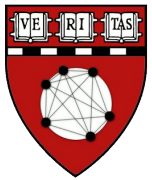
Quo Vadis Workshop 2016

Software installation
Intro to Computing on Linux



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Welcome!
Quo Vadis Workshop 2016


Pete Meyer


Ilyas Hamdi


Mick Timony


Andrew Morin


Justin O' Connor


Michelle Ottaviano


Saythyda Corrado

Carol Herre
Rob DiCamillo

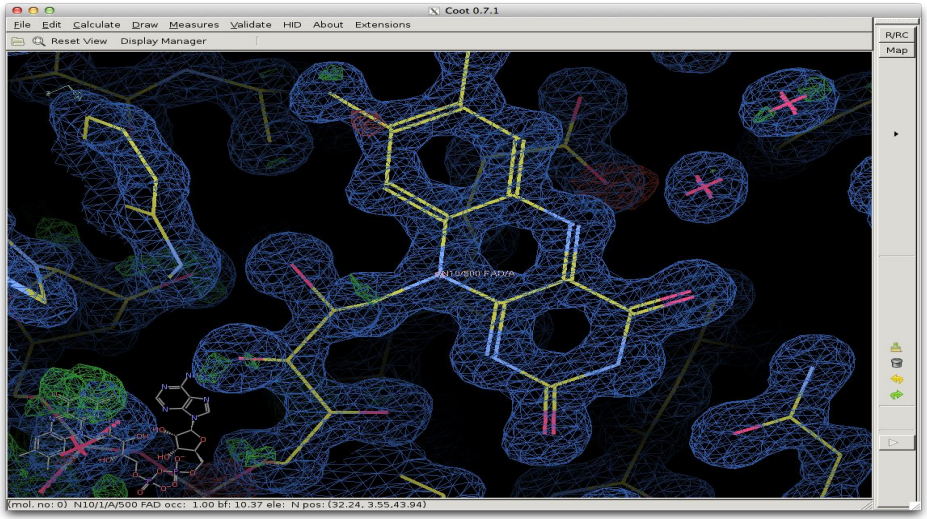

Piotr
Sliz

SBGrid : Structural Biology Research Computing

Who we are:

Non-profit Consortium based in BCMP @HMS focused on Structural Biology computing

Structural Biologists, IT pros, software engineers, programmers, software policy advocates, postdocs, students



Quo Vadis Workshop 2016 - 22 May 2016

Software Installation for QV2016

Intro to Linux Computing

Quo Vadis Workshop 2016

CCP4 : (COOT, iMosflm, ...)

DIALS :

XDS : (XDSGUI, XDSSTAT, XDSViewer)

Software for QV2016

https://sbgrid.org/wiki/sbgrid-qv2016-installation

1) Download the script :

```
curl -o sbgrid-qv2016 https://sbgrid.org/wiki/sbgrid-qv2016
```

2) Make executable and execute :

```
chmod +x sbgrid-qv2016
./sbgrid-qv2016
```

3) Load the environment :

```
source /programs/sbgrid.shrc    (sbgrid.cshrc in tcsh)
```

Software for QV2016

Installing updates:

```
./$HOME/programs/share/bin/sbgrid-qv2016
```

Datasets for QV2016

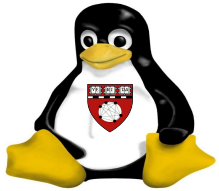
Datasets can be downloaded via rsync

```
rsync -av rsync://data.sbgrid.org/10.15785/SBGRID/$id
```

(where $id is replaced by the dataset ID).

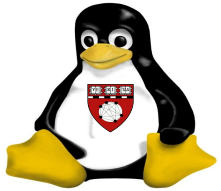
Quo Vadis Workshop 2016 - 22May16

Intro to Linux Computing



- Introduction to Linux
  - Why Linux?
- The Linux interface
  (Understanding the Shell)
- Scientific Computing on linux -
  - Sysadmin’s tips and tools for computing and research

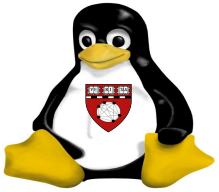
Linux



Linux is an open-source operating systems modeled on UNIX developed by Linux Torvalds in 1991.

> Comp.os.minix
>
> *Hello everybody out there using minix - I'm doing a (free) operating system (just a hobby, won't be big and professional like gnu) for 386(486) AT clones. …*

Linux

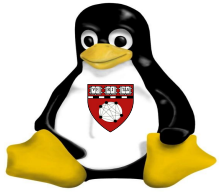


The GNU (Gnu's Not Unix) was an effort to develop free and open source OS and applications.

Torvalds developed 'kernel' and combined it with software from Richard Stallman @ MIT.

GNU's Not Unix

Linux

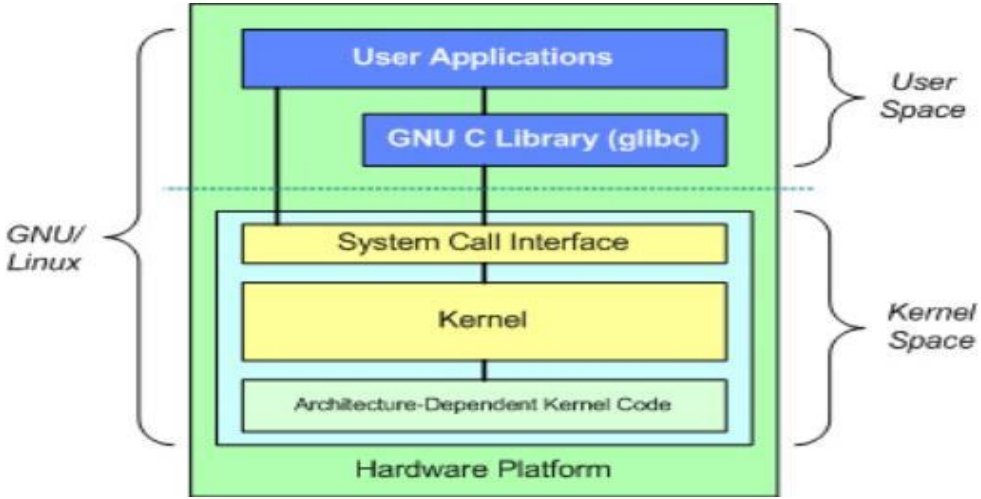


Multi-user, multi-tasking

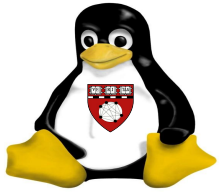
Many users on the same machine at once, running many programs

Multi-platform

runs on many different processor types



Linux



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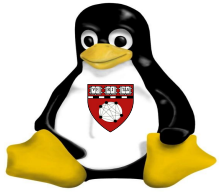
Linux is a Unix-like system free of proprietary software for which source code is available and freely distributed

Linux



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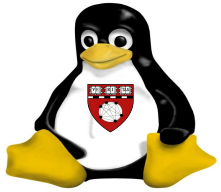
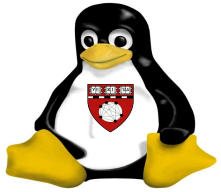


But why did Linux succeed?
(and not HURD, BSD, Minux, etc …)

- Decentralized Development
- Pragmatic (Not an academic or ideological exercise)
- Technological Superiority
- Luck?

Linux



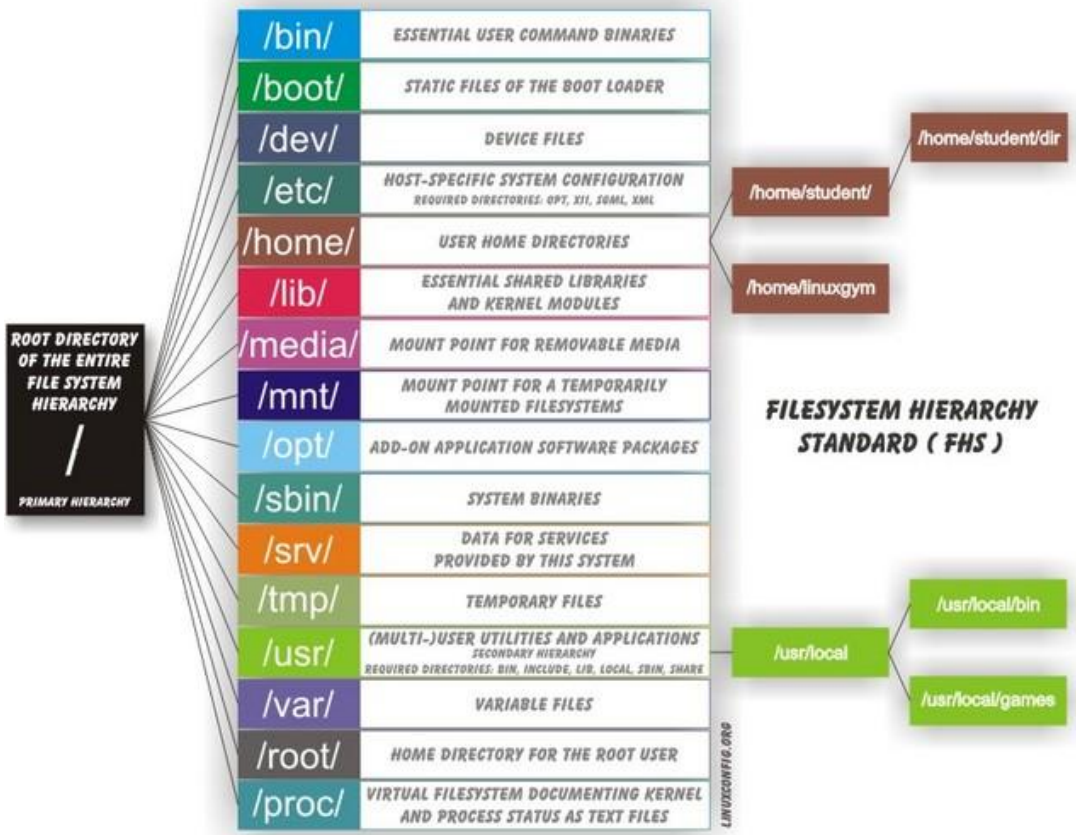
"Everything is a file"

Defining features of *nix

Resources (documents, directories, keyboards, printers, storage, network communications, etc)

Are simple streams of bytes exposed through the filesystem name space

The Filesystem Hierarchy Standard (FHS) defines the directory structure and directory contents.



The Shell

The ‘shell’ is the Command Line Interface for Linux

This is an program that interprets what you type, keeps track of programs on the system, etc.

Common Shells:

tcsh : exTended C SHell
bash : Bourne Again SHell
ksh : Korn SHell
csh : C SHell (early popular shell)
sh : the original shell, often a synonym for bash now

The Shell : Commands

Navigation (cd, pwd, ls)

Manipulating Files (cp, rm, mv, mkdir)

Search (grep, find)

Permissions (chmod, chown, chgrp)

Job Control (jobs, ps, fg, bg, nohup)

http://linuxcommand.org/lc3_learning_the_shell.php

The Shell : The Environment

The shell environment is configured globally per user in files and startup scripts

- Settings for variables
- Function definitions
- Aliases

Except for the reserved Shell special parameters variable names can be set by the user

Quotes remove special meaning from one or multiple characters

The Shell : The Environment

- The ‘printenv’ command

The Shell : The Environment

The ‘printenv’ command

Shell variables:

- PATH
  - Where executables can be found
- HOME
  - User’s home directory
- USER
  - User’s username
- SHELL
  - Default shell setting

The Shell : The Environment

The ‘printenv’ command

Shell variables:

PS1
Shell prompt settings

LD_LIBRARY_PATH
Primary search path for library directories

...

The Shell : The Environment

The ‘alias’ command

An alias is a shortcut or abbreviation.

Great for avoiding typing a long command sequences

Aliases do NOT get passed to scripts (sub-shells)

The Shell : The Environment

Functions: The ‘declare -f’ command

Functions are subroutines :
a code block (list of commands) that implements a set of operations.

The Shell : stdout stdin stderr

---

stdout :

Output from commands
written to the screen

stdin :

Input for commands
usually come from the keyboard

stdin :

Error messages from processes
usually written to the screen

The Shell : stdout stdin stderr

Pipe (|):

stdout of one command to stdin of another command

Output Redirection (>):

stdout of a command to a file

Output Appending (>>):

stdout of a command appending to a file

Input Redirection (<):

stdin of a command from a file

Use “-” to read this from standard input

The Shell : stdout stdin stderr

Stderr redirection

For tcsh

```
&> filename
```

For bash

```
2>&1 filename
```

The Shell : stdout stdin stderr

Most Linux (*nix) commands can be strung together

Example:

How many image files do I have?

```
ls -l *img | wc
```

How many image files do I have that are not have ‘native’ in the name?

```
ls -l *img | grep -v “native” | wc
```

The Shell : stdout stdin stderr

Most Linux (*nix) commands can be strung together

Example:

A list of all my image files :

```
ls *img > my_images.txt
```

A list of all my images sorted in reverse numerical order?

```
ls -l *img | sort -rn -k 9 > sorted_files.txt
```

The Shell script

Shell scripts are text files of variables, functions, and commands

A ‘shebang’ (#!/bin/bash, …) is required to indicate which interpreter the OS programs loader should use

Conditional expressions: if/else, case
Loops: for, while, until

http://tldp.org/HOWTO/Bash-Prog-Intro-HOWTO.html

Scientific Computing: tools, tips and tricks

- Getting there and moving data
- What resources does this computer have (and what is it doing)?
- Reproducibility and collaboration

Scientific Computing: tools, tips and tricks

SSH

provides a secure channel (encrypted) over an unsecured network in a client-server architecture

- remote command-line login
- remote command execution
- any network service can be secured with SSH.

Scientific Computing: SSH

SSH public-key authentication allows login and command execution without passwords based on a public/private key pair

Setup: create keys, set a password

```
ssh-keygen -t rsa
```

Public key goes on the remote server in your .ssh directory in the file $HOME/.ssh/authorized_keys

Private key stays in $HOME/.ssh

Ssh-agent manages keys - typically running by default on most Linuxes

Use ssh-add command to add key, No more passwords!

Scientific Computing: SSH

SSH public-key authentication allows login and command execution without passwords based on a public/private key pair

Use ssh -X to forward X11 for graphics access

Scientific Computing: Moving data with rsync

---

rsync

- Transfers only changes in a file tree
- Local and remote synchronization of data file and directories

```
rsync -rv /my/files/here/ /my/files/over_there/
```

- Can be run over ssh for secure transfer

```
rsync -rv /my/files/here/ remote.server.org:/my/files/over_there/
```

- Ideal for data backup

```
man rsync
```

For more info

Scientific Computing: Hardware

CPU, Storage,memory,usb and pci

- cpuinfo or cat /prog/cpu
- df or lsblk
- free
- lsusb
- lspci

Scientific Computing: What is running

CPU and memory use, jobs, IO

- top, uptime
- ps
- sar

Scientific Computing: history

---

history

The shell records all commands.
This record can be accessed with the ‘history’ command.

Some relevant variables:

HISTSIZE
Define number of commands

HISTFILE
Define file

HISTCONTROL=ignoredups
Ignore duplicates

Scientific Computing: Terminal multiplexer

Tmux (or screen)

A terminal multiplexer is terminal-based program that gives the user

- Ability to detach and reattach sessions from a terminal
  - Sessions persist on the remote machine
  - A terminal session can be accessed from multiple machines
  - Persist through network disconnection

- Multiple separate login sessions inside a single terminal window

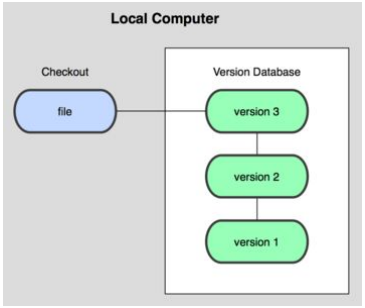
Scientific Computing: Version Control

VCS

Version control systems are designed for software development, are are great for scientific computing projects

Version control software keeps track of every modification to the code

Earlier versions of code are retained and can be accessed



Scientific Computing: Version Control

Git / hg / svn

Preserves the modification history of scripts and configuration files *‘stream of snapshots’*

Allows branching for new projects, ideas and experimentation

Designed for collaboration (labs)

Github, bitbucket, etc.

Scientific Computing: Getting started with git

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https://git-scm.com/book/en/v1/Getting-Started