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Bioinformatics 101 – Lecture 2

Introduction to command line

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ICBR Bioinformatics Core

Computing environments

- Standalone application – for local, interactive use;
- Command-line – local or remote, interactive use;
- Cluster oriented: remote, not interactive, highly parallelizable.



Command-line basics

- Commands are typed at a *prompt*. The program that reads your commands and executes them is the *shell*.
- Interaction style originated in the 70s, with the first visual terminals (connections were *slow...*).
- A command consists of a program name followed by *options* and/or *arguments*.
- Syntax may be obscure and inconsistent (but efficient!).



Command-line basics

- Example: to view the names of files in the current directory, use the “ls” command (short for “list”)

ls plain list

ls -l long format (size, permissions, etc)

ls -l -t sort newest to oldest

ls -l -t -r reverse sort (oldest to newest)

ls -lrt options can be combined (in this case)

- Command names and options are case sensitive!



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File System

- Unix systems are centered on the *file system*. Huge tree of directories and subdirectories containing all files.
- *Everything* is a file. Unix provides *a lot* of commands to operate on files.
- File extensions are not necessary, and are not recognized by the system (but may still be useful).
- Please do *not* put spaces in filenames!

Permissions

- Different privileges and permissions apply to different areas of the filesystem.
- Every file has an *owner* and a *group*. A user may belong to more than one group.
- Permissions specify read, write, and execute privileges for the owner, the group, everyone else. Example:
 - ```
ls -l qmonitor
-rwxr-x--- 1 ariva riva 68 Sep 15 2015 qmonitor
```



# Filesystem commands

- `pwd`      where are we?
- `cd`        move around the filesystem
- `ls`        view contents of directory
- `mkdir`    create new directory
- `chmod`    change file permissions
- `cp`        copy files
- `mv`        move files
- `rm`        delete files (use with caution!)
- `rmdir`    remove (empty) directory

Every user has a *home* directory. “`cd`” with no arguments takes you back there.



# Working with text files

- Plain text files are the “lingua franca” of Unix systems.
- Most files are structured, either in a simple way (rows and columns, comma- or tab-delimited) or complex (e.g. XML, JSON).
- Text files can be created manually with an editor (e.g. nano, vi) or generated by other programs.



# Working with text files

## Viewing files:

- `file` show type of file
- `cat` display contents of a file
- `more` display contents better
- `less` display contents even better
- `head` display top (10) lines
- `tail` display last (10) lines



# Working with text files

Finding information on or in files:

- `wc`      count rows / words / chars in file
- `grep`    print rows containing text / pattern
- `cut`      select columns from delimited file
- `diff`     display differences between two files
- `find`     search for files matching tests (file name, size, modification date, etc).



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# Working with text files

## Other file operations...

- `sort` sort file lines (alphabetically, numerically, based on one or more fields)
- `uniq` detect (and remove / print / count) duplicate lines
- `split` split a file into chunks
- `paste` join files side by side
- `shuf` shuffle file lines

More advanced processing can be accomplished with `sed`, `awk`.



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# Other useful commands

- `echo` display message
- `screen` run multiple terminals over one connection
- `watch` execute a command periodically
- `man` get help on a command
- `gzip` compress files
- `gunzip` uncompress files
- `zcat/zmore/zgrep` view / search compressed files
- `zip` create zip archive
- `time` measure command execution time
- `wget` download file given URL (http, ftp, etc)



# Scripting

The real power of unix commands lies in *scripting*:

- Sequences of commands can be saved to a file and repeated easily.
- Shell syntax supports variables and control structures (conditionals, loops, etc). Simple but powerful.
- Basic Unix philosophy: simple building blocks can be easily combined to create new complex tools.



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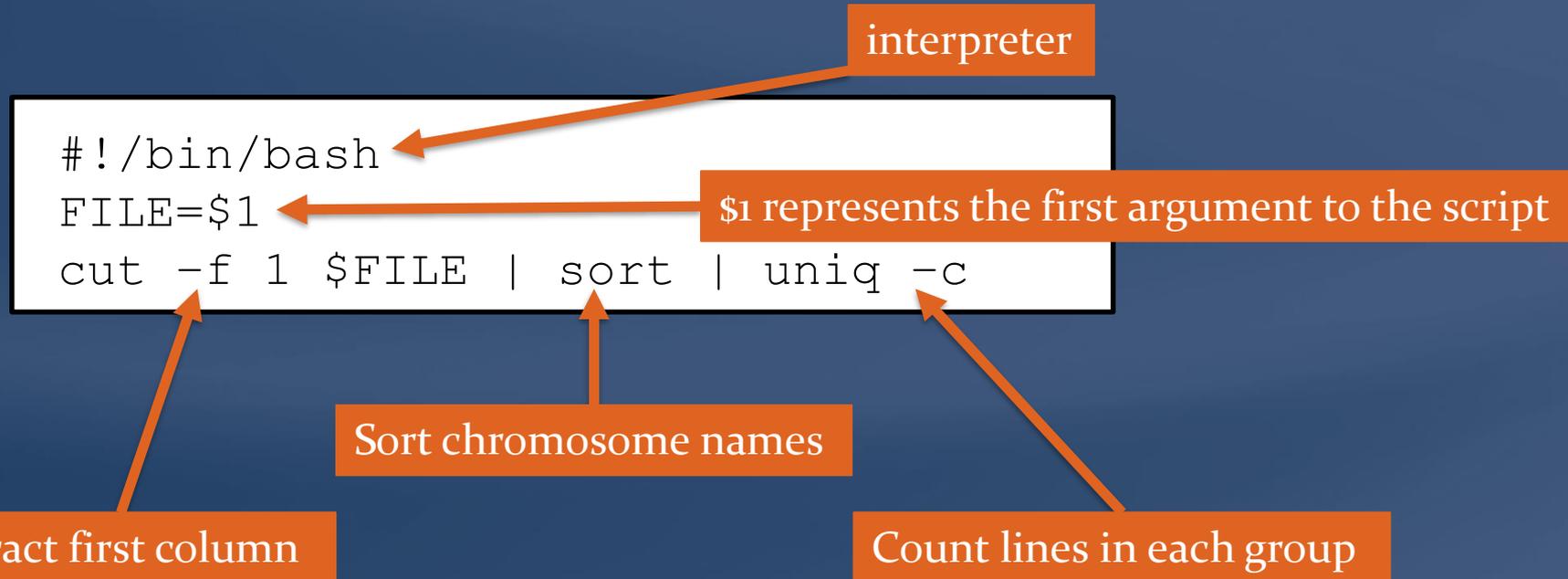
# Pipelining and redirection

- Pipelining: the output of a program can be directed to another program with the | (pipe) operator. Complex sequences of commands can be created easily.
- Redirection:
  - < read command input from a file
  - > send command output to a file
  - >> append command output to a file
- General form:  
`command1 < file1 | command2 > file3`



# Scripting example

- Given a tab-delimited file with chromosome names in the first column, the following script prints the number of occurrences of each chromosome:



# How to create a script

- Use a text editor (e.g. nano, vim) to create the file. Use any name, extension not necessary (but .sh is a good choice).
- Make the script executable:  

```
chmod +x scriptname
```
- Put script in a directory that is in your PATH, or call it with full pathname.



# Cluster-oriented approach

- Extension of shell scripting: the same commands are executed *in parallel* on a large number of nodes, with different arguments.
- The *scheduler* manages job submission and execution according to priorities, policies, available resources, and current usage.
- HiPerGator is a cluster computer with approx. 50,000 cores and several PB of memory. It uses *slurm* as the job scheduler.



# Modules

- Software on HiPerGator is organized into *modules*.  
Module commands:

- `module load <name>` Load named module
- `module spider <patt>` Show matching module(s)
- `module unload <name>` Unload named module
- `module purge` Unload all modules

The **dibig\_tools** module provides access to several useful commands. For example: `cut`, a more powerful version of `cut`.