Lecture 06 - Git discussion, review, and extension

# some logistics

- quizzes were worth too much and so I'm fixing that by increasing the weight on the group project
- messed up good & bads last week, but will do it on this Wednesday; put names on them!
- exercises due the following tutorial to allow for help at office hours
- orthogonal design to a point...





#### How does Git work?

- ► A set of functions that allow tracking of progress in a project and facilitate collaboration.
- Sets up a hidden directory that stores information about changes in a working directory.

```
git init

git add file_names
git commit -m "custom commit message"
```

 Use Git to commit each version of the shell script developed below when answering questions 2 - 4. Print your Git log for this shell script and turn it in with your answers below.

Write a shell script that does NOT use a loop, but writes the atom number and element with the lowest value in the fifth column of each .pdb file to a text file. Once you have a shell script that works, write the contents of that script below.

cd data-shell/molecules

git init

```
#!/usr/bin/env bash
# a script for pulling the atom with the minimum value is
# usage ./pdbScript.sh
cat cubane.pdb | grep ATOM | sort -n -k 5 | head -n 1 |
tr -s " " | cut -d " " -f 3.5 >> results.txt
cat propane.pdb | grep ATOM | sort -n -k 5 | head -n 1 |
tr -s " " | cut -d " " -f 3,5 >> results.txt
```

git add -A

git commit -m "added shell script without a for loop"

Revise the shell script from above so that it DOES use a loop. Once you have a shell script that works, write the contents of that script below.

```
#!/usr/bin/env bash

# a script for pulling the atom with the minimum value is
# usage ./pdbScript.sh

for file in "$@"
do
   cat $file | grep ATOM | sort -n -k 5 | head -n 1 |
   tr -s " " | cut -d " " -f 3,5 >> results.txt
done
```

git add -A

git commit -m "added a for loop to pdbScript.sh"

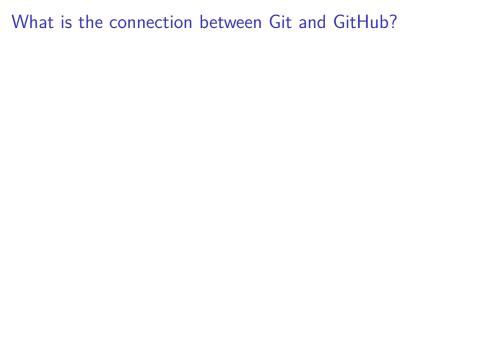
4. Revise the shell script from above so that it can take an argument from the user to determine which column from the .pdb files we are using to pick an atom. Once you have a shell script that works, write the contents of that script below.

```
git log
git diff HEAD 'hash from previous commit'
git checkout 'hash from previous commit'
-- pdbScript.sh
```

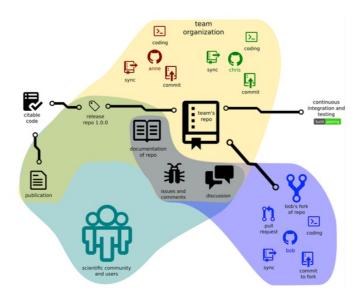
```
#!/usr/bin/env bash
# a script for pulling the atom with the minimum value is
# usage ./pdbScript.sh column_number
 cat cubane.pdb | grep ATOM | sort -n -k $1 | head -n 1
tr -s " " | cut -d " " -f 3.5 >> results.txt
cat propane.pdb | grep ATOM | sort -n -k $1 | head -n 1
tr -s " " | cut -d " " -f 3,5 >> results.txt
```

git add -A

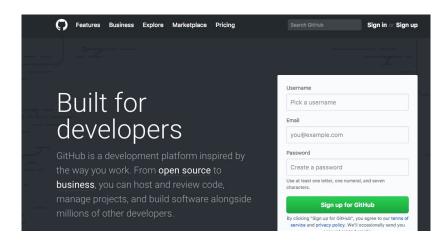
git commit -m "added argument to pbsScript.sh
for selecting the column number but got rid of
the for loop"



#### What is the connection between Git and GitHub?



# Sign up for GitHub...



# Sign up for GitHub...



0 \*

0 \*

0 \*

0 \*

**New repository** 

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# Sign up for GitHub...



Add a bio

**L** University of Notre Dame

siones20@nd.edu

@ http://www.nd.edu/~sjones20

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Shell 🛊 1

Tools for interacting with the General Lake Model (GLM) in R

R

KF-code

peaksND

R tool for processing of amplified fragment length polymorphism data generated by ABI sequencers

Forked from ctsolomon/KF-code

Kalman Filter analysis of lake C models

LakeMetabolizer

Forked from GLEON/LakeMetabolizer

methaneEcosystemModel

Collection of Lake Metabolism Functions

## function review

```
git config
git init
git add
git commit
git status
git log
git checkout
```