

# CS107 / AC207

## SYSTEMS DEVELOPMENT FOR COMPUTATIONAL SCIENCE

### LECTURE 0

Thursday, September 2nd 2021

# OUTLINE

- Teaching Staff
- Course Policies
- History of Unix and Class Motivation
- Linux

# TEACHING STAFF



- **Head instructor:** Fabian Wermelinger (PhD, ETH Zürich)
- Lecturer in Computational Science
- **Research interests:** Fluid Mechanics, compressible multiphase flows, high performance computing, software development
- **Hobbies:** Vinyl records, cooking (love the wok!), reading, ice hockey

# TEACHING FELLOWS



- Sehaj Chawla (Head TF)
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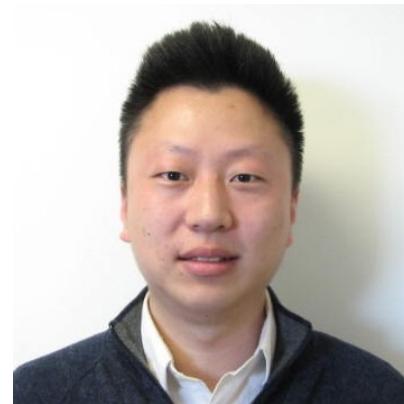
- Connor Capitolo
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# COURSE POLICIES

- **Sign up for Piazza:** <http://piazza.com/harvard/fall2021/cs107>
- **Sign up for GitHub:** <https://www.github.com>
  - Add the teaching staff GitHub user `cs107-sys-dev` as a collaborator on your course repository when you create it. Click on "Settings" and then "Manage Access" in the left panel.
- **Understand roles of main course sites:**
  - Main class site: <https://harvard-iacs.github.io/2021-CS107/>
  - Canvas: Grades
  - Piazza: All course announcements and discussions
  - GitHub: All assignment submissions (homework, project, pair-programming exercises)
- **Helpline:** [cs107-sys-dev@lists.fas.harvard.edu](mailto:cs107-sys-dev@lists.fas.harvard.edu)
- **Homework re-grading requests:** Send them to [cs107-sys-dev@lists.fas.harvard.edu](mailto:cs107-sys-dev@lists.fas.harvard.edu). See the [Course Flow](#) section on the main class site.

We will be working in the command line. If you are a Windows user, please install the "[Windows Subsystem for Linux](#)" on your OS (choose [Ubuntu](#) if you are not sure about which Linux).

Alternatively we provide an Ubuntu based docker image. You can obtain it with

```
$ docker pull cs107sysdev/ubuntu
```

# CLASS COMPONENTS

- 7 Homeworks (25%)
- Participation (25%)
- Final project (50%)

## PARTICIPATION

- Pair-programming sections account for 20% (you must attend one section per week)
- Posting on [Piazza](#) (questioner and/or responder)
- Engaging in class discussions

# PAIR-PROGRAMMING SECTIONS

- We practice coding and command-line usage with pair-programming sections
- There are multiple sections per week, you must attend **one**
- We are using Zoom for these sections
- Pair-programming exercises are not difficult and designed to be completed during the section
- If there were issues and you can not finish during the section, TFs can make a note and you are allowed to hand in the completed exercise **one week after the last section of the cycle**. Make use of the office hours for more help.
- The deadline for handing in PP exercises is one week after the last PP-section of a cycle. The start of a PP cycle is Friday morning (new PP-exercise will be available by then). The last section of that cycle is on the following Thursday morning. *The hand-in deadline is the Thursday in the following week*. Every PP-cycle we have sections on **Friday, Monday, Wednesday and Thursday**.
- See "Pair-Programming Sections" on [our class website](#) for more details
- The tool we are using to connect with programming mates is [tmate](#)

# PROJECT

- You will work in groups of 3 to 4 people (assigned by teaching staff)
- You will add to your library throughout the semester
- The project is guided by two milestones
- Project topic: automatic differentiation
  - Evaluate derivatives of single-variate ( or multi-variate) scalar (or vector) functions
  - Computes the result to *machine precision*
  - Applications: neural networks and back-propagation, Hamiltonian Monte Carlo methods, compute Jacobians (e.g. for coordinate transformations), ...

# PROGRAMMING AND HOMEWORK 0 REFRESHMENT

- The homework, pair-programming exercises and project will be using the Python programming language
- Please spend a few minutes on [Homework 0](#) to refresh your mind (will not be graded)

## C/C++ PROGRAMMING PRIMER

I will be offering a voluntary C/C++ mini-class in calendar **week 42 and 43** if you are interested to dig into the very basics of a widely used programming language. See the [main class site](#) for more info.

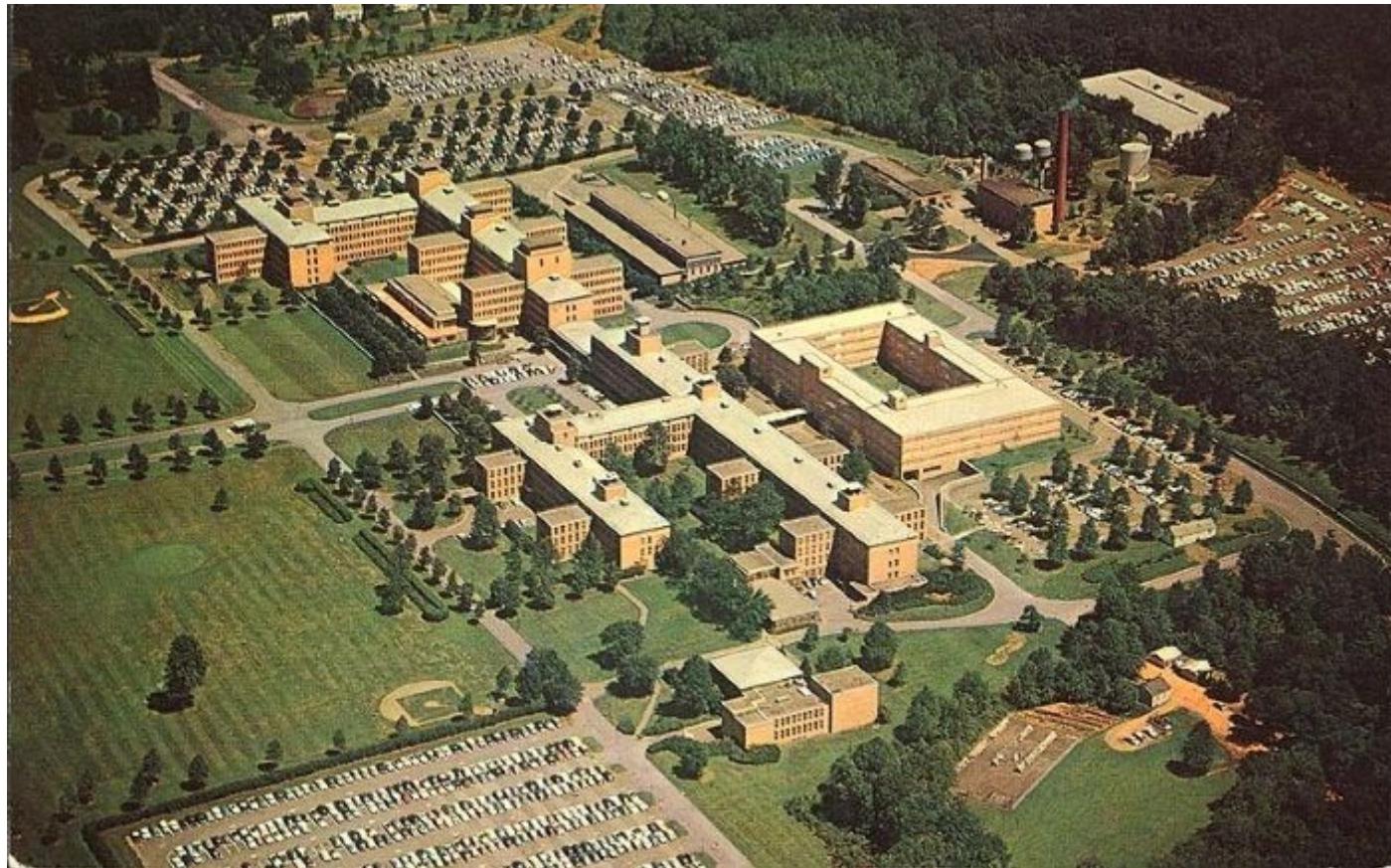
*CS205: If you plan on taking this class you must be familiar with the basics of C or C++ at the beginning of the class.*

# **DO YOU HAVE QUESTIONS ABOUT THE COURSE POLICIES?**

- Class syllabus: <https://harvard-iacs.github.io/2021-CS107/pages/syllabus.html>
- Coursework: <https://harvard-iacs.github.io/2021-CS107/pages/coursework.html>

# HISTORY OF UNIX

# WHERE IT ALL BEGAN...



Bell Labs, Murray Hill, NJ, 1961

# BELL TELEPHONE LABORATORIES

...was what Google is today (somehow)...

...but WAY more influential!

- 9 Nobel Prizes have been awarded for work completed at Bell Labs
- 5 Turing Awards went to Bell Labs, *one was for Unix*
- Transistors have been invented there
- C and C++ originate from Bell Labs
- Information theory ([Claude Shannon](#))
- The Bourne shell ([Steve Bourne](#))
- Error-correcting-code ([Richard Hamming](#))
- The list goes on...

# UNIX

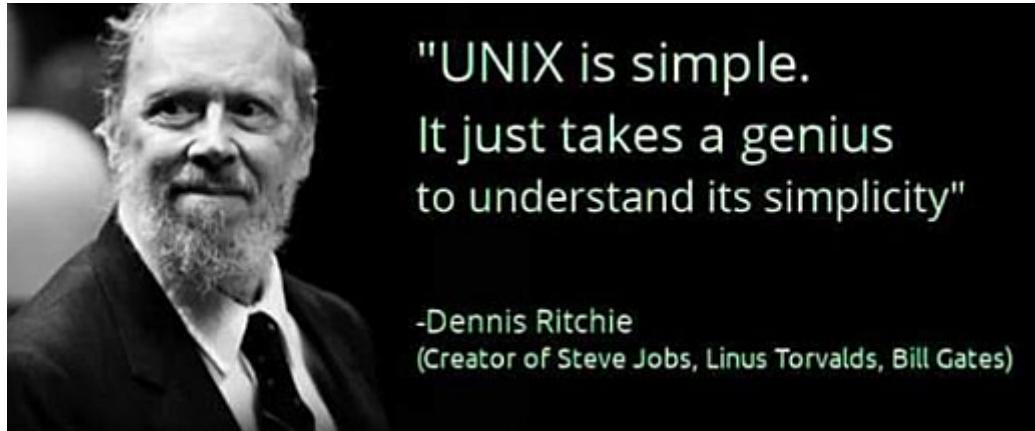
- Is based on the ideas of **MULTICS** (developed at MIT)
- **Time-Sharing Operating System (OS)**: many users *share* the same computing resources at the same time
- **The kernel** is responsible to manage the available resources (hardware) and coordinates the different user requests to grant them computing resources
- Some **interface** is required to communicate with the kernel

# UNIX



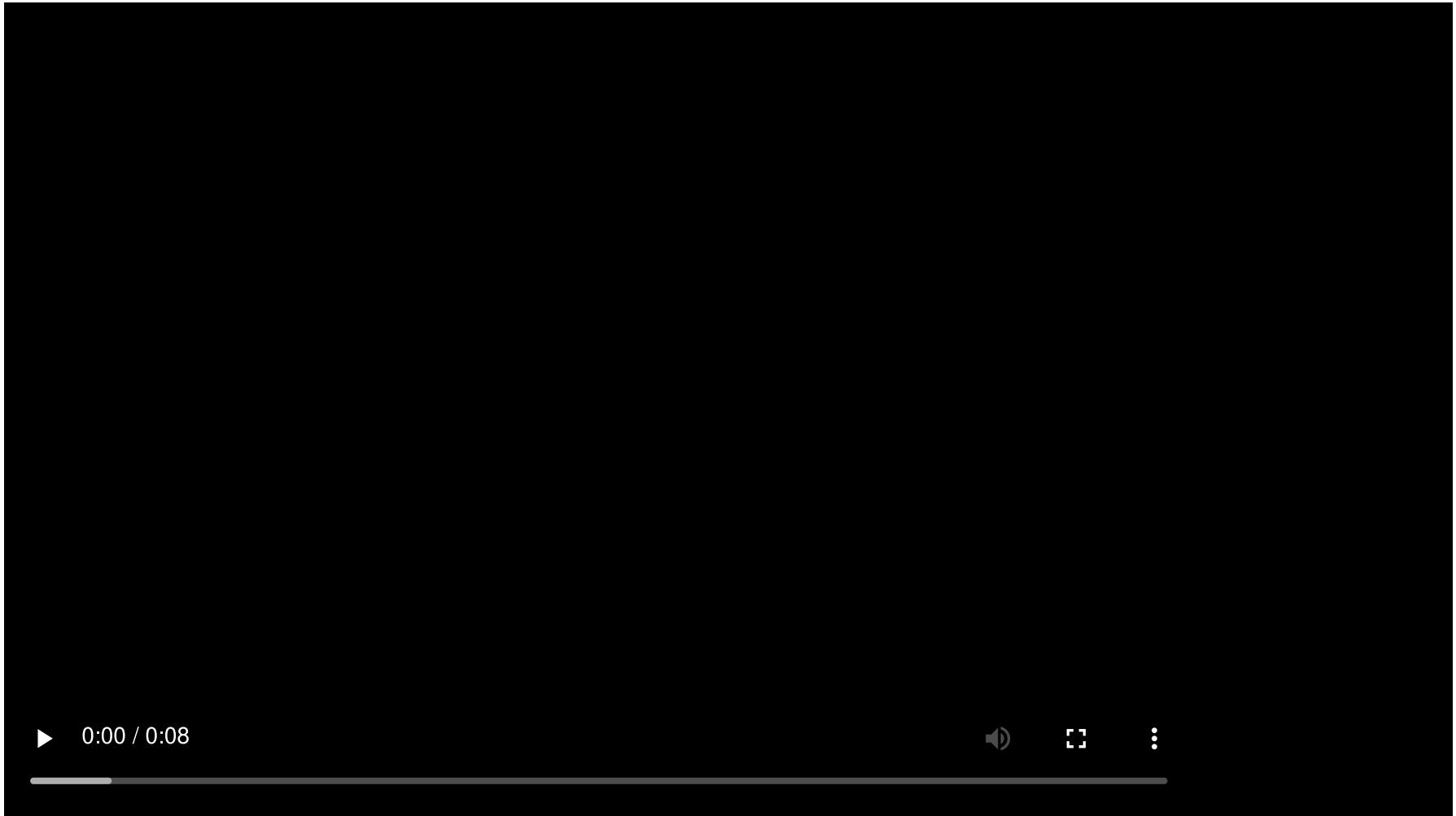
Dennis Ritchie (standing) and Ken Thompson operating a PDP-11 computer with Unix at Bell Labs (1972)

# SO DO WE STILL USE UNIX TODAY?



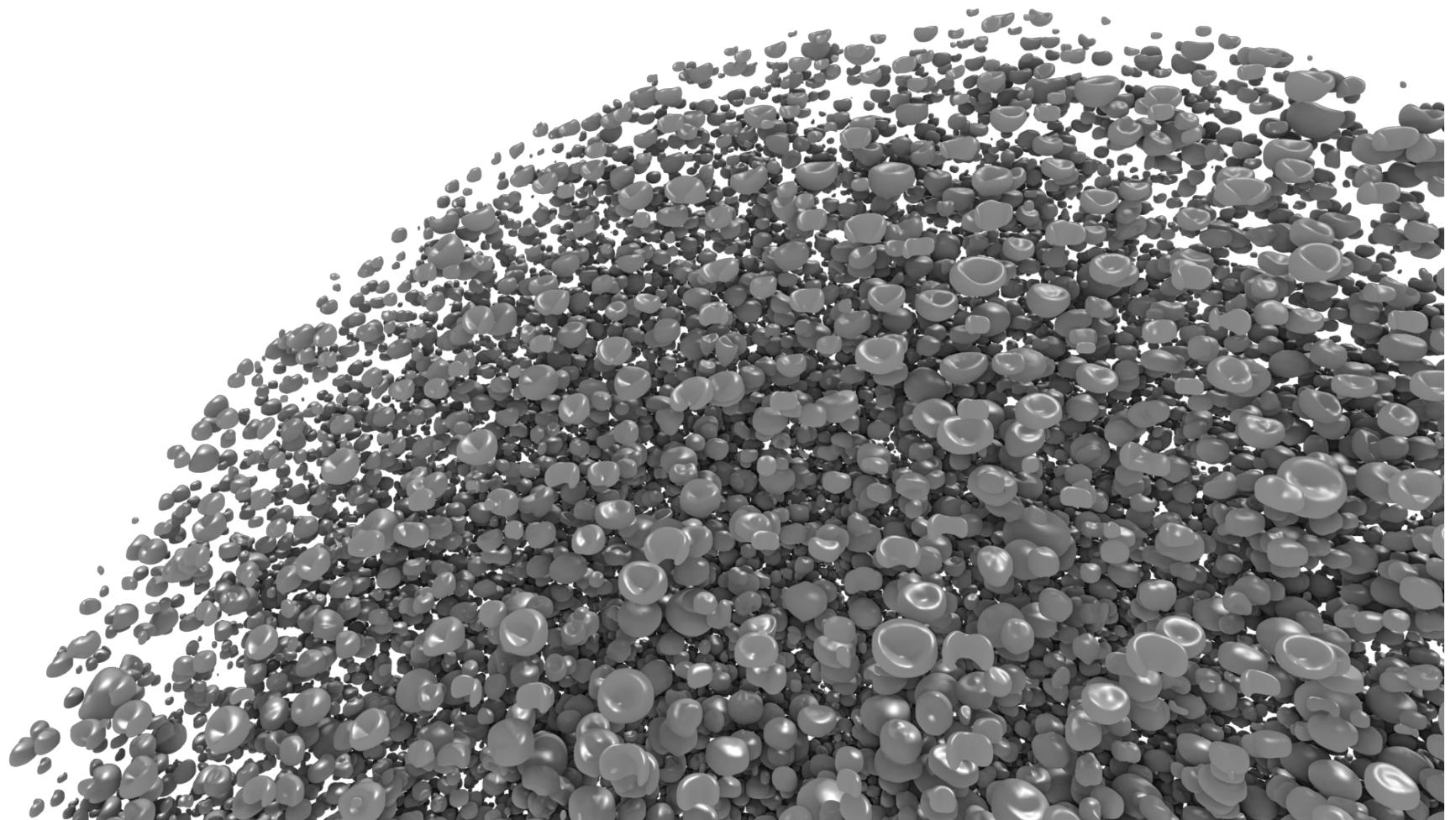
- Do you have an Android or maybe iPhone? You use Unix
- MacBook's OSX is based on Unix
- Stream Netflix? Not without Unix...
- Your research?

# MOTIVATION



Compressible turbulent channel flow with air bubbles

# MOTIVATION



Cloud cavitation collapse with 50'000 air bubbles

# WHY UNIX/LINUX?

- Many research codes are developed and maintained in Unix/Linux systems (including the previous examples)
- Unix/Linux is an ideal development platform (it was designed by Bell Labs for this purpose as well as necessity for time-sharing )
- Very stable and reliable due to its long existence

# WHY UNIX/LINUX?

- The 500 most powerful supercomputers in the world use a Unix-like OS (<https://top500.org/>)
- Remote resources at companies like Google, Facebook or Nvidia use a Unix-like OS almost certainly



Summit Supercomputer (ORN)

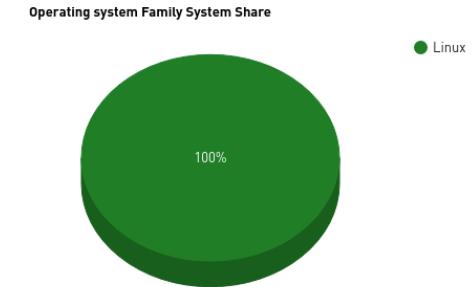
TOP500 Release

June 2021

Category

Operating system Family

Submit

A screenshot of a web interface for the TOP500 supercomputer list. It shows dropdown menus for selecting the release date (set to June 2021) and category (set to "Operating system Family"). A "Submit" button is at the bottom.

Linux OS share for top500

# UNIX VS. LINUX

- Unix is licensed and you actually have to pay to use it.
- Linux was first developed by [Linus Torvalds](#) and first released in 1991.
- Linux is based on the same ideas of Unix, but it *does not* contain any code from Unix. It is licensed under the [GNU General Public License](#) and therefore **free software**.
- You often see GNU/Linux - GNU stands for "GNU is not Unix".

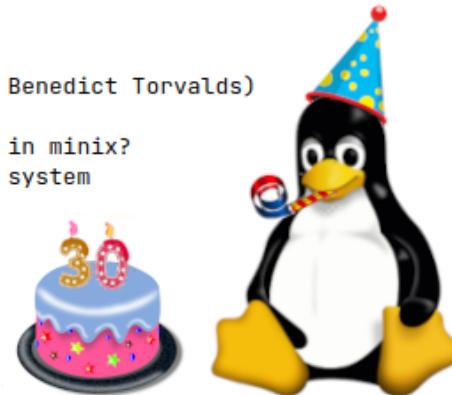
# LINUX

Big Birthday Party last week!

## Happy 30th birthday Linux

From: torvalds@klaava.Helsinki.FI (Linus Benedict Torvalds)  
Newsgroups: comp.os.minix  
Subject: What would you like to see most in minix?  
Summary: small poll for my new operating system  
Message-ID:  
**Date: 25 Aug 91 20:57:08 GMT**  
Organization: University of Helsinki

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. This has been brewing since april, and is starting to get ready. I'd like any feedback on things people like/dislike in minix, as my OS resembles it somewhat (same physical layout of the file-system (due to practical reasons) among other things).

I've currently ported bash(1.08) and gcc(1.40), and things seem to work. This implies that I'll get something practical within a few months, and I'd like to know what features most people would want. Any suggestions are welcome, but I won't promise I'll implement them :-(

Linus (torvalds@kruuna.helsinki.fi)

PS. Yes - it's free of any minix code, and it has a multi-threaded fs. It is NOT portable (uses 386 task switching etc), and it probably never will support anything other than AT-harddisks, as that's all I have :-(.

# LINUX

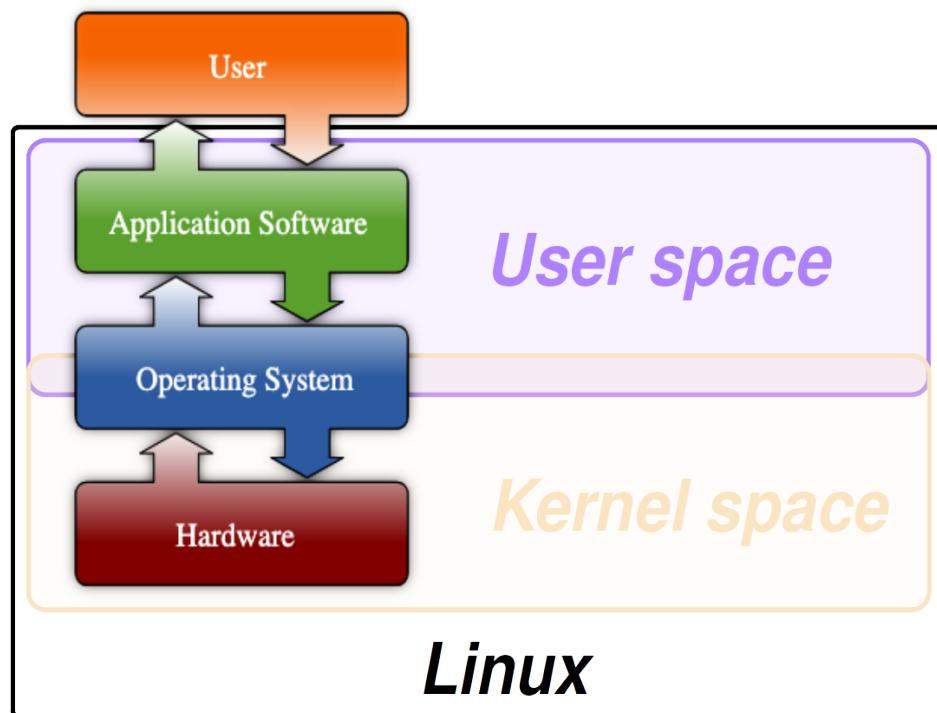
"Linux" is a broad term. In most cases it refers to the **kernel** which is the code responsible to manage hardware resources. This happens in the so called "*kernel space*".

On top of the kernel space, there is a "*user space*" where applications run (with less permissions). Many different **Linux distributions** exist, they combine kernel, libraries and programs to make the system usable. Examples are:

- [Ubuntu](#) (easy to get started with Linux)
- [Debian](#) (completely free, i.e. no proprietary hardware drivers)
- [CentOS](#) (often used on servers or HPC systems)
- [Arch Linux](#) (for the advanced user)

# LINUX

How do you interface with the system?



User *input* and system *output*



Ken and Dennis in 1972

Fun fact: Unix/Linux commands have short names because you had to apply quite some force to type on the Teletype Model 33 terminal...

# LINUX

## How do you interface with the system?

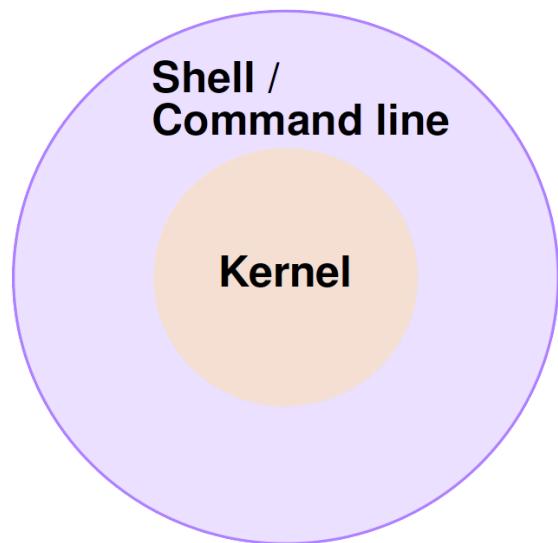
- Today mostly Graphical User Interface (GUI) dominated by **mouse** and **keyboard** input.
- The classical Textual User Interface (TUI) still exists and is dominated by **keyboard** input primarily.

Discuss with your neighbors:

- Which interface do you prefer? GUI or textual?
- Which of the two do you think is more efficient in terms of navigation through files, for example?
- Can you think of advantages a GUI might have over a TUI or vice versa?

# LINUX

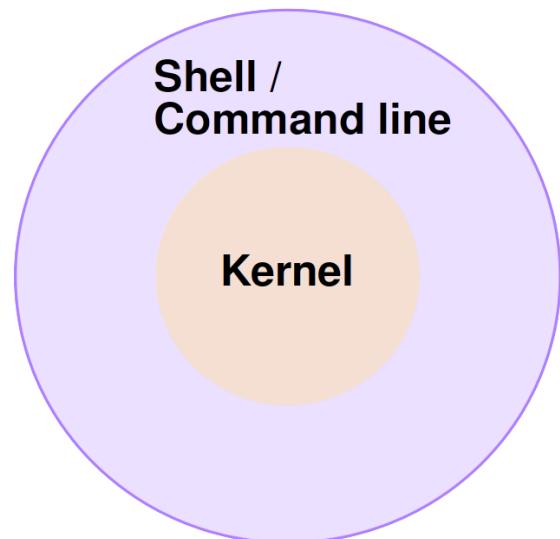
## How do you interface with the system?



- *Applications* that run in user space communicate with the kernel.
- These applications can be isolated programs (e.g. allocating memory in C++ using the new operator involves the kernel) or a textual interface where you can enter commands *interactively*.
- This textual interface is called *command line*, the application where you enter commands is called a *shell*.

# LINUX

## How do you interface with the system?



- Everything in Unix/Linux is either a *process* or a *file*
- A process is a running application
  - Each process has a unique process ID (PID)
  - Processes may have different priorities and can live for a short time or run indefinitely
- A file is a sequence of bytes in memory
  - It stores data (long-term)
  - Files can be created by users or processes
  - Text files (ASCII) or binary files
  - Executable applications/programs are files itself

# THE SHELL

The shell basically does four things repeatedly:

1. Display the prompt and command output
2. Read commands
3. Process commands (can be a sequence of many)
4. Execute commands

Example for listing the contents of a directory:

```
$ ls -la                                # ls is the list command, -la are options
total 16
drwxr-xr-x 4 fabs fabs 4096 Aug 23 12:33 .
drwxr-xr-x 4 fabs fabs 4096 Aug 23 12:32 ..
drwxr-xr-x 2 fabs fabs 4096 Aug 23 12:33 dir1
drwxr-xr-x 2 fabs fabs 4096 Aug 23 12:33 dir2
-rw-r--r-- 1 fabs fabs    0 Aug 23 12:33 file1
-rw-r--r-- 1 fabs fabs    0 Aug 23 12:33 file2
```

# THE SHELL

- All user interaction with the system is through the shell
  - E.g. create files or directories, list all contents of current directory, ...
- There are different kinds of shells, the two main families are:
  - **Bourne shell:** bash, zsh (on Mac OSX) or ksh
  - **C shell:** csh, tcsh
- To remotely access a shell session you can use ssh (secure shell, more on it later)

# COMMON LINUX TERMINOLOGY

Time-sharing introduces *accounts*, which are associated with:

1. A username and password
2. A user and group ID (uid/gid)
3. A home directory (\$HOME)
4. A preference for your login shell

**Example:** who am I and what are my ID's?

```
$ whoami  
fabs  
$ id  
uid=1000(fabs) gid=1000(fabs) groups=1000(fabs),985(video),986(uucp),991(lp),995(audio),998(wheel)
```

# FILES AND DIRECTORIES

- A file simply is a sequence of bytes in memory and it stores your data
- Every file has a *filename* associated to it
- Filenames (or directory names) are *case-sensitive* in Linux:

```
$ ls -l
-rw-r--r-- 1 fabs fabs    0 Aug 23 12:33 file1  # a file
-rw-r--r-- 1 fabs fabs    0 Aug 23 12:33 File1  # not the same file as 'file1'
```

- Directories are a special kind of files (they hold information about other files inside the directory)
- Think of a directory as a container for other files
  - On Mac or Windows they are often called *folders*

# THE LINUX FILESYSTEM

- Unix (and Linux) uses a hierarchical system of files and directories
- The top level in the hierarchy is called the *root*, denoted by a "/" (forward slash)

```
$ ls /  
bin dev etc lib lost+found opt root sbin sys usr  
boot efi home lib64 mnt proc run srv tmp var
```

- */bin*: contains system critical executable programs
  - */etc*: contains system configuration files
  - */root*: home directory of the system administrator
  - */usr*: contains applications accessible to all users
  - */home*: contains the home directories of all users
- The full *pathname* of a file includes all directories up to the root of the file system:

```
$ ls /home/fabs/harvard/CS107/file1  
/home/fabs/harvard/CS107/file1
```

# ABSOLUTE AND RELATIVE PATHS

- **Absolute** pathnames start at the root of the file system. In the following /home/fabs is an absolute path:

```
$ pwd          # pwd: print working directory  
/home/fabs
```

- **Relative** pathnames are specified in relation to the current working directory:

```
$ ls ..        # list the contents of the parent directory which is /home.  
fabs
```

# SPECIAL DIRECTORY NAMES

- The placeholder for the *current* directory is a dot ".":

```
$ pwd      # print the path of the current working directory  
/home/fabs/harvard/CS107  
$ ls .    # list the contents of the current directory  
dir1 dir2 file1 file2
```

- The placeholder for the *parent* directory is ".." (note that 'parent' implies relative):

```
$ ls ..    # list the contents of the parent directory  
CS107
```

- The tilde "~" will expand to your home directory:

```
$ ls ~      # list the contents of the home directory  
Desktop Documents Downloads Music Pictures Public Templates Videos
```

# OVERVIEW OF BASIC LINUX COMMANDS

## UNIX / LINUX CHEAT SHEET



### FILE SYSTEM

**ls** — list items in current directory  
**ls -l** — list items in current directory and show in long format to see permissions, size, and modification date  
**ls -a** — list all items in current directory, including hidden files  
**ls -F** — list all items in current directory and show directories with a slash and executables with a star  
**ls dir** — list all items in directory dir  
**cd dir** — change directory to dir  
**cd ..** — go up one directory  
**cd /** — go to the root directory  
**cd ~** — go to your home directory  
**cd -** — go to the last directory you were just in  
**pwd** — show present working directory  
**mkdir dir** — make directory dir  
**rm file** — remove file  
**rm -r dir** — remove directory dir recursively  
**cp file1 file2** — copy file1 to file2  
**cp -r dir1 dir2** — copy directory dir1 to dir2 recursively  
**mv file1 file2** — move (rename) file1 to file2  
**ln -s file link** — create symbolic link to file  
**touch file** — create or update file  
**cat file** — output the contents of file  
**less file** — view file with page navigation  
**head file** — output the first 10 lines of file  
**tail file** — output the last 10 lines of file  
**tail -f file** — output the contents of file as it grows, starting with the last 10 lines  
**vim file** — edit file  
**alias name 'command'** — create an alias for a command

### SYSTEM

**shutdown** — shut down machine  
**reboot** — restart machine  
**date** — show the current date and time  
**whoami** — who you are logged in as  
**finger user** — display information about user  
**man command** — show the manual for command  
**df** — show disk usage  
**du** — show directory space usage  
**free** — show memory and swap usage  
**whereis app** — show possible locations of app  
**which app** — show which app will be run by default

### COMPRESSION

**tar cf file.tar files** — create a tar named file.tar containing files  
**tar xf file.tar** — extract the files from file.tar  
**tar czf file.tar.gz files** — create a tar with Gzip compression  
**tar xzf file.tar.gz** — extract a tar using Gzip  
**gzip file** — compresses file and renames it to file.gz  
**gzip -d file.gz** — decompresses file.gz back to file

### PROCESS MANAGEMENT

**ps** — display your currently active processes  
**top** — display all running processes  
**kill pid** — kill process id pid  
**kill -9 pid** — force kill process id pid

### SEARCHING

**grep pattern files** — search for pattern in files  
**grep -r pattern dir** — search recursively for pattern in dir  
**grep -rn pattern dir** — search recursively for pattern in dir and show the line number found  
**grep -r pattern dir --include='\*.ext'** — search recursively for pattern in dir and only search in files with .ext extension  
**command | grep pattern** — search for pattern in the output of command  
**find file** — find all instances of file in real system  
**locate file** — find all instances of file using indexed database built from the updatedb command. Much faster than find  
**sed -i 's/day/night/g' file** — find all occurrences of day in a file and replace them with night - s means substitute and g means global - sed also supports regular expressions

### PERMISSIONS

**ls -l** — list items in current directory and show permissions  
**chmod ugo file** — change permissions of file to ugo - u is the user's permissions, g is the group's permissions, and o is everyone else's permissions. The values of u, g, and o can be any number between 0 and 7.  
7 — full permissions  
6 — read and write only  
5 — read and execute only  
4 — read only  
3 — write and execute only  
2 — write only  
1 — execute only  
0 — no permissions

**chmod 600 file** — you can read and write - good for files  
**chmod 700 file** — you can read, write, and execute - good for scripts  
**chmod 644 file** — you can read and write, and everyone else can only read - good for web pages  
**chmod 755 file** — you can read, write, and execute, and everyone else can read and execute - good for programs that you want to share

### NETWORKING

**wget file** — download a file  
**curl file** — download a file  
**scp user@host:file dir** — secure copy a file from remote server to the dir directory on your machine  
**scp file user@host:dir** — secure copy a file from your machine to the dir directory on a remote server  
**scp -r user@host:dir dir** — secure copy the directory dir from remote server to the directory dir on your machine  
**ssh user@host** — connect to host as user  
**ssh -p port user@host** — connect to host on port as user  
**ssh-copy-id user@host** — add your key to host for user to enable a keyed or passwordless login  
**ping host** — ping host and output results  
**whois domain** — get information for domain  
**dig domain** — get DNS information for domain  
**dig -x host** — reverse lookup host  
**lsof -i tcp:1337** — list all processes running on port 1337

### SHORTCUTS

**ctrl+a** — move cursor to beginning of line  
**ctrl+f** — move cursor to end of line  
**alt+f** — move cursor forward 1 word  
**alt+b** — move cursor backward 1 word

# COMMANDS YOU SHOULD GET FAMILIAR WITH

`ls` — list items in current directory

`ls -l` — list items in current directory and show in long format to see permissions, size, and modification date

`ls -a` — list all items in current directory, including hidden files

`ls -F` — list all items in current directory and show directories with a slash and executables with a star

`ls dir` — list all items in directory dir

`cd dir` — change directory to dir

`cd ..` — go up one directory

`cd /` — go to the root directory

`cd ~` — go to your home directory

`cd -` — go to the last directory you were just in

`pwd` — show present working directory

`mkdir dir` — make directory dir

`rm file` — remove file

`rm -r dir` — remove directory dir recursively

`cp file1 file2` — copy file1 to file2

`cp -r dir1 dir2` — copy directory dir1 to dir2 recursively

`mv file1 file2` — move (rename) file1 to file2

`ln -s file link` — create symbolic link to file

`touch file` — create or update file

`cat file` — output the contents of file

`less file` — view file with page navigation

`head file` — output the first 10 lines of file

`tail file` — output the last 10 lines of file

`tail -f file` — output the contents of file as it grows, starting with the last 10 lines

`vim file` — edit file

`alias name 'command'` — create an alias for a command

# THE LIST COMMAND

The list command "ls" displays the contents of directories:

```
$ man ls # get the manual page for ls
LS(1)                               User Commands                               LS(1)

NAME
    ls - list directory contents

SYNOPSIS
    ls [OPTION]... [FILE]...

DESCRIPTION
    List information about the FILEs (the current directory by default). Sort entries
    alphabetically if none of -cftuvSUX nor --sort is specified.
...
...
```

## Some ls examples:

ls	List files in the current directory
ls .	List files in the current directory
ls ..	List files in the parent directory
ls ~	List files in your home directory
ls /	List files in the root directory
ls /usr	List files in the /usr directory

# COMMAND LINE OPTIONS

- Almost all commands use *options* to customize their behavior.
- There are many options for the `ls` command, for example:
  - `-l`: *long* format
  - `-a`: *all*, shows hidden files in addition to regular files

```
$ ls
dir1 dir2 file1 file2
$ ls -a # note: hidden filenames start with a '.'
. .. dir1 dir2 file1 file2 .hidden_file
$ ls -la
total 16
drwxr-xr-x 4 fabs fabs 4096 Aug 23 16:05 .
drwxr-xr-x 4 fabs fabs 4096 Aug 23 12:32 ..
drwxr-xr-x 2 fabs fabs 4096 Aug 23 12:33 dir1
-rw-r--r-- 1 fabs fabs     0 Aug 23 12:33 file1
-rw-r--r-- 1 fabs fabs     0 Aug 23 16:05 .hidden_file
```

- The `drwxr-xr-x` or `-rw-r--r--` describe the file type and permissions relative to the file owner, group and everybody else.  
**Why do we care about permissions? Because of time-sharing system - there are other users too...**

# GENERAL COMMAND LINE FOR THE LIST COMMAND

- The general form is always given in the man page:

```
$ man ls # get the manual page for ls
LS(1)                               User Commands                               LS(1)

NAME
    ls - list directory contents

SYNOPSIS
    ls [OPTION]... [FILE]...
```

- The arguments in [...] brackets are *optional*. If arguments are required, they will not be enclosed in such brackets.
- Options can be combined, e.g., "ls -l -a" is the same as "ls -la".
- The ellipsis "..." mean that this argument may occur multiple times. For example, "ls -l . ~ /usr" lists the **current**, **home** and **/usr** directories in long format.

# RECAP

- Course intro
- History of Bell Labs and Unix
- Linux and different ways to interface with the system
- Looked at common Unix/Linux terminology
- Intro to the ls command and its options and arguments
- All Linux commands are documented in manual pages (more next week)

## SUGGESTED OPTIONAL READING/LISTENING

- B. W. Kernighan, *UNIX: A History and a Memoir*, Independently published, 2019
- Check out Episode 1 and 2 of Season 1 from the [Command Line Heroes](#) podcast

# UPCOMING SEMINAR SERIES AT IACS

The IACS hosts Seminar Series with interesting talks from researchers in Computational Science!

- Checkout the upcoming events here: <https://iacs.seas.harvard.edu/>
- They are free to join and will be held via Zoom
- You need to register to attend a series

*Upcoming talk is by Katherine Yelick of UC Berkeley*