HBC
Harvard Chan Bioinformatics Core

Shell for Bioinformatics

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

Harvard Chan Bioinformatics Core

in collaboration with

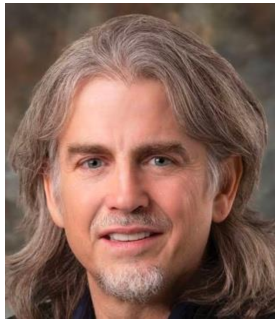
HMS Research Computing

Introductions!

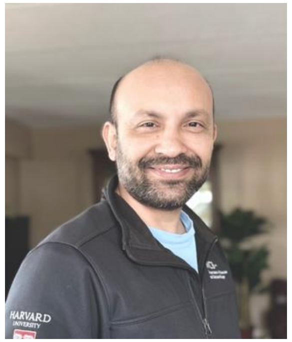
Shannan Ho Sui
Director

Meeta Mistry
Associate Director

Lorena Pantano
Director of Bioinformatics Platform



John Quackenbush
Faculty Advisor



Upen Bhattarai

Heather Wick

Will Gammerdinger

Noor Sohail

Alex Bartlett

Elizabeth
Partan

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James Billingsley

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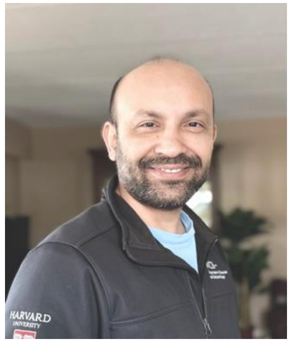

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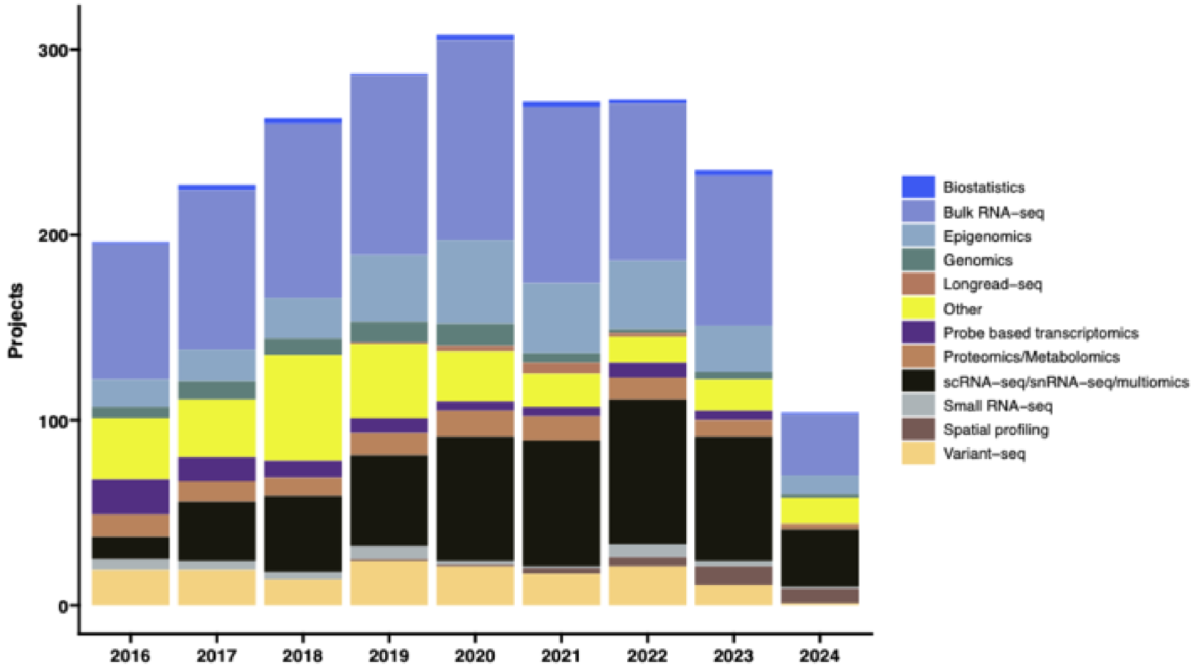
Consulting

- Transcriptomics: Bulk, single cell, small RNA
- Epigenomics: ChIP-seq, CUT&RUN, ATAC-seq, DNA methylation
- Variant discovery: WGS, resequencing, exome-seq and CNV
- Multiomics integration
- Spatial biology
- Experimental design and grant support



https://bioinformatics.sph.harvard.edu/services

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CFAR
HARVARD UNIVERSITY
CENTER FOR AIDS RESEARCH

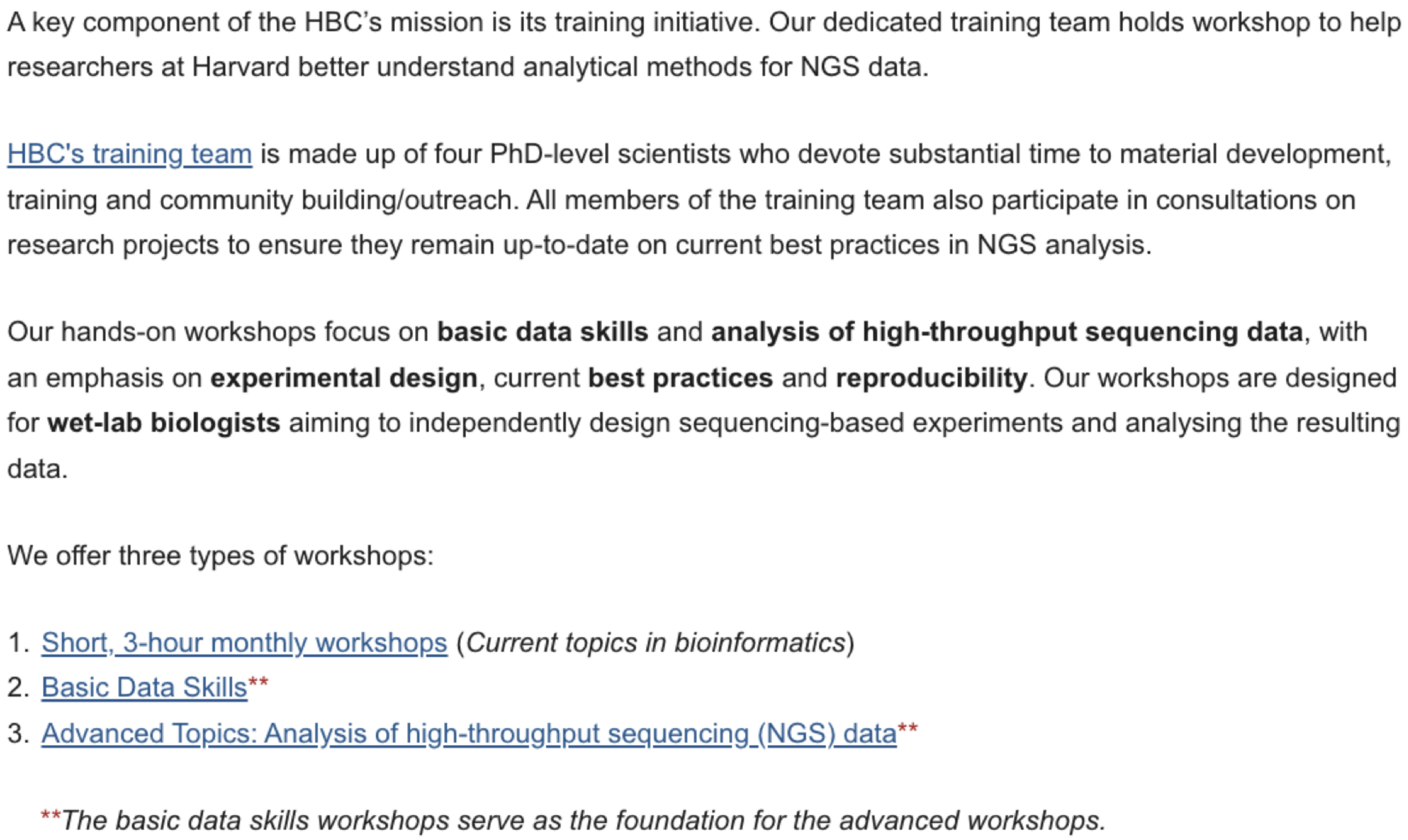
HARVARD
T.H. CHAN
SCHOOL OF PUBLIC HEALTH

NIEHS

HARVARD
CATALYST
THE HARVARD CLINICAL AND TRANSLATIONAL SCIENCE CENTER

HARVARD
MEDICAL SCHOOL

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.

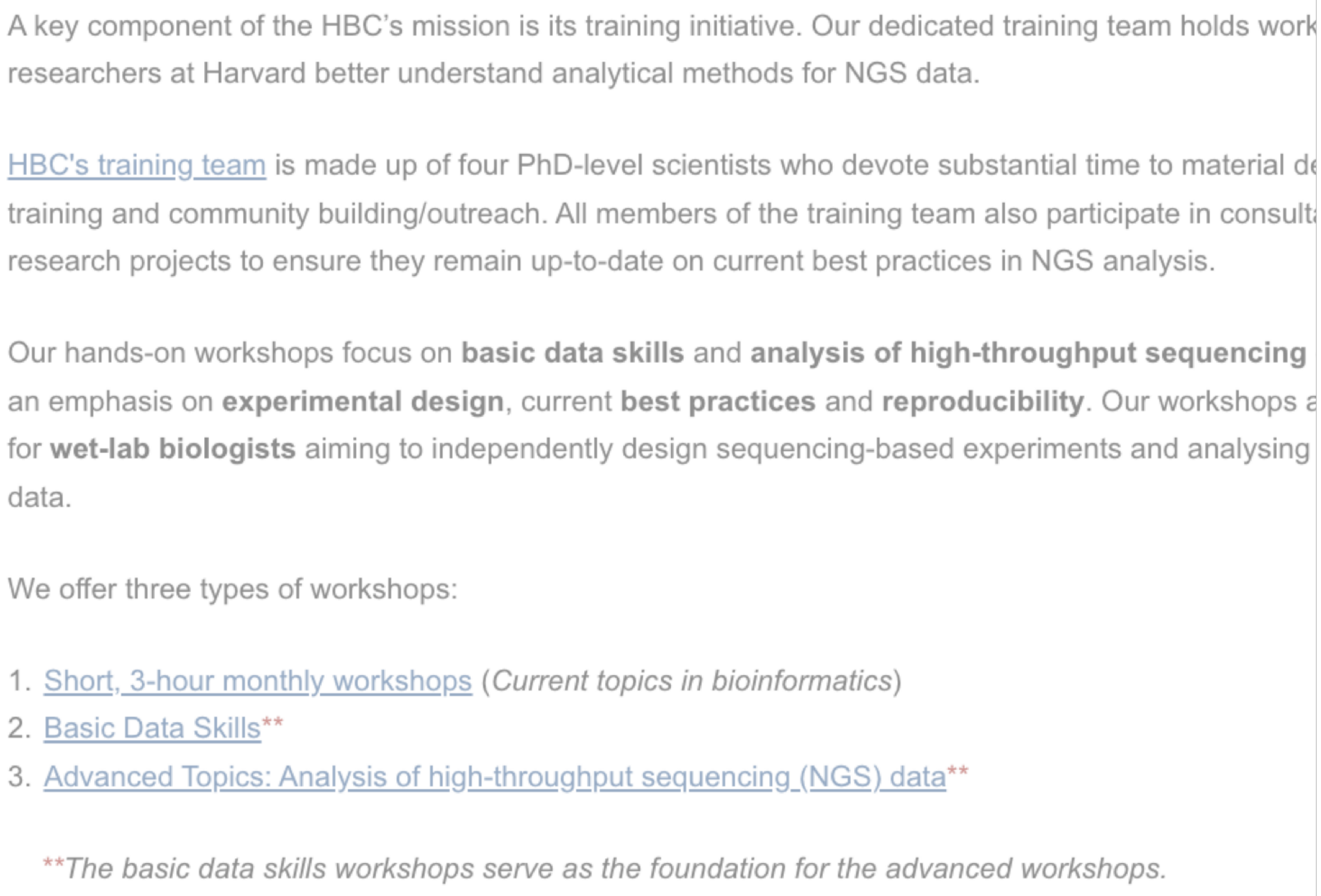
We offer three types of workshops:

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.*

https://bioinformatics.sph.harvard.edu/training

Training



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DF/HCC DANA-FARBER / HARVARD CANCER CENTER

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HARVARD MEDICAL SCHOOL

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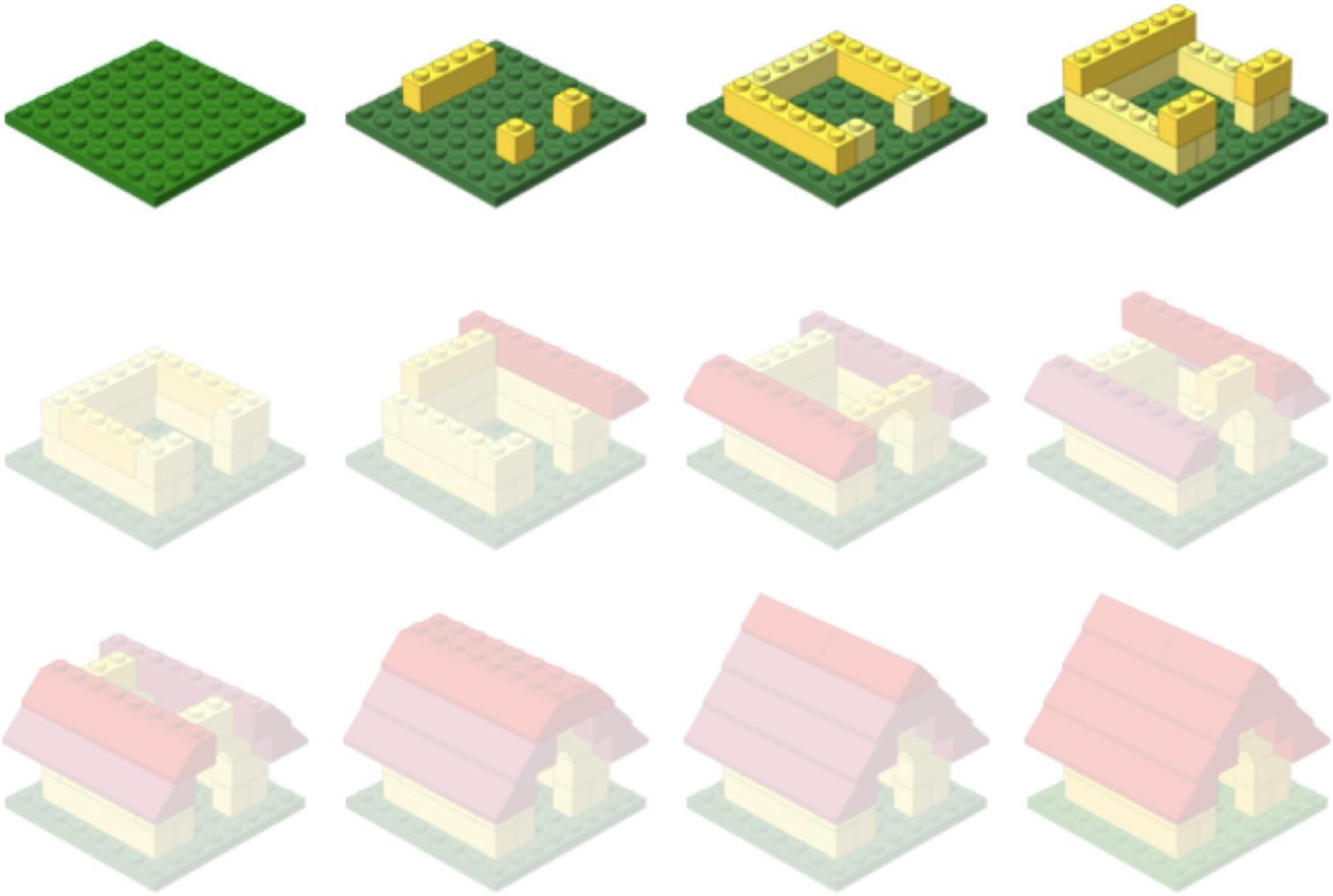
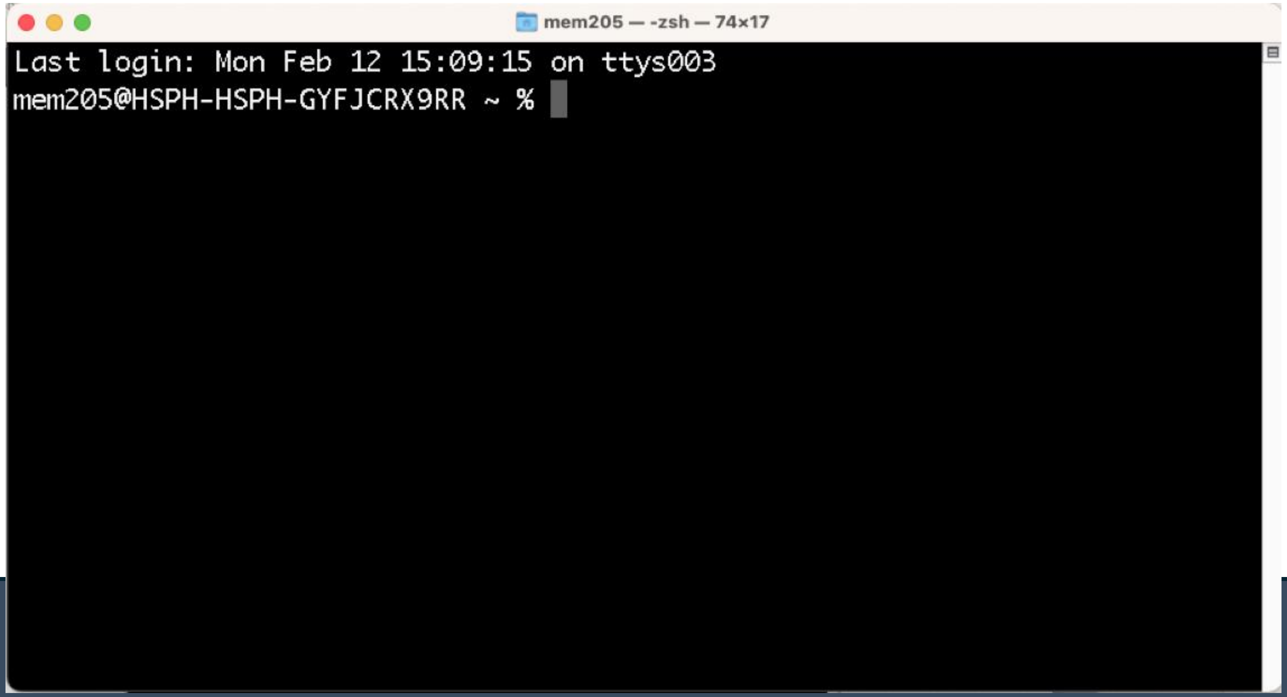
Workshop scope



Learning Bioinformatics

What is shell?



```
Last login: Mon Feb 12 15:09:15 on ttys003
mem205@HSPH-HSPH-GYFJCRX9RR ~ %
```

- Shell is a program that allows users to control Unix/Linux OS with text commands

Terminology

- **Unix/Linux** - The operating systems of High Performance Computers (HPC)

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- **Shell** - A program that allows users to control Unix/Linux OS with text commands
- **Bash** - The most prevalent kind of shell

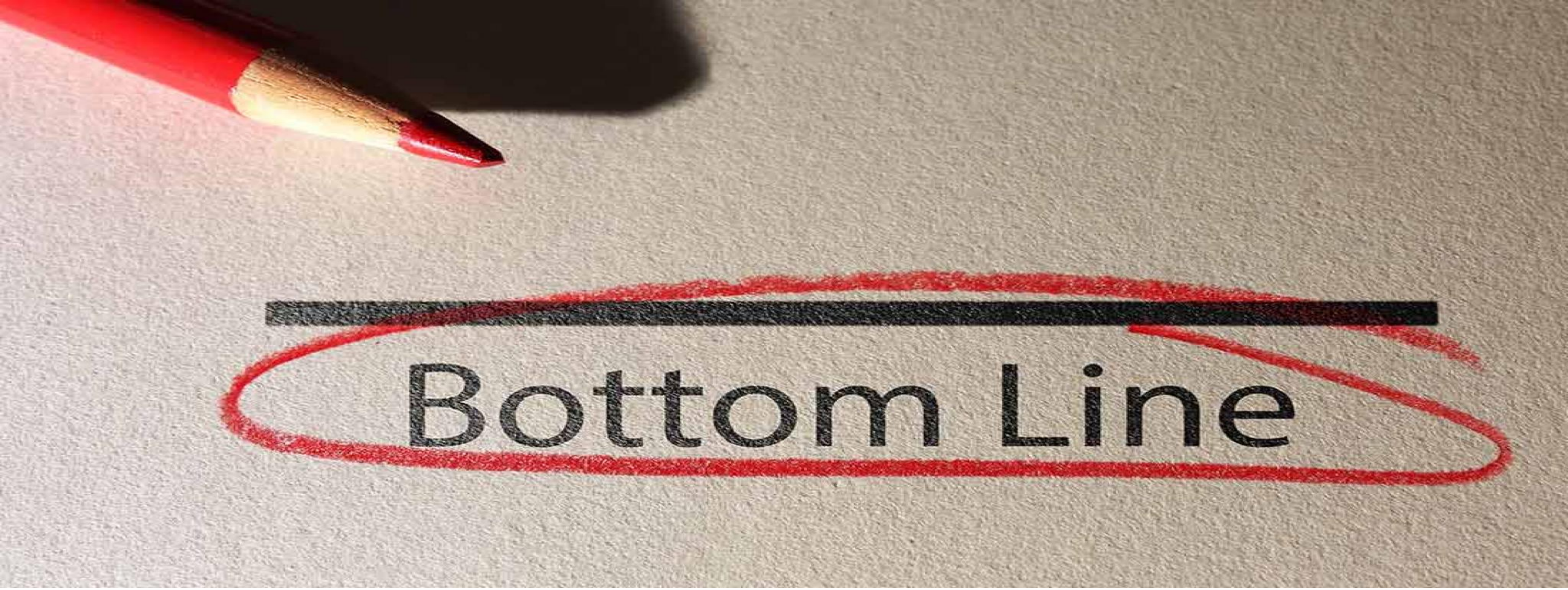


Image source: Balboa Capital Blog

If you plan to process raw high throughput sequencing data yourself, you will need to learn shell.

1. You need more resources than what is available on your laptop

- Sequence data files are LARGE
- Processing these data require increased CPU and memory
- High performance compute clusters have the necessary resources!

2. Many bioinformatics tools are only available as command-line tools

10XGenomics/
cellranger

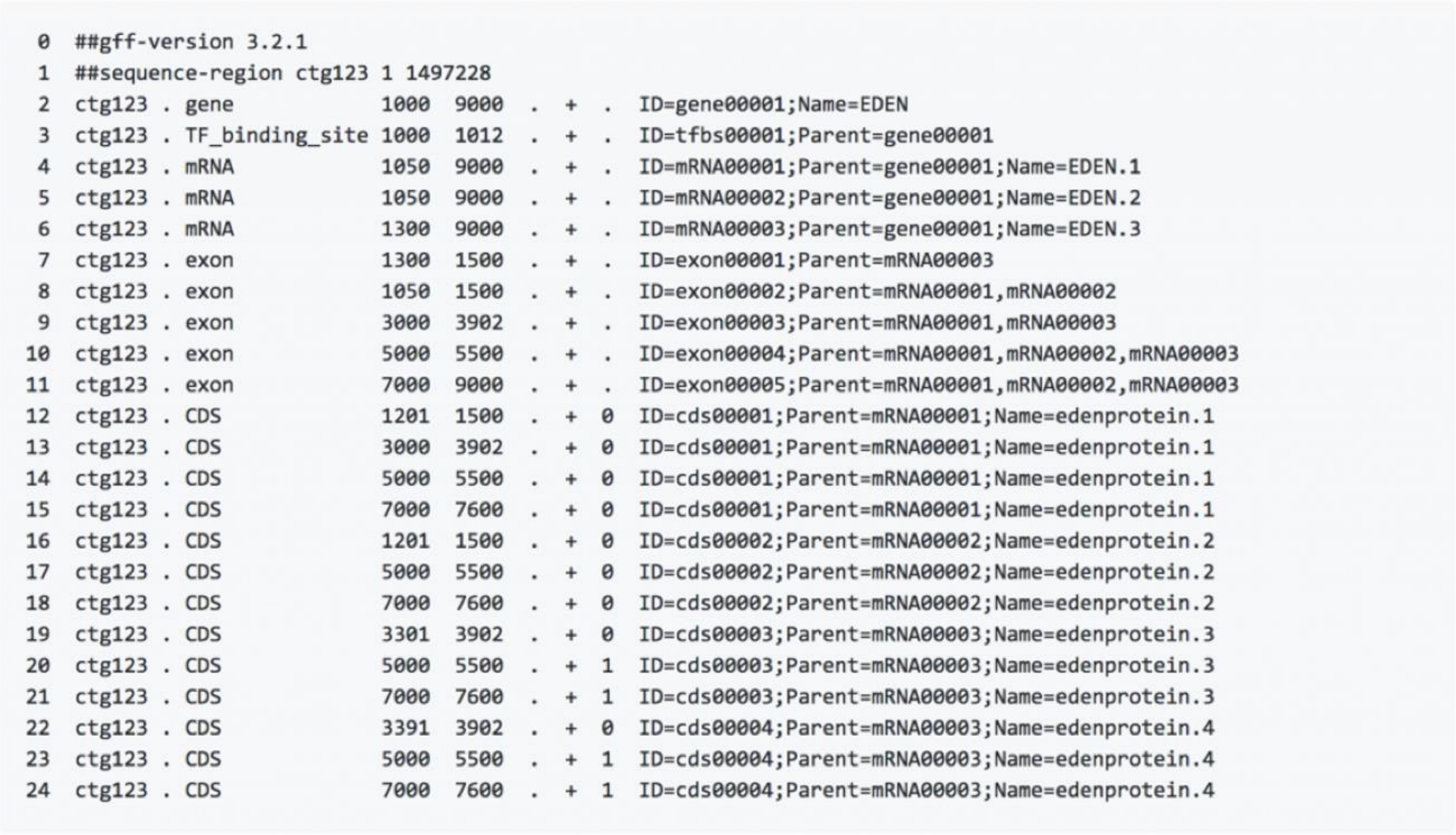
10x Genomics Single Cell Analysis

3. Many genomics filetypes are binary

- Binary files are not human readable
- Binary files need an interpreter

4. There are many useful commands that can help work with enormous data files

- Commands for easily viewing files: less, cat, head, tail



```
##gff-version 3.2.1
##sequence-region ctg123 1 1497228
ctg123 . gene             1000  9000  .  +  .  ID=gene00001;Name=EDEN
ctg123 . TF_binding_site  1000  1012  .  +  .  ID=tfbs00001;Parent=gene00001
ctg123 . mRNA             1050  9000  .  +  .  ID=mRNA00001;Parent=gene00001;Name=EDEN.1
ctg123 . mRNA             1050  9000  .  +  .  ID=mRNA00002;Parent=gene00001;Name=EDEN.2
ctg123 . mRNA             1300  9000  .  +  .  ID=mRNA00003;Parent=gene00001;Name=EDEN.3
ctg123 . exon             1300  1500  .  +  .  ID=exon00001;Parent=mRNA00003
ctg123 . exon             1050  1500  .  +  .  ID=exon00002;Parent=mRNA00001,mRNA00002
ctg123 . exon             3000  3902  .  +  .  ID=exon00003;Parent=mRNA00001,mRNA00003
ctg123 . exon             5000  5500  .  +  .  ID=exon00004;Parent=mRNA00001,mRNA00002,mRNA00003
ctg123 . exon             7000  9000  .  +  .  ID=exon00005;Parent=mRNA00001,mRNA00002,mRNA00003
ctg123 . CDS              1201  1500  .  +  0  ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
ctg123 . CDS              3000  3902  .  +  0  ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
ctg123 . CDS              5000  5500  .  +  0  ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
ctg123 . CDS              7000  7600  .  +  0  ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
ctg123 . CDS              1201  1500  .  +  0  ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
ctg123 . CDS              5000  5500  .  +  0  ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
ctg123 . CDS              7000  7600  .  +  0  ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
ctg123 . CDS              3301  3902  .  +  0  ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
ctg123 . CDS              5000  5500  .  +  1  ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
ctg123 . CDS              7000  7600  .  +  1  ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
ctg123 . CDS              3391  3902  .  +  0  ID=cds00004;Parent=mRNA00003;Name=edenprotein.4
ctg123 . CDS              5000  5500  .  +  1  ID=cds00004;Parent=mRNA00003;Name=edenprotein.4
ctg123 . CDS              7000  7600  .  +  1  ID=cds00004;Parent=mRNA00003;Name=edenprotein.4
```

5. Automation is the name of the game

- Launch many jobs with one command
- Code is used and reused to iterate tasks over multiple files
- Parallelization to complete tasks using multiple cores and increase speed!

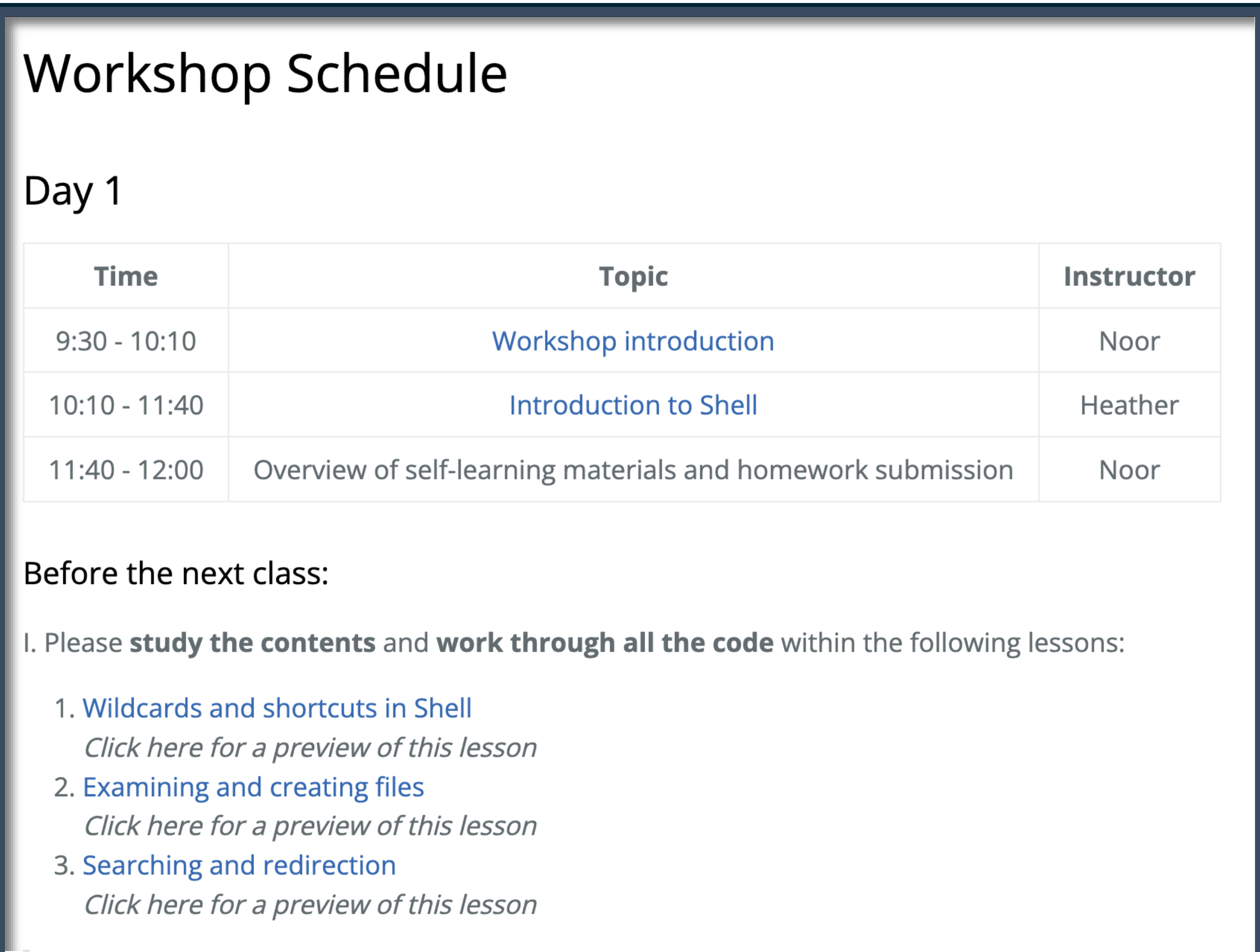
This could be you watching your analysis run!

Learning Objectives

- Navigate around the command line interface (bash/shell)
- Create and manipulate text files
- Submit jobs to a high-performance computing cluster

Logistics

Course schedule



Workshop Schedule

Day 1

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

Before the next class:

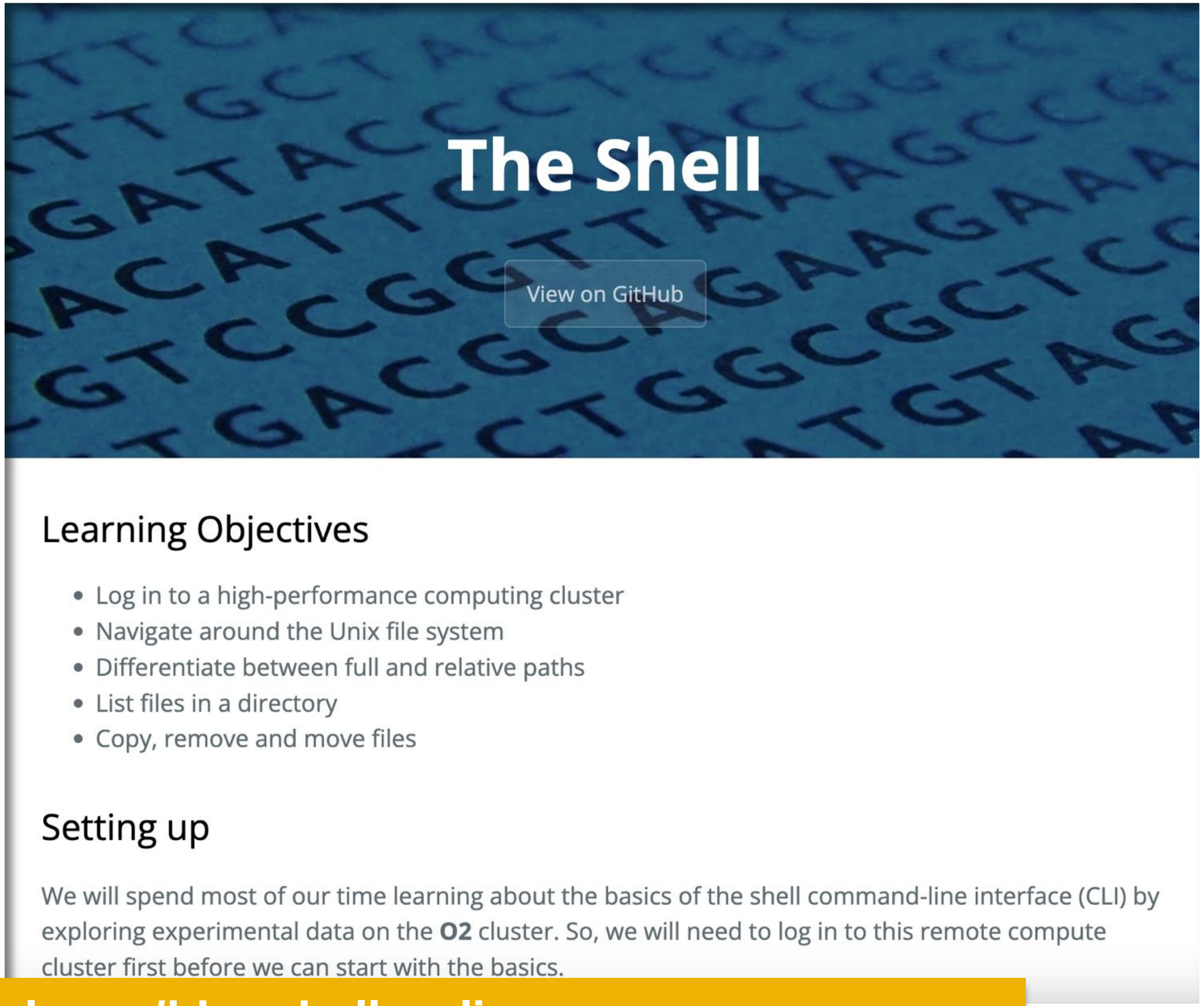
I. Please **study the contents** and **work through all the code** within the following lessons:

1. Wildcards and shortcuts in Shell
   Click here for a preview of this lesson
2. Examining and creating files
   Click here for a preview of this lesson
3. Searching and redirection
   Click here for a preview of this lesson

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

Course materials

- We continuously update our materials to reflect changes in the field/software



Learning Objectives

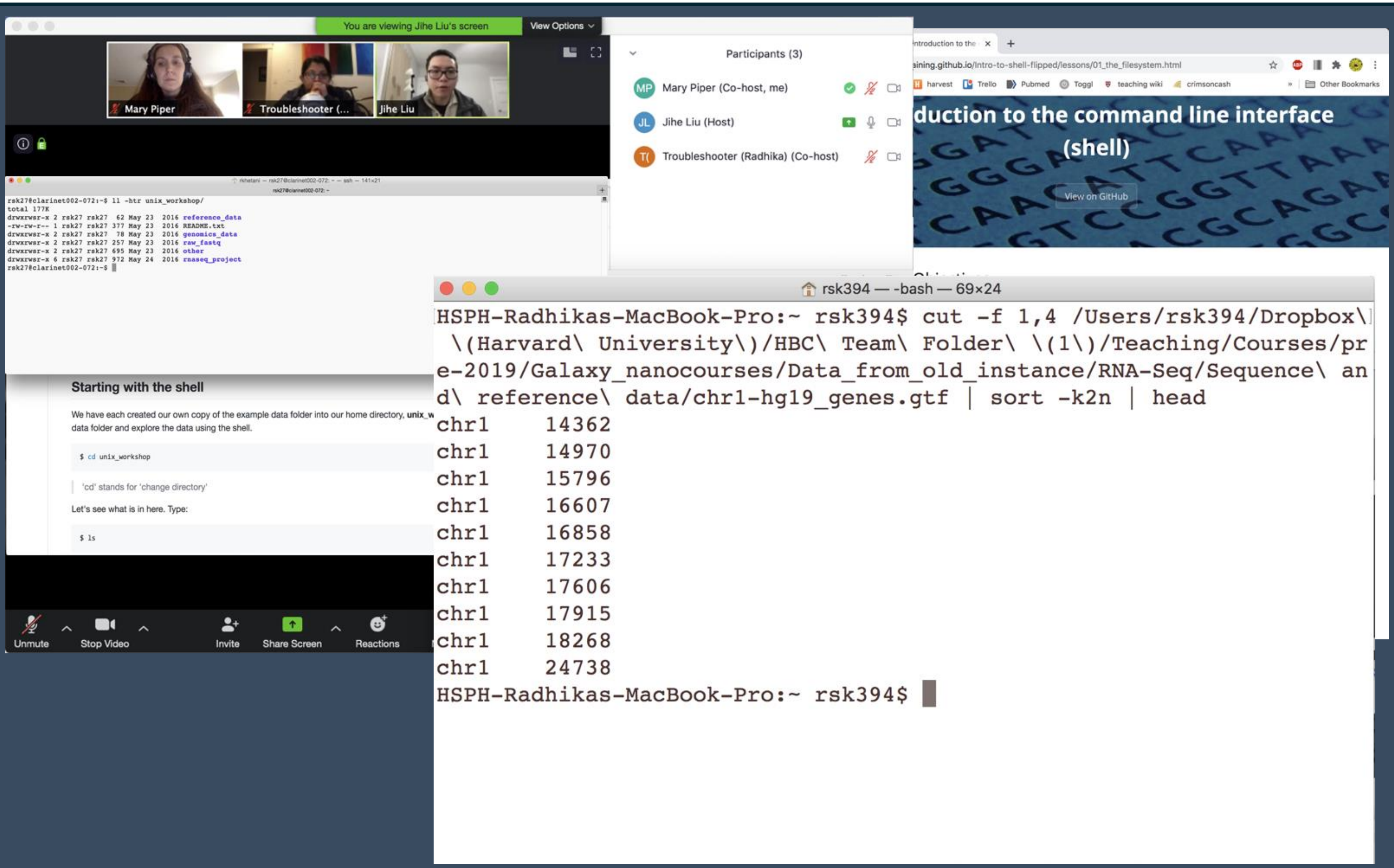
- Log in to a high-performance computing cluster
- Navigate around the Unix file system
- Differentiate between full and relative paths
- List files in a directory
- Copy, remove and move files

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.

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

Single Screen & 3 Windows



```
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:~$
```

Starting with the shell

We have each created our own copy of the example data folder into our home directory, **unix_w** data folder and explore the data using the shell.

```
$ cd unix_workshop
```

> 'cd' stands for 'change directory'

Let's see what is in here. Type:

```
$ ls
```

```
HSPH-Radhikas-MacBook-Pro:~ rsk394$ cut -f 1,4 /Users/rsk394/Dropbox\
 \(Harvard\ University\)/HBC\ Team\ Folder\ \(1\)/Teaching/Courses/pr
e-2019/Galaxy_nanocourses/Data_from_old_instance/RNA-Seq/Sequence\ an
d\ reference\ data/chr1-hg19_genes.gtf | sort -k2n | head
chr1    14362
chr1    14970
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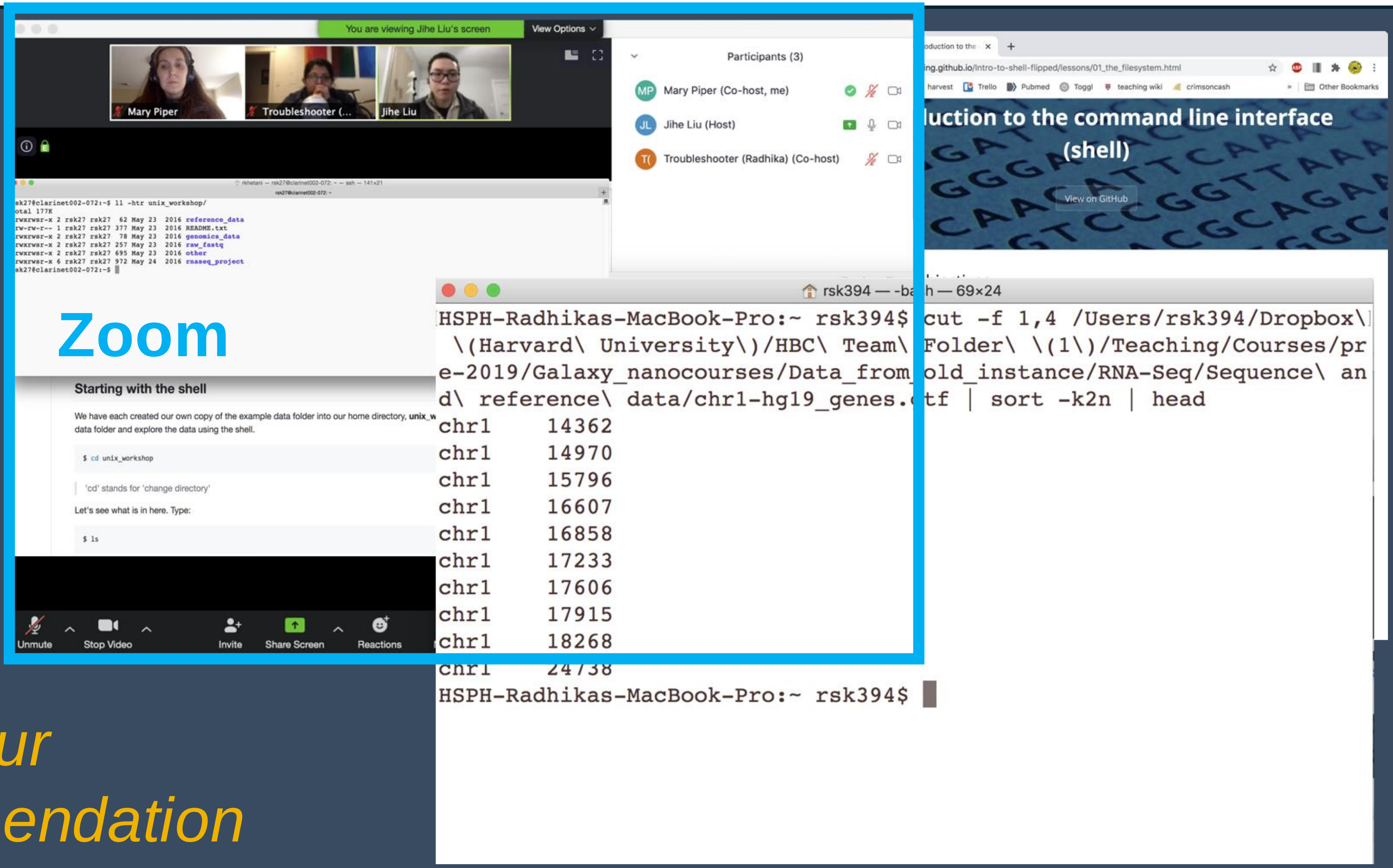
Single Screen & 3 Windows



Zoom

```
sk27@clarinet002-072:~$ ll -htr unix_workshop/
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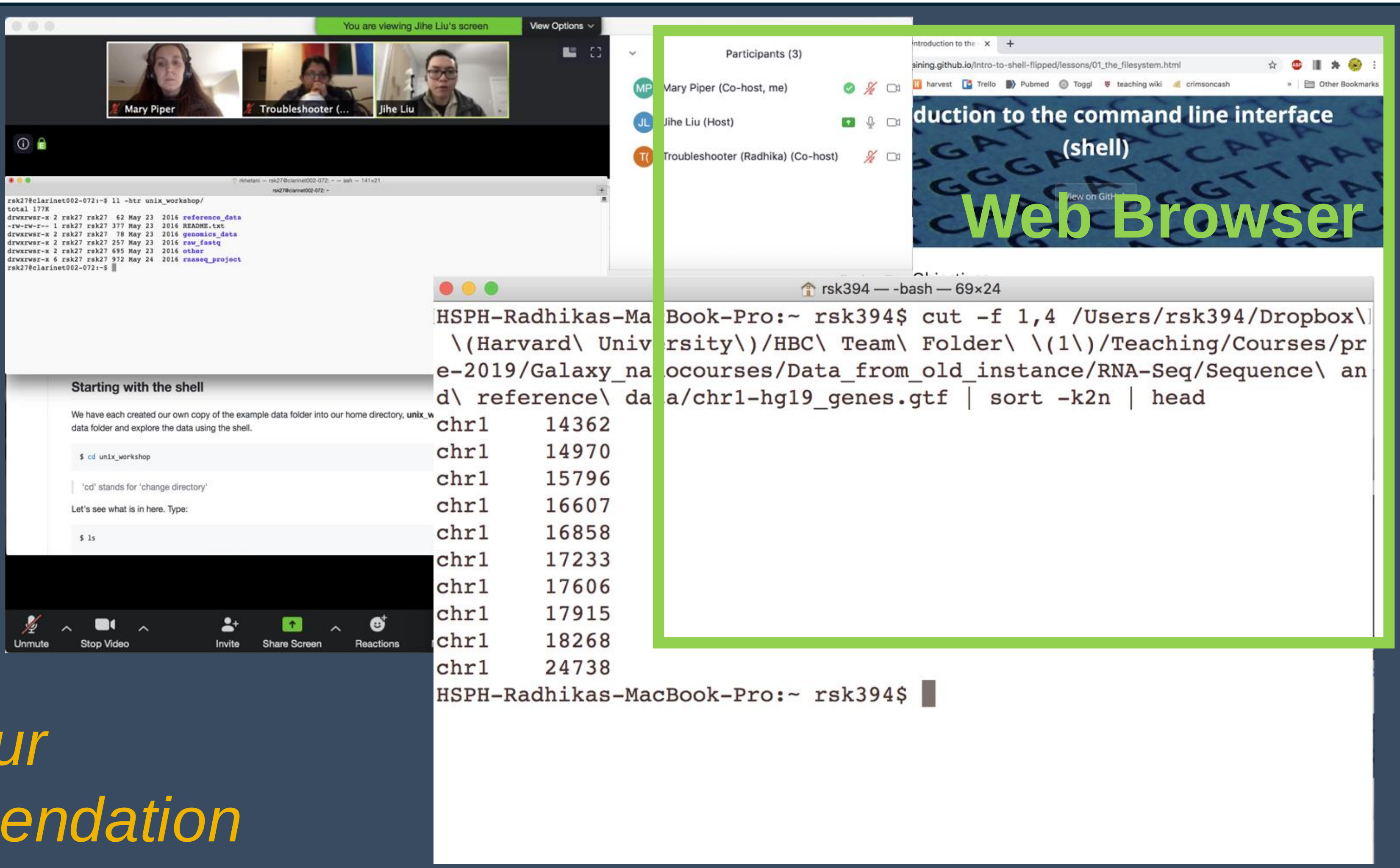
Our Recommendation

Single Screen & 3 Windows



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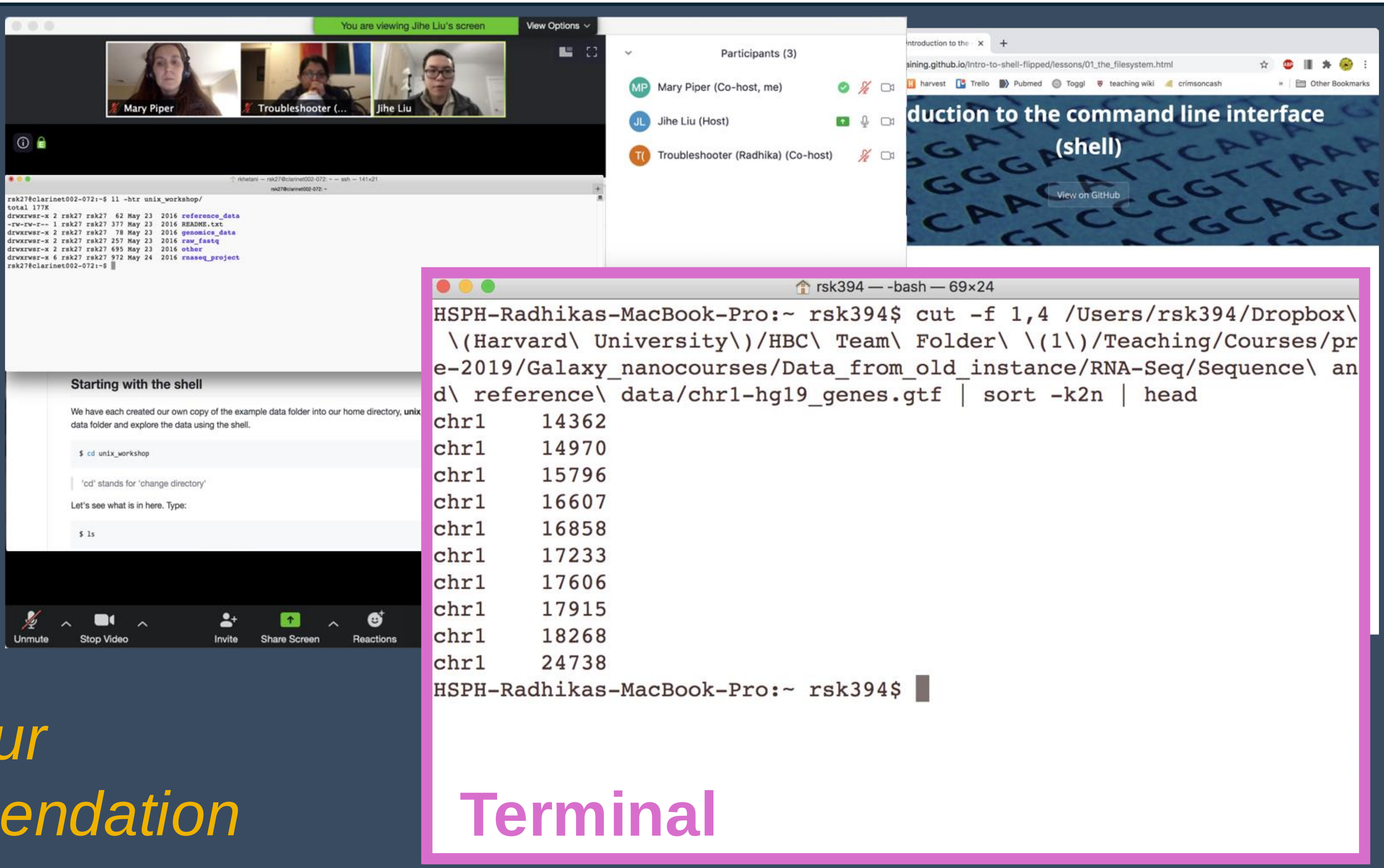
```

Web Browser

Our Recommendation

Single Screen & 3 Windows



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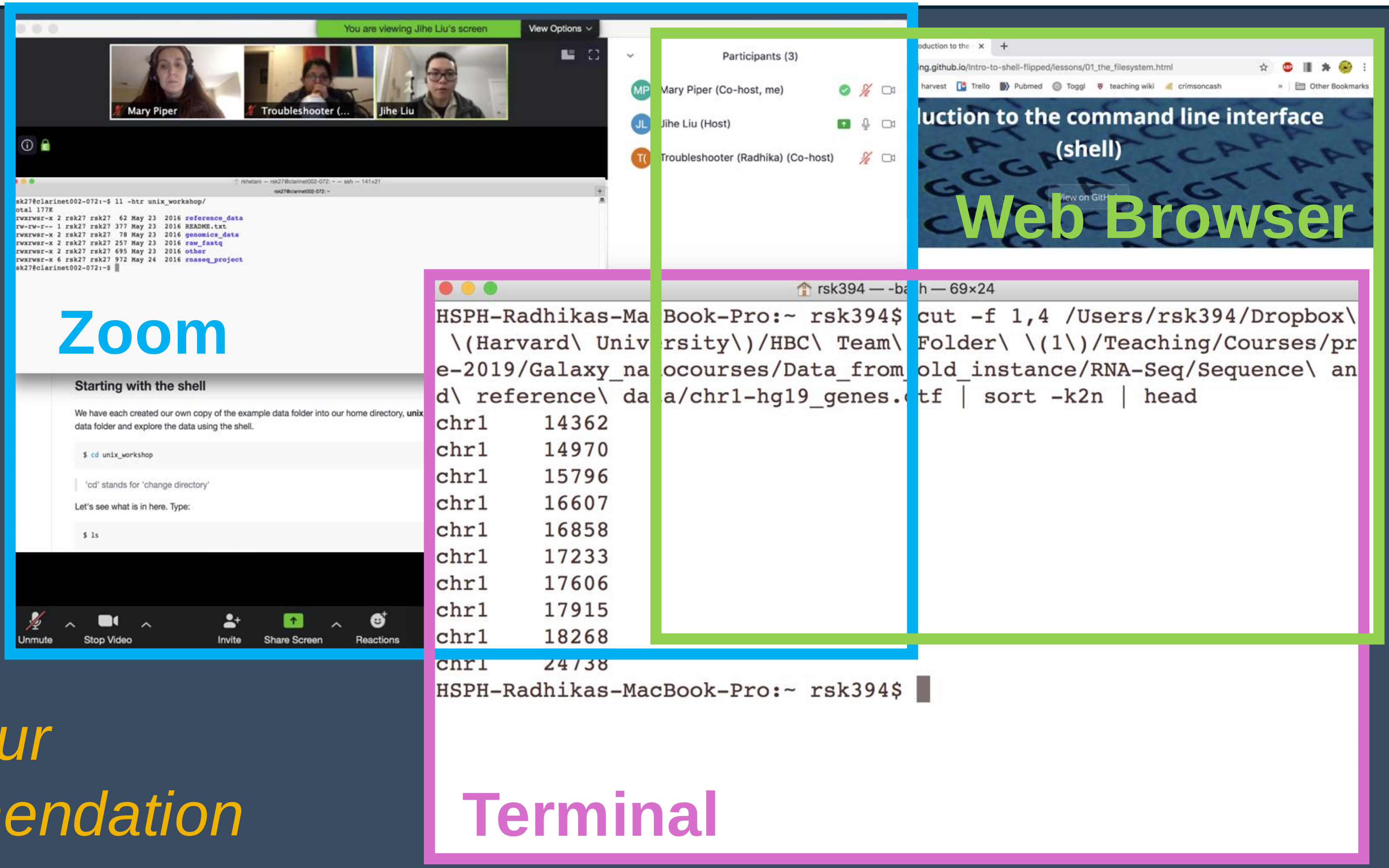
Terminal

Our Recommendation

Single Screen & 3 Windows



rkhetani — rsk27@clarinet002-072: ~ — ssh — 141×21

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```

rsk394 — -bash — 69×24

```
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HSPH-Radhikas-MacBook-Pro:~ rsk394$
```

Our Recommendation

Course participation

- 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!**

Course participation

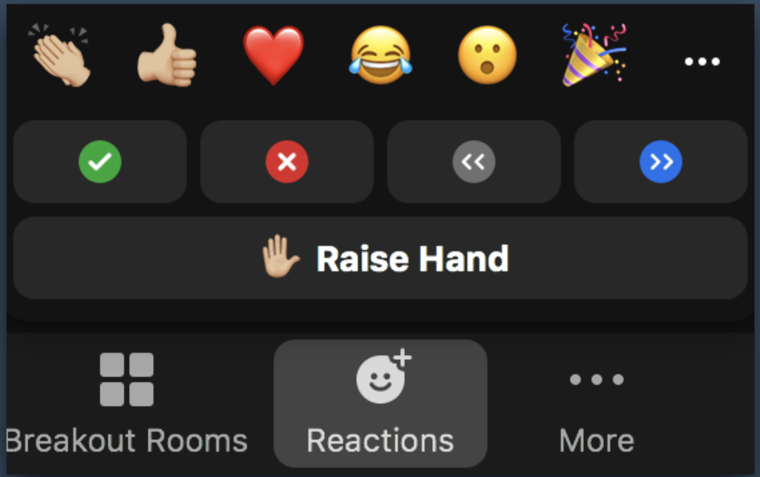
- At-home lessons and exercises after each session
- Cover material not previously discussed
- Provides us feedback to help pace the course appropriately
- 3-5 hours to complete
- Homework load is heavier in the beginning of this workshop series and tapers off

Using AI for Assignments

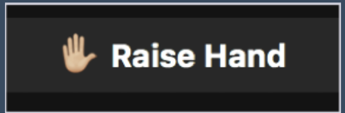
- Do
  - Try to resolve error messages with it
  - Test code written by AI on a dataset where you have expected results
  - Take the time to review the generated code line-by-line
- Don’t
  - Implement it in replacement to learning
  - Write code that you don’t understand
  - Assume the output from an AI process is correct

Odds & Ends

- Quit/minimize all applications that are not required for class
- Are you all set?
  - ✓ = "agree", "I'm all set"
  - ✗ = "disagree", "I need help"



Odds & Ends

- Questions for the presenter?
  - Post the question in the Chat window OR
  -  when the presenter asks for questions
  - Let the Troubleshooter know

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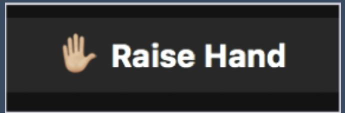
  - 

when the presenter asks for questions
  - Let the Troubleshooter 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

Contact Us

HBC
Harvard Chan Bioinformatics Core

- *HBC training team:* hbctraining@hsph.harvard.edu
- *HBC consulting:* bioinformatics@hsph.harvard.edu
- *O2 (HMS-RC):* rchelp@hms.harvard.edu