McGill initiative in Computational Medicine

UNIX basics and introduction to HPC

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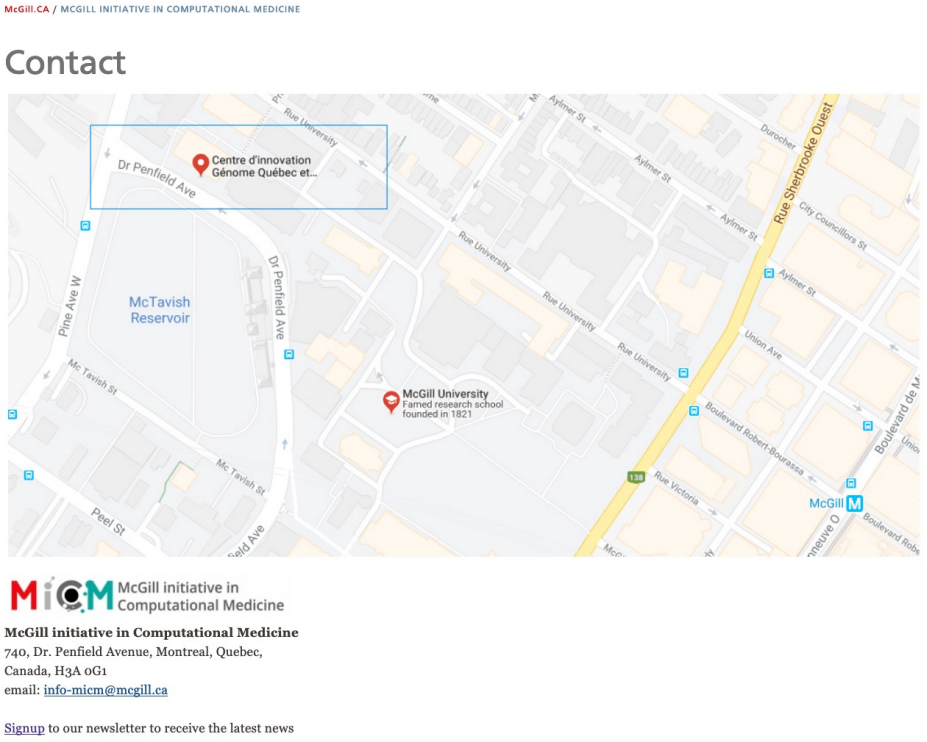
20-Septemer-2021

McGill initiative in Computational Medicine

Mission : aims to deliver inter-disciplinary research programs and empower the use of data in health research and health care delivery



https://www.mcgill.ca/micm

Workshop outline

1. UNIX operating system
   File system structure
   File management
   Built-in commands

2. Variables
   Pipes, loops and conditional statements
   Shell scripting
   Text processing and pattern matching

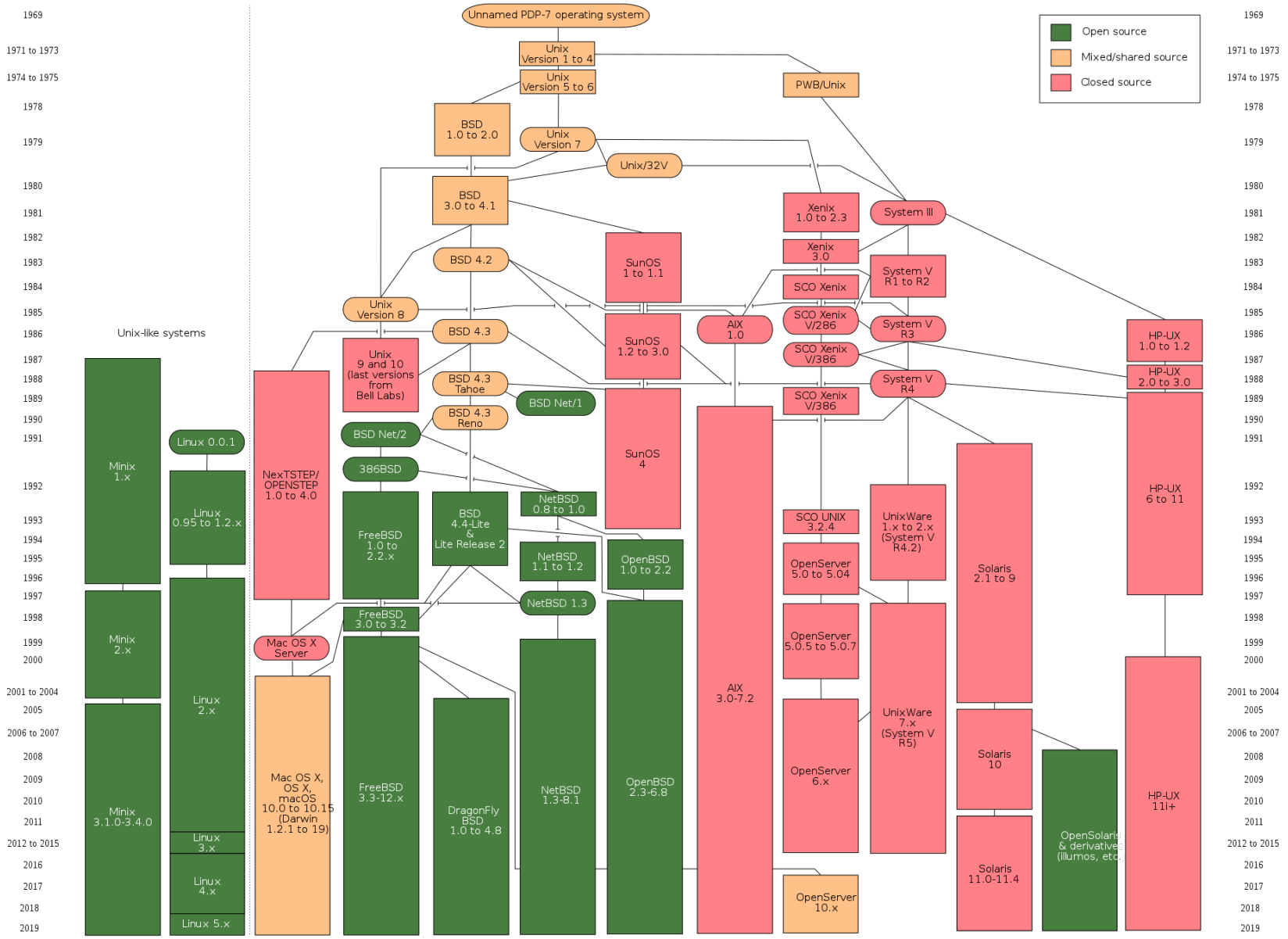
3. What is HPC?
   Compute Canada
   Servers, clusters, and supercomputers
   Submitting jobs to a cluster

Dennis Ritchie (standing) and Ken Thompson (seating) at Bell Labs, 1960's

https://www.bell-labs.com/institute/blog/invention-unix/#gref

UNIX Operating system

- General purpose
- Multiuser
- Interactive
- Resource-efficient
- Hierarchical file system
- Compatibility (files, devices, processes)
- Time sharing



https://en.wikipedia.org/wiki/Unix#/media/File:Unix_history-simple.svg

The Single UNIX® Specification History & Timeline

1969	**The Beginning**	The history of UNIX starts back in 1969, when Ken Thompson, Dennis Ritchie and others started working on the "little-used PDP-7 in a corner" at Bell Labs and what was to become UNIX.
1971	**First Edition**	It had an assembler for a PDP-11/20, file system, fork(), roff and ed. It was used for text processing of patent documents.
1972	**First UNIX Installations**	The first installations had 3 users, no memory protection, and a 500 KB disk.
1973	**Fourth Edition**	It was rewritten in C. This made it portable and changed the history of OS's.
1975	**Sixth Edition**	UNIX leaves home. Also widely known as Version 6, this is the first to be widely available outside of Bell Labs. The first BSD version (1.x) was derived from V6.
1979	**Seventh Edition**	It was an "improvement over all preceding and following Unices" [Bourne]. It had C, UUCP and the Bourne shell. It was ported to the VAX and the kernel was more than 40 Kilobytes (K).
1980	**Xenix**	Microsoft introduces Xenix. 32V and 4BSD introduced.
1982	**System III**	AT&T's UNIX System Group (USG) release System III, the first public release outside Bell Laboratories. SunOS 1.0 ships. HP-UX introduced. Ultrix-11 introduced.
1983	**System V**	Computer Research Group, UNIX System Group (USG) and a third group merge to become UNIX System Development Lab. AT&T announces UNIX System V, the first supported release. Installed base 45,000.
1984	**4.2BSD**	University of California at Berkeley releases 4.2BSD, includes TCP/IP, new signals and much more. X/Open formed.
1984	**SVR2**	System V Release 2 introduced. At this time there are 100,000 UNIX installations around the world.
1986	**4.3BSD**	4.3BSD released, including internet name server. SVID introduced. NFS shipped. AIX announced. Installed base 250,000.
1987	**SVR3**	System V Release 3 including STREAMS, TLI, RFS. At this time there are 750,000 UNIX installations around the world. IRIX introduced.
1988		POSIX.1 published. Open Software Foundation (OSF) and UNIX International (UI) formed. Ultrix 4.2 ships.
1989		AT&T UNIX Software Operation formed in preparation for spinoff of UNIX development group. Motif 1.0 ships.
1989	**SVR4**	UNIX System V Release 4 ships, unifying System V, BSD and Xenix. Installed base 1.2 million.
1990	**XPG3**	X/Open launches XPG3 Brand. OSF/1 debuts. Plan 9 from Bell Labs ships.

"The Single UNIX Specification brings all the benefits of a single standard operating system, namely application and information portability, scalability, flexibility and freedom of choice for customers"

Allen Brown, President and CEO, The Open Group

The Story of the License Plate...

In 1983 Digital Equipment Corporation (DEC) was ramping up their engineering group to create and ship their first UNIX system product.

One of the stalwarts of the group was Armando P. Stettner. Armando was a UNIX system devotee. He lived and he breathed the UNIX system. When he got his new car, it was natural that he got vanity license plates that said "UNIX" on them. And it only made it better that the state motto of New Hampshire was "Live Free or Die".

Armando often got requests from people along the lines of "When will we be able to get our UNIX system license directly from DEC?" And Armando kept saying "Real Soon Now" (RSN).

Armando was going to a conference and he was dreading having to say "RSN" many more times, so he had a bright idea. Amando went prepared to give out "UNIX licenses". On stage, when the question came up, "When will we be able to get our UNIX system license directly from DEC?", Armando yelled "Right Now!" and produced facsimilies of his license plate, holding it up for all to see. It was an almost perfect likeness of his license plate, with the trademark "UNIX" in the middle of it, but instead of having "Live Free or Die" across the bottom of the plate (as in the real case), it had it across the top. Across the bottom was the trademark acknowledgement.

DEC made UNIX license plates up in small numbers and handed them out at events. They usually ran out. The demand for the license plates never did abate. People saw them on an office wall, or heard about them somewhere, and wanted one of their own.

Armando left the state for the sunny climes of California, and had taken his car and license plate with him. Or so many people thought.

In 1989 Jon 'maddog' Hall was purchasing a new car, a Jeep Wrangler. And of course the license plate had to be relevant. So Jon, a long time DEC employee and UNIX system guru, submitted his application with many variations and the clerk said "I think we can give you your first choice...." and gave him the temporary paper plates (to be used on the car until the metal plates were manufactured) with "UNIX" on them. And so it has been ever since. Jon's Jeep has been the holder of the UNIX license plate.

The Open Group thanks Jon "maddog" Hall for sharing the story of the UNIX license plate.

The UNIX Brand

The UNIX Brand is used to identify products that have been certified as conforming to the Single UNIX Specification, initially UNIX 93, followed subsequently by UNIX 95, UNIX 98 and now UNIX 03.

UNIX is a registered trademark of The Open Group in the United States and other countries.

1991		UNIX System Laboratories (USL) becomes a company - majority-owned by AT&T. Linus Torvalds commences Linux development. Solaris 1.0 debuts.
1992	**SVR4.2**	USL releases UNIX System V Release 4.2 (Destiny). October - XPG4 Brand launched by X/Open. December 22nd - Novell announces intent to acquire USL. Solaris 2.0 and HP-UX 9.0 ship.
1993	**4.4BSD**	4.4BSD the final release from Berkeley. June 16 - Novell acquires USL
Late 1993	**SVR4.2MP**	Novell decides to get out of the UNIX business. Rather than sell the business as a single entity, Novell transfers the rights to the UNIX trademark and the specification to X/Open Company. COSE Initiative delivers "Spec 1170" to X/Open for fasttrack. In December Novell ships SVR4.2MP , the final USL OEM release of System V
1994	**Single UNIX Specification**	BSD 4.4-Lite eliminated all code claimed to infringe on USL/Novell. As the owner of the UNIX trademark, X/Open introduces the Single UNIX Specification (formerly Spec 1170) which separates the UNIX trademark from any actual code stream itself, thus allowing multiple implementations.
1995	**UNIX 95**	X/Open introduces the UNIX 95 branding program for implementations of the Single UNIX Specification. Novell sells UnixWare business to SCO. Digital UNIX introduced. UnixWare 2.0 ships. OpenServer 5.0 debuts.
1996		The Open Group forms as a merger of the Open Software Foundation (OSF) and X/Open. UnixWare 2.1, HP-UX 10.20 and IRIX 6.2 ship.
1997	**Single UNIX Specification, Version 2**	The Open Group introduces Version 2 of the Single UNIX Specification, including support for realtime, threads and 64-bit and larger processors. The specification is made freely available on the web. IRIX 6.4, AIX 4.3 and HP-UX 11 ship.
1998	**UNIX 98**	The Open Group introduces the UNIX 98 family of brands, including Base, Workstation and Server. First UNIX 98 registered products shipped by Sun, IBM and NCR. The Open Source movement starts to take off with announcements from Netscape and IBM. UnixWare 7 and IRIX 6.5 ship.
1999	**UNIX at 30**	The UNIX system reaches thirty. Solaris 7 ships. Linux 2.2 kernel released. The Open Group and the IEEE commence joint development of a revision to POSIX and the Single UNIX Specification. First LinuxWorld conferences. Dot com fever on the stock markets. Tru64 UNIX ships.
2001	**Single UNIX Specification, Version 3**	Version 3 of the Single UNIX Specification unites IEEE POSIX, The Open Group and the industry efforts. Linux 2.4 kernel released. The value of procurements of open systems referencing the UNIX brand exceeds $55 billion. AIX 5L ships.
2003	**ISO/IEC 9945**	The core volumes of Version 3 of the Single UNIX Specification are approved as an international standard. "Westwood" test suites shipped for UNIX 03 brand. Solaris 9.0 E ships. Linux 2.6 kernel released.

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Making standards work™

https://unix.org/license-plate.html

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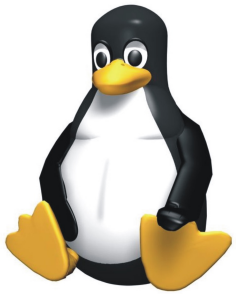
How it started

How it's going



Linux
Operating System

ANDROID

Parts

The kernel

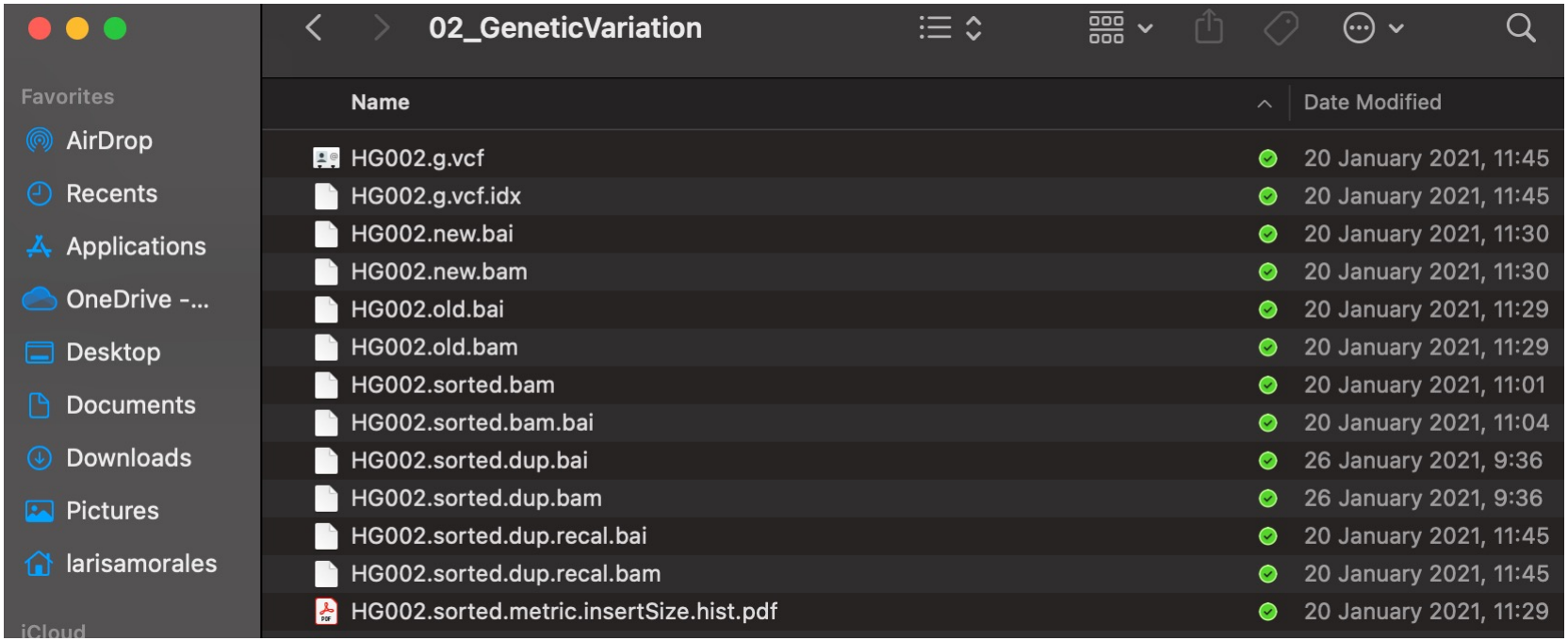
- The core of the operating system
- Manages processes' time, memory and resources
- Handles file storage
- Responds to system calls

The shell

- Let's the user communicate with the kernel
- Command line interpreter (CLI)
- Executes the instructions requested by the user (commands)

In UNIX
everything is a file or a
process!

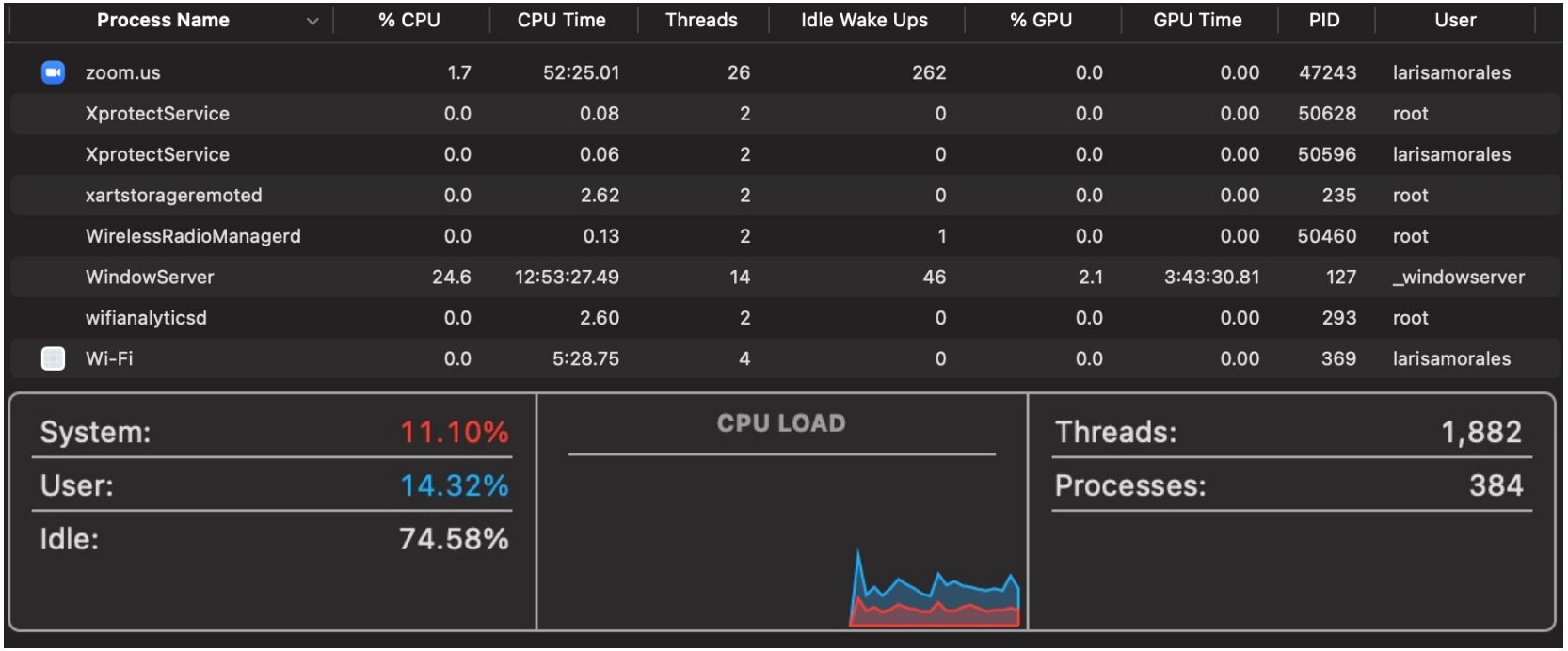
Files


02_GeneticVariation
Favorites
AirDrop
Recents
Applications
OneDrive -...
Desktop
Documents
Downloads
Pictures
larisamorales
iCloud
Name
Date Modified
HG002.g.vcf
20 January 2021, 11:45
HG002.g.vcf.idx
20 January 2021, 11:45
HG002.new.bai
20 January 2021, 11:30
HG002.new.bam
20 January 2021, 11:30
HG002.old.bai
20 January 2021, 11:29
HG002.old.bam
20 January 2021, 11:29
HG002.sorted.bam
20 January 2021, 11:01
HG002.sorted.bam.bai
20 January 2021, 11:04
HG002.sorted.dup.bai
26 January 2021, 9:36
HG002.sorted.dup.bam
26 January 2021, 9:36
HG002.sorted.dup.recal.bai
20 January 2021, 11:45
HG002.sorted.dup.recal.bam
20 January 2021, 11:45
HG002.sorted.metric.insertSize.hist.pdf
20 January 2021, 11:29

Files

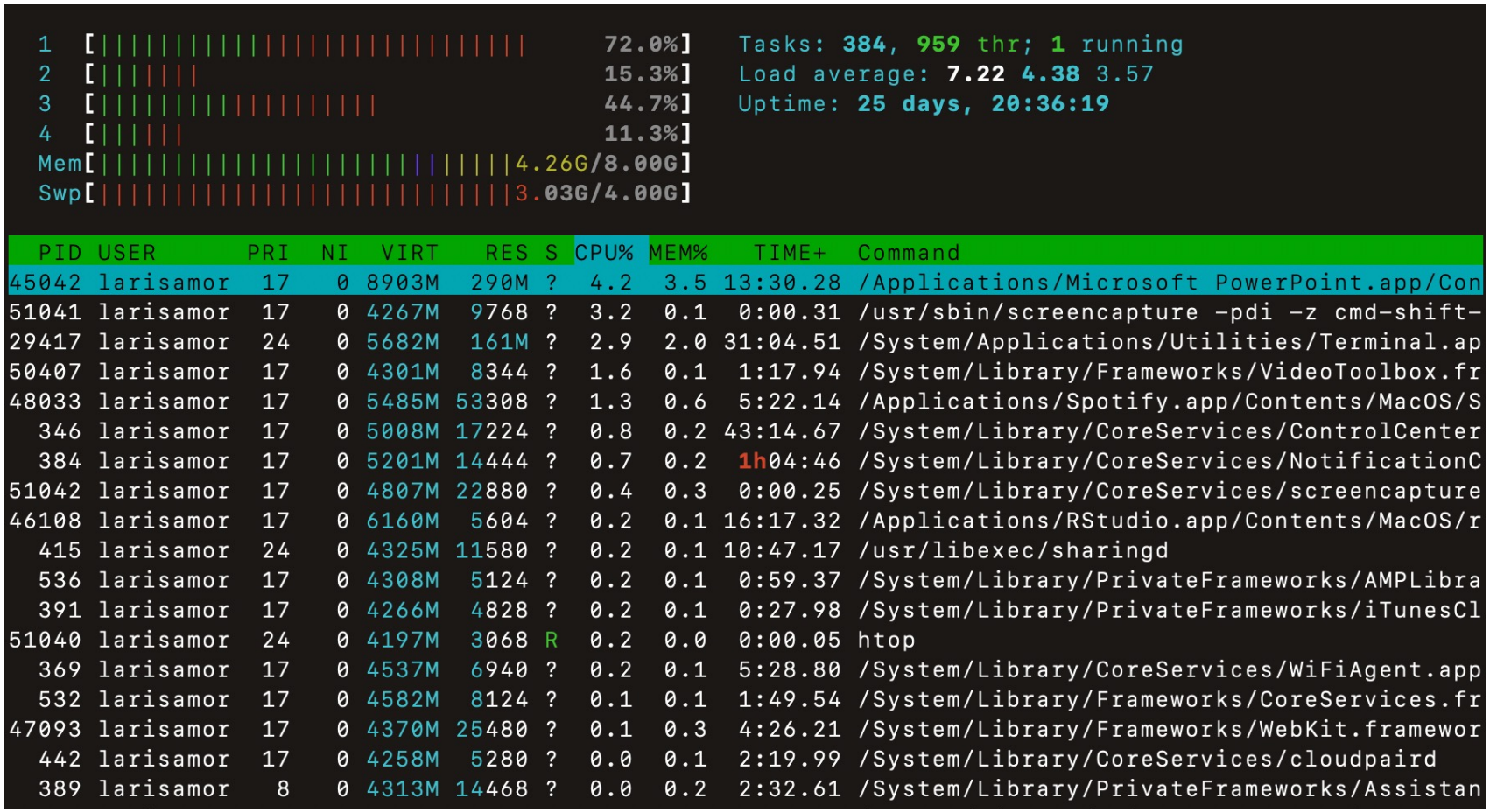
```
total 132464
-rw-r--r--@ 1 larisamorales  staff     75629 Jan 20  2021 HG002.g.vcf
-rw-r--r--@ 1 larisamorales  staff     44048 Jan 20  2021 HG002.g.vcf.idx
-rw-r--r--@ 1 larisamorales  staff     21584 Jan 20  2021 HG002.new.bai
-rw-r--r--@ 1 larisamorales  staff     78169 Jan 20  2021 HG002.new.bam
-rw-r--r--@ 1 larisamorales  staff     21584 Jan 20  2021 HG002.old.bai
-rw-r--r--@ 1 larisamorales  staff     76424 Jan 20  2021 HG002.old.bam
-rw-r-----@ 1 larisamorales  staff  17803945 Jan 20  2021 HG002.sorted.bam
-rw-r-----  1 larisamorales  staff   1350440 Jan 20  2021 HG002.sorted.bam.bai
-rw-r--r--@ 1 larisamorales  staff   1350440 Jan 26  2021 HG002.sorted.dup.bai
-rw-r--r--@ 1 larisamorales  staff  17956229 Jan 26  2021 HG002.sorted.dup.bam
-rw-r--r--@ 1 larisamorales  staff   1350440 Jan 20  2021 HG002.sorted.dup.recal.bai
-rw-r--r--@ 1 larisamorales  staff  24793574 Jan 20  2021 HG002.sorted.dup.recal.bam
-rw-r--r--@ 1 larisamorales  staff     32357 Jan 20  2021 HG002.sorted.metric.insertSize.hist.pdf
```

Processes

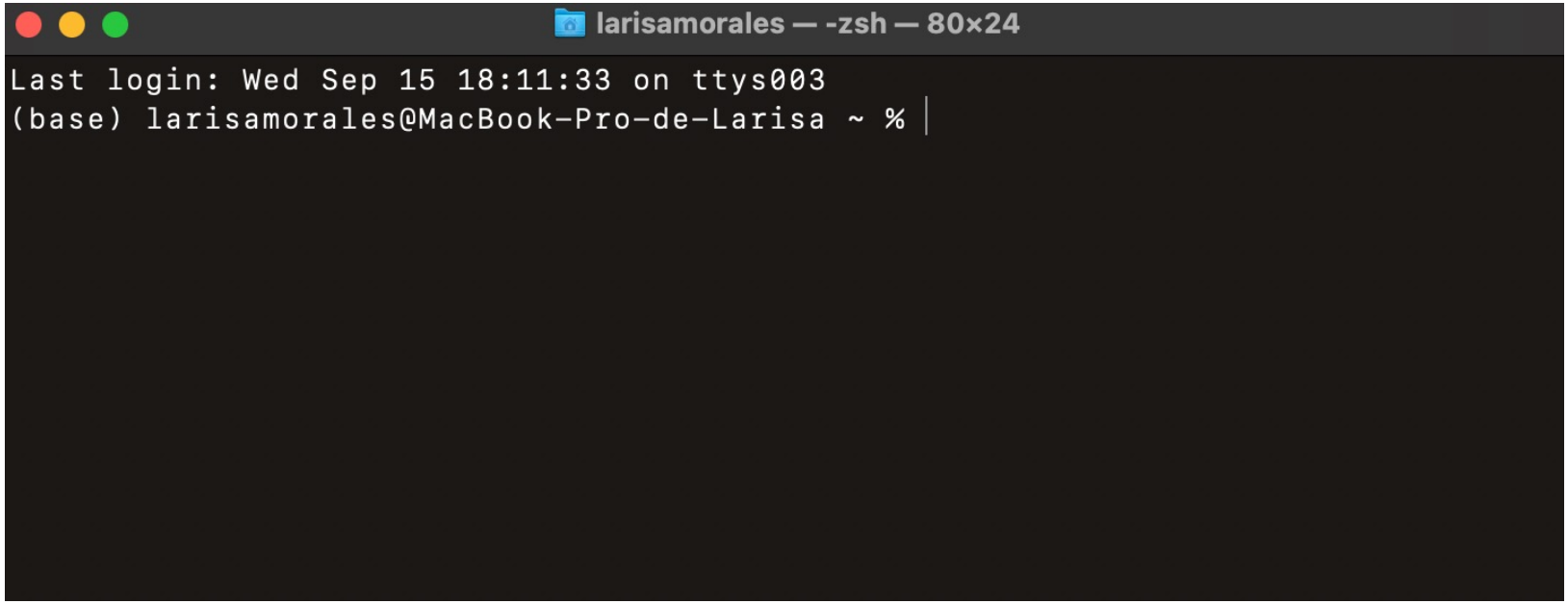


Process Name	% CPU	CPU Time	Threads	Idle Wake Ups	% GPU	GPU Time	PID	User
zoom.us	1.7	52:25.01	26	262	0.0	0.00	47243	larisamorales
XprotectService	0.0	0.08	2	0	0.0	0.00	50628	root
XprotectService	0.0	0.06	2	0	0.0	0.00	50596	larisamorales
xartstorageremoted	0.0	2.62	2	0	0.0	0.00	235	root
WirelessRadioManagerd	0.0	0.13	2	1	0.0	0.00	50460	root
WindowServer	24.6	12:53:27.49	14	46	2.1	3:43:30.81	127	_windowserver
wifianalyticsd	0.0	2.60	2	0	0.0	0.00	293	root
Wi-Fi	0.0	5:28.75	4	0	0.0	0.00	369	larisamorales

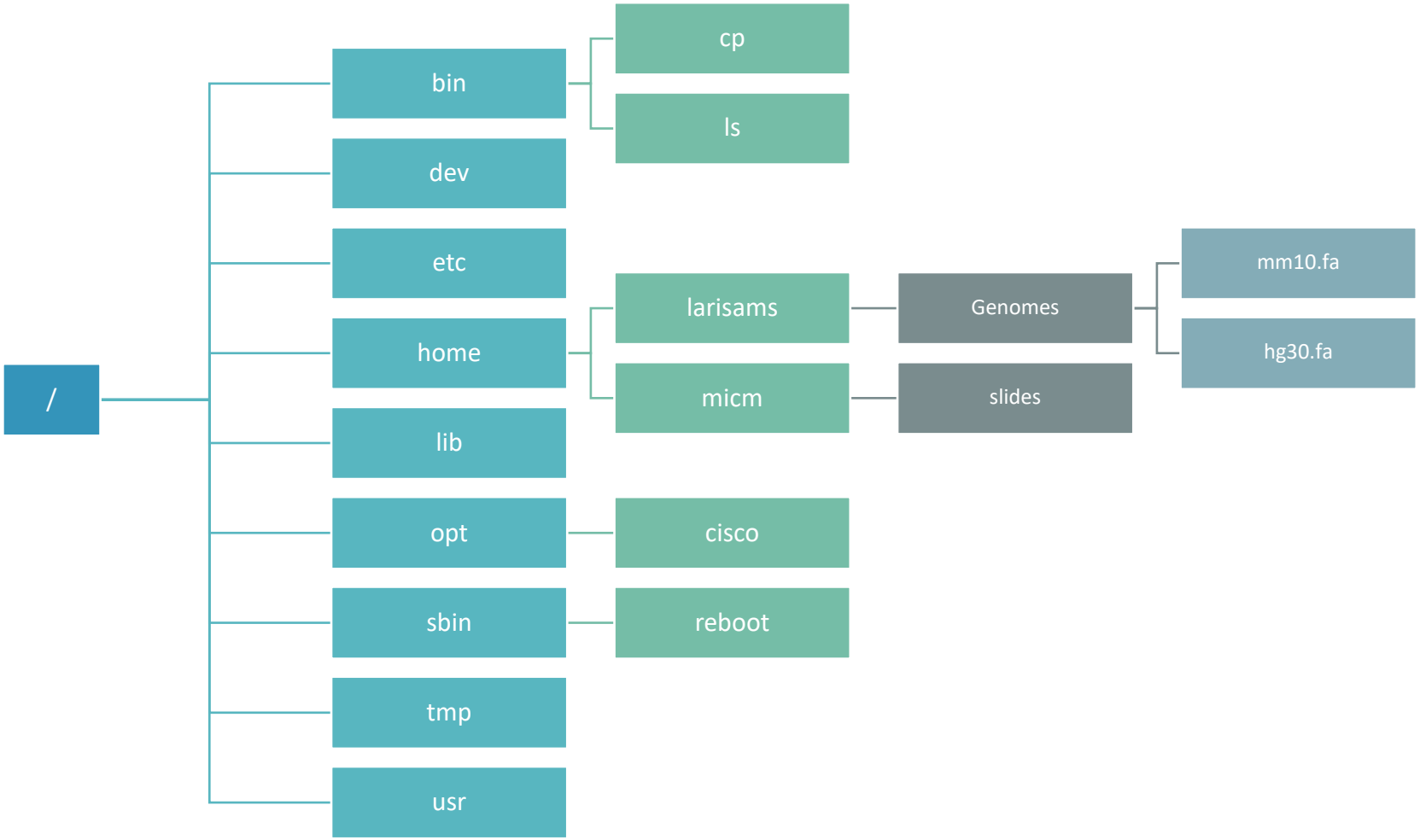
Processes


1 [||||||||||||||||||||||||| 72.0%]
2 [|||||||| 15.3%]
3 [|||||||||||||||||| 44.7%]
4 [|||||| 11.3%]
Mem[||||||||||||||||||||||||||||4.26G/8.00G]
Swp[||||||||||||||||||||||||||||3.03G/4.00G]
Tasks: 384, 959 thr; 1 running
Load average: 7.22 4.38 3.57
Uptime: 25 days, 20:36:19
PID USER PRI NI VIRT RES S CPU% MEM% TIME+ Command
45042 larisamor 17 0 8903M 290M ? 4.2 3.5 13:30.28 /Applications/Microsoft PowerPoint.app/Con
51041 larisamor 17 0 4267M 9768 ? 3.2 0.1 0:00.31 /usr/sbin/screencapture -pdi -z cmd-shift-
29417 larisamor 24 0 5682M 161M ? 2.9 2.0 31:04.51 /System/Applications/Utilities/Terminal.ap
50407 larisamor 17 0 4301M 8344 ? 1.6 0.1 1:17.94 /System/Library/Frameworks/VideoToolbox.fr
48033 larisamor 17 0 5485M 53308 ? 1.3 0.6 5:22.14 /Applications/Spotify.app/Contents/MacOS/S
346 larisamor 17 0 5008M 17224 ? 0.8 0.2 43:14.67 /System/Library/CoreServices/ControlCenter
384 larisamor 17 0 5201M 14444 ? 0.7 0.2 1h04:46 /System/Library/CoreServices/NotificationC
51042 larisamor 17 0 4807M 22880 ? 0.4 0.3 0:00.25 /System/Library/CoreServices/screencapture
46108 larisamor 17 0 6160M 5604 ? 0.2 0.1 16:17.32 /Applications/RStudio.app/Contents/MacOS/r
415 larisamor 24 0 4325M 11580 ? 0.2 0.1 10:47.17 /usr/libexec/sharingd
536 larisamor 17 0 4308M 5124 ? 0.2 0.1 0:59.37 /System/Library/PrivateFrameworks/AMPLibra
391 larisamor 17 0 4266M 4828 ? 0.2 0.1 0:27.98 /System/Library/PrivateFrameworks/iTunesCl
51040 larisamor 24 0 4197M 3068 R 0.2 0.0 0:00.05 htop
369 larisamor 17 0 4537M 6940 ? 0.2 0.1 5:28.80 /System/Library/CoreServices/WiFiAgent.app
532 larisamor 17 0 4582M 8124 ? 0.1 0.1 1:49.54 /System/Library/Frameworks/CoreServices.fr
47093 larisamor 17 0 4370M 25480 ? 0.1 0.3 4:26.21 /System/Library/Frameworks/WebKit.framewor
442 larisamor 17 0 4258M 5280 ? 0.0 0.1 2:19.99 /System/Library/CoreServices/cloudpaird
389 larisamor 8 0 4313M 14468 ? 0.0 0.2 2:32.61 /System/Library/PrivateFrameworks/Assistan

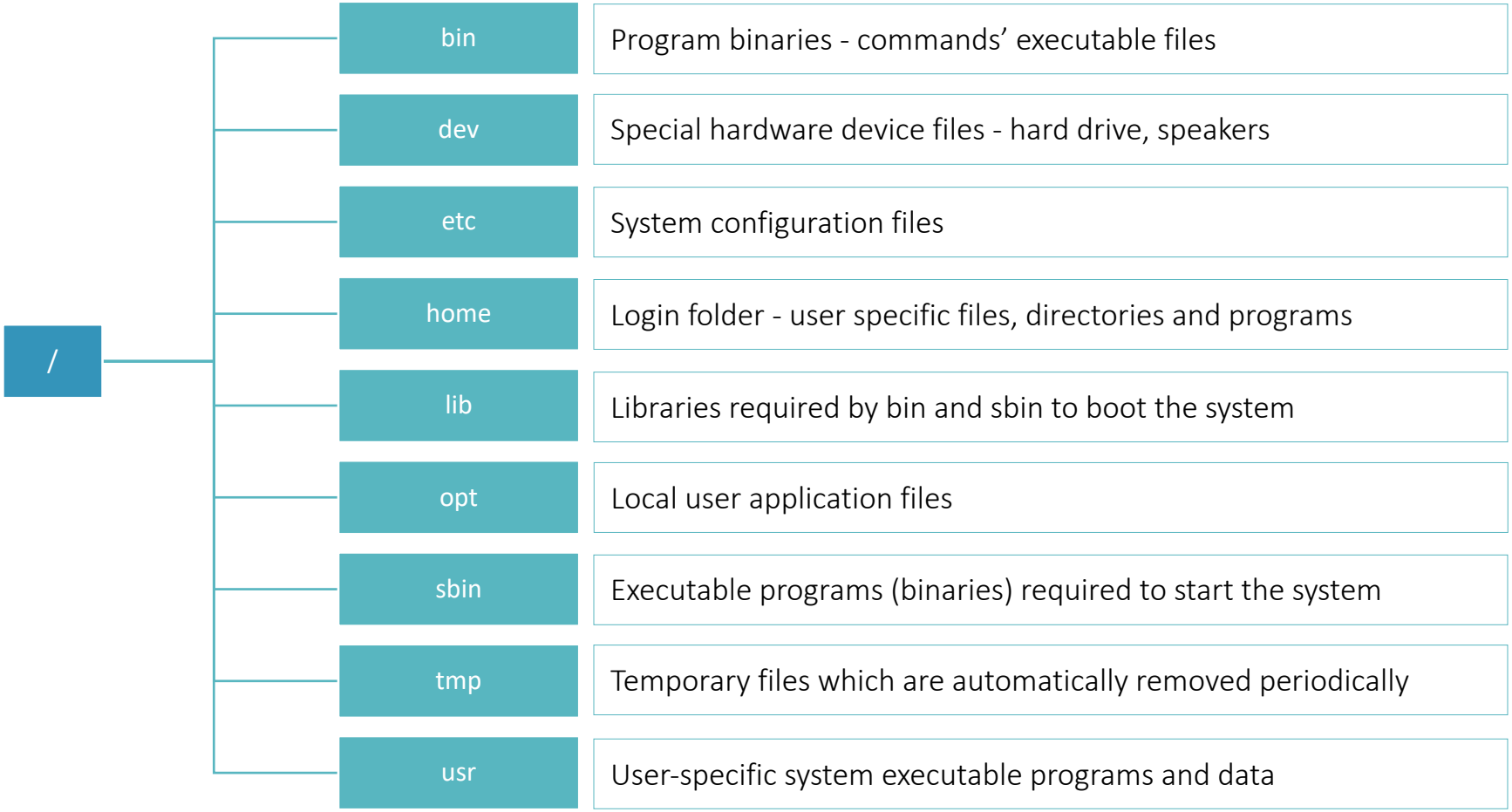
The shell terminal



File system structure



File system structure



Hands on

1. Create a directory called folder1