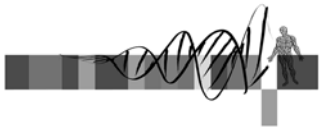

Unix, Perl and BioPerl

I: Introduction to Unix for Bioinformatics

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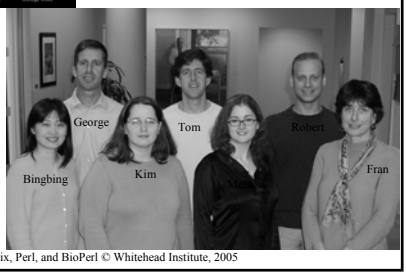
WIBR Bioinformatics and Research Computing

http://web.wi.mit.edu/bio



BaRC Bioinformatics and Research Computing

- Training
  - Train Whitehead scientists on the use of bioinformatics and graphics tools
- Education
  - Teach courses about theory behind bioinformatics tools and graphics concepts
- Consulting
  - Advise scientists on ways of analyzing data and designing graphics images
- Collaboration
  - Build new bioinformatics tools
  - Use bioinformatics tools to analyze research data
  - Publish papers in the area of bioinformatics with Whitehead scientists

Introduction to Unix for Bioinformatics

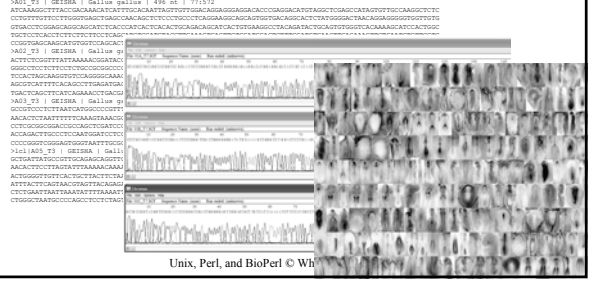
- Why Unix?
- The Unix operating system
- Files and directories
- Ten required commands
- Input/output and command pipelines
- Supplementary information
  - X windows
  - EMBOSS
  - Shell scripts

Objectives

- Get around on a Unix computer
- Run bioinformatics programs "from the command line"
- Design potential ways to streamline data manipulation and analysis with scripts

Why Unix (for me)?

- GEISHA, the *Gallus gallus* (chicken) EST and in situ hybridization (ISH) database



Why Unix (in general)?

- Features: multiuser, multitasking, network-ready, robust
- Others use it – and you can benefit from them (open source projects, etc.)
- Good programming and I/O tools
- Scripts can be easily re-run
- Types: Linux, Solaris, Darwin, etc.
- Can be very inexpensive

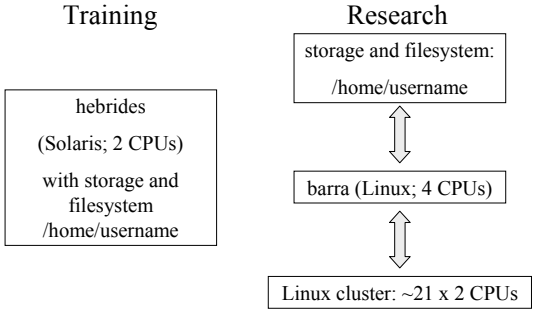
Why Unix for Bioinformatics?

- Good for manipulating lots of data
- Many key tools written for Unix
- Don't need to re-invent the wheel
- Unix-only packages: EMBOSS, BioPerl
- Unix tools with other OSs: Mac (OS X) & PC (Cygwin)

Unix O.S.

- kernel
  - managing work, memory, data, permissions
- shell:
  - working environment and command interpreter
  - link between kernel and user
  - choices: tcsh, etc.
  - History, filename completion [tab], wildcard (*)
  - Shell scripts to combine commands
- filesystem
  - ordinary files, directories, special files, pipes

WIBR BaRC systems

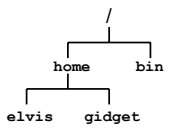


Logging in

- ssh (secure shell; for encrypted data flow)
  `ssh -l user_name hebrides.wi.mit.edu`
- passwd: to change your passwd
- logging out
  `logout`

Intro to files and directories

- Arranged in a branching tree
- Root of tree at "/" directory
- User elvis lives at /home/elvis (on 'hebrides')
- No spaces allowed
- Full vs. relative pathnames
  - At his home, Elvis' home dir is "."
  - To get to /home/gidget, go up and back down: (../gidget relative to /home/elvis)
- Anywhere, your home directory is "~".



Intro to Unix commands

- Basic form is

command_name options argument(s)

examples:

```
mv old_data new_data
blastall -p blastn -i myFile.seq -e 0.05
  -d nt -T T -o myFile.out
```

- Use history (↑, ↓, !*num*) to re-use commands
- Cursor commands: ^A(beginning) and ^E (end)
- To get a blank screen: `clear`
- For info about a command: `man` *command*

Key commands p. 1

- **Where am I?**

```
elvis@hebrides[1]% pwd
/home/elvis
```

- **What's here?**

```
elvis@hebrides [2]% ls
A01.fa

elvis@hebrides [3]% ls -a
.     .cshrc       A01.fa
..    .twmrc

elvis@hebrides [4]% ls -l
-rw-r--r--  1 elvis musicians  1102 Jun 19 10:45 A01.fa
```


Key commands p. 2

- Change directories:

```
cd ../gidget
/home/gidget
```

- Make a new directory:

```
mkdir spleen
```

- Remove a directory (needs to be empty first):

```
rmdir spleen
```


File permissions

- Who should be reading, writing, and executing files?
- Three types of people: user (u), group (g), others (o)
- 9 choices (rwx or each type of person; default = 644)

0 = no permission	4 = read only
1 = execute only	5 = r + x
2 = write only	6 = r + w
3 = x + w	7 = r + w + x

- Setting permissions with chmod:

chmod 744 myFile or **chmod u+x myFile**

```
-rwxr--r--  1 elvis musicians  110 Jun 19 10:45 myFile
chmod 600 myFile
-rw-------  1 elvis musicians  110 Jun 19 10:45 myFile
```


Key commands p.3

- Copying a file:

```
cp [OPTION]... SOURCE DEST
Ex: cp mySeq seqs/mySeq
```

- Moving or renaming a file:

```
mv [OPTION]... SOURCE DEST
Ex: mv mySeq seqs/mySeq
```

- Looking at a file (one screenful) with 'more'

```
Ex: more mySeq
```

(Spacebar a screenful forward,
<enter> a line forward; ^B a screenful back; q to exit)

Key commands (summary)

ssh	**mkdir**	**cp**
pwd	**mvdir**	**mv**
ls	**chmod**	**more**
cd		

To get more info (syntax, options, etc.):
man ***command***

Input/output redirection

- Defaults: stdin = keyboard; stdout = screen
- To modify,
  `command < inputFile > outputFile`
- input examples
  `sort < my_gene_list`
- output examples
  `ls > file_name` (make new file)
  `ls >> file_name` (append to file)
  `ls foo >& file_name` (stderr **too**)

Pipes (command pipelines)

- In a pipeline of commands, the output of one command is used as input for the next
- Link commands with the "pipe" symbol: |
  ex1: **`ls *.fa | wc -l`**
  ex2: **`grep '^>' *.fa | sort`**

Managing jobs and processes

- Run a process in the foreground (fg):
  `command`
- Run a process in the background (bg):
  `command` **`&`**
- Change a process (fg to bg):
  1. suspend the process: **`^Z`**
  2. change to background: **`bg`**

Managing jobs and processes (cont.)

- See what's running (ps)

```
elvis@hebrides[1]% ps –u user_name
   PID TTY      TIME CMD
22541 pts/22   0:00 perl
22060 pts/22   0:00 tcsh
```

- Stop a process:

`kill` ***`PID`***

ex: ***`kill 22541`***

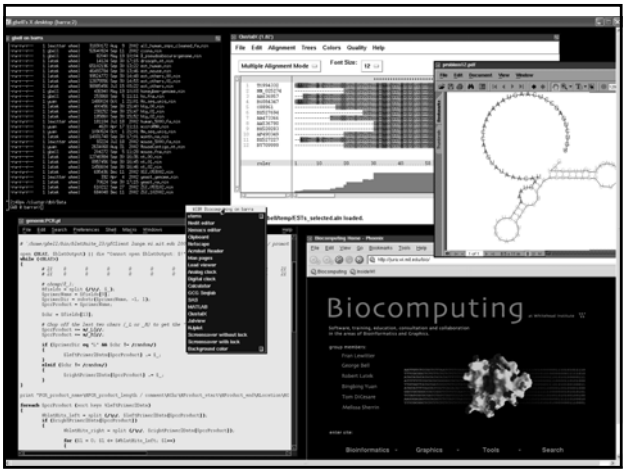
Text editors

- emacs, vi (powerful but unfriendly at first); pico
- nedit, xemacs (easier; X windows only)
- desktop text editors (BBEdit; TextPad) + sftp

Supplementary information

X Windows

- method for running Unix graphical applications
- still allows for command-line operation
- see help pages for getting started
- some applications with extensive graphics:
  - EMBOSS
  - R
  - Matlab
  - ClustalX + TreeView
- Requires a fast network/internet connection



EMBOSS

- The European Molecular Biology Open Software Suite
- List of programs at http://www.hgmp.mrc.ac.uk/Software/EMBOSS/Apps/
- ex: Smith-Waterman local alignment (`water`)
- Programs have two formats: interactive and one-line
- Conducive to embedding in scripts for batch analysis
- Traditionally command-line but web interfaces are becoming available

EMBOSS examples

- needle: Needleman-Wunsch global alignment
  `needle seq1.fa seq2.fa -auto -outfile seq1.seq2.needle`
- dreg: regular expression search of a nucleotide sequence
  `dreg -sequence mySeq.tfa -pattern GGAT[TC]TAA -outfile mySeq_dreg.txt`

Shell script example

```
#!/bin/csh
# alignSeqs.csh: align a pair of sequences

# Check to make sure you get two arguments (sequence
   files)
if ($#argv != 2) then
   echo "Usage: $0 seq1 seq2"; exit 1
endif

# Local alignment
set localOut=$1.$2.water.out
water $1 $2 -auto -outfile $localOut
echo Wrote local alignment to $localOut

# Global alignment
set globalOut=$1.$2.needle.out
needle $1 $2 -auto -outfile $globalOut
echo Wrote global alignment to $globalOut
```


Some other helpful commands

- rm: remove (delete) files ex: **`rm myOldfile`**
- cat: concatenate files
  `ex: cat *.seq > all_seq.tfa`
- alias: create your own command shortcuts
  `ex: alias myblastx blastall -p blastx -d nr`
- find: find a lost file (ex: look for files with the .fa extension)
  `ex: find . -name \*.fa`
- diff, comm: compare files or lists
- sort: sort (alphabetically/numerically) lines in a file
- uniq: get list of non-redundant lines
- grep: search a file for a text pattern
- tar: combine files together for storage or transfer
- sftp: transfer files between machines
- gzip & gunzip: compress or uncompress a file

Summary

- Why Unix?
- The Unix operating system
- Files and directories
- Ten required commands
- Input/output and command pipelines
- X windows, EMBOSS, and shell scripts

Exercises

- compress, move, and uncompress sequence files
- make a multiple sequence file
- create a BLAST database
- run BLAST on your database
- extract a sequence from the database