

# **RGGS Comparative Genomics 2 – Informatics (Session 1)**

Jose Barba

Gerstner Scholar in Bioinformatics & Computational Biology

## **Session 1 outline**

- **Personal backgrounds and research interests**
- **Course overview**
- **Reproducibility and organization in computational biology**
- **Introduction to Unix and Unix-like operating systems**
- **Basic navigation in the terminal**

## Course overview

- This project-based course introduces computational tools for interpreting molecular sequencing data, focusing on genome and transcriptome assembly, comparative analyses (both de novo and reference-based), and phylogenomic inference.
- The course emphasizes documentation, reproducibility, and computational proficiency.
- Students will address experimental questions starting from raw data, relevant to their research, with the goal of laying a foundation for a publishable final product.
- [https://github.com/josebarbamontoya/rggs\\_comparative\\_genomics\\_2](https://github.com/josebarbamontoya/rggs_comparative_genomics_2)

# Reproducibility and organization in computational biology

- **Reproducibility**

- Documentation: Maintain comprehensive documentation for every step of the analysis, including code, parameters, and software versions. Tools like **GitHub**, **Jupyter Notebooks**, or **RMarkdown** can integrate code with narrative text, making it easier to follow the analysis.
- Version control: Use version control systems like **Git** to track changes in scripts and collaborate with others. This ensures that any modification can be traced back and the exact state of the code at any point in time can be recovered.

# Reproducibility and organization in computational biology

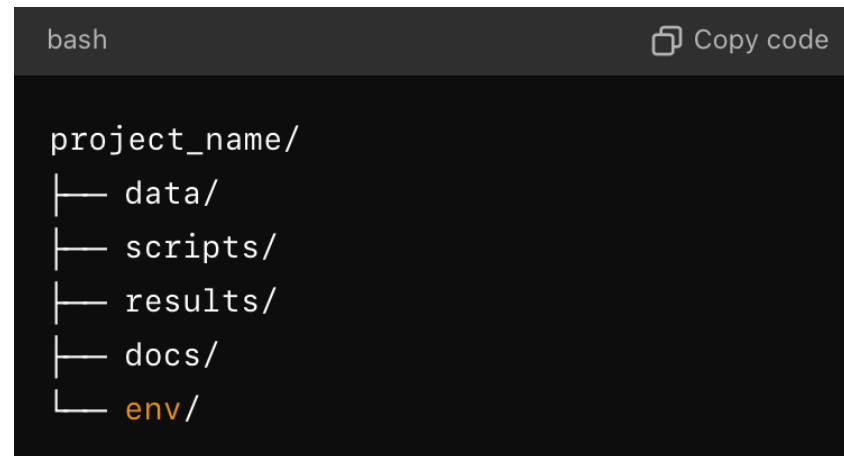
- **Reproducibility**

- Containerization: Employ containerization tools such as **Docker** or **Singularity** to encapsulate the computational environment. This includes software, libraries, and dependencies, ensuring that the analysis can be replicated on different systems without compatibility issues.
- Automated workflows: Tools like **Snakemake** or **Nextflow** help automate and standardize workflows. They ensure that the entire analysis pipeline can be executed in a controlled manner, reducing human error and making the process more reproducible.
- Data management: Organize raw and processed data systematically, using consistent naming conventions and directory structures (e.g., **Globus**). Data should be stored with appropriate metadata, making it easier to understand and reuse.

# Reproducibility and organization in computational biology

- **Organization**

- Project Structure: Adopt a standardized directory structure for projects. A common approach is to separate raw data, processed data, scripts, and results into distinct directories. For example:

A terminal window with a dark background. The title bar shows 'bash' on the left and a 'Copy code' button on the right. The terminal content shows a directory tree for 'project\_name/'. The tree has five subdirectories: 'data/', 'scripts/', 'results/', 'docs/', and 'env/'. The 'env/' directory is highlighted in orange.

```
bash                                                                    Copy code

project_name/
├─ data/
├─ scripts/
├─ results/
├─ docs/
└─ env/
```

- Naming Conventions: Use clear and consistent naming conventions for files, variables, and functions. This makes it easier to understand the purpose of each component in your project.

# Reproducibility and organization in computational biology

- **Organization**

- Modular Code: Write modular code that separates different parts of the analysis into functions or classes. This not only makes the code more readable but also reusable for other projects.
- Backups and Data Integrity: Regularly back up your data and use versioned storage to ensure data integrity. This is especially important for long-term projects where data may be accessed or reused after extended periods.
- Collaboration: Foster a collaborative environment by sharing code, data, and documentation with colleagues. Use platforms like **GitHub** or **GitLab** to collaborate efficiently on code and data.

# Introduction to Unix and Unix-like operating systems

- **Unix is a multiuser, multitasking OS originally developed in the 1960s-70s at AT&T's Bell Labs**
- **Its key features include:**
  - Multitasking: Unix can execute multiple processes simultaneously.
  - Multiuser: Multiple users can access the system concurrently without interfering with each other.
  - Portability: Unix was designed to be portable to different machines and hardware configurations.
  - Security and permissions: It has a strong security model with user permissions and file access controls.
  - Text-based interface: Unix uses a command-line interface (terminal) for user interactions, which is efficient for many tasks.



# Introduction to Unix and Unix-like operating systems

- **Unix-like operating systems behave similarly to Unix but are not directly derived from the original Unix source code**
  - macOS: Apple's operating system for Mac computers, which is built on a Unix-based foundation.
  - Linux: A widely used Unix-like system with various distributions such as Ubuntu, Fedora, and Debian. Known for its open-source nature and flexibility.

# Introduction to Unix and Unix-like operating systems

- Key Concepts

- Filesystem hierarchy: Unix-like systems organize files and directories in a hierarchical structure, starting from the root directory `/`, home directory `~`.
- Shell: The command-line interface where users can execute commands. Common shells include `bash`, `sh`, and `zsh`.
- Commands: Basic commands include `ls` (list directory contents), `cd` (change directory), `cp` (copy files), `mv` (move files), and `rm` (remove files).
- Processes: Unix-like systems handle multiple processes, and tools like `ps` and `top`, `htop` help monitor them.
- Permissions: Files and directories have permissions (read, write, execute) that control access for the owner, group, and others like `chmod`.

# Basic navigation in the terminal

- Using the command line interface involves executing commands to navigate directories, view/edit/create files, among other tasks

|   |  |
|---|--|
| Archiving and Compression   | File Space and Disk Usage  |
| <b>tar</b> - Archive files into a tarball (or extract them)       | <b>df</b> - Display disk space usage                                   |
| <b>zip/unzip</b> - Compress and extract files in zip format       | <b>du</b> - Estimate file space usage                                  |
| File and Directory Operations                                     | Networking and Remote Operations                                       |
| <b>cd</b> - Change directory                                      | <b>scp</b> - Secure copy, used for transferring files between hosts    |
| <b>ls</b> - List files and directories                            | <b>sftp</b> - Securely transfer files between computers over a network |
| <b>pwd</b> - Print working directory                              | <b>ssh</b> - Secure shell, used for logging into a remote machine      |
| <b>mkdir</b> - Make directory                                     | <b>wget</b> - Download and transfer data from remote servers           |
| <b>mv</b> - Move or rename files or directories                   | Process Management   |
| <b>cp</b> - Copy files or directories                             | <b>ps</b> - Display information about running processes                |
| <b>rm</b> - Remove files or directories                           | <b>kill</b> - Terminate processes by ID                                |
| <b>rmdir</b> - Remove directory                                   | Terminal Utilities   |
| <b>touch</b> - Create an empty file or update a file's timestamp  | <b>clear</b> - Clear the terminal screen                               |
| <b>cat</b> - Concatenate and display file contents                | <b>man</b> - Display manual for a command                              |
| File and Directory Search   | <b>help</b> - Show information about built-in shell commands           |
| <b>find</b> - Search for files and directories within a hierarchy | Text Processing  |
| <b>grep</b> - Search for patterns within text                     | <b>awk</b> - Pattern scanning and processing language                  |
| File Permissions and Ownership                                    | <b>echo</b> - Display a line of text or variables                      |
| <b>chmod</b> - Change file permissions                            | <b>nano</b> - Text editor  |
| <b>chown</b> - Change file owner and group                        | <b>vi</b> - Text editor  |

# Basic navigation in the terminal

- **Some links for useful tutorial on basic navigation commands**
  - Unix basic commands: <https://sandbox.bio/tutorials/terminal-basics/>
  - Unix shell: <https://swcarpentry.github.io/shell-novice/01-intro.html>
  - Data exploration with awk: <https://sandbox.bio/tutorials/awk-intro>