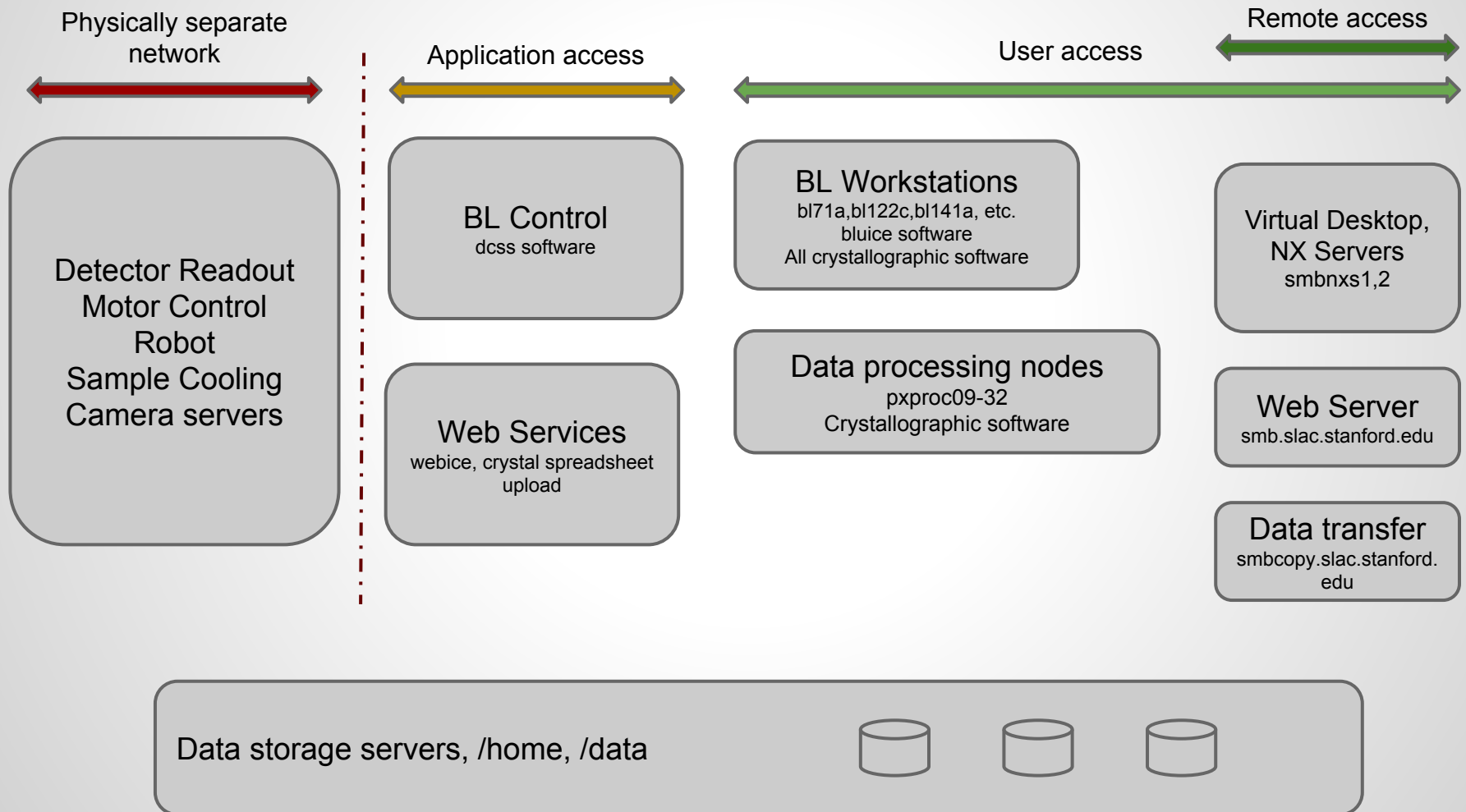# Macromolecular Crystallography Computer Environment

Brief Orientation

Introduction

- SSRL PX Group Computers
  - General layout - network, hostnames
  - Some technical details
  - Usage advice and policies
- Short Unix command line tutorial
- Further Documentation
  - http://smb.slac.stanford.edu/
  - Links to versions of this presentation at http://smb.slac.stanford.edu/facilities/computing/

General layout

Physically separate network

Application access

Remote access

User access

Detector Readout
Motor Control
Robot
Sample Cooling
Camera servers

BL Control
dcss software

Web Services
webice, crystal spreadsheet upload

BL Workstations
bl71a,bl122c,bl141a, etc.
bluice software
All crystallographic software

Data processing nodes
pxproc09-32
Crystallographic software

Virtual Desktop, NX Servers
smbnxs1,2

Web Server
smb.slac.stanford.edu

Data transfer
smbcopy.slac.stanford.edu

Data storage servers, /home, /data

Overview

- SSRL PX Beamlines is it's own Auth Domain
  - Separate SLAC, LCLS or other SSRL beamlines
  - Prior registration with SSRL user portal required
- Linux is used exclusively as OS.
  - Redhat/CentOS 6.9
- Network storage only
  - /home/<username>
  - /data/<username>
  - Available from all computers

Remote Access

- \>95% of experiments are done remotely
- NoMachine Servers - Virtual Desktop
  - smbnxs1, smbnxs2 (smbnxs3 - RapiData only)
- Free Client (nomachine.com)
  - Windows, Mac, Linux, iOS, Android
  - Keep the client updated
  - Use the "Enterprise Client"
- Reliable and responsive
  - Applications continues to run if connection is lost
  - Disconnect at the lab and reconnect from home.

At the Beamline

- 2 or 3 Workstations at each beamline
  - bl71a, bl122b, bl141c, etc.
  - Same desktop and resources as when using the NoMachine virtual desktop.
  - Graphics heavy tasks like coot and pymol are the only ones that benefit from using a local workstation.
  - Allows connection of USB drives for data backup.

Data processing

- 24 nodes dedicated to data processing
  - pxproc[09-16] 8 core / 16 thread, 24GB
  - pxproc[17-32] 24 core / 48 thread, 128GB
  - Available via ssh from the NX server.
- Crystallography software packages
  - Environment for crystallography software automatically setup for users.
  - Development or older versions may be available via the 'module' command.

Data Storage

- Home disk - /home/rapidata - $HOME
  - Small capacity - 12TB
  - Fast - 24, 15,000rpm, spindles
  - NO Data Files Here! They will be deleted!
  - Backed up daily, snapshots every 2-3 hours
- Data disk(s) - /data/rapidata
  - Large capacity - 500TB+
  - Slow for writing lots of small files
  - Good for reading/writing large files
  - No backups, data will be deleted when disk fills up.
  - For best performance, keep file count below 10,000 per directory

Backup your data

- Remote
  - scp, sftp, rsync

    example using rsync from your home computer to pull data from SSRL

    ```
    rsync -avP rapidata@smbcopy.slac.stanford.edu:/data/rapidata/Lyso /MyLocalDisk/
    ```

- Local
  - External disk (USB, FireWire)

These slides are available at:
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)

All credit to James Holton for putting together the remaining slides

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!

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

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
```