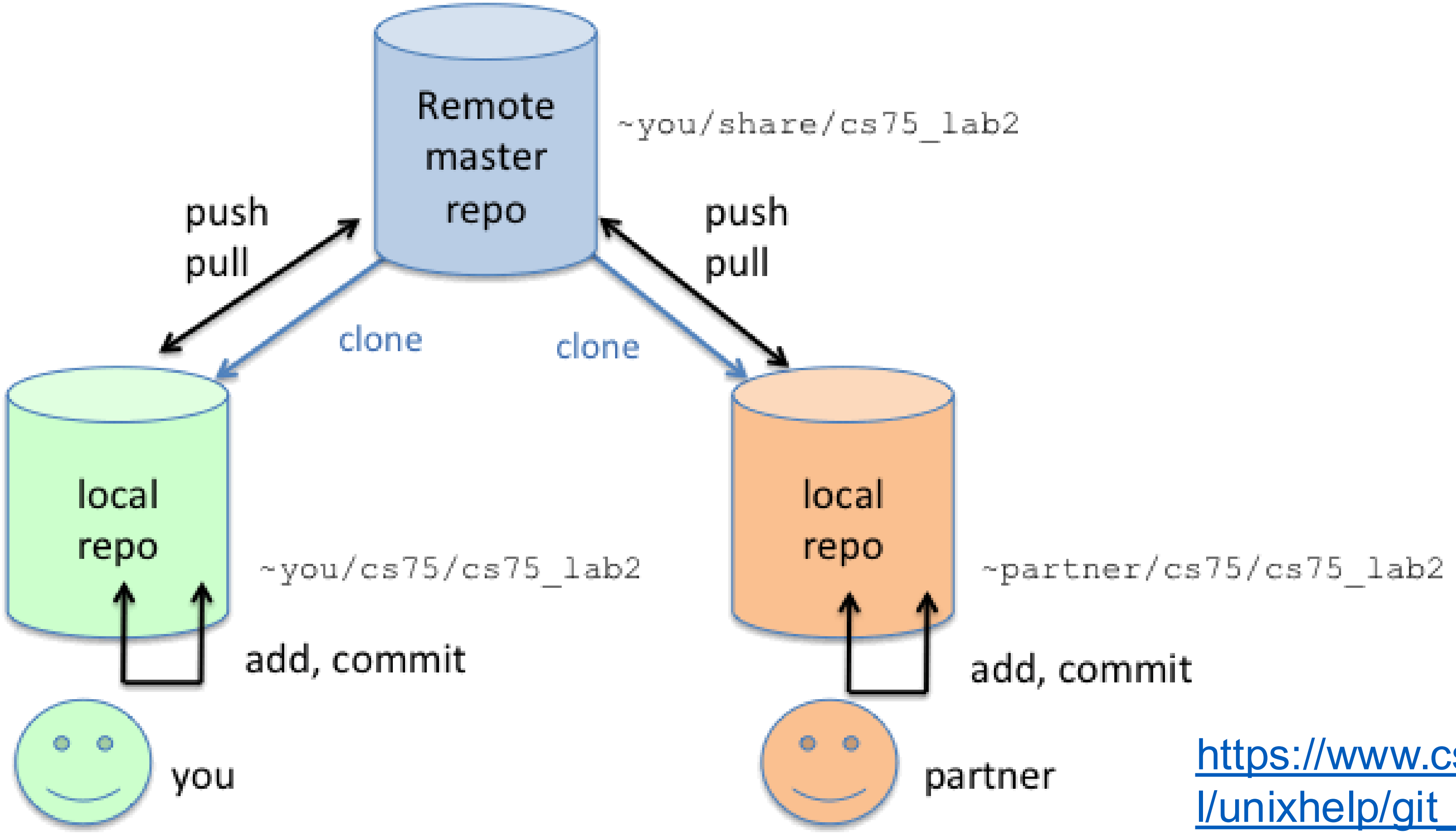
Basic concepts in git: Nodes and trees

You can also start splits call branches

And when you finish an idea you can merge them together



Basic concepts in git: Local and remote

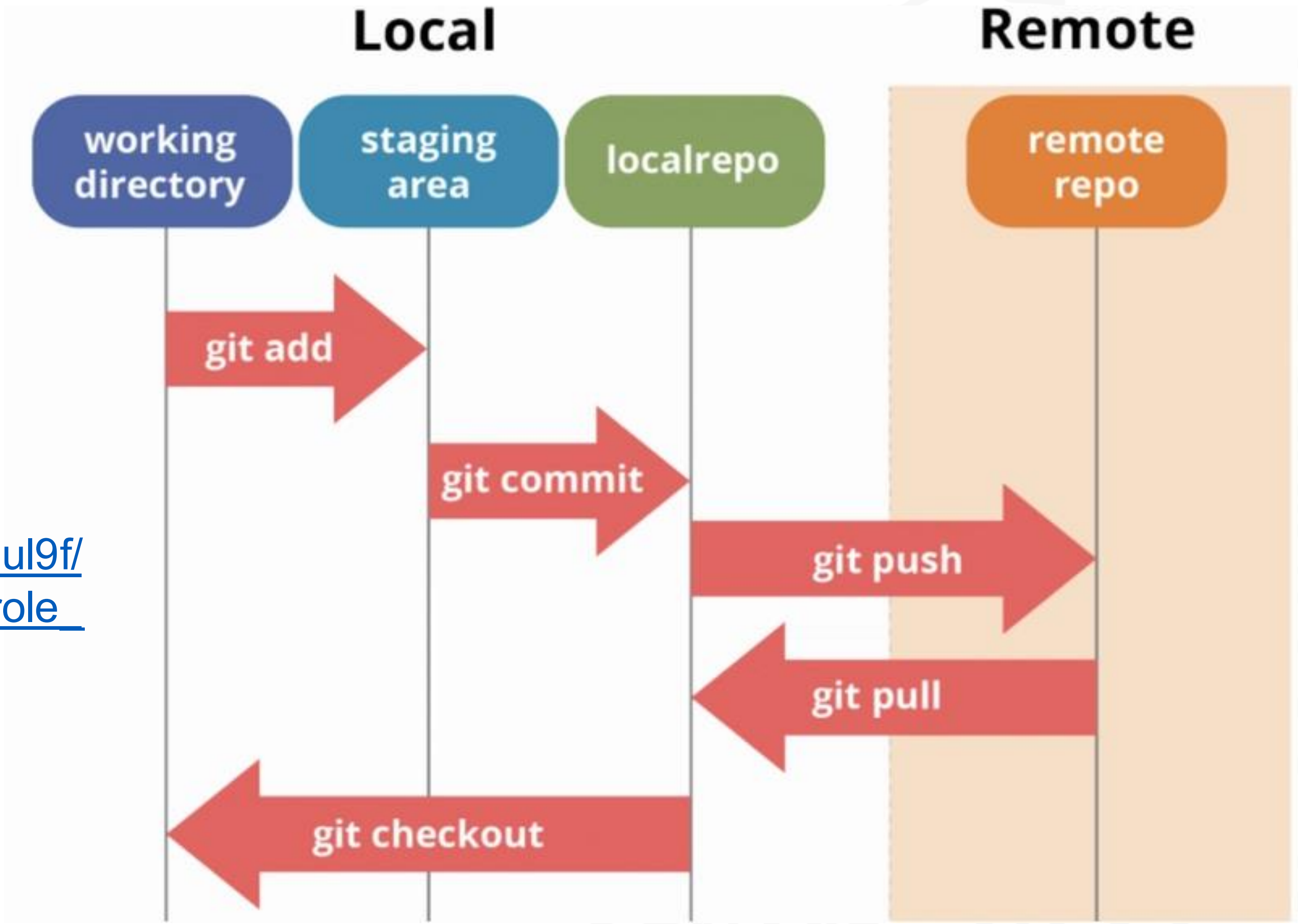


https://www.cs.swarthmore.edu/~newhall/unixhelp/git_create.php

GitHub workflow

Basics:
https://dev.to/mollynem/git-github--workflow-fundamentals-5496

Advanced:
https://www.reddit.com/r/git/comments/99ul9f/git_workflow_diagram_showcasing_the_role_of/



To get familiar with the setup, we will practice GitHub in today’s lab