http://bl831.als.lbl.gov/~jamesh/powerpoint/unix_commands.ppt

Slightly more advanced:
http://bl831.als.lbl.gov/~jamesh/elves/manual/tricks.html

# Basic unix commands
# that everyone should know

## (Even if you have a mac)

# What the ~*&?!

~     "tilde" indicates your home directory: `/home/you`

*     "star": wildcard, matches anything

?     wildcard, matches any one character

!     History substitution, do not use

&     run a job in the background, or redirect errors

#%     special characters for most crystallography programs

` \ ( [ " '     back-quote, backslash, etc. special to shell

_     underscore, use this instead of spaces!!!

# Where am I?

# pwd

Print name of the "current working directory"

This is the default directory/folder where the shell program will look first for programs, files, etc.  It is "where you are" in Unix space.

# What is a directory?

## /home/yourname/whatever

Directories are places you put files.  They are represented as words connected by the "/" character.  On Windows, they use a "\", just to be different. On Mac, they are called "folders". Whatever you do…

**DO NOT PUT SPACES**

In directory/file names!

# What have we here?

# `ls`

List contents of the current working directory

`ls -l`     - long listing, with dates, owners, etc.
`ls -lrt`   - above, but sorted by time
`ls -lrt /home/yourname/something`
          - long-list a different directory

# Go somewhere else?

# **cd**

Change the current working directory

```
cd /tmp/yourname/
            - go to your temporary directory
cd -        - go back to where you just were
cd          - no arguments, go back "home"
            "home" is where your login starts
```

# A new beginning…

# **mkdir**

Create a new directory.

```
mkdir ./something    - make it
cd ./something       - go there
ls                   - check its is empty
```

# How do I get help?

# man

Display the manual for a given program

```
man ls     - see manual for the "ls" command
man tcsh   - learn about the C shell
man bash   - learn about that other shell
man man    - read the manual for the manual
```

to return to the command prompt, type "q"

# Move it!

# **mv**

Move or rename a file.  If you think about it, these are the same thing.

```
mv stupidname.txt bettername.txt
```
- change name
```
mv stupidplace/file.txt ../betterplace/file.txt
```
- same name, different directory
```
mv stupidname_*.img bettername_*.img
```
Will not work! Never ever do this!

# Copy machine

# cp

Copy a file.  This is just like "`mv`" except it does not delete the original.

```
cp stupidname.txt bettername.txt
```
     - change name, keep original
```
rm stupidname.txt
```
     - now this is the same as "`mv`"

# "Permission denied" !?

# **chmod**

Change the "permission" of a file.

```
chmod a+r filename.txt
```
 - make it so everyone can read it
```
chmod u+rwx filename.txt
```
 - make it you can read/write/execute it
```
chmod -R u+rw /some/random/place
```
 - make it so you can read/write everything under
   a directory

# Destroy! Destroy!

# rm

Remove a file forever.  There is no "trash" or "undelete" in unix.

```
rm unwanted_file.txt
```
- delete file with that name
```
rm -f /tmp/yourname/*
```
- forcefully remove everything in your temporary directory.

Will not prompt for confirmation!

# less is more

# more

Display the contents of a text file, page by page

`more filename.txt` – display contents

`less filename.txt` – many installs now have a replacement for "`more`" called "less" which has nicer search features.

to return to the command prompt, type "`q`"

# After the download…

# **gunzip**

File compression and decompression

```
gunzip ~/Downloads/whatever.tar.gz
```
        - decompress
```
gzip ~/Downloads/whatever.tar
```
        - compress, creates file with `.gz` extension

# Where the %$#& is it?

# `find`

Search through directories, find files

```
find ./ -name 'important*.txt'
```
- look at everything under current working directory
with name starting with "`important`" and ending in "`.txt`"

```
find / -name 'important*.txt'
```
- will always find it, but take a very long time!

# Control! Control! You must learn Control!

# `<Ctrl>-C`

Stop jobs that are running in the foreground.  Note: <Ctrl> is that key on the keyboard that says "Ctrl".

`<Ctrl>-Z`    - get prompt back, but don't kill the job

`bg`              - after <Ctrl>-Z, put job in background

`fg`              - I changed my mind! come back to foreground

`<Ctrl>-A`    - go to beginning of the line

# Did I run out of disk space?

# `df du`

Check how much space is left on disks

`df` - look at space left on all disks

`df .` - look at space left in the current working directory

`du -sk . | sort -g`

- add up space taken up by all files and subdirectories, list biggest hog last

# Why so slow?

# `ps top`

Look for programs that may be eating up CPU or memory.

`top`    - list processes in order of CPU usage

`jobs`   - list jobs running in background of current terminal

`ps -fHu yourname`

     - list jobs belonging to your account in order of what spawned what (leave out the H on a mac)

# Die Die Die!

## **kill**

Stop jobs that are running in the background

```
kill %1      - kill job [1], as listed in "jobs"
kill 1234  - kill job listed as 1234 by "ps" or "top"
kill -9 1234 - that was not a suggestion!
kill -9 -g 1234 – seriously kill that job and the
                 program that launched it
```

# too… much… typing!



1) Make sure X11 is running

2) Select some text with mouse

3) Move mouse over to your terminal

4) Hit middle mouse button

5) No keyboard required!

# How to run DIALS:

source /Applications/dials-v1-7-2/dials_env.csh

xia2 mosflm_beam_centre=151.4,144.8
/home/data/data2016/SERCAT-Sun/MM/MLYS/

dials.reciprocal_space_viewer

# How to run DIALS the hard way:

% dials.import /home/ …. /MLYS/

% dials.find_spots datablock.json nproc=8

% dials.reciprocal_space_viewer datablock.json strong.pickle &

% dials.image_viewer datablock.json &

% dials.generate_mask untrusted.polygon=1958,2024,0,2005,0,2151,1956,2125 untrusted.circle=1964,2073,200

% open –t datablock.json

# How to run DIALS the hard way:

% open -t datablock.json

<span style="color:green">Change origin to -144.8,151.4,-200</span>

<span style="color:green">edit mask = mask.pickle</span>

% dials.find_spots datablock.json nproc=8

% dials.index datablock.json strong.pickle \
    space_group=P21 \
    unit_cell=27.28,62.44,59.82,90,90.615,90

% dials.integrate experiments.json indexed.pickle

% dials.image_viewer integrated.pickle \
    integrated_experiments.json

# How to run DIALS the hard way:

% dials.export integrated_experiments.json
    integrated.pickle

% pointless hklin integrated.mtz hklout ptls.mtz |
    tee pointless.log

% egrep "Best|twin" pointless.log

% echo "refine parallel" |\

    aimless hklin ptls.mtz hklout amls.mtz |\

    tee aimless.log

% truncate hklin amls.mtz hklout truncated.mtz

% phenix.autosol truncated.mtz

# How to run XDS:

cd

mkdir –p processing/SERCAT-Sun/MM/MLYS

cd processing/SERCAT-Sun/MM/MLYS

ln –sf /home/data/data2016/SERCAT-Sun/MM/MLYS/ ./data


xdsgui &


firefox https://strucbio.biologie.uni-
        konstanz.de/xdswiki/index.php/XDSGUI &