

Intro to computation

Emily Jane McTavish

Life and Environmental Sciences
University of California, Merced

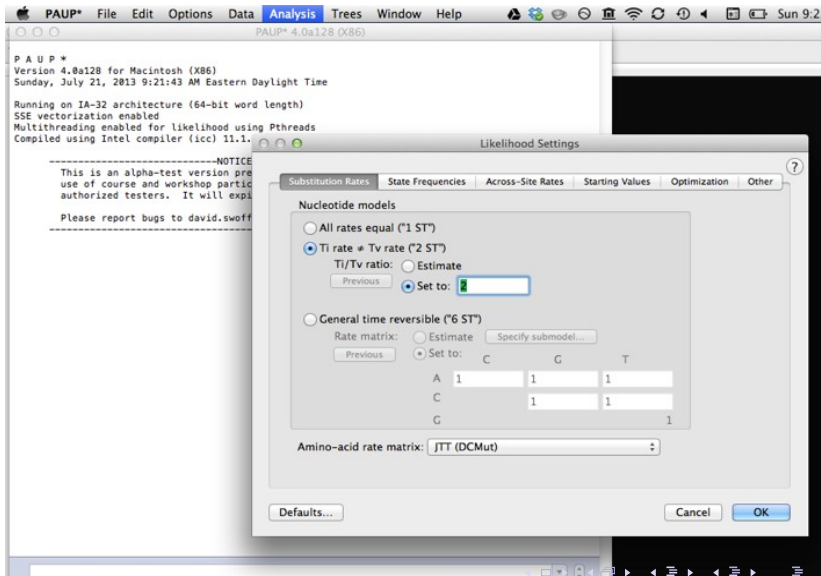
`ejmctavish@ucmerced.edu`, `twitter:snacktavish`

(With thanks to Jeet Sukumaran for the exercise)

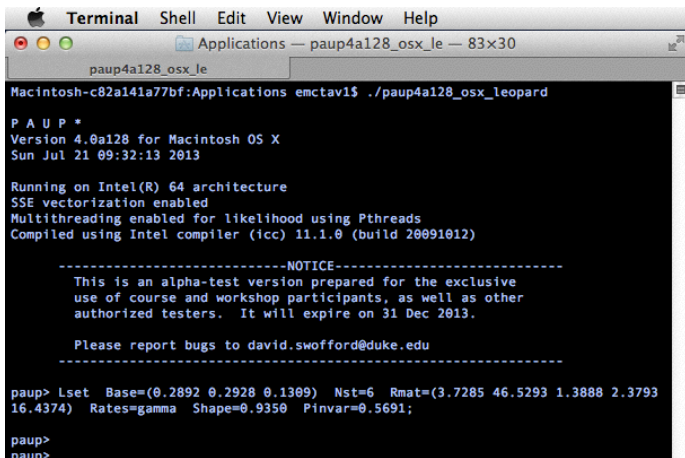
There are many ways to interact with your computer



Graphical User Interface (GUI)



Command line



```
Terminal  Shell  Edit  View  Window  Help
Applications — paup4a128_osx_le — 83x30
paup4a128_osx_le
Macintosh-c82a141a77bf:Applications emctav1$ ./paup4a128_osx_leopard

P A U P *
Version 4.0a128 for Macintosh OS X
Sun Jul 21 09:32:13 2013

Running on Intel(R) 64 architecture
SSE vectorization enabled
Multithreading enabled for likelihood using Pthreads
Compiled using Intel compiler (icc) 11.1.0 (build 20091012)

-----NOTICE-----
This is an alpha-test version prepared for the exclusive
use of course and workshop participants, as well as other
authorized testers.  It will expire on 31 Dec 2013.

Please report bugs to david.swofford@duke.edu
-----

paup> Lset Base=(0.2892 0.2928 0.1309) Nst=6 Rmat=(3.7285 46.5293 1.3888 2.3793
16.4374) Rates=gamma Shape=0.9350 Pinvar=0.5691;

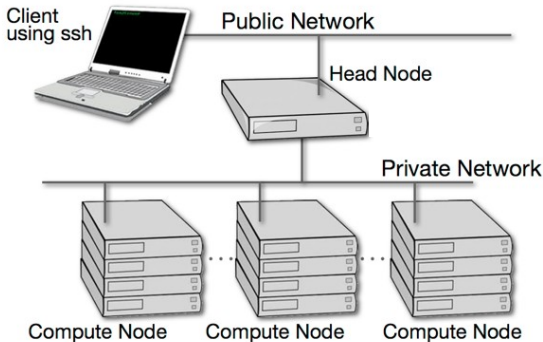
paup>
paup>
```

Why do things the hard way?

Advantages of command line

- Ease of repetition
- Batch processing
- Cluster computing
- Sometimes you just have to!

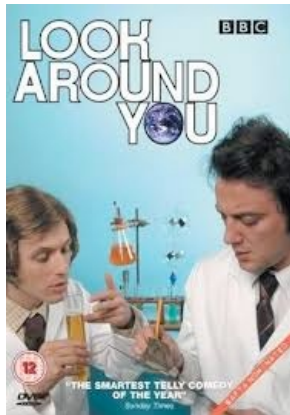
Cluster computing



www.udel.edu -

Open Terminal

Welcome to the command line!

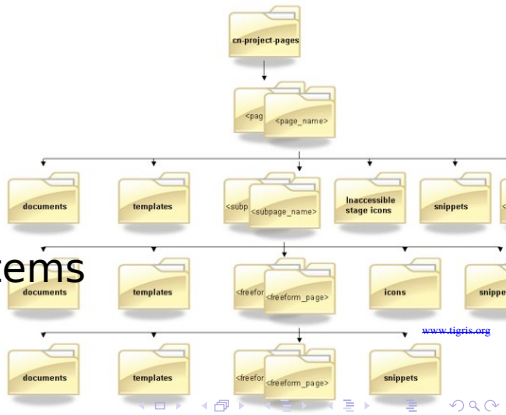


Directory Structure

`cd` to move around

`mkdir` to make a new directory

`pwd` to check where you are



/class/emctavish/items

Directory Structure

absolute paths start with '/'

relative paths are relative to your current working directory.

. refers to the directory you are in

.. is the directory above

Running programs: need to tell the computer where they are! (i.e /Applications/paup)

Special Characters

A space in bash denotes a new argument, so don't use it in filenames

* and ? are wildcard match characters

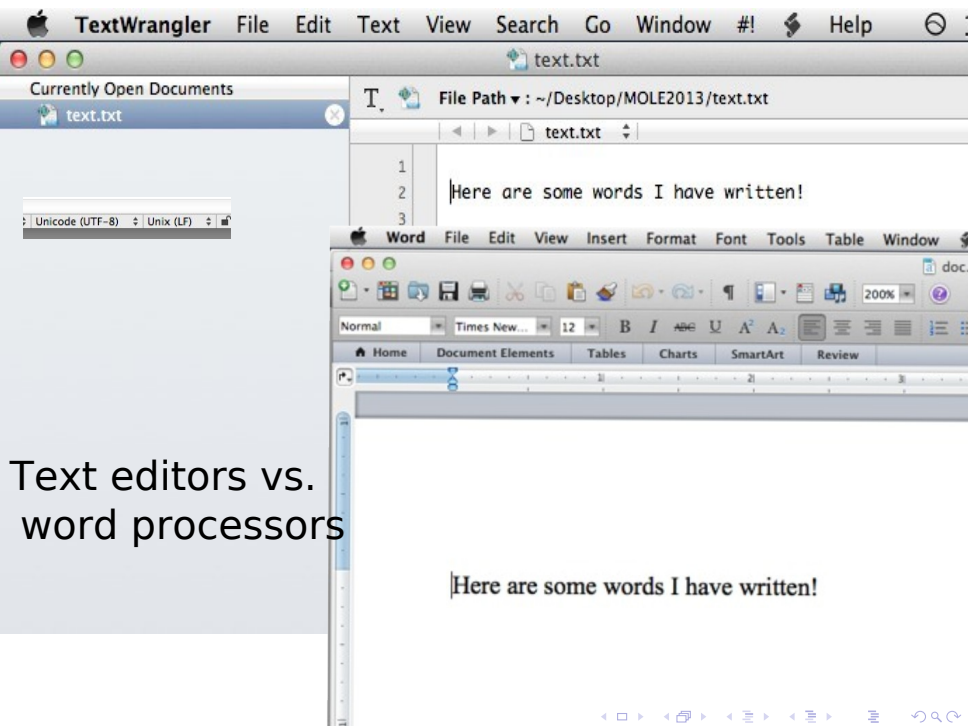
Basic syntax is:

```
command -options arguments
```

e.g.

```
ls -ltr /class/
```

```
cp from to
```



TextWrangler File Edit Text View Search Go Window #! Help

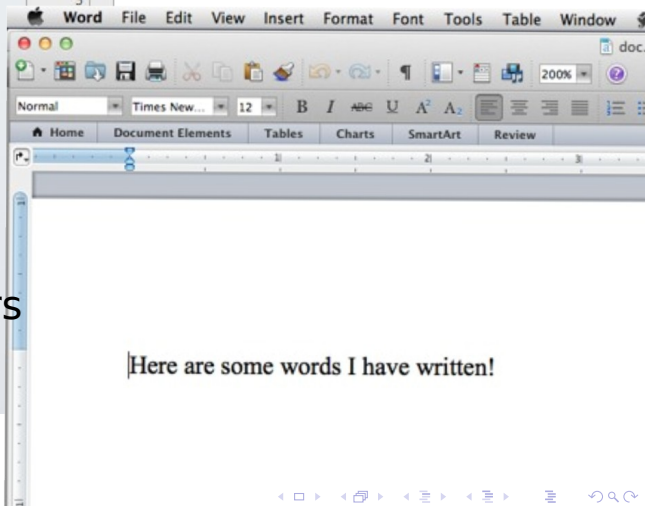
Currently Open Documents

text.txt

Unicode (UTF-8) Unix (LF)

File Path: ~/Desktop/MOLE2013/text.txt

1
2 Here are some words I have written!
3



Here are some words I have written!

Text editors vs.
word processors



bash

```
Macintosh-c82a141a77bf:MOLE2013 emctav1$ head text.txt
Here are some words I have written!
Macintosh-c82a141a77bf:MOLE2013 emctav1$
```



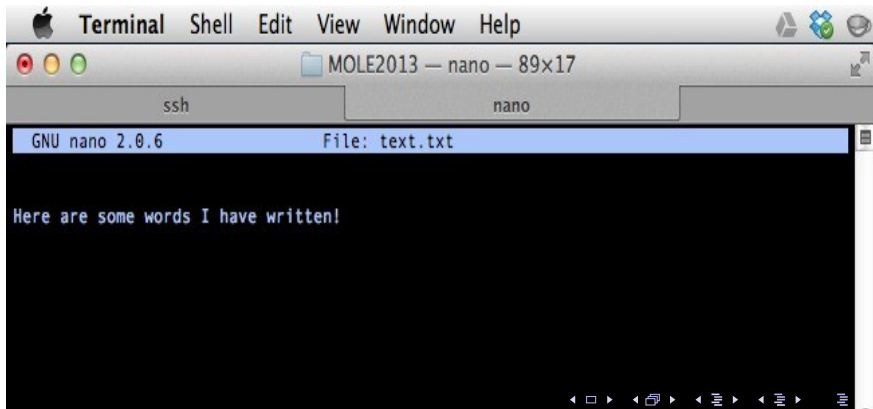
bash

```
??;5?????l?(?X???B??f:MOLE2013 emctav1$ head doc.docx
?"M?25h>?$??S?) /))6:?????|7'??M0?@??&??f??]?'??pP<*???v
"?|h75)????6Sf?????c??'??I?(zi?N??)f??_,?
?l????????:0T[?"?p'??tn??&? QS?X????!.???,?_WF?L8W()???
??}'????F?????G????? ?Y,K??c??? ?sB`
????Ih??/YfS
????Y9??wr???F???JB?/?R?;"?+Z(?e?daU?=????????<I?H?<4?e??:bG@
0???n?#?W?????H:#o???h{?JuLG?
?&?????_?ao?? .8??t????q????Uc??H<2??l???o??P!Jc?word.
4?Is?L???[e[???H????l??vHr???{0?????,?=7V?Z?x??+?P????~;??? :RZ??
?
r??\/?WI
l'?rB(?T?-H?N?B?Kj?R027d C??xX?I?QG??6???X?3U{j?N?eh??xE?PR?:?sF??B?I???1?lwz?
:U>'A?^??b??[?si3?gh6)???5??? '??~--?? ??H?C???n ???]??0???$J<[?J?Q5ub#J??/?v0???U?)?
[?<?>???sf?
?eR&?R?????p??>{[?I?e?o?S?G? ?8\B?iI????Ys?J?|'??3?*--[?????/'M?[?_p6+7 ?%??C7%2B?[?i??_uP%8??o
?? L????P!hu? word/_rels/document.xml.rels ?(????N?0??H???;qR? T?@?78??:????^~???T??Z?%K?+?|
[?7770??-??ix??0?????H?3PT"?wpC??_T?Bi???d5?;?{ok???7BU8?G?q]????
```

nano

nano < lename>

use Ctrl-X to exit and save



The screenshot shows a macOS Terminal window with the title bar 'Terminal' and menu items 'Shell', 'Edit', 'View', 'Window', and 'Help'. The window contains a nano text editor session. The top status bar of the editor shows 'GNU nano 2.0.6' and 'File: text.txt'. The main editing area is black with white text that reads 'Here are some words I have written!'. The bottom status bar of the editor shows various navigation icons. The window's title bar also indicates the current file is 'MOLE2013' and the editor is in 'nano' mode with dimensions '89x17'.

```
GNU nano 2.0.6 File: text.txt
Here are some words I have written!
```

```
[emctavish@class02 ~]$
```

```
>
```

The prompt

```
P A U P *  
Portable version 4.0b10 for Unix  
Sun Jul 27 13:52:25 2014
```

```
-----NOTICE-----  
This is a beta-test version. Please report any crashes,  
apparent calculation errors, or other anomalous results.  
There are no restrictions on publication of results obtained  
with this version, but you should check the WWW site  
frequently for bug announcements and/or updated versions.  
See the README file on the distribution media for details.  
-----
```

```
paup>
```


Local vs. remote

```
[emctavish@class02 ~]$
```

```
ejmctavish@pym:~$
```

Ctrl-C



tab ↑



An Exercise: Writing and Viewing a Tree by Hand

- ① Make sure you have:
 - ▶ A *good* text editor installed.
 - ▶ *FigTree* (or some other tree visualizer of choice).
- ② Create a subdirectory for all our labs, e.g. `"$HOME/projects/GradPhylo"`.
- ③ Create a work subdirectory within this directory for this particular lab, e.g. `"lab-01"`.
- ④ Using a command line text editor (nano or or personal favorite) create a simple Newick tree file using a text editor, e.g. `"simple.newick"`.
- ⑤ This tree should reflect the real topological relationships of at least 4 species.
- ⑥ Visualize it in *FigTree*.
- ⑦ Export as a NEXUS file.
- ⑧ Open this second file in a text editor and edit the tip labels.
- ⑨ Visualize it again.

HPC Assignment:

Write and submit a job submission script for the cluster that will run on the fastq queue.

It should have the job name, 'test244' followed by the job id, print output to a file test244.log, and it should run whoami, and concatenate the contents of the file 'hello_tree.txt' in the in the qsb244 directory into the output.

Upload your submission script and the output log file to catcourses.