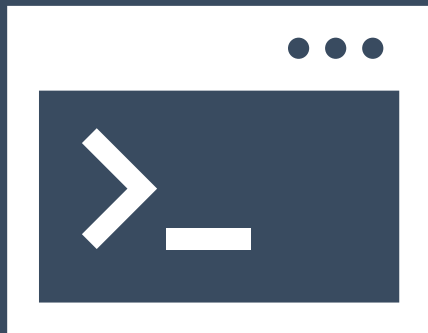


Shell for Bioinformatics

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



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



Emma Berdan



James Billingsley



Zhu Zhuo



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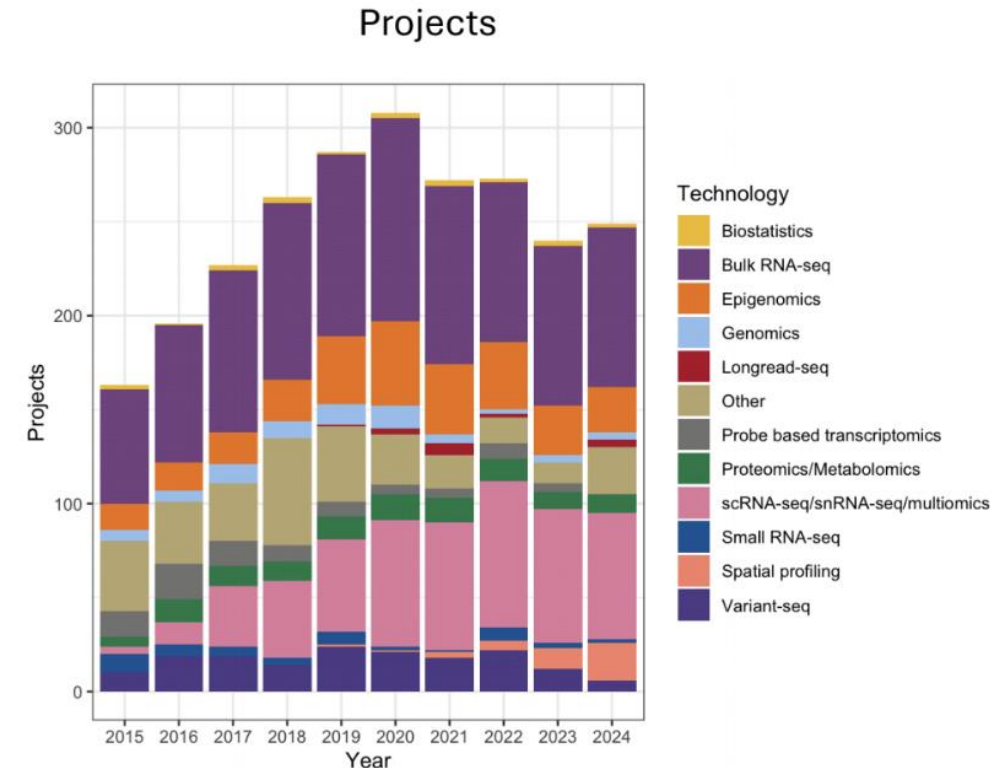
Zhu Zhuo



Maria Simoneau

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



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SCHOOL OF PUBLIC HEALTH

NIEHS



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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](#)**
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***The basic data skills workshops serve as the foundation for the advanced workshops.*

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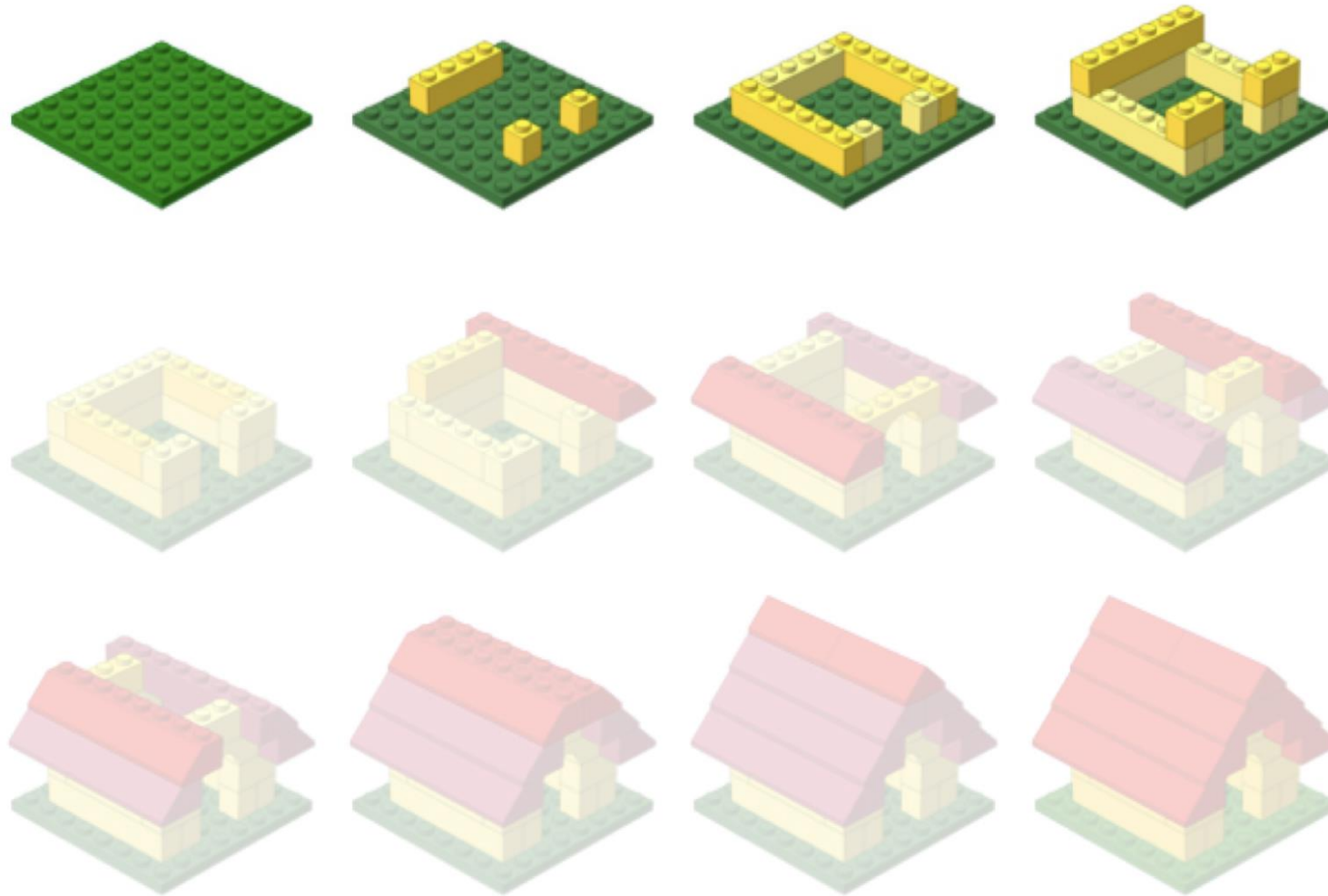


THE HARVARD CLINICAL
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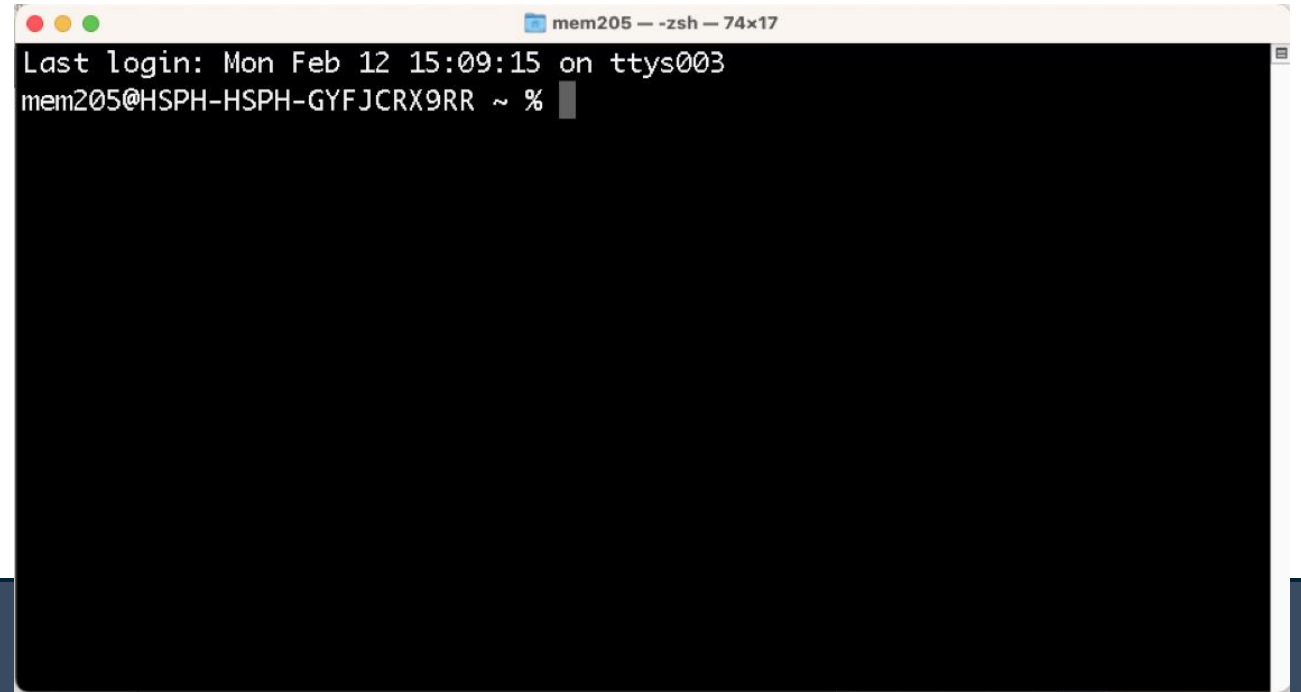
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Workshop scope



Learning Bioinformatics

What is shell?



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

Terminology

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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



Bottom Line

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

10x
GENOMICS™

staraligner



SAMtools



3. Many genomics filetypes are binary



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

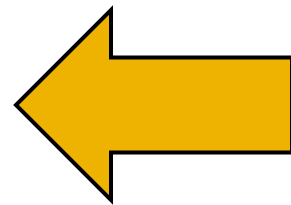
4. There are many useful commands that can help work with enormous data files

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

```
0 ##gff-version 3.2.1
1 ##sequence-region ctg123 1 1497228
2 ctg123 . gene 1000 9000 . + . ID=gene00001;Name=EDEN
3 ctg123 . TF_binding_site 1000 1012 . + . ID=tfbs00001;Parent=gene00001
4 ctg123 . mRNA 1050 9000 . + . ID=mRNA00001;Parent=gene00001;Name=EDEN.1
5 ctg123 . mRNA 1050 9000 . + . ID=mRNA00002;Parent=gene00001;Name=EDEN.2
6 ctg123 . mRNA 1300 9000 . + . ID=mRNA00003;Parent=gene00001;Name=EDEN.3
7 ctg123 . exon 1300 1500 . + . ID=exon00001;Parent=mRNA00003
8 ctg123 . exon 1050 1500 . + . ID=exon00002;Parent=mRNA00001,mRNA00002
9 ctg123 . exon 3000 3902 . + . ID=exon00003;Parent=mRNA00001,mRNA00003
10 ctg123 . exon 5000 5500 . + . ID=exon00004;Parent=mRNA00001,mRNA00002,mRNA00003
11 ctg123 . exon 7000 9000 . + . ID=exon00005;Parent=mRNA00001,mRNA00002,mRNA00003
12 ctg123 . CDS 1201 1500 . + 0 ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
13 ctg123 . CDS 3000 3902 . + 0 ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
14 ctg123 . CDS 5000 5500 . + 0 ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
15 ctg123 . CDS 7000 7600 . + 0 ID=cds00001;Parent=mRNA00001;Name=edenprotein.1
16 ctg123 . CDS 1201 1500 . + 0 ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
17 ctg123 . CDS 5000 5500 . + 0 ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
18 ctg123 . CDS 7000 7600 . + 0 ID=cds00002;Parent=mRNA00002;Name=edenprotein.2
19 ctg123 . CDS 3301 3902 . + 0 ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
20 ctg123 . CDS 5000 5500 . + 1 ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
21 ctg123 . CDS 7000 7600 . + 1 ID=cds00003;Parent=mRNA00003;Name=edenprotein.3
22 ctg123 . CDS 3391 3902 . + 0 ID=cds00004;Parent=mRNA00003;Name=edenprotein.4
23 ctg123 . CDS 5000 5500 . + 1 ID=cds00004;Parent=mRNA00003;Name=edenprotein.4
24 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-materials>

Course materials

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



The Shell

[View on GitHub](#)

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-materials>

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
- ❖ Name tags
- ❖ Post-its
 - ❖  green - I am all set
 - ❖  red - I need time/help
- ❖ Quit/minimize all applications that are not required for class
- ❖ Phones on vibrate/silent
- ❖ Bathrooms

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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