

Introduction to the command-line interface (shell)

Harvard Chan Bioinformatics Core
in collaboration with
HMS Research Computing

<https://tinyurl.com/hbc-shell-online>



Shannan Ho Sui
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Victor Barrera



Amelie Jule



Zhu Zhuo



James Billingsley



Radhika Khetani
Director of Education



Meeta Mistry



Will Gammerdinger



Emma Berdan



Sergey Naumenko



Maria Simoneau



We are hiring!
Email bioinformatics@hspf.harvard.edu
for more information



Peter Kraft
Faculty Advisor

Introductions!



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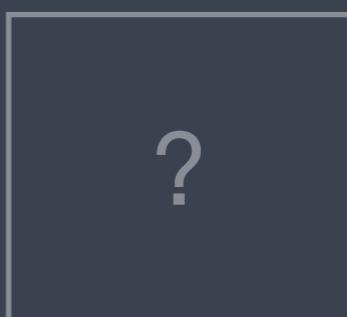
Emma Berdan



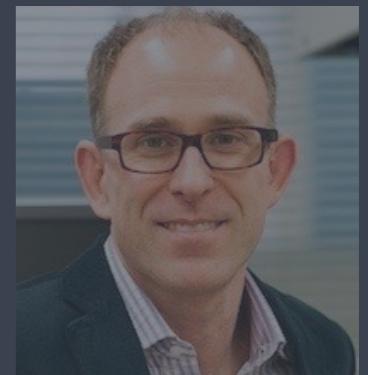
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Peter Kraft
Faculty Advisor

Consulting

- Experimental design help
- RNA-seq analysis: bulk, single cell, small RNA
- ChIP-seq and ATAC-seq analysis
- Genome-wide methylation
- WGS, resequencing, exome-seq and CNV studies
- QC & analysis of gene expression arrays
- Functional enrichment analysis
- Grant support

<http://bioinformatics.sph.harvard.edu/>



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NIEHS



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AND TRANSLATIONAL
SCIENCE CENTER



Training

A key component of the HBC's mission is its training initiative. Our dedicated training team holds workshop to help researchers at Harvard better understand analytical methods for NGS data.

HBC's training team is made up of four PhD-level scientists who devote substantial time to material development, training and community building/outreach. All members of the training team also participate in consultations on research projects to ensure they remain up-to-date on current best practices in NGS analysis.

Our hands-on workshops focus on **basic data skills** and **analysis of high-throughput sequencing data**, with an emphasis on **experimental design**, current **best practices** and **reproducibility**. Our workshops are designed for **wet-lab biologists** aiming to independently design sequencing-based experiments and analysing the resulting data.

We offer three types of workshops:

1. Short, 3-hour monthly workshops (*Current topics in bioinformatics*)
2. Basic Data Skills**
3. Advanced Topics: Analysis of high-throughput sequencing (NGS) data**

***The basic data skills workshops serve as the foundation for the advanced workshops.*

<http://bioinformatics.sph.harvard.edu/training/>

<https://hbctraining.github.io/main/>

Training

A key component of the HBC's mission is to train researchers at Harvard and beyond.

HBC's training team is made up of scientists, educators, and community based organizations involved in research projects to ensure that our training is relevant and effective.

Our hands-on workshops are designed to provide an emphasis on **experimental design** and **informatics**, as well as training for **wet-lab biologists** and **bioinformaticians** to work with NGS data.

We offer three types of workshops:

1. Short, 3-hour monthly workshops
2. Basic Data Skills**
3. Advanced Topics: Analysis of high-throughput sequencing data

**The basic data skills workshop is designed for researchers who have no experience with NGS data analysis.



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Our dedicated training team holds workshops to help researchers learn how to analyze and interpret NGS data.

In addition to devote substantial time to material development, the training team also participate in consultations on best practices in NGS analysis.

Workshops focus on the analysis of high-throughput sequencing data, with an emphasis on **experimental design**, **informatics**, and **reproducibility**. Our workshops are designed to provide hands-on training for conducting experiments and analysing the resulting NGS data.

informatics)

NGS) data**

and **reproducibility** for the advanced workshops.

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<https://hbctraining.github.io/main/>

Training

A key component of the HBC's mission is to support researchers at Harvard by providing training.

HBC's training team is made up of scientists who provide training and community building for research projects to ensure the quality of our work.

Our hands-on workshops focus on **bioinformatics**, with an emphasis on **experimental design** and **data analysis**. We also provide training for **wet-lab biologists** aiming to understand their data.

We offer three types of workshops:

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2. Basic Data Skills**
3. Advanced Topics: Analysis of high-throughput sequencing data

**The basic data skills workshop is designed for researchers who have no prior experience with bioinformatics.



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Our dedicated training team holds workshops to help researchers learn how to analyze high-throughput sequencing (NGS) data.

The training team also devote substantial time to material development, and our training team also participate in consultations on best practices in NGS analysis.

Workshops focus on the analysis of high-throughput sequencing data, with an emphasis on **experimental design**, **data quality**, and **reproducibility**. Our workshops are designed to help researchers understand the principles of sequencing-based experiments and analysing the resulting data.

bioinformatics)

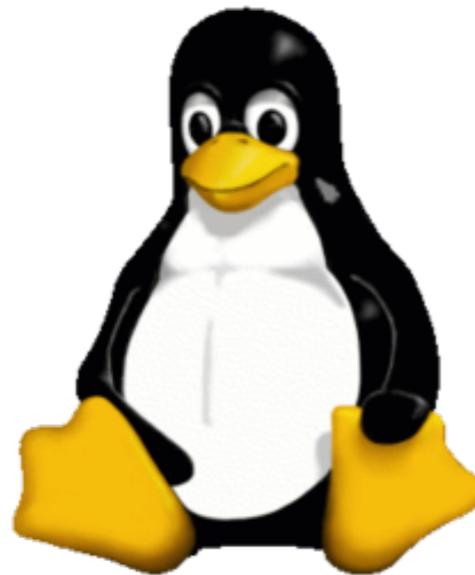
basic data skills (e.g., NGS) data**

and **advanced topics** (e.g., for the advanced workshops).

<http://bioinformatics.sph.harvard.edu/training/>

<https://hbctraining.github.io/main/>

Workshop scope



```
rkhetani — rsk27@clarinet002-072: ~ — ssh — 75x51
rsk27@clarinet002-072:~$ ll -htr unix_workshop/
total 177K
drwxrwsr-x 2 rsk27 rsk27 62 May 23 2016 reference_data
-rw-rw-r-- 1 rsk27 rsk27 377 May 23 2016 README.txt
drwxrwsr-x 2 rsk27 rsk27 78 May 23 2016 genomics_data
drwxrwsr-x 2 rsk27 rsk27 257 May 23 2016 raw_fastq
drwxrwsr-x 2 rsk27 rsk27 695 May 23 2016 other
drwxrwsr-x 6 rsk27 rsk27 972 May 24 2016 rnaseq_project
rsk27@clarinet002-072:~$
```

“Unix is user-friendly.

It's just very selective about who its friends are.”

The Unix command-line interface

- ◆ Unix is a stable, efficient and powerful operating system
- ◆ It can easily coordinate the use and sharing of a computer's (or a system's) resources, i.e. built to allow multi-user functionality
- ◆ Can easily handle complex and repetitive tasks easily on large and small datasets
- ◆ Usually, written commands are used to work with this OS, instead of the pointing and clicking used with operating systems like Windows and OSX

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Bioinformatics:

- ◆ A lot of NGS-analysis tools are created for the Unix OS
- ◆ High-performance compute clusters which are necessary to analyze large datasets require a working knowledge of Unix

Linux

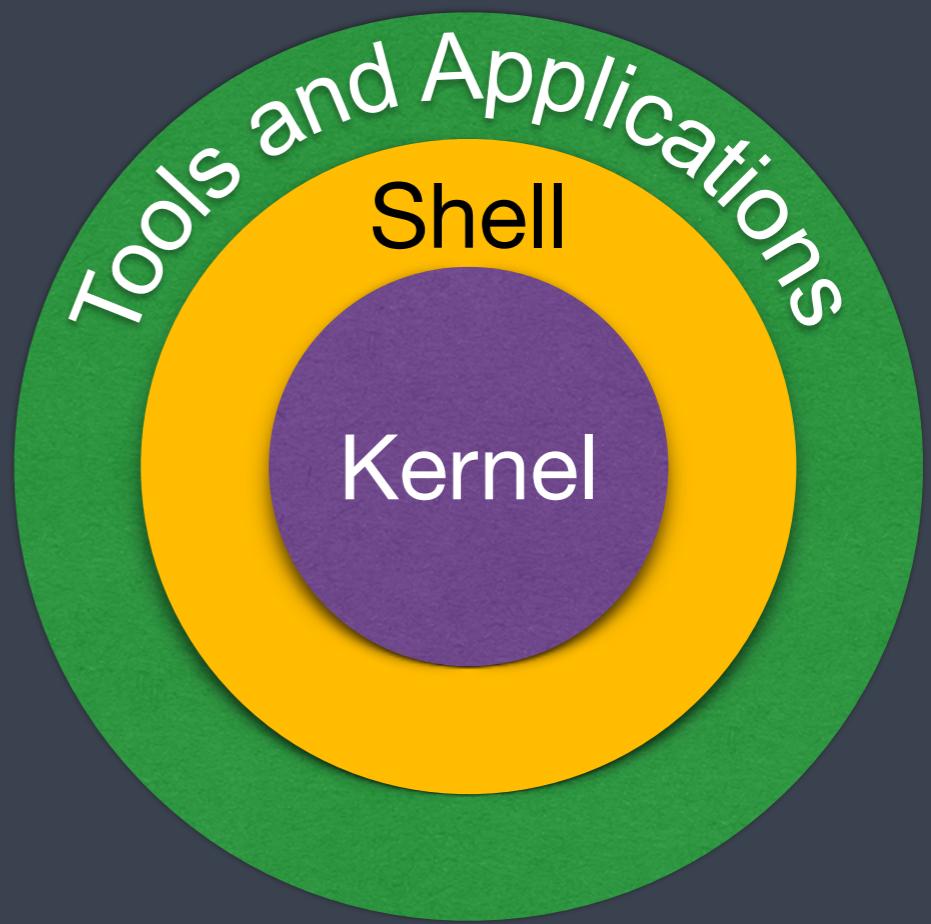
- ❖ Linux is a free, open-source operating system based on Unix
- ❖ It has the same components as the original, but the open source community is involved in active development of various distinct distributions of Linux



Components

The Unix/Linux system is functionally organized at 3 levels:

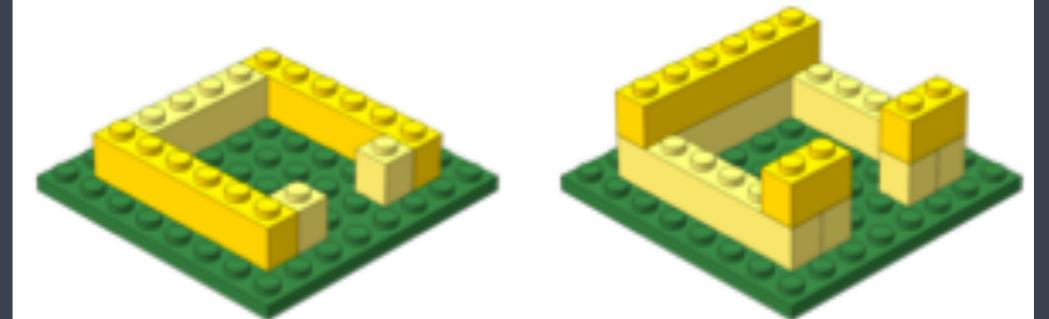
- ◆ **The kernel**, which schedules tasks and manages storage: *the brain of the system*
- ◆ **The shell**, *an interpreter* that helps interprets our input for the kernel
- ◆ **Utilities, tools and applications**, which use the shell to communicate with the kernel



The “shell”

- ◆ The shell is **an interpreter**
- ◆ It is independent of the operating system
- ◆ Dozens of shells have been developed throughout UNIX history, and a lot of them are still in use
- ◆ The most commonly used shell is **bash**

Learning Objectives



- ✓ Learn what a “shell” is and become comfortable with the command-line interface
 - Find your way around a filesystem using written commands
 - Work with small and large data files
 - Become more efficient when performing repetitive tasks
- ✓ Understand what a computational cluster is and why we need it

Logistics

Course webpage

<https://tinyurl.com/hbc-shell-online>

Course schedule online

Workshop Schedule

Day 1

Time	Topic	Instructor
9:30 - 10:10	Workshop introduction	Meeta
10:10 - 11:40	Introduction to Shell	Mary
11:40 - 12:00	Overview of self-learning materials and homework submission	Jihe

Before the next class:

1. Please **study the contents** and **work through all the code** within the following lessons:

- Wildcards and shortcuts in Shell
- Examining and creating files
- Searching and redirection
- Shell scripts and variables in Shell

NOTE: To run through the code above, you will need to be **logged into O2** and **working on a compute node** (i.e. your command prompt should have the word `compute` in it).

1. Log in using `ssh rc_trainingXX@o2.hms.harvard.edu` and enter your password (replace the "XX" in the username with the number you were assigned in class).
2. Once you are on the login node, use `srun --pty -p interactive -t 0-2:30 --mem 1G`

Course materials online



Introduction to the command line interface (shell)

[View on GitHub](#)

Learning Objectives

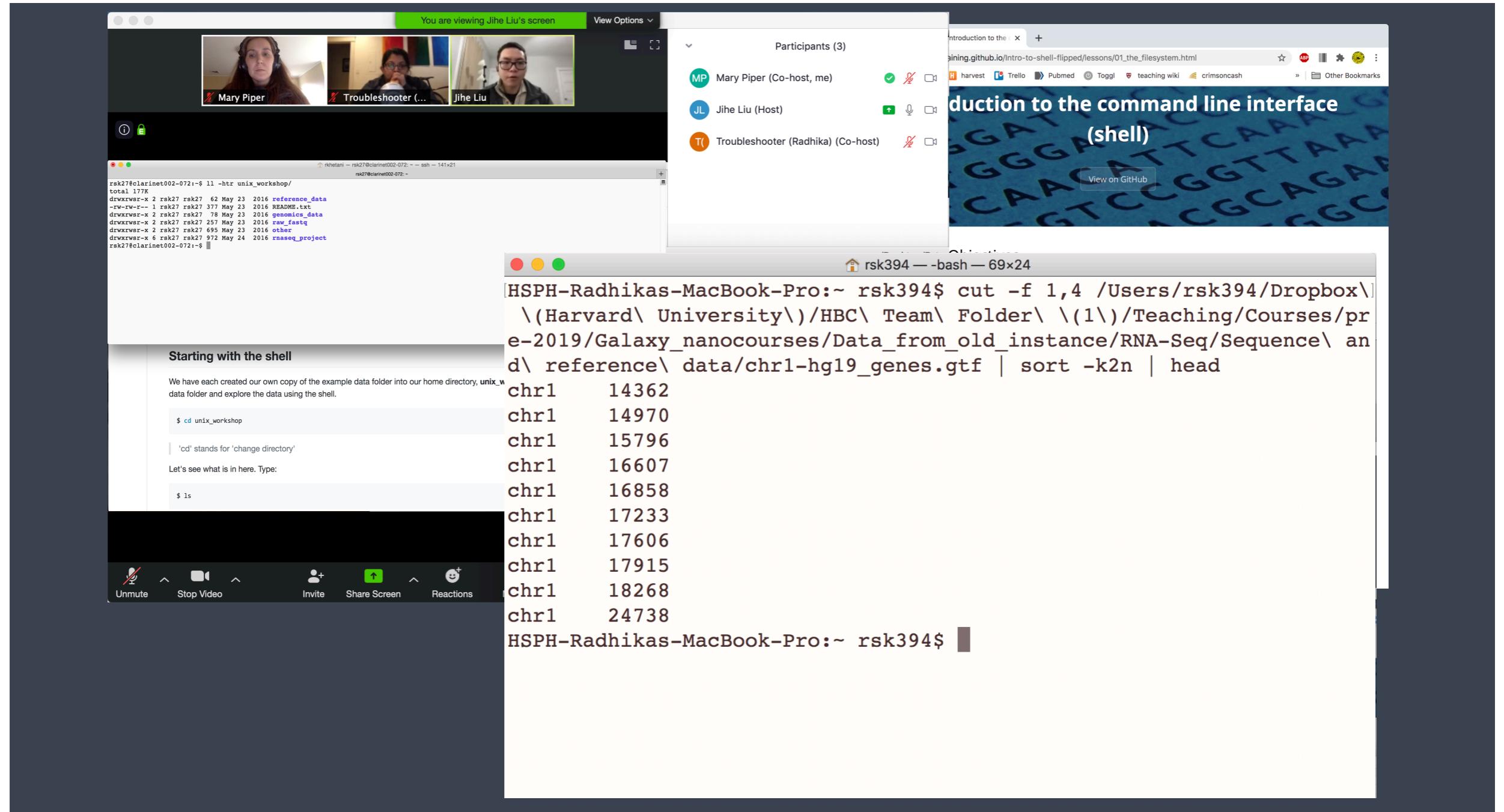
- How do you access the shell?
- How do you use it?
 - Getting around the Unix file system
 - looking at files
 - manipulating files
 - automating tasks
- What is it good for?

Setting up

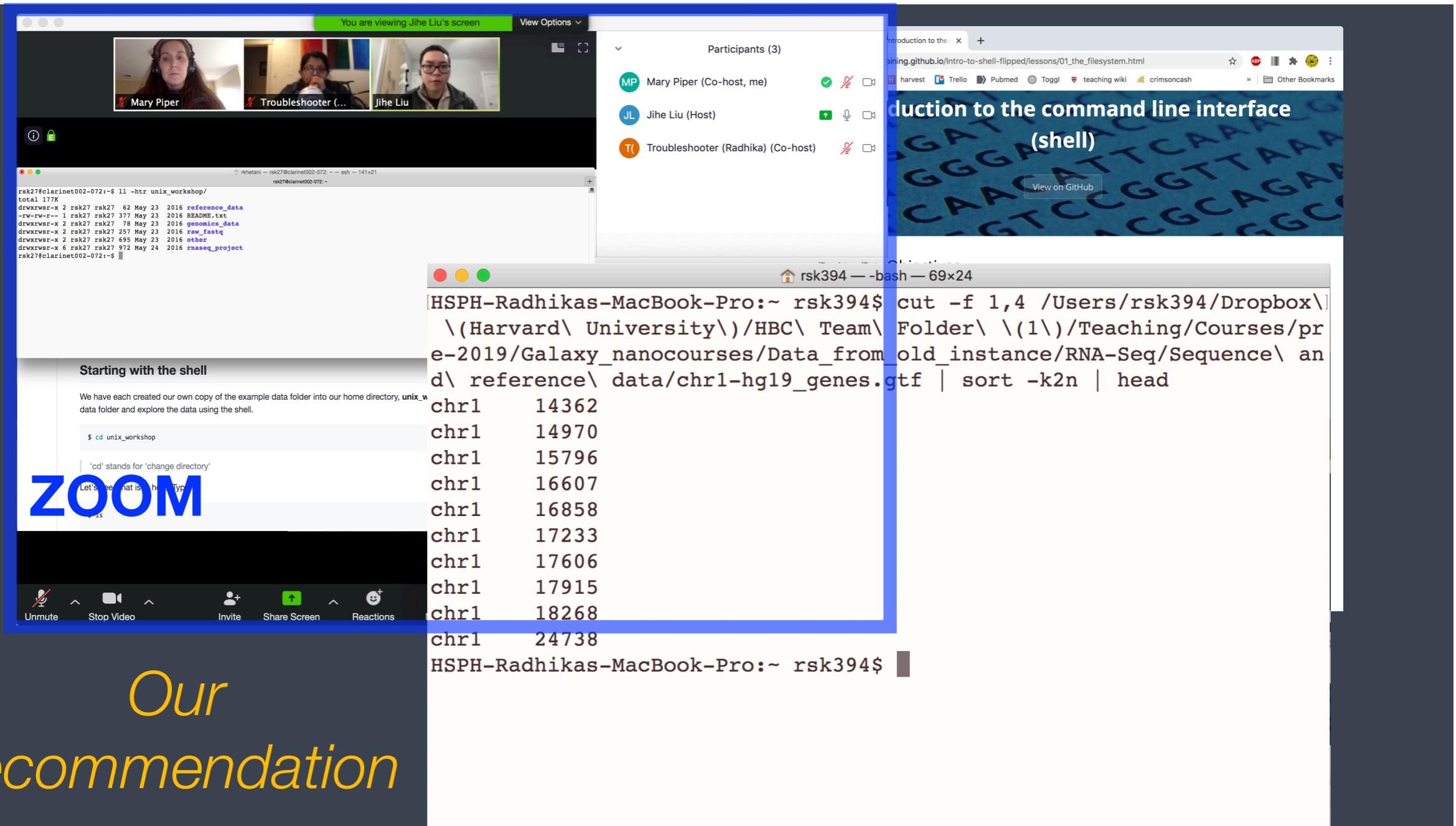
We will spend most of our time learning about the basics of the shell command-line interface (CLI) by exploring experimental data on the **O2** cluster. So, we will need to log in to this remote compute cluster first before we can start with the basics.

Let's take a quick look at the basic architecture of a cluster environment and some cluster-specific jargon prior to logging in.

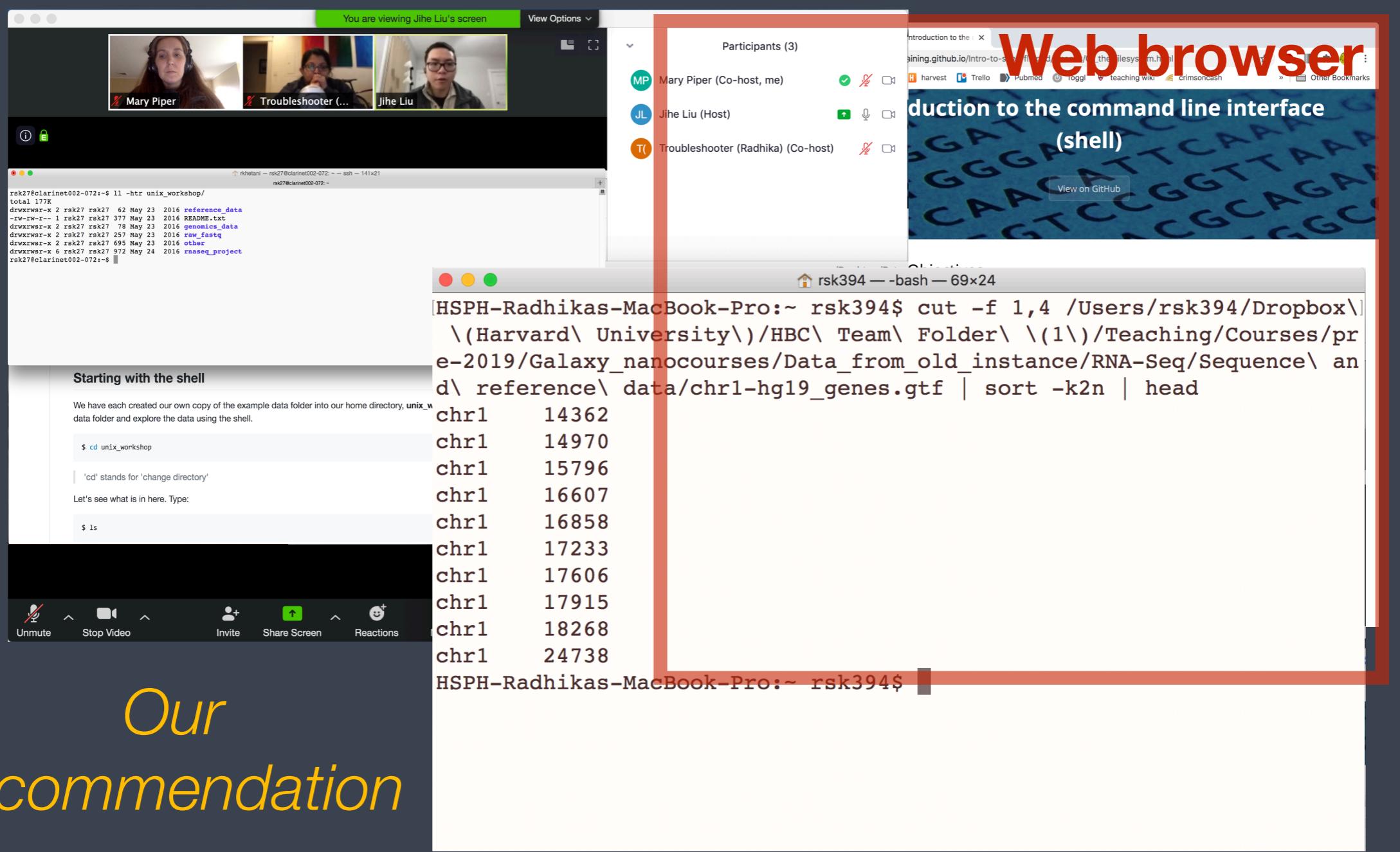
Single screen & 3 windows?



Single screen & 3 windows?



Single screen & 3 windows?



Single screen & 3 windows?

The image shows a video conference interface with three main windows:

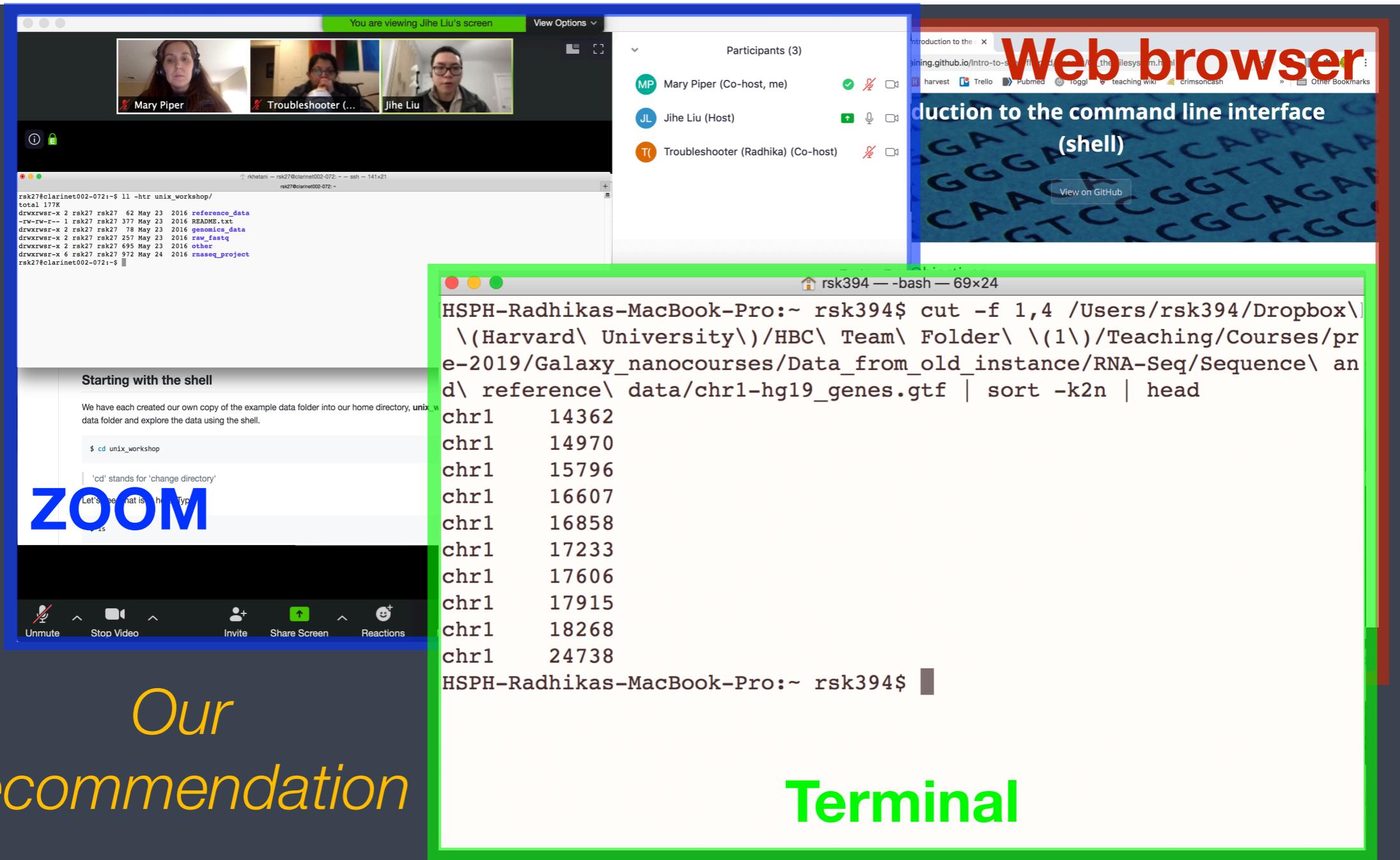
- Video Feed:** Shows three participants: Mary Piper, Troubleshooter (Radhika), and Jihe Liu.
- Participants List:** Shows three participants: Mary Piper (Co-host, me), Jihe Liu (Host), and Troubleshooter (Radhika) (Co-host).
- Terminal Session:** A green-highlighted window showing a command-line interface. The command run is:

```
rsk394 — bash — 69x24
HSPH-Radhikas-MacBook-Pro:~ rsk394$ cut -f 1,4 /Users/rsk394/Dropbox\(\Harvard\ University\)/HBC\ Team\ Folder\ \((1\))/Teaching/Courses/pre-2019/Galaxy_nanocourses/Data_from_old_instance/RNA-Seq/Sequence\ and\ reference\ data/chr1-hg19_genes.gtf | sort -k2n | head
chr1    14362
chr1    14970
chr1    15796
chr1    16607
chr1    16858
chr1    17233
chr1    17606
chr1    17915
chr1    18268
chr1    24738
```

Our recommendation

Terminal

Single screen & 3 windows?



Course participation

- ▶ Please keep your videos on, we would love to see your faces!
- ▶ Mandatory review of self-learning lessons and assignments
- ▶ Attendance required for all classes
- ▶ Your questions and active participation drive learning
- ▶ We look forward to all of your questions!



Homework and Expectations

- ❖ At-home lessons and exercises after each session
- ❖ Cover material not previously discussed
- ❖ Provides us feedback to help pace the course appropriately
- ❖ 3-5 hours to complete
- ❖ Homework load is heavier in the beginning of this workshop series and tapers off

Odds and Ends (1/2)

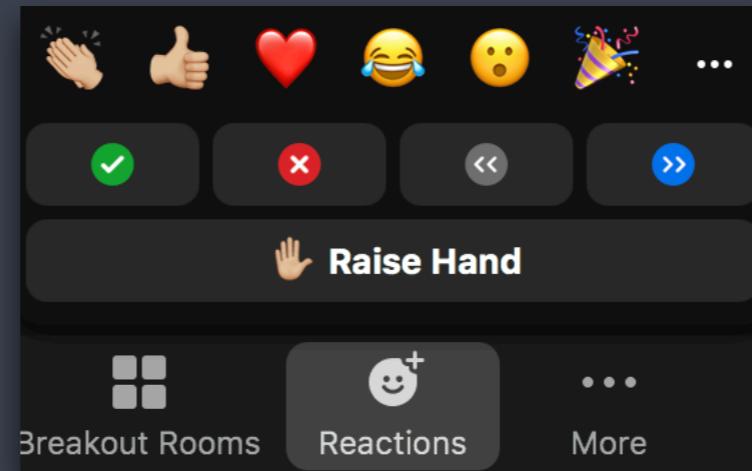
- ❖ Quit/minimize all applications that are not required for class

Odds and Ends (1/2)

- ❖ Quit/minimize all applications that are not required for class
- ❖ Captioning is available upon request

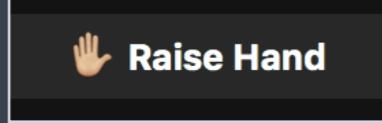
Odds and Ends (1/2)

- ❖ Quit/minimize all applications that are not required for class
- ❖ Captioning is available upon request
- ❖ Are you all set?
 - ▶  = "agree", "I'm all set" (equivalent to a **green post-it**)
 - ▶  = "disagree", "I need help" (equivalent to a **red post-it**)



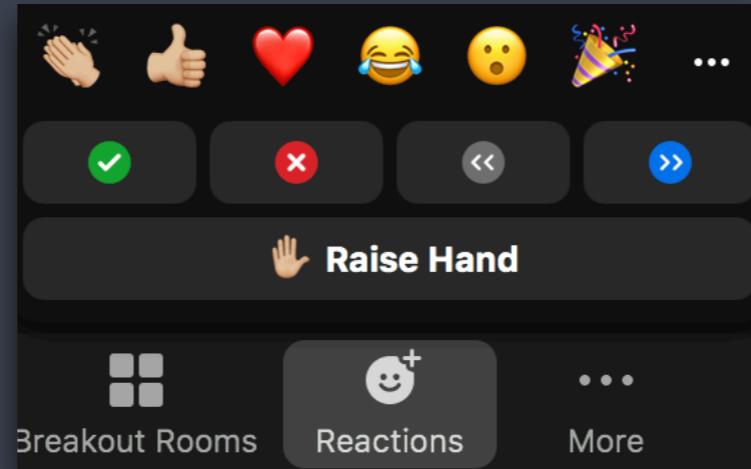
Odds and Ends (2/2)

- ❖ Questions for the presenter?

- Post the question in the Chat window OR
-  when the presenter asks for questions
- Let the Moderator know

- ❖ Technical difficulties with software?

- Start a private chat with the Troubleshooter with a description of the problem.



Thanks!

- Kathleen Chappell and Andy Bergman from HMS-RC
- [Data Carpentry](#)

These materials have been developed by members of the teaching team at the [Harvard Chan Bioinformatics Core \(HBC\)](#). These are open access materials distributed under the terms of the [Creative Commons Attribution license \(CC BY 4.0\)](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.



Contact us!

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Twitter

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HMS-RC: @hms_rc