

USING THE BRIDGES-2 SUPERCOMPUTER

Observations, Information, & How You Can Waste Less Time than Me

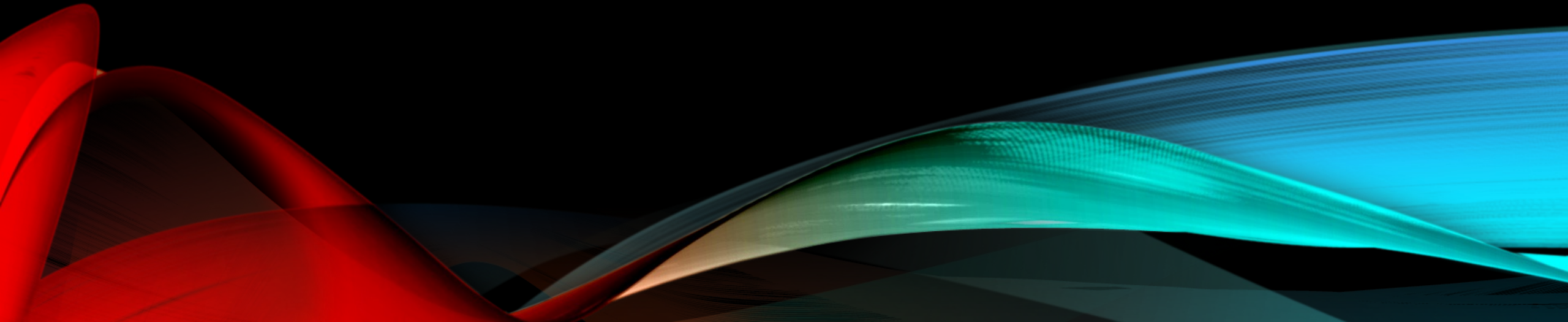
Anna Cobb

GOALS OF THIS PRESENTATION

1. Understand the awesome power of supercomputers
2. Know that you can pretty easily access some really nice ones nearby
3. Feel like you could easily learn how to use it
4. Feel cool because it is cool to talk about supercomputers



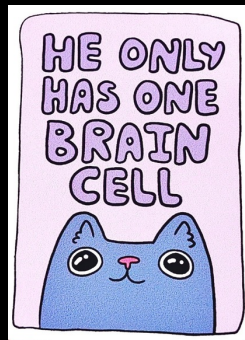
SUPERCOMPUTING INTRODUCTION AND THE POWER OF PITTSBURGH'S BRIDGES-2



High performance computing!
High performance computing!
High performance computing!

WHAT IS SUPERCOMPUTING?

“A supercomputer is a computer with a high level of performance as compared to a general-purpose computer.” (Wikipedia)



the already incredible modern laptop



the supercomputer

IS SUPERCOMPUTING RIGHT FOR ME?

THE SIGNS:

- You are propping your laptop open while it's in your backpack so that it won't go to sleep and will continue running code
 - There's actually a better solution to this: it's called amphetamine
- Your code takes days or large parts of days to run/you're doing intensive simulations
 - Agent-based models, working with really giant datasets, CFD, biophysics stuff
- You want to learn; it's a cool thing to know!

BRIDGES-2 IS A SUPERCOMPUTER AT THE PSC

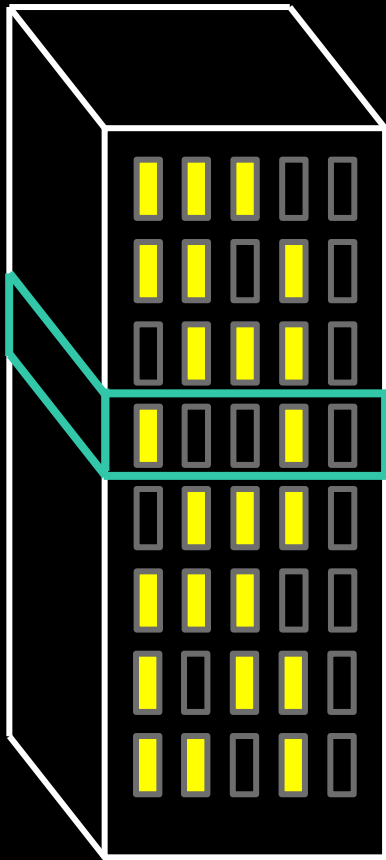
Pittsburgh Supercomputing Center (PSC) computing resources:

- Anton 2: special purpose for biomolecular simulation
- Neocortex: high performance AI
- Bridges-2:
 - 3 types of nodes
 1. Regular Memory (RM):
128 cores, 256 GB RAM
 2. Extreme Memory (EM):
96 cores, 4 TB RAM
 3. GPU:
40 cores, 512 GB RAM

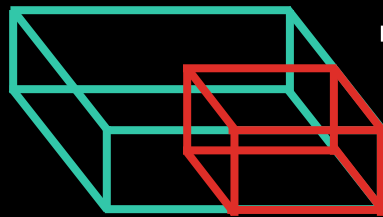


NODES, CORES, CPU'S, OH MY!

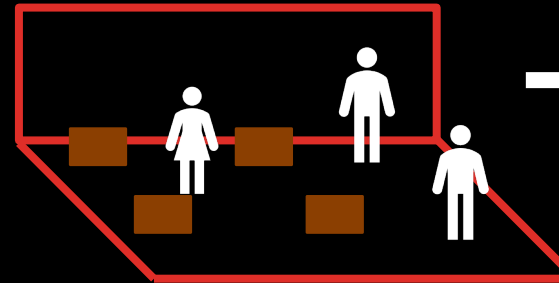
giant office building =
rack of nodes



floor of office building =
1 node



office on the floor =
1 CPU



worker in the office =
1 core



PUTTING THE POWER OF SUPERCOMPUTERS INTO CONTEXT

Macbook Air M1 Specs

- 8-core CPU
- 8-core GPU
- 8 GB unified memory (RAM)



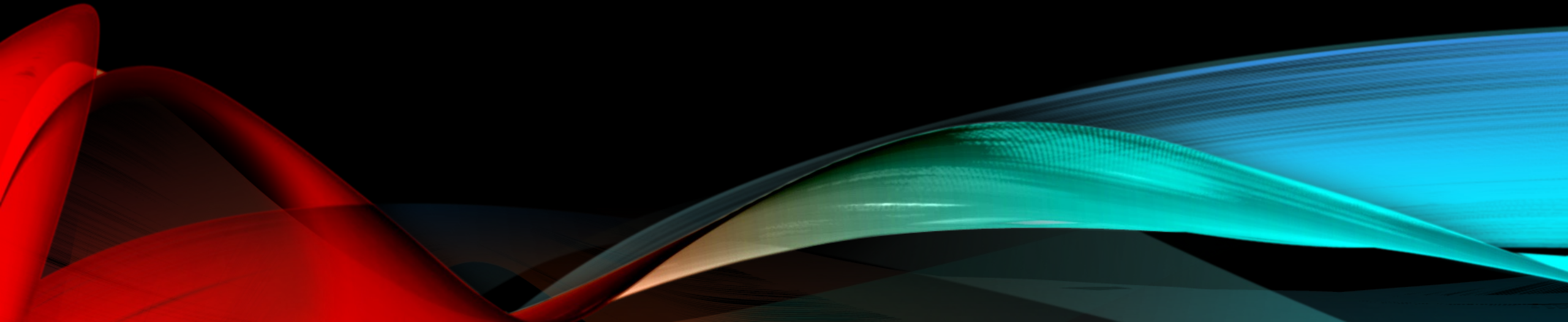
Bridges 2 Specs

- 1 RM node = 2 CPUs = 128 cores
→ 64-core CPUs
- 1 RM node = 256 GB RAM
(except for 16 special nodes
which have 512 GB!)

...and you can use as many as
you need!



GETTING ACCESS TO PSC RESOURCES



ACCESS: THE FRUSTRATING YET FRIENDLY ALLOCATIONS PROVIDER

- ACCESS is much like trying to get supercomputer access from your grandma: they make you follow all the rules so you can be safe (annoying) but provide massive amounts of info and respond to emails very quickly!
 - No fun email forwards though☹



Image Credits:
<https://www.nytimes.com/2020/09/01/style/shirley-curry-skyrim-youtube.html>

WHAT'S THE PROCESS FOR GETTING ~ACCESS~?



Decide what allocation type is right for you

Apply for your allocation type

Exchange your credits for service units (SUs) on specific resources

Allocation Type	Credits*
Explore	400,000
Discover	1,500,000
Accelerate	3,000,000
Maximize	N/A

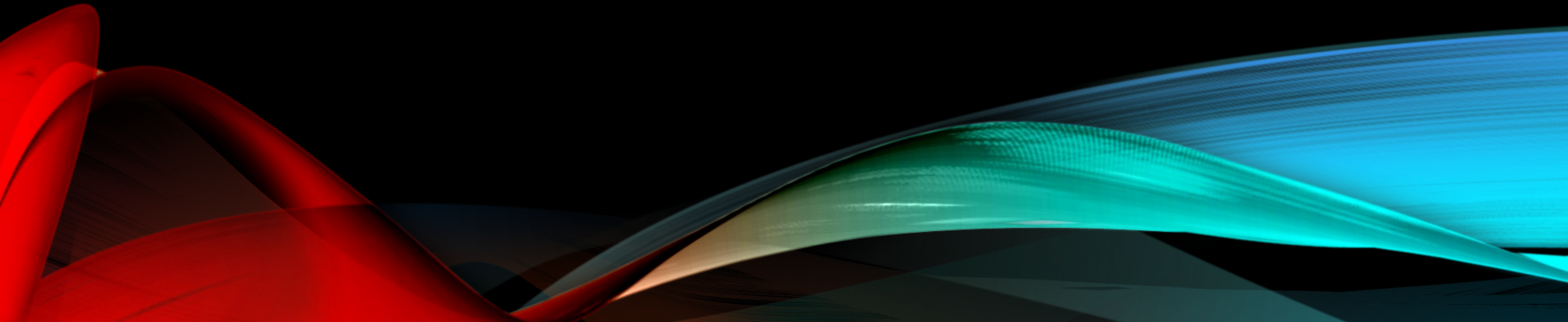
e.g., for Explore:

- Overview of research Q's & how you intend to use supercomputing resources
- CVs for PI & co-PI's—you can be a PI!
- Letter of collaboration if you, as graduate student, are PI

For Bridges-2 RM:

- 1 SU = 1 core-hour (1 hour of computation with 1 core)
- Note: you have to submit an exchange request each time you exchange ACCESS credits for SUs

ACTUALLY USING BRIDGES-2



THE PROCESS

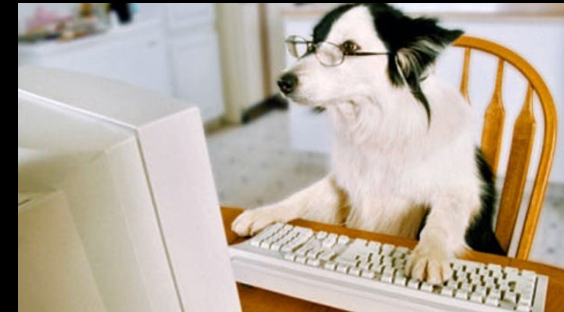
You write your code you want to run on the SC



You write the batch file needed to run your code on the SC



You interface with the SC to submit your batch file



your job (and code) are executed



your job gets scheduled and goes in the queue



WHAT DOES A BATCH FILE LOOK LIKE?

```
#!/bin/bash
```

Specs

```
#SBATCH -N 1                # number of nodes
#SBATCH -p RM
#SBATCH -t 30:00:00
#SBATCH --ntasks-per-node=128 # number of cores per node
#SBATCH --mail-type=ALL      # send email when job ends
#SBATCH --mail-user=acobb
```

Code to
be run

```
cd /jet/home/acobb/
export PATH="$PATH:/jet/home/acobb/my_modules/julia-1.7.0/bin"
export JULIA_NUM_THREADS=128 → Multithreading—go even faster!
julia --project='/jet/home/acobb/V4' small_taxis_ICE_SC_no_AP_driver_position.jl
```

QUICK CAVEAT ON MULTITHREADING

- To use multiple CPU cores, your code needs to have been written to use multiple threads. Otherwise, no point in requesting multiple cores! (as far as I know). More info on this can be found on this [Princeton website](#)
- Example:

```
Threads.@threads for i in 1:length(taxis) # for those taxis that need a route calculation,  
                                         # calculate route and reset their queue number  
    idx = trunc{Int, taxis[i]}  
    V[i] = OSM.plan_route(model[idx].pos, model[idx].destination, model)  
    model[idx].route = V[i]  
    model[idx].queue = model[idx].queue - 10000  
end
```

RUNNING BATCH JOBS

- All you have to do is type these commands into the shell:
 - > sbatch myjob.sh
 - An output file is automatically created that basically contains everything that would've been printed out in your command window/terminal
 - when your job(s) is done, you get notified!
- You may be wondering: what if I request more time/nodes/cores than I actually need?
 - You only get charged for what you use!

Slurm 2:29 PM
Slurm Job_id=18626653 Name=n...
This message has no content.

Slurm 2:29 PM
Slurm Job_id=18626654 Name=n...
This message has no content.

Slurm 2:14 PM
Slurm Job_id=18651443 Name=c...
This message has no content.

• **Slurm** 2:08 PM
Slurm Job_id=18651443 Name=c...
This message has no content.

• **Slurm** 2:08 PM
Slurm Job_id=18651421 Name=c...
This message has no content.

• **Slurm** 2:05 PM
Slurm Job_id=18651421 Name=c...
This message has no content.

• **Slurm** 2:04 PM
Slurm Job_id=18651361 Name=c...
This message has no content.

• **Slurm** 2:02 PM
Slurm Job_id=18651361 Name=c...
This message has no content.

• **Slurm** 1:56 PM
Slurm Job_id=18651301 Name=c...
This message has no content.

• **Slurm** 1:55 PM
Slurm Job_id=18651301 Name=c...
This message has no content.

USING SSH TO INTERFACE

- SSH (secure shell):
 - Allows for secure access to computer over unsecured network
 - For Macs: can just use your terminal
 - For Windows: I believe you may need to install a ssh client (PutTY is a popular one)

```
annacobb — acobb@br012:~ — ssh acobb@bridges2.psc.edu — 80x34
Last login: Mon Aug 21 07:58:05 on ttys002
[(base) annacobb@Annas-MacBook-Pro-3 ~ % ssh acobb@bridges2.psc.edu
acobb@bridges2.psc.edu's password:
***** W A R N I N G *****
You have connected to br012.ib.bridges2.psc.edu, a login node of Bridges 2.

This computing resource is the property of the Pittsburgh Supercomputing Center.

It is for authorized use only. By using this system, all users acknowledge
notice of, and agree to comply with, PSC policies including the Resource Use
Policy, available at http://www.psc.edu/index.php/policies. Unauthorized or
improper use of this system may result in administrative disciplinary action,
civil charges/criminal penalties, and/or other sanctions as set forth in PSC
policies. By continuing to use this system you indicate your awareness of and
consent to these terms and conditions of use.

LOG OFF IMMEDIATELY if you do not agree to the conditions stated in this warning

***** W A R N I N G *****

For documentation on Bridges 2, please see www.psc.edu/resources/bridges-2/user-
guide/
Please contact help@psc.edu with any comments/concerns.
Last login: Fri Aug 25 10:00:13 2023 from cmu-secure-128-237-82-10.nat.cmu.net

Projects
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Project: eng230003p [Default charging account] PI: Anna Cobb
Extreme Memory      89 SU remain of 3,000 SU      Active: Yes
Regular Memory      109,467 SU remain of 385,687 SU    Active: Yes
Ocean /ocean/projects/eng230003p 53.56G used of 101G

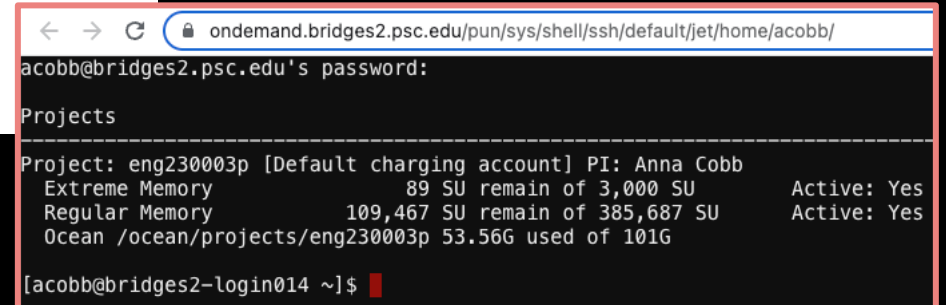
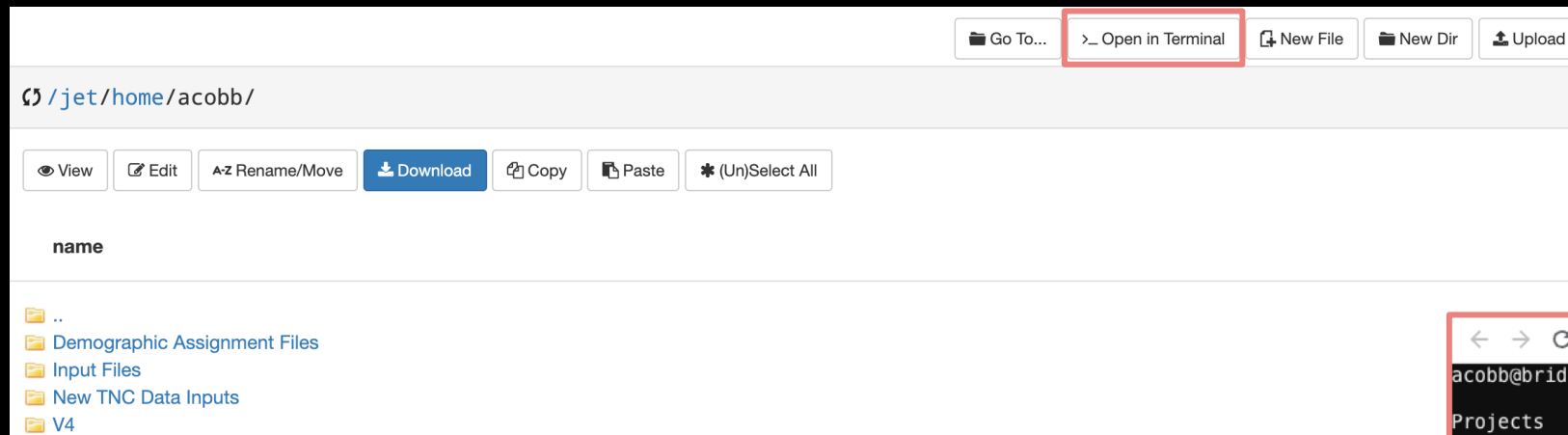
[acobb@bridges2-login012 ~]$
```

The only command needed to connect with Bridges-2

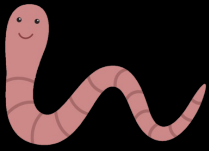
Some good info about your remaining SUs & storage

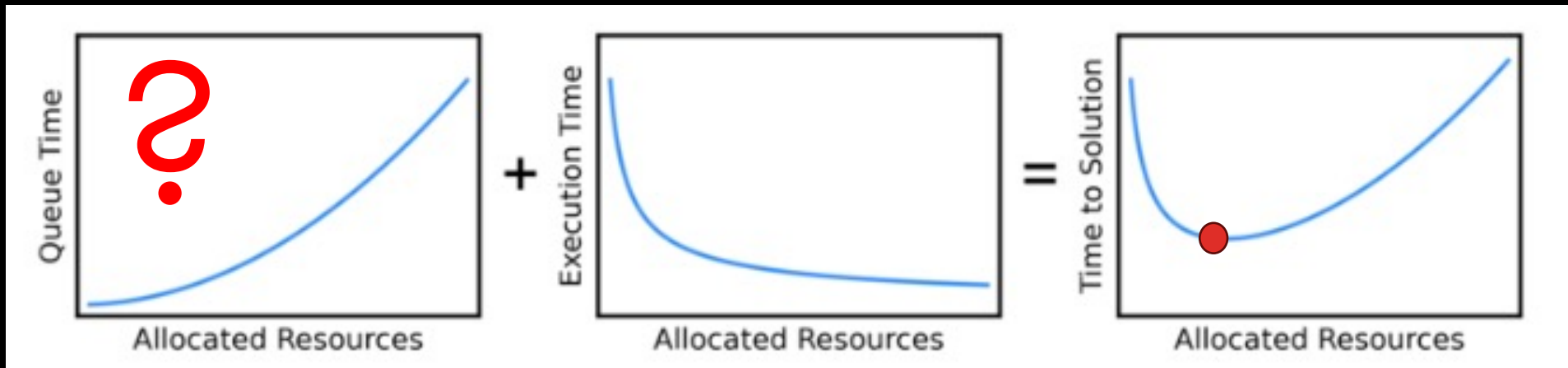
USING ONDEMAND TO INTERFACE

- OnDemand is a gift that we honestly do not deserve
 - Lovely, built-in commands (particularly the file editor)
 - Batch jobs still run through shell (in browser)
 - But do not, under any circumstances, connect to eduroam!



HOW DO JOBS GET SCHEDULED?

- Meet SLURM 
 - Simple Linux Utility for Resource Management (SLURM) Workload Manage: free & open-source job scheduler
 - takes in your batch (AKA “job”) files and puts them in order with everyone else’s to get executed



~optimization~

ADDITIONAL FEATURES OF BRIDGES-2

- Built-in Bridges-2 software:
 - RStudio
 - iJulia
 - Jupyter Notebook
 - However, as far as I know you can install whatever you want using an executable
- Usage is funded by NSF (you can use Bridges-2 for free as an academic researcher!)
- You can also exchange your allocated credits for storage (I currently have 100 GB)
- It can be accessed from anywhere! (through both OnDemand & your local shell)

RESOURCES

- [Bridges-2 User Guide](#): extremely helpful for using Bridges-2
 - [Link to OnDemand](#): this is in the OnDemand section of the user guide
- [Princeton's supercomputing website](#): great for general knowledge
- [ACCESS allocations website](#): this is where you actually have to do stuff



QUESTIONS?