PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

Introduction to Linux

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Our goal

- Practical introduction to the use of Linux

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- Working using a terminal

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- Environment variables

Historical overview

- Two physical/logical layers:
  - hardware: physical components
  - software: instructions (on a set of data) for a computer
- Originally, instructions written in the physical format
- Idea: write instructions according to rules close to the programmer

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- High-level languages, independent on the hardware

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- UNIX was the name of the project
- Computers communicate each other because they share the same "language" (a part the kernel, see next slides)
- 70s and 80s: UNIX not usable on microcomputers (like PCs), too slow

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- The Linux project has grown into a mature and powerful OS
- Linux is developed and distributed under the GNU General Public License (GPL)
- The GNU project (www.gnu.org) was founded in 1984 with the goal of developing high quality, free software
- GNU is a recursive acronym for "GNU's Not UNIX''

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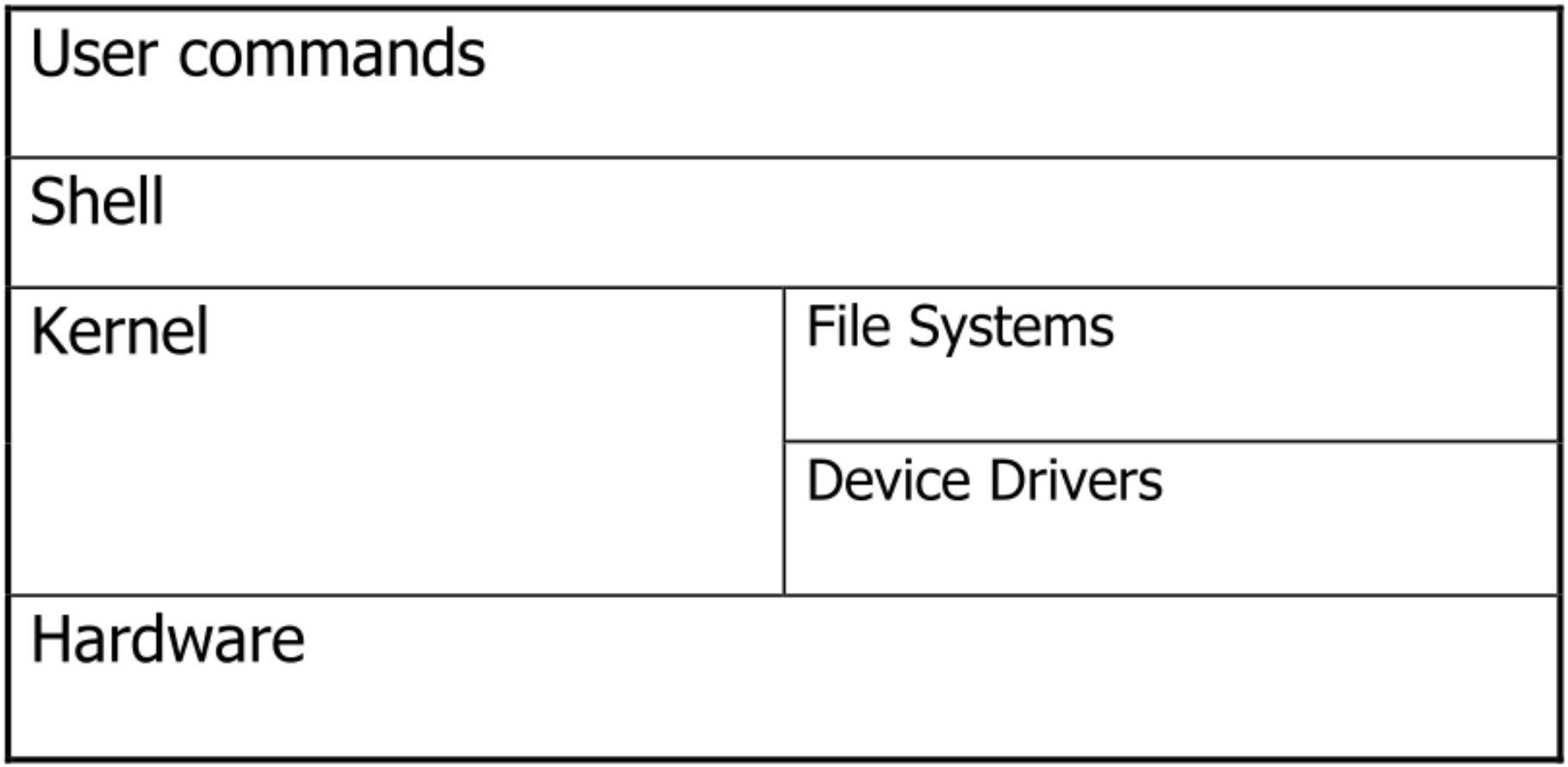
- They all use the Linux kernel:
  - Ubuntu
  - Fedora
  - SuSe Linux
  - Debian
  - CentOS
  - ...
- Compatible each other

The Linux system



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- The kernel manages the hardware resources for the rest of the system

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- Bash is popular and easy to use

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- They allow software to interact with a device driver

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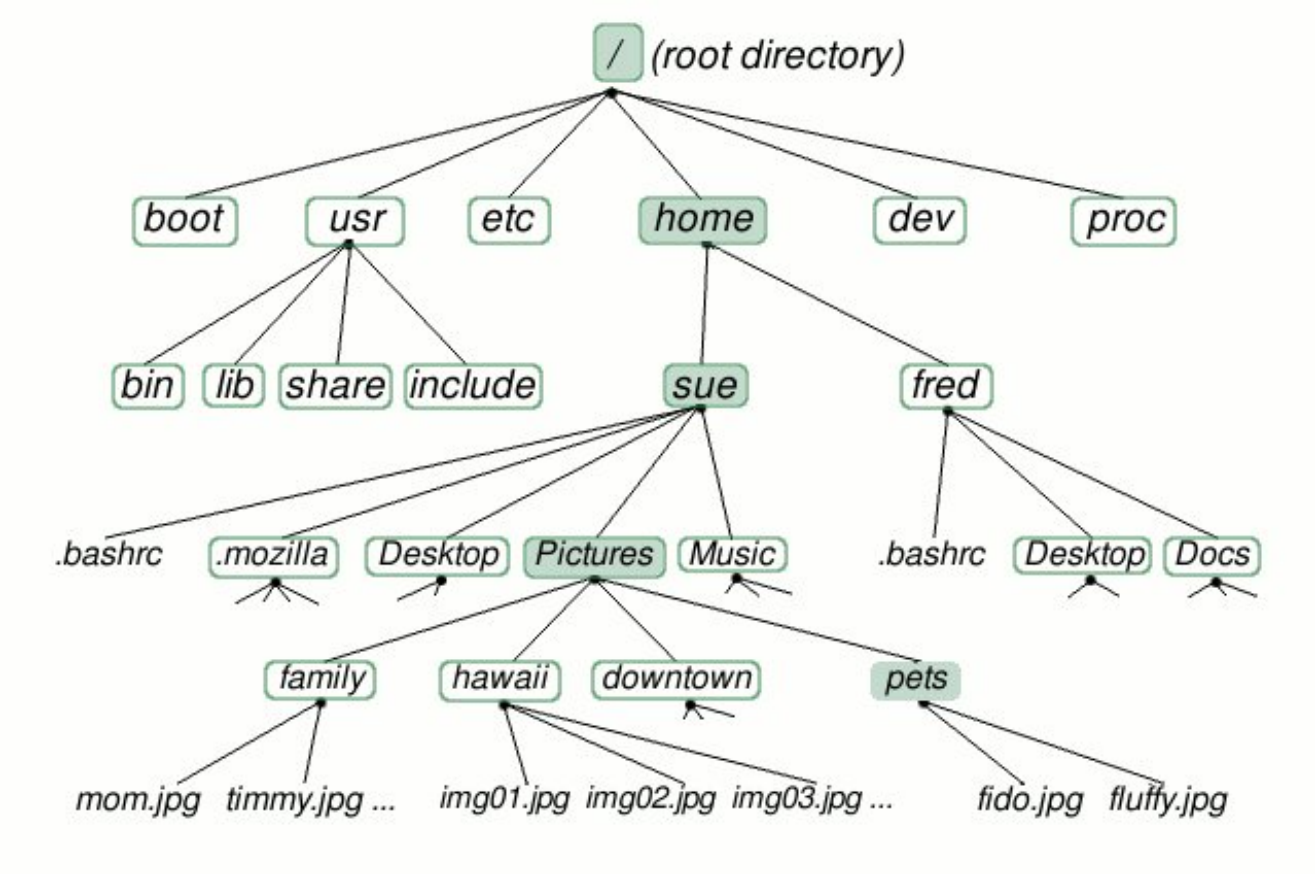
- Only one root (/)



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- /var → various other files: mail, web server etc.
- /opt → extra software

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- To copy files locally, use Bitvise SFTP

How to launch a Linux command

- Synopsis of any Linux command:
  command name options (flags) arguments

Text editors

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- vi (vim) $\rightarrow$ vimtutor
  Open a terminal and type vimtutor

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- man: manual and info of commands

Special file names

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- / → The root directory
- . → The current directory
- .. → The parent (previous) directory
- ~ → My home directory

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- grep: find and display a string in a given file

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- find: searches for files in a directory hierarchy
- bc -l: calculator

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- which: locates a command

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- chmod, chown and chgrp

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