Introduction

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FAU

2025-10-07: Computers in Geosciences

GeoZentrum Nordbayern

Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
Instructor	Chris and Sebastian	Adam	Adam and Wolfgang	Adam	Adam
Morning	9:30-12:00	9:00-11:00 **11:00 – 12:00 Msc Welcome event @ GeoZentrum!**	9:00 – 16:00	9:00-12:00	9:00-12:00
Afternoon	13:00-16:00	13:00-16:00	13:00-16:00 (Wolfgang)	13:00-16:00	13:00-16:00

https://tinyurl.com/ywwwxmey

Objectives

1. Experience with **raster** and **vector graphics**
2. Better understand **programming** and FOSS
3. Execute, understand, and modify **R scripts**
4. Write **basic R code**, see the capabilities
5. Essentials of the **BASH** Shell/Language

Discussions

1. What do we/you use computers for?

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2. In (geo)sciences what do you use computers for? What kind of software?

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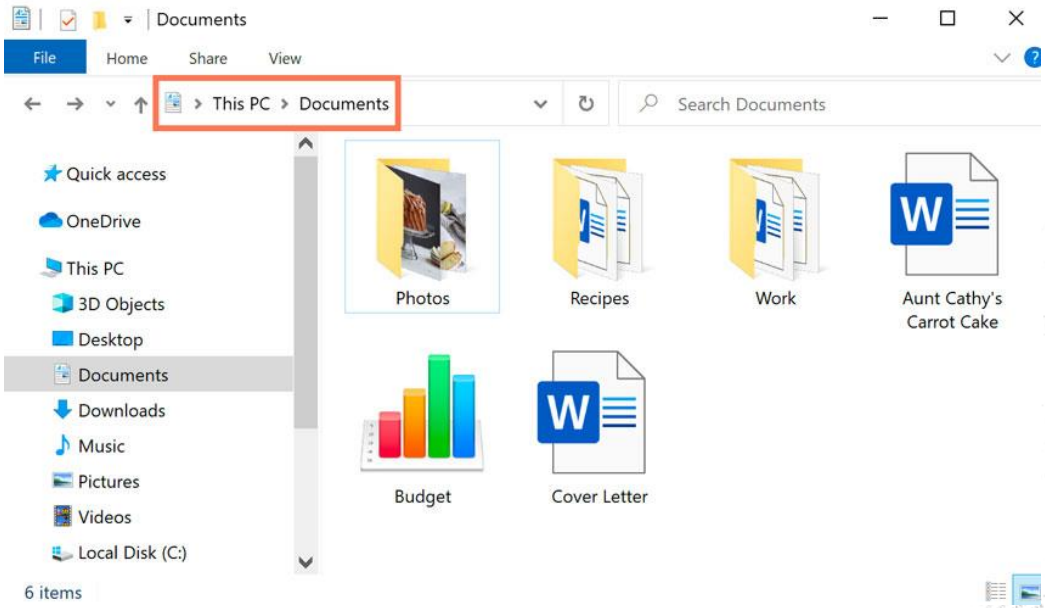
1. What do we/you use computers for?

2. In (geo)sciences what do you use computers for? What kind of software?

Presentation
Publishing, Typesetting
Multimedia consumption
Internet Browsing
Email, Communication
Graphics Vector, Raster, 3D
Software Development
Data Processing/Analysis
Statistical Analysis and Modelling
Computation
GIS
Web Design
File management

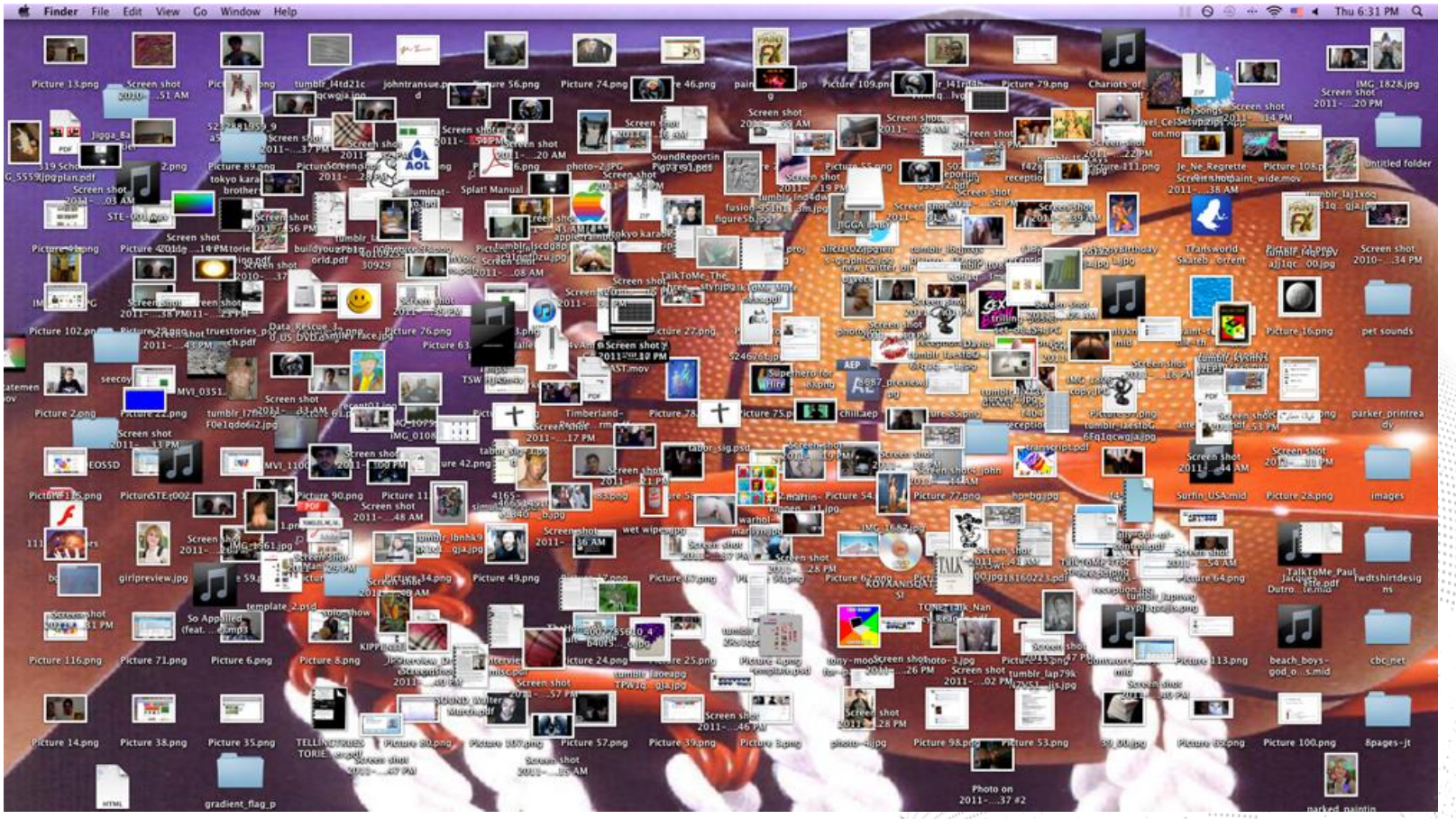
Files and directories

The practical point of view



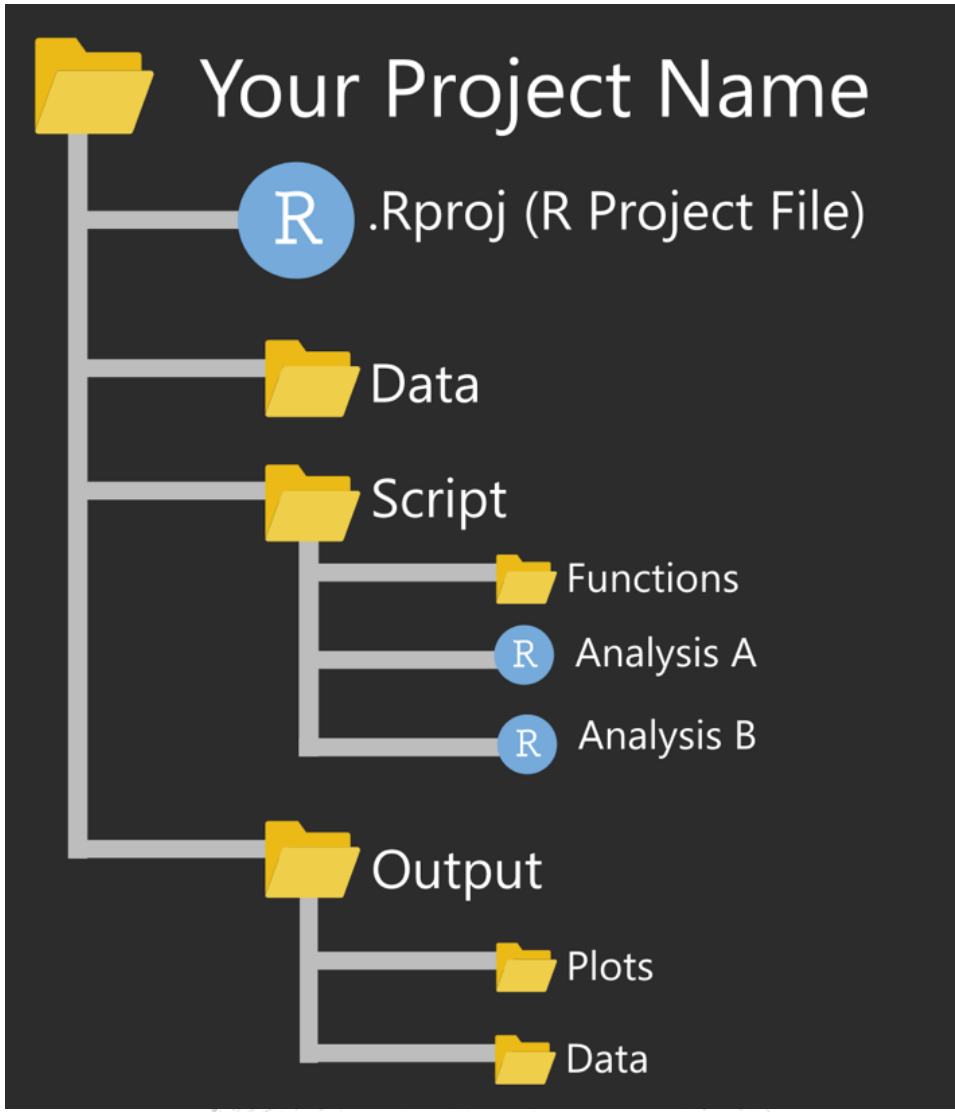
(Almost) everything that you work on is in a file.

Avoid this!

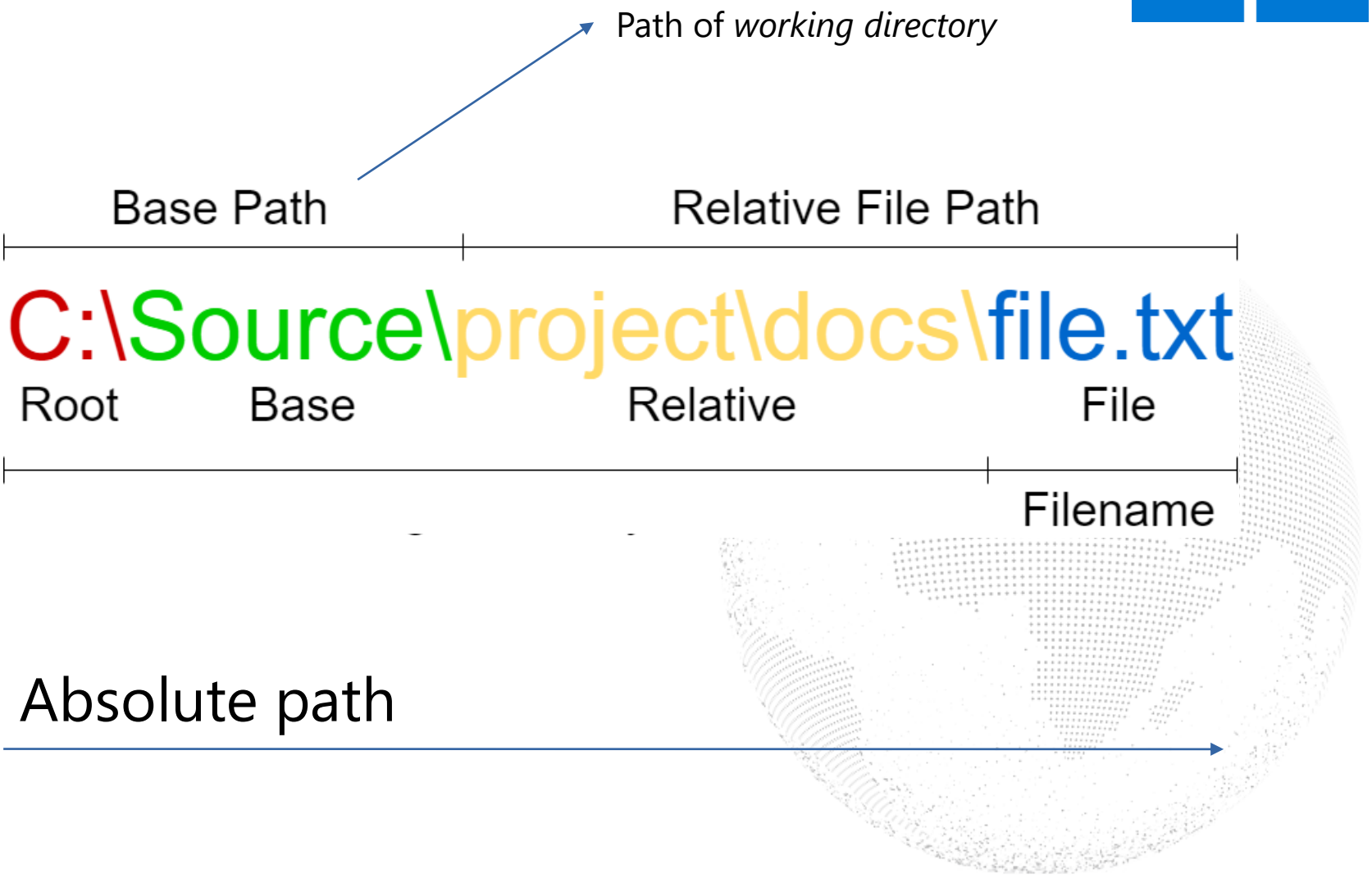


Solution: hierarchy

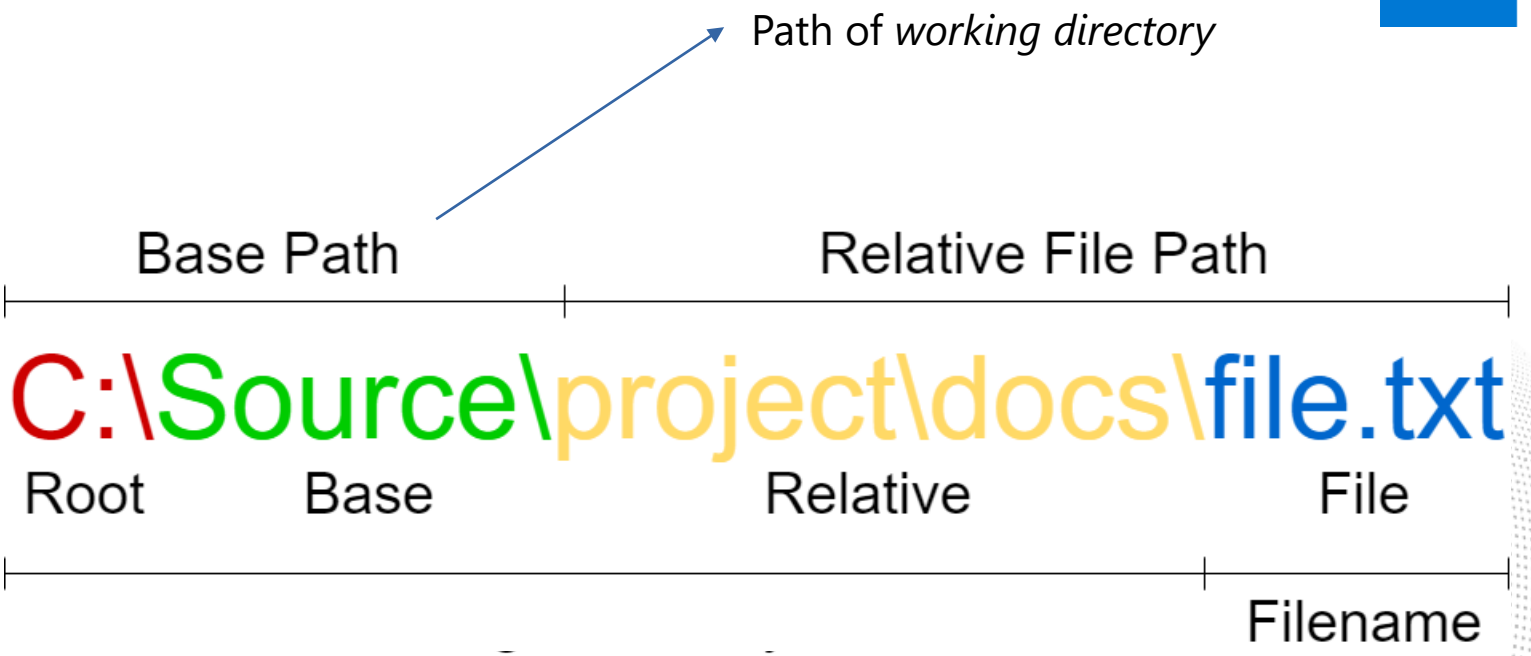
- **Regular file**: cannot contain other files
- **Directory**: special file, does not store anything but **other files (can be empty)**
- Directories **do not actually contain data,** this is just an abstract representation, just references to other files
- Copying vs Moving (renaming) speed difference!



The file's path



The file's path



Note: Things are easier if this does not have any spaces!

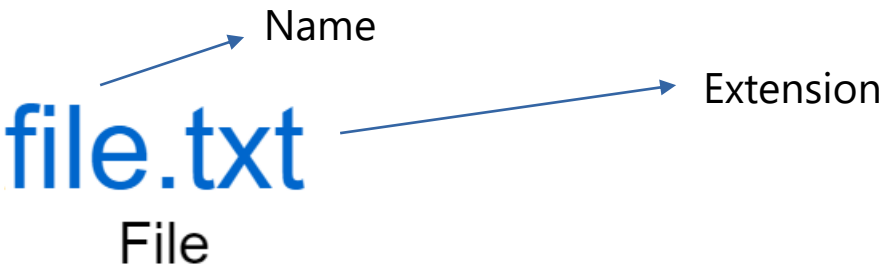
No Spaces?

- Systematic rules to represent text with one word
- Variable/Object names - Language dependent conventions

Naming Convention	Example Format
Pascal Case	PascalCase
Camel Case	camelCase
Snake Case	snake_case
Kebab Case	kebab-case
Flat Case	flatcase
Upper Flat Case	UPPERFLATCASE
Pascal Snake Case	Pascal_Snake_Case
Camel Snake Case	camel_Snake_Case
Screaming Snake Case	SCREAMING_SNAKE_CASE
Train Case	Train-Case
Cobol Case	COBOL-CASE

The file's extension

Files don't need to have an extension!

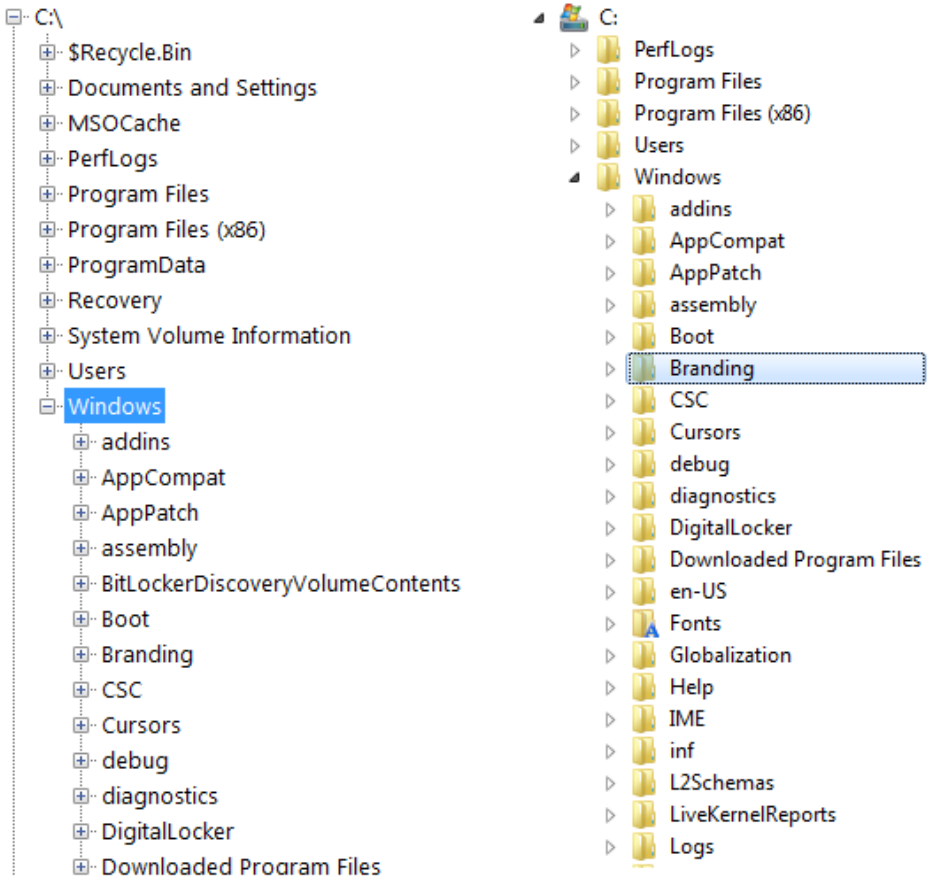


a)The file extension indicates to the operating system (and you!) how to handle the file.

b) This is not a hard constraint! Changing the extension will not make the file's contents different in any way!

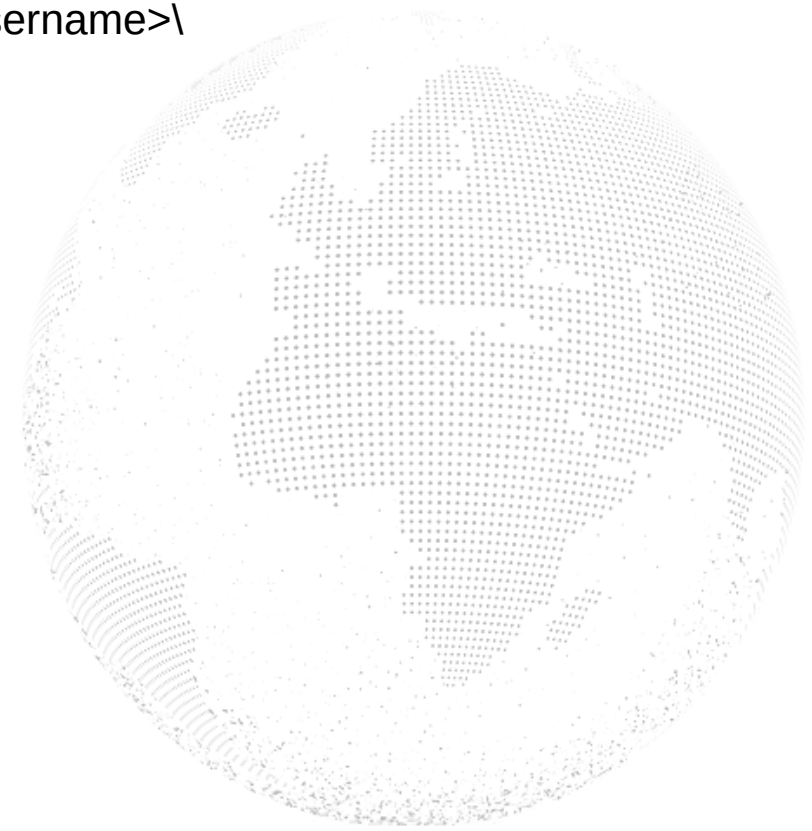
Windows - files

- Files are data items on storage devices
- Multiple roots e.g. C:, each correspond to a **partition**
- Paths use the characteristic **backslash** \ character to depict nestedness
- Directories are called “**Folders**”
- Executables: filename.exe
- Total path to “Branding”:
- `C:\Windows\Branding`
- Case insensitive!
- FAT32 and NTFS



Windows - files

- Paths Always present, if you don’t see it
- To make the directory hierarchy novice-friendly, Windows creates “aliases” that look nice, but are not functional!
- User’s home directory is by default: C:\Users\<Username>\
- Desktop: C:\Users\<Username>\Desktop
- The program to view files is “Explorer.exe”

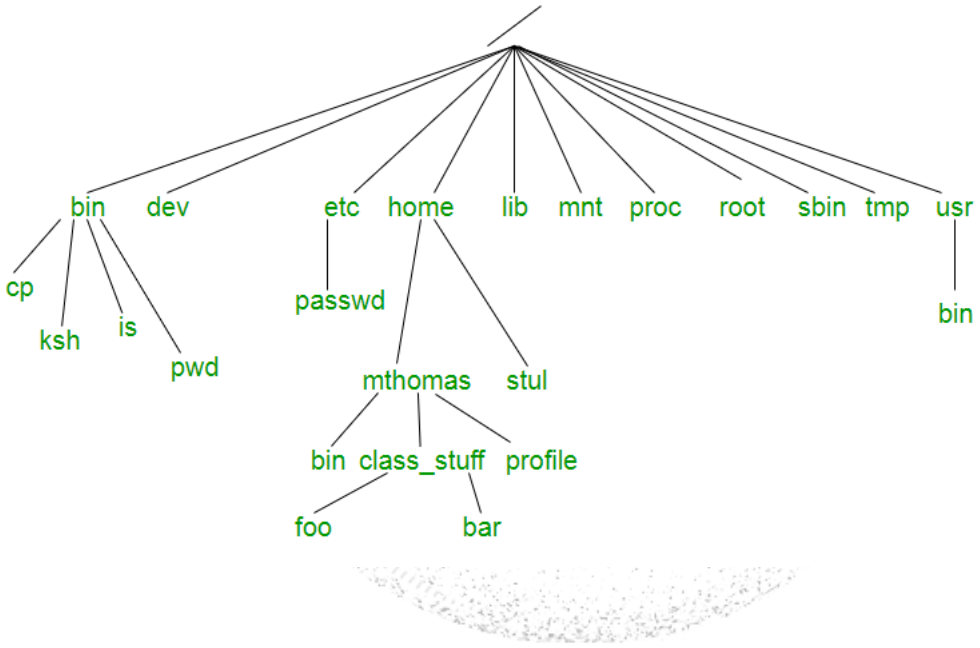


UNIX File system

UNIX®
A Standard of The Open Group®

- Shared for UNIX and UNIX-like systems (GNU/Linux, macOS, Android)
- More abstract: everything in the computer is represented by a file
- ~ Standard directory names
- Nestedness coded with forward slash : /
- File can be anything
- Executables don’t have extensions
- Complete path to “bar”
- `/home/mthomas/class_stuff/bar`
- Case sensitive!

macOS



Archives

Excellent for storing and transmitting files – entire directory structures

Two processes:

a) creating an **archive**: one file from multiple files

b) employing **lossless compression**: algorithm to make decrease the size of a file

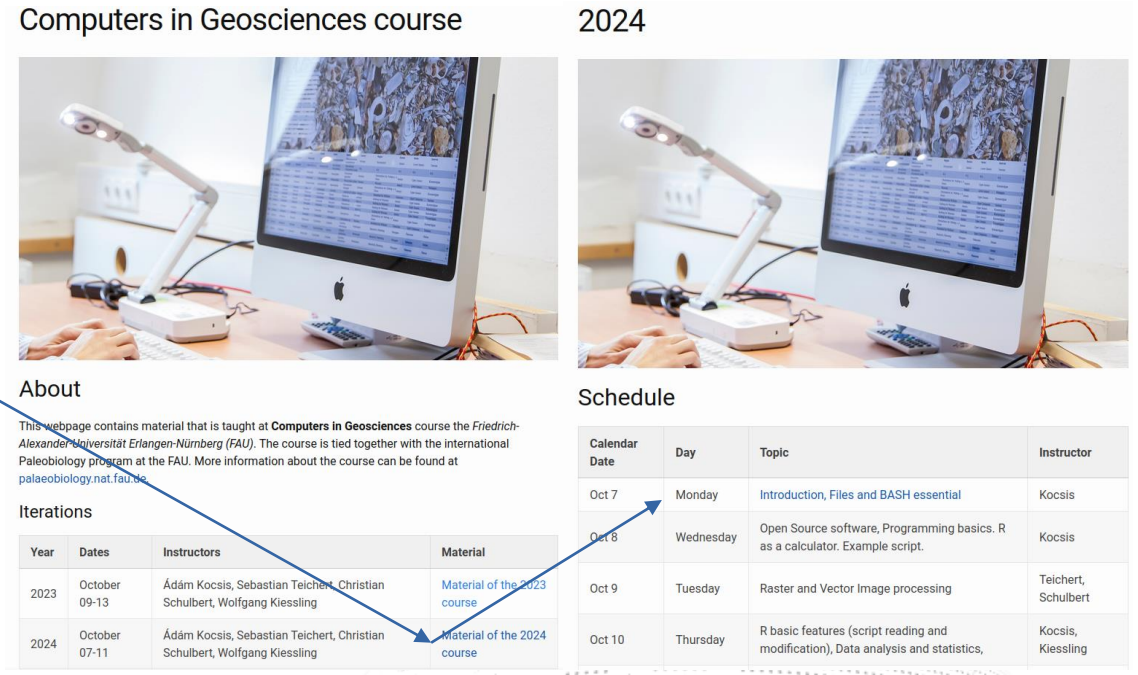
Examples: zip, rar, gzip, bzip2, tgz (e.g. .tar.gz)

Compression is everywhere!

- Often part of I/O (input/output)
- Multimedia (codecs)

Exercise

- Go to this page
- Download **data.zip**
- Uncompress the file!
- Copy contents into a new directory (e.g. day_1) in this class' directory!



Computers in Geosciences course 2024

About

This webpage contains material that is taught at **Computers in Geosciences** course the *Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*. The course is tied together with the international Paleobiology program at the FAU. More information about the course can be found at palaeobiology.nat.fau.de.

Iterations

Year	Dates	Instructors	Material
2023	October 09-13	Ádám Kocsis, Sebastian Teichert, Christian Schulbert, Wolfgang Kiessling	Material of the 2023 course
2024	October 07-11	Ádám Kocsis, Sebastian Teichert, Christian Schulbert, Wolfgang Kiessling	Material of the 2024 course

Schedule

Calendar Date	Day	Topic	Instructor
Oct 7	Monday	Introduction, Files and BASH essential	Kocsis
Oct 8	Wednesday	Open Source software, Programming basics. R as a calculator. Example script.	Kocsis
Oct 9	Tuesday	Raster and Vector Image processing	Teichert, Schulbert
Oct 10	Thursday	R basic features (script reading and modification), Data analysis and statistics,	Kocsis, Kiessling

Hints and tips for file management

- Keep all your stuff together (separate partition!)
- Logical hierarchy
- Make it portable (Windows!)
- Regularly spend time on organizing and cleaning files
- Naming and grouping: self-explanatory – make it for somebody else (you!)
- Avoid spaces in paths
- Cloud backups!

Novice- vs Expert-friendly tools

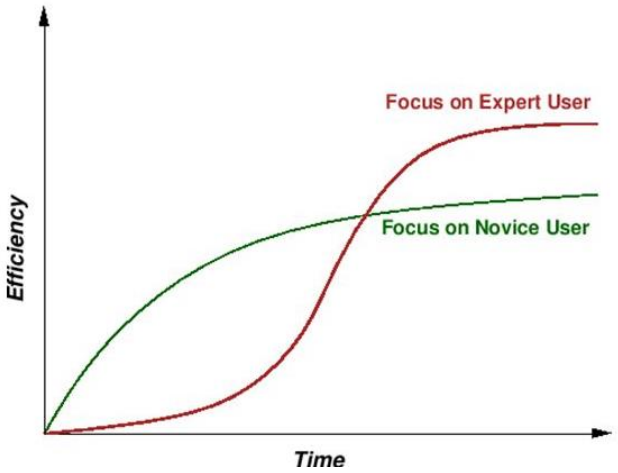
No program is perfectly user-friendly! Depending on the task at hand:

Novice-friendly

- Graphical User Interface (GUI)
- No or very basic training
- Quick learning
- Lower final efficiency
- Visually appealing

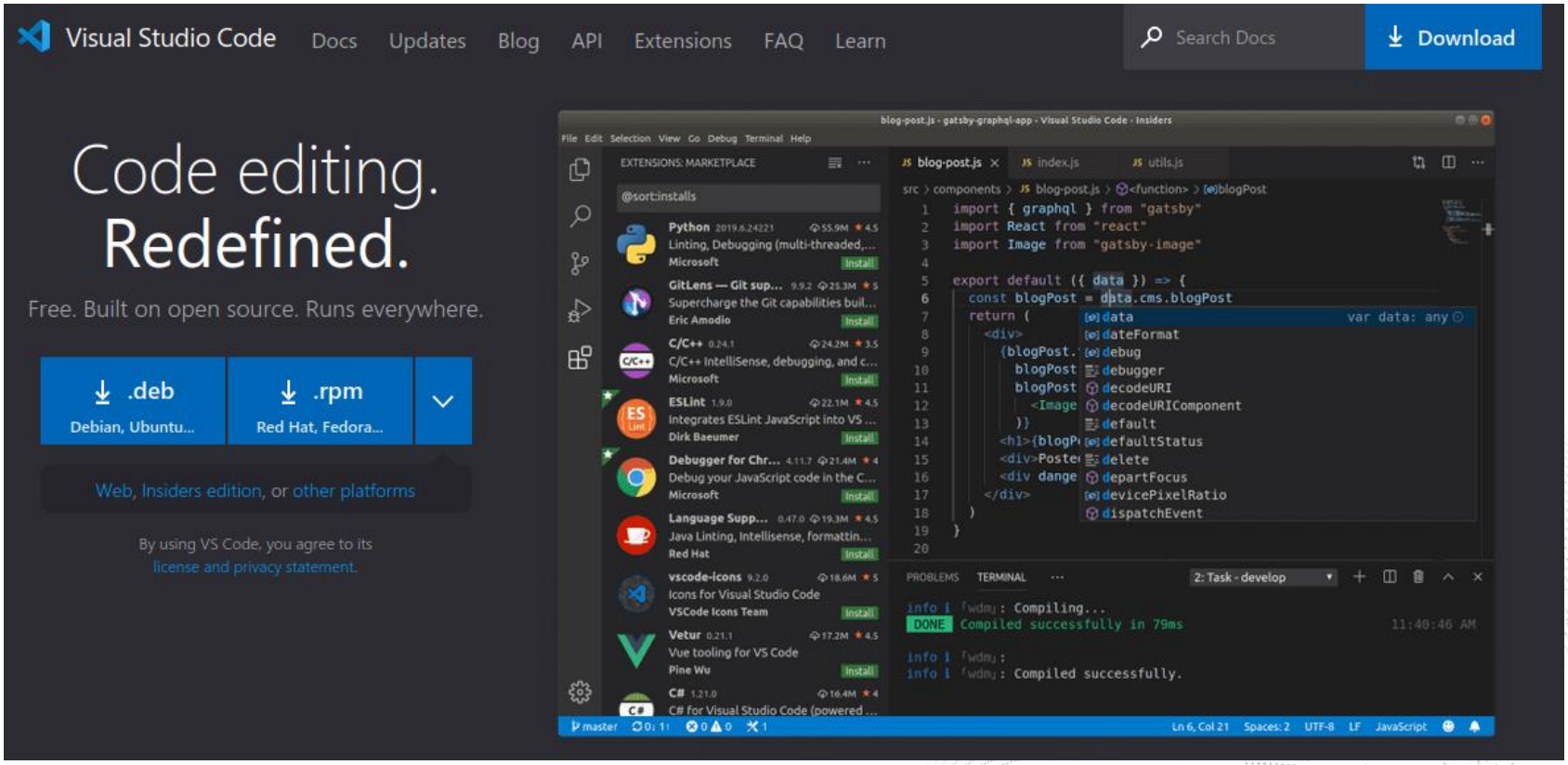
Expert-friendly

- Command Line Interpreter (CLI) or **Text-based** interface
- Education/training is necessary
- Eventually higher efficiency
- Visuals: usually invisible!
- Programmable



Working with text is essential

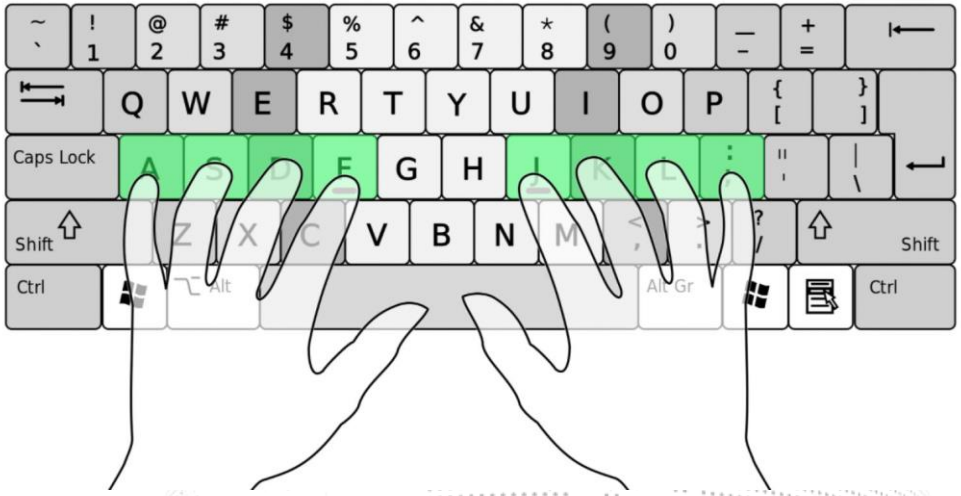
Recommendation: get a code editor!



https://code.visualstudio.com/

Working with text is essential

Recommendation: learn to touch type, if you don't know



Loads of resources available online!

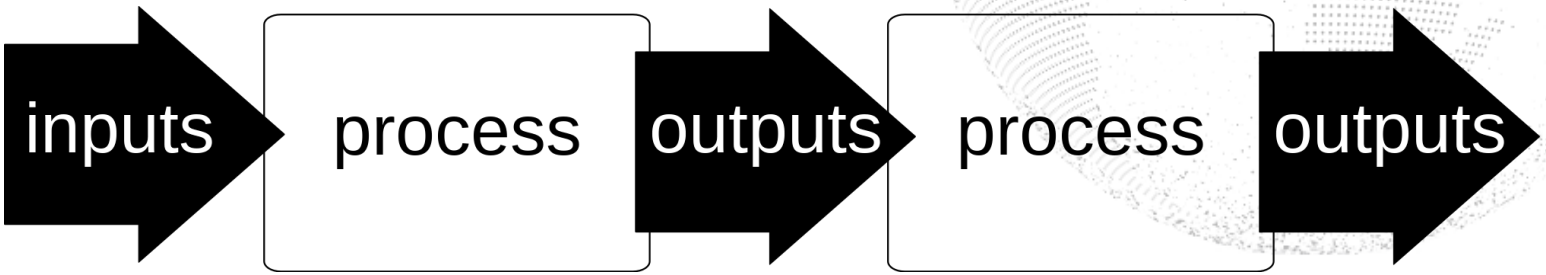
e.g. https://keybr.com

R consolidation course!

Enter data < Write instructions

Why text? Universal language

- Easy to connect processes / programs



Why text? Text is actually numbers

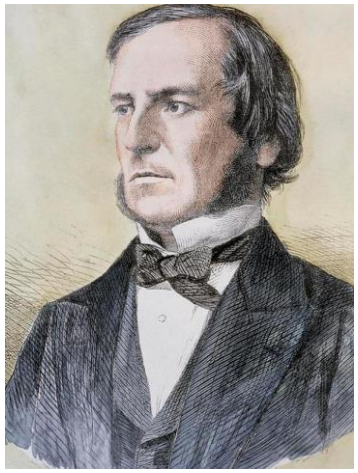
Perfect balance between simplicity and complexity

- Text can be represented with numbers, e.g. ASCII: https://www.ascii-code.com/

DEC	OCT	HEX	BIN	Symbol	HTML Number	HTML Name	Description
32	040	20	00100000	SP	&#32;		Space
33	041	21	00100001	!	&#33;	&excl;	Exclamation mark
34	042	22	00100010	"	&#34;	&quot;	Double quotes (or speech marks)
35	043	23	00100011	#	&#35;	&num;	Number sign
36	044	24	00100100	$	&#36;	&dollar;	Dollar
37	045	25	00100101	%	&#37;	&percnt;	Per cent sign
38	046	26	00100110	&	&#38;	&amp;	Ampersand
85	125	55	01010101	U	&#85;		Uppercase U
86	126	56	01010110	V	&#86;		Uppercase V
87	127	57	01010111	W	&#87;		Uppercase W
88	130	58	01011000	X	&#88;		Uppercase X
89	131	59	01011001	Y	&#89;		Uppercase Y
90	132	5A	01011010	Z	&#90;		Uppercase Z
91	133	5B	01011011	[	&#91;	&lsqb;	Opening bracket
92	134	5C	01011100	\	&#92;	&bsol;	Backslash
93	135	5D	01011101	]	&#93;	&rsqb;	Closing bracket
94	136	5E	01011110	^	&#94;	&Hat;	Caret - circumflex
95	137	5F	01011111	_	&#95;	&lowbar;	Underscore
96	140	60	01100000	`	&#96;	&grave;	Grave accent
97	141	61	01100001	a	&#97;		Lowercase a
98	142	62	01100010	b	&#98;		Lowercase b

Binary code: 0 and 1

Why binary?



George Boole

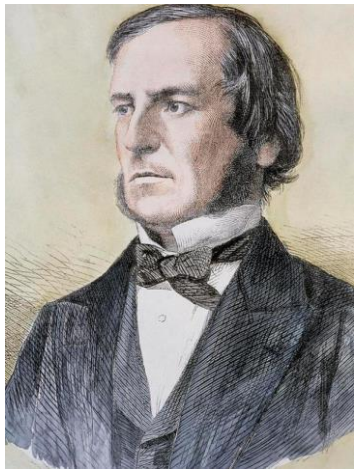
Simplest way to record information

- As type of data: True: (1) and False (0)
- Basis of scientific hypothesis testing – Hypothesis is a statement about reality, that can be answered with true or false. e.g.
- **It is raining outside.** (TRUE/FALSE?)
- Boolean Algebra (Logic)
- Easy to make machines the process information

Boolean algebra

The logical AND operation

Input 1	Input 2	operation	Result
True	True	AND (&)	True
True	False	AND (&)	False
False	True	AND (&)	False
False	False	AND (&)	False



George Boole

A: True

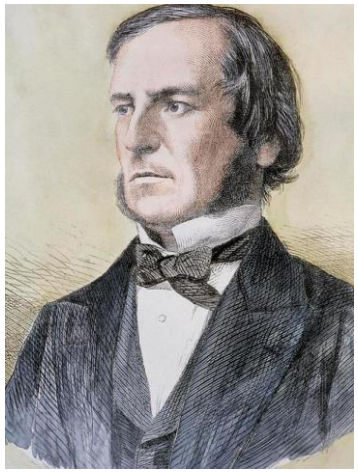
B: False

A & B = ?

Boolean algebra

The logical OR operation

Input 1	Input 2	operation	Result
True	True	OR (|)	True
True	False	OR (|)	True
False	True	OR (|)	True
False	False	OR (I)	False



George Boole

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Boolean algebra

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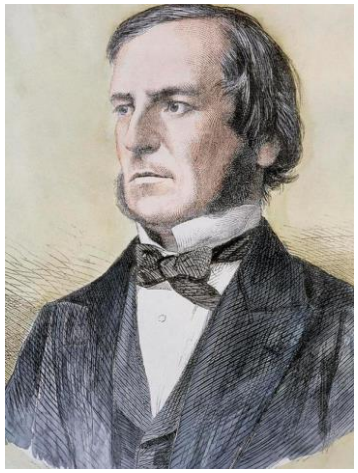
False	False	OR (I)	False



George Boole

A: True

B: False

A | B = ?

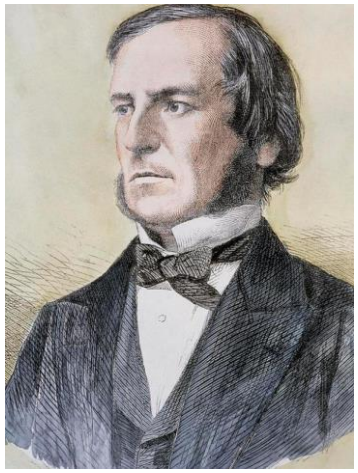
C: True

(A & B) | C = ?

Boolean algebra

The logical NOT operation

Input 1	operation	Result
True	NOT (!)	False
False	NOT (!)	True



George Boole

A: True

!A = ?

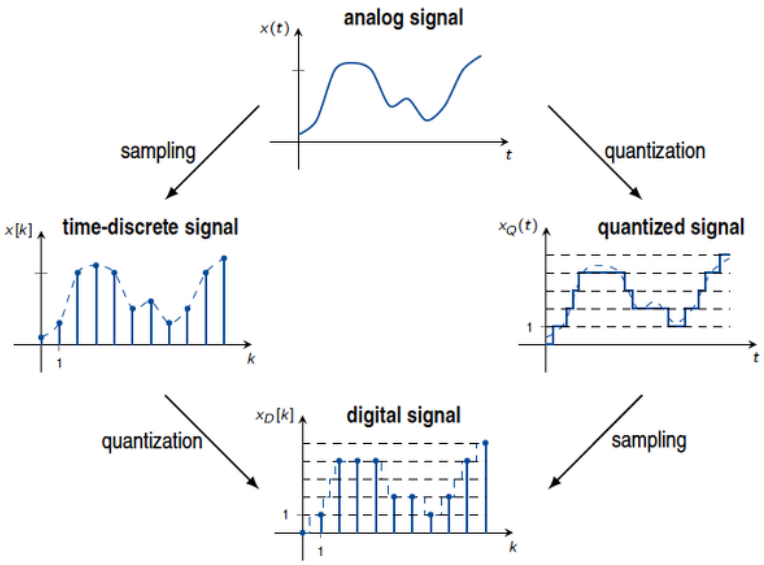
B: True

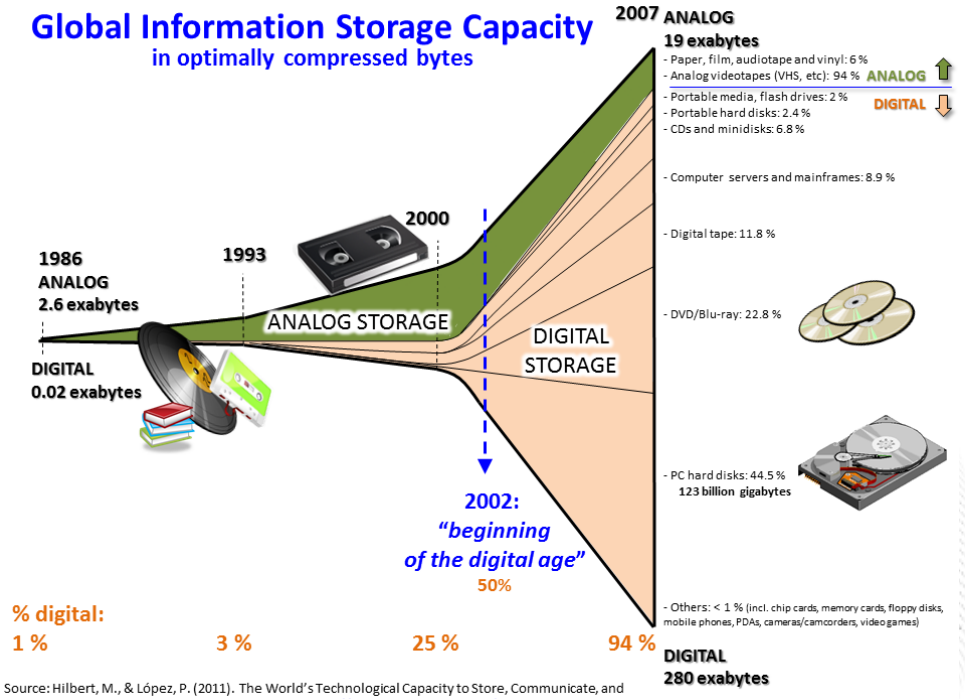
C: True

!(A & B) | C = ?

Digital vs Analogue information

Used to build up elementary building blocks of computers





Source: Hilbert, M., & López, P. (2011). The World's Technological Capacity to Store, Communicate, and Compute Information. *Science*, 332(6025), 60 –65. http://www.martinhilbert.net/WorldInfoCapacity.html

Computing and programming

- The concept of calculation: how much is 651/7?

You have 651 balls.

1. You go through them one-by one.
2. You put every 7th ball in a bin.
3. After done, count the balls. (divisor)

Computing and programming

- The concept of calculation: how much is 651/7?

  You have 651 balls.

  1. You go through them one-by one.
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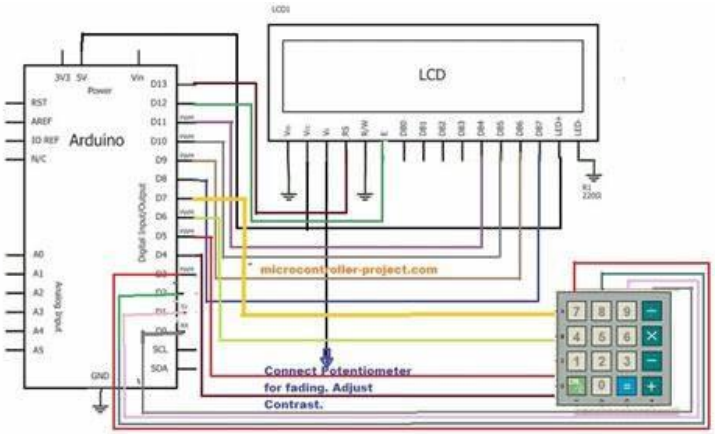
- You can do this with electricity

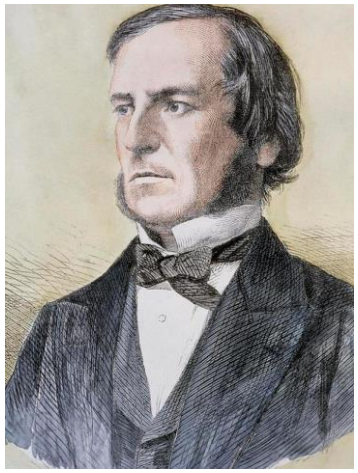


Logic Gates

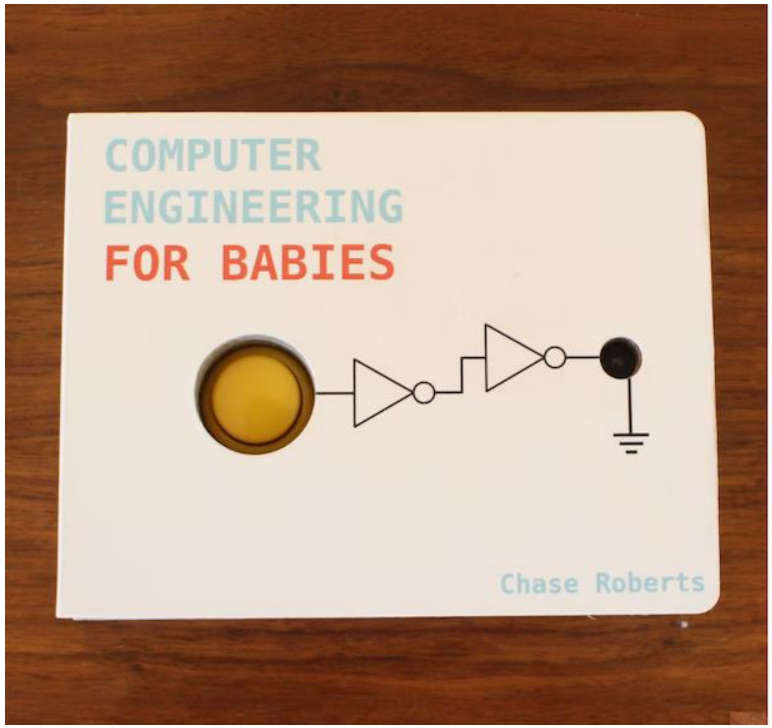
Boolean algebra is relatively simple to implement with physics

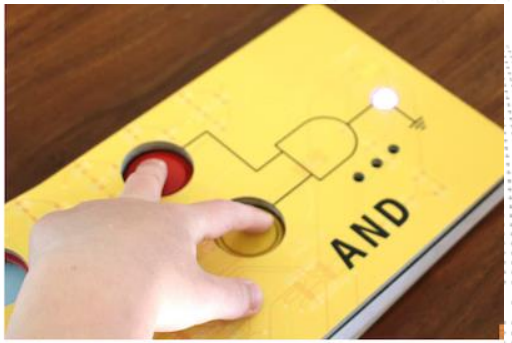
True: Electricity!

False: No electricity.



George Boole

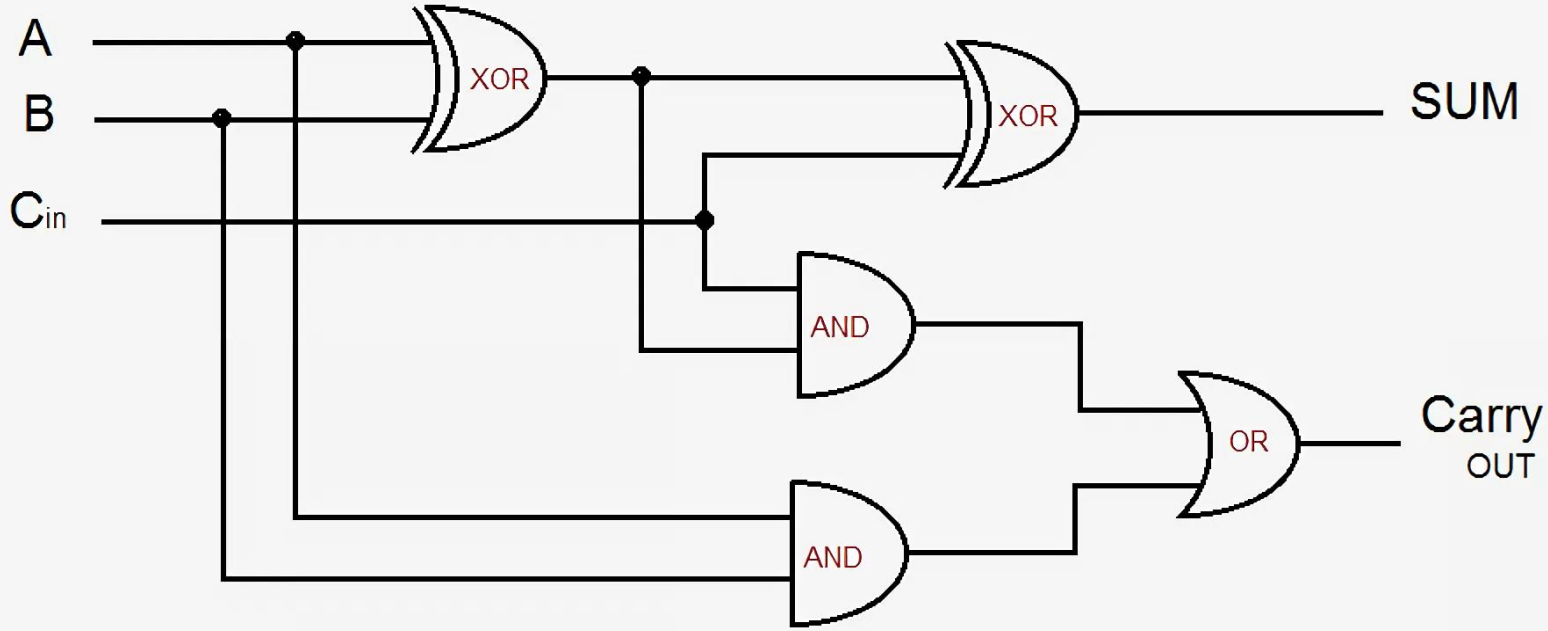


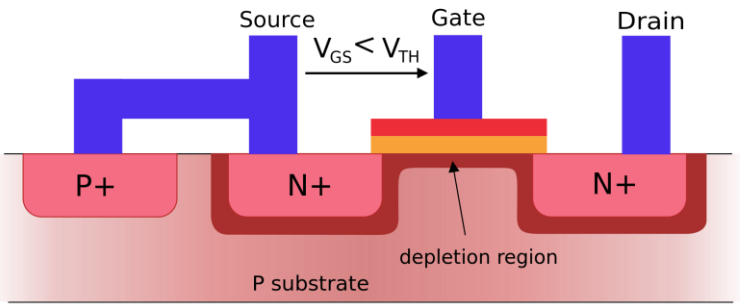


https://www.youtube.com/watch?v=_ldfWkZgX1Y

Logic Gates

Used to build up elementary building blocks of computers





Transistors...

https://en.wikipedia.org/wiki/MOSFET

Computing and programming

- The concept of calculation: how much is 651/7?

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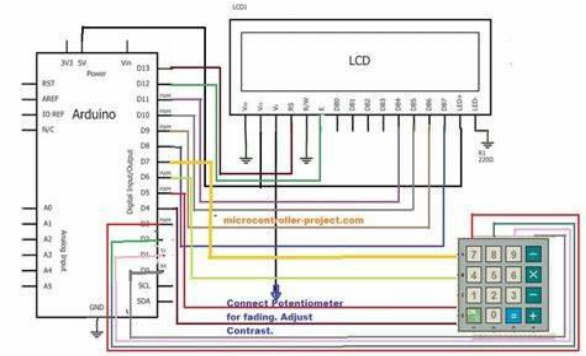
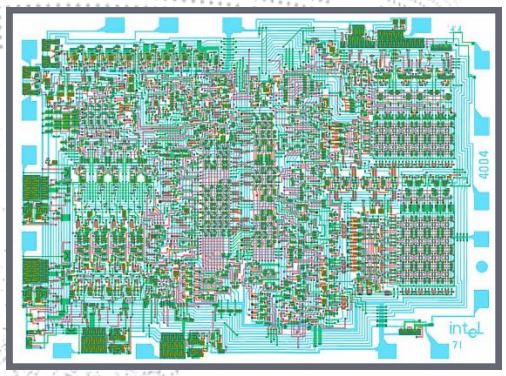


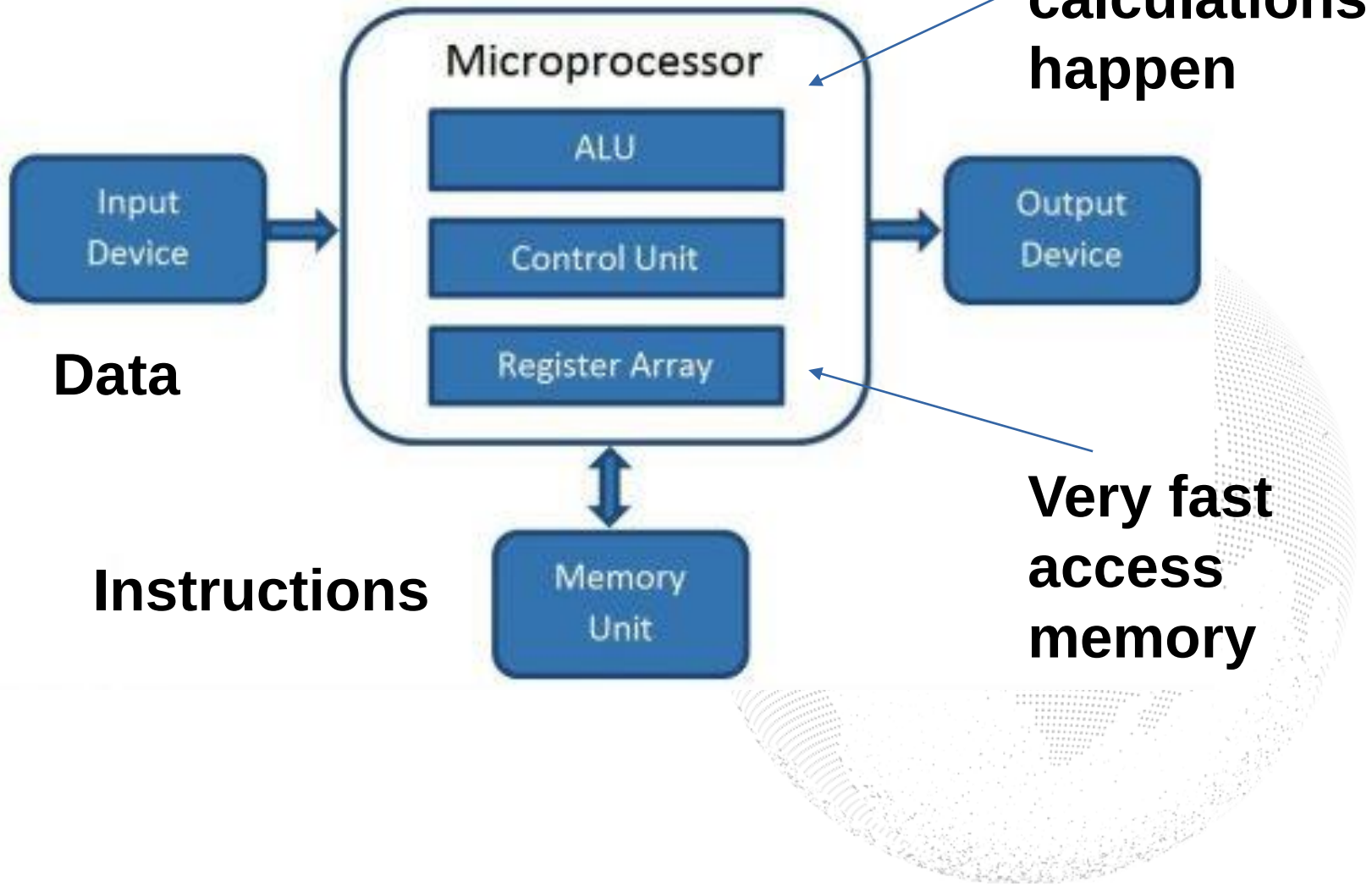
- You can do this with electricity

- Use instructions to define a machine that calculates numbers that represent something else (programmable computer)



https://www.youtube.com/shorts/i2k6jHHzK4s

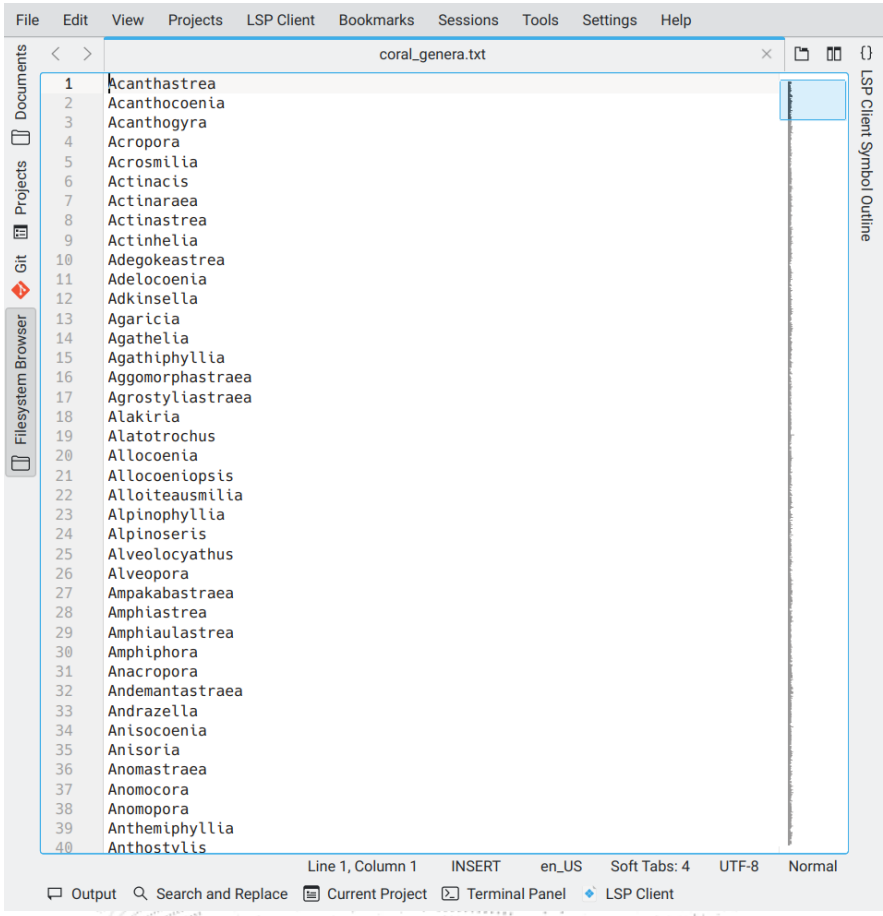
Building up more complex things



Structured text data types

List of entries

- The simplest thing ever
- Convention is to use .txt
- Entries are separated by new lines
- coral_genera.txt



Structured text data types

(csv) Comma-Separated Values

- Frequently used to represent tabular data
- Rows in lines
- Values separated by commas
- Example: corals.csv

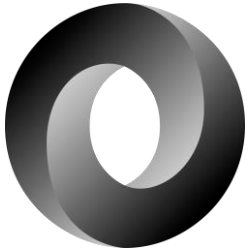
```
"10422","occ","","","601","Phacops sp.","genus","21701","","Phacops","genus","21701","Pragian","","410.8","407.6","60918"
"10438","occ","","","602","Proetida indet.","order","21062","","Proetida","order","21062","Pragian","","410.8","407.6","27289"
"10439","occ","","","602","Phacops sp.","genus","21701","","Phacops","genus","21701","Pragian","","410.8","407.6","27289"
"10440","occ","","","602","Leonaspis sp.","genus","19814","","Leonaspis","genus","19814","Pragian","","410.8","407.6","27289"
"10558","occ","","","605","Dalmanites sp.","genus","21523","","Dalmanites","genus","21523","Emsian","","407.6","393.3","60970"
"10559","occ","","","605","Phacops sp.","genus","21701","","Phacops","genus","21701","Emsian","","407.6","393.3","60970"
"10567","occ","","","606","Leonaspis sp.","genus","19814","","Leonaspis","genus","19814","Emsian","","407.6","393.3","60984"
"10568","occ","","","606","Phacopida indet.","order","21421","","Phacopida","order","21421","Emsian","","407.6","393.3","60984"
"10569","occ","","","606","Dechenella sp.","genus","21144","","Dechenella","genus","21144","Emsian","","407.6","393.3","60984"
"10573","occ","","","607","Basidechenella ? sp.","genus","21087","","Basidechenella","genus","21087","Emsian","","407.6","393.3","60984"
"10574","occ","","","607","Otarion sp.","genus","21275","","Otarion","genus","21275","Emsian","","407.6","393.3","60984"
"10575","occ","","","607","Proetida indet.","order","21062","","Proetida","order","21062","Emsian","","407.6","393.3","60984"
"10576","occ","","","607","Terataspis sp.","genus","19765","","Terataspis","genus","19765","Emsian","","407.6","393.3","60984"
"10577","occ","","","607","Leonaspis sp.","genus","19814","","Leonaspis","genus","19814","Emsian","","407.6","393.3","60984"
"10631","occ","","","608","Phacops sp.","genus","21701","","Phacops","genus","21701","Emsian","","407.6","393.3","13441"
"10683","occ","","","612","Phacopida ? indet.","order","21421","","Phacopida","order","21421","Eifelian","","393.3","387.7","17056"
"10704","occ","","","613","Phacopida ? indet.","order","21421","","Phacopida","order","21421","Eifelian","","393.3","387.7","61511"
"10716","occ","","","614","Otarion sp.","genus","21275","","Otarion","genus","21275","Eifelian","","393.3","387.7","272"
"10745","occ","","","616","Leonaspis sp.","genus","19814","","Leonaspis","genus","19814","Eifelian","","393.3","387.7","61110"
"10746","occ","","","616","Proetus sp.","genus","21327","","Proetus","genus","21327","Eifelian","","393.3","387.7","61110"
"10784","occ","","","619","Otarion sp.","genus","21275","","Otarion","genus","21275","Eifelian","Givetian","393.3","382.7","61512"
"10811","occ","","","621","Proetida ? indet.","order","21062","","Proetida","order","21062","Eifelian","Givetian","393.3","382.7","61512"
"10820","occ","","","622","Dechenella sp.","genus","21144","","Dechenella","genus","21144","Eifelian","Givetian","393.3","382.7","61512"
"10971","occ","","","627","Dechenella sp.","genus","21144","","Dechenella","genus","21144","Givetian","","387.7","382.7","841"
"10972","occ","","","627","Phacops sp.","genus","21701","","Phacops","genus","21701","Givetian","","387.7","382.7","841"
"10973","occ","","","627","Greenops sp.","genus","21588","","Greenops","genus","21588","Givetian","","387.7","382.7","841"
"10974","occ","","","627","Trimerus sp.","genus","21805","","Trimerus","genus","21805","Givetian","","387.7","382.7","841"
"11038","occ","","","632","Proetus sp.","genus","21327","","Proetus","genus","21327","Frasnian","","382.7","372.2","61501"
"11099","occ","","","640","Trimerocephalus sp.","genus","21804","","Trimerocephalus","genus","21804","Late Devonian","","382.7","358.9","60994"
```

Some structured text “languages”

(csv) Comma-Separated Values (variants)

- Separator can be different - e.g. semicolon (;) or white-space (\t, \s)
- Semicolon-separated example: stages.csv
- Tab-delimited: penguins.tab

Structured text data types

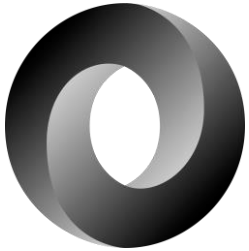


(JSON) JavaScript Object Notation

- Text-based format of key-value pairs

```
{
 “firstname”: “Adam”,
 “lastname”: “Kocsis
 }
```

Structured text data files

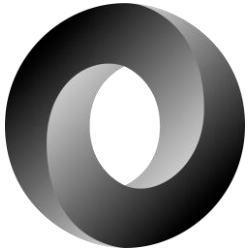


(JSON) JavaScript Object Notation

- Text-based format of key-value pairs
- Allows hierarchical structuring, multiple values/keys (‘array’)
- Can be made complicated, but very straightforward

```
{
  "firstName": "John",
  "lastName": "Smith",
  "isAlive": true,
  "age": 27,
  "address": {
    "streetAddress": "21 2nd Street",
    "city": "New York",
    "state": "NY",
    "postalCode": "10021-3100"
  },
  "phoneNumbers": [
    {
      "type": "home",
      "number": "212 555-1234"
    },
    {
      "type": "office",
      "number": "646 555-4567"
    }
  ],
  "children": [
      "Catherine",
      "Thomas",
      "Trevor"
  ],
  "spouse": null
}
```

Structured text data files



(YAML) Yet Another Markup Language

- Similar Text-based format that allows hierarchical structuring
- Key-value pairs
- Similar to JSON

```yaml
- name: Computers in Geosciences
  nickname: Computers in Geosciences
  ref: computers
  group:
    - key
    - wahl
  short: "Usually just called the ‘<i>computers course
  note:  "As many other courses in the Paleobiology ma
  more: "Essential tasks on the computer including ima
  evaluation: "Attendance and participation is require
  administrator: kocsis
  instructors:
    - kiessling
    - teichert
    - kocsis
  ects: 5
  campo: "https://www.campo.fau.de:443/qisserver/pages
  studon: "https://www.studon.fau.de/crs1321742.html"
  photos:
  thumbnail: "images/courses/thumbnails/computers.jpg"
  image:
    title: "images/courses/big/computers.jpg"
  form: "1 week block course."
  type: "practical"
```

Structured text data files

HTML (Hypertext Markup Language)

- Used to structure webpages, based on ‘tags’
- Also used for interface development

```
<!DOCTYPE html>
<html>
  <head>
    <meta charset="UTF-8">
    <title>Title goes here</title>
  </head>
  <body>

  </body>
</html>
```

CSS (Cascading Style Sheets)

- Adding formatting to webpages

Structured text data files

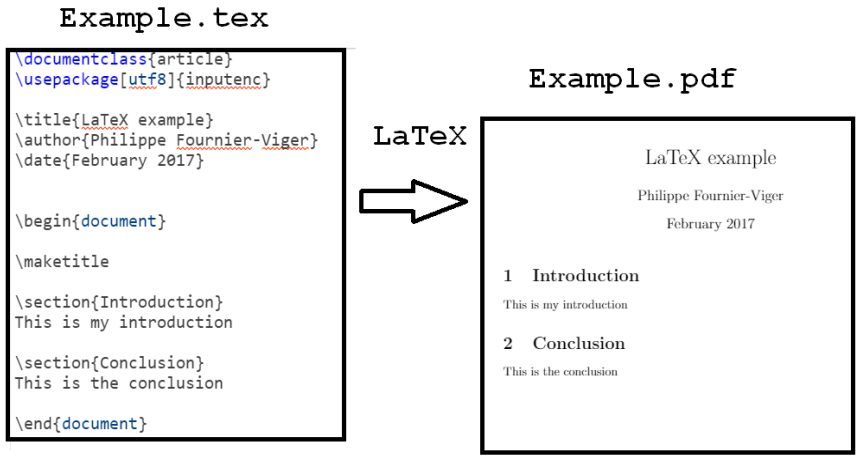
XML (eXtensible Markup Language)

- Storing Arbitrary Data
- Very similar to HTML
- Many file formats are based on this (OOXML, e.g. MS Office)

Structured text data files

TeX/LaTeX

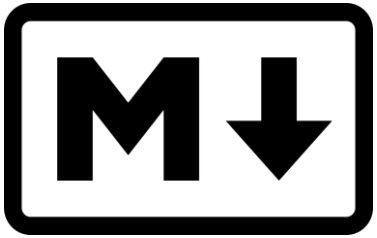
- Markup language for typesetting documents (e.g. creating .pdf files)
- LaTeX is a generalized implementation
- Excellent for mathematical expressions



$$^{w}\phi = {}^{w}f^{-1}({}^{0}f({}^{0}\phi))$$

Programs: MikTex, Tex Live

Structured text data files



Markdown

- Developed for easier web development
- Very clean and easy syntax
- Frequently used in ‘literate programming’*
- Various flavors (e.g. R-markdown)

*Methodology that combines programming with a documentation language

Free & Open Source Software

Ádám T. Kocsis (adam.kocsis@fau.de)

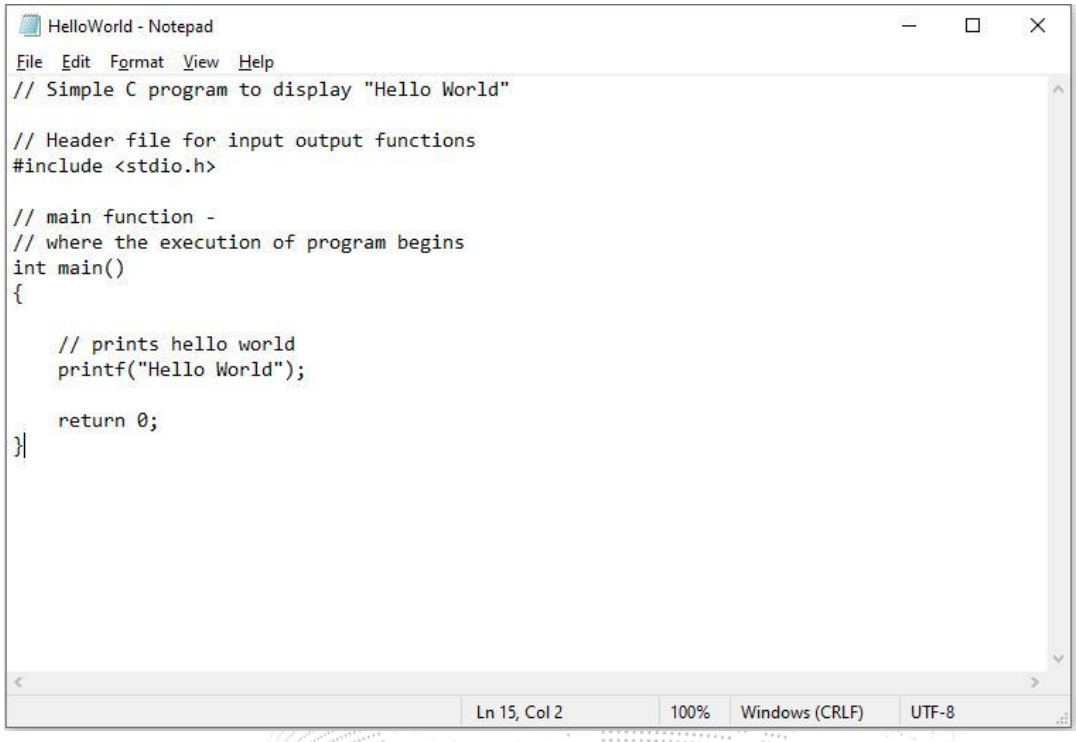
FAU

GeoZentrum Nordbayern

How are application software built?

The source code

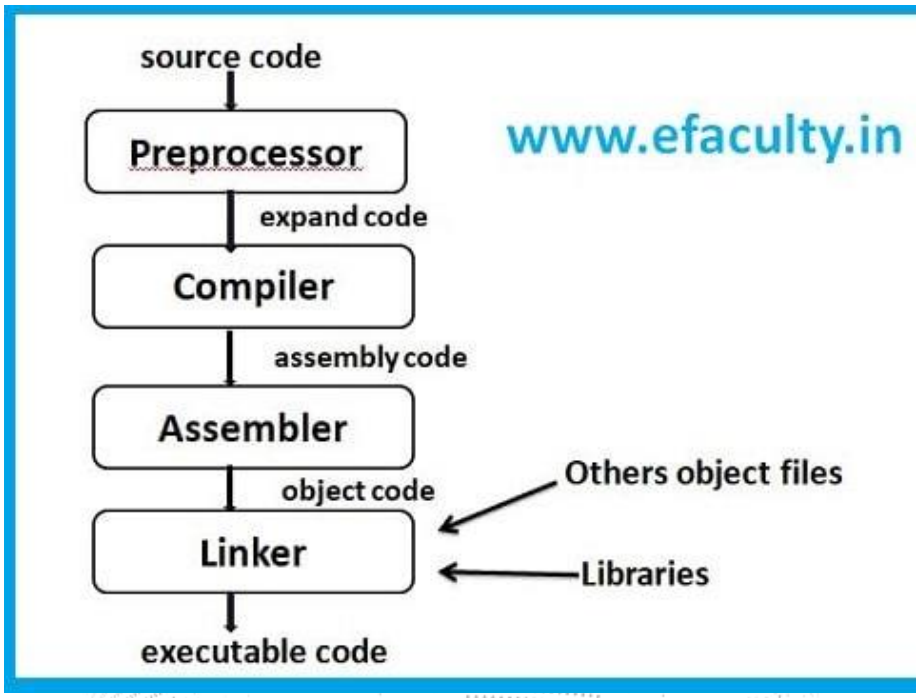
- Human-readable
- A language of some sort



How are application software built?

The building process (*sensu lato* compilation)

- Translate the source code to executable
- One way deal, i.e. irreversible process – the exact source code cannot be recreated!



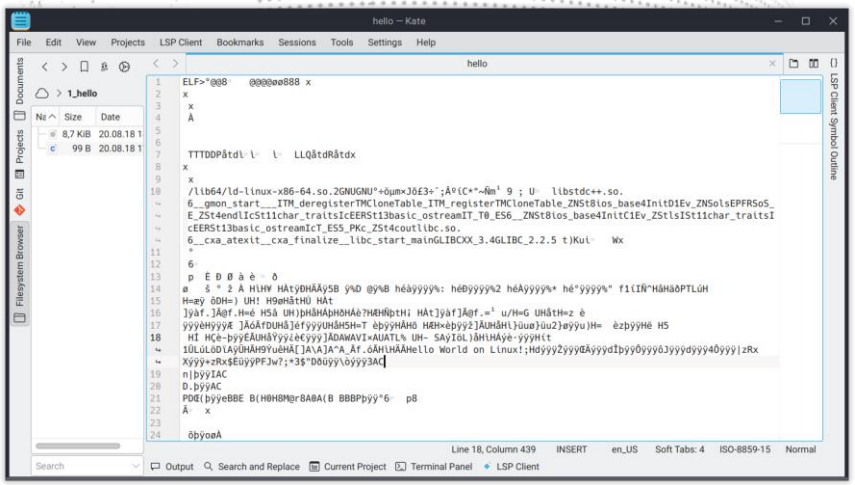
How are application software built?

Result: **binary executable**

- Modification is limited
- What the program does is cryptic (almost black box)
- Specific to Operating System and Architecture!

Download selection

- gplates_2.3.0_win64.exe
- gplates_2.3.0_win64.zip
- gplates_2.3.0_Darwin-x86_64.dmg
- gplates_2.3.0_ubuntu-18.04-amd64.deb
- gplates_2.3.0_ubuntu-20.04-amd64.deb
- gplates_2.3.0_ubuntu-20.10-amd64.deb
- gplates_2.3.0_ubuntu-21.04-amd64.deb
- gplates_2.3.0_ubuntu-21.10-amd64.deb
- gplates_2.3.0_ubuntu-22.04-amd64.deb
- gplates_2.3.0_ubuntu-22.10-amd64.deb
- gplates_2.3.0_ubuntu-23.04-amd64.deb
- gplates_2.3.0_src.zip
- gplates_2.3.0_src.tar.bz2



Free and Open Source Software?

Result

- You don’t need to use binaries from the authors (no charge or restrictions)
- You can modify the program’s behavior
- You can see what the program does

SOURCEFORGE

GitHub

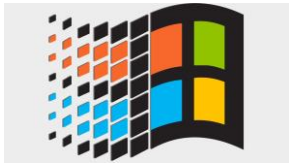
Original paradigm

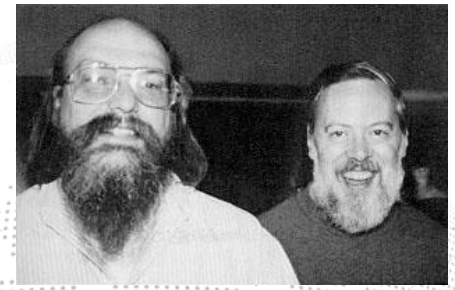
Software only for specific hardware!

- No transferability
- Apple still does this

Same Hardware → Different Software

- Proprietary operating systems
- Expensive, opaque
- **UNIX** (1969, AT&T Bell Labs)





Ken Thompson and
Dennis Ritchie

UNIX®

A Standard of The Open Group®

AIX

XENIX

solaris

BSD

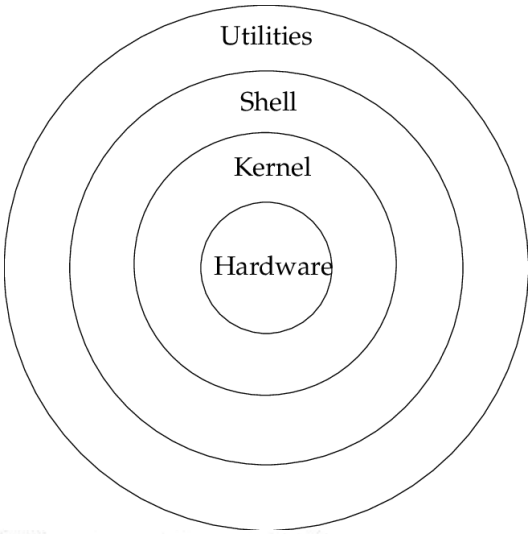
hp UX

A Free operating system?

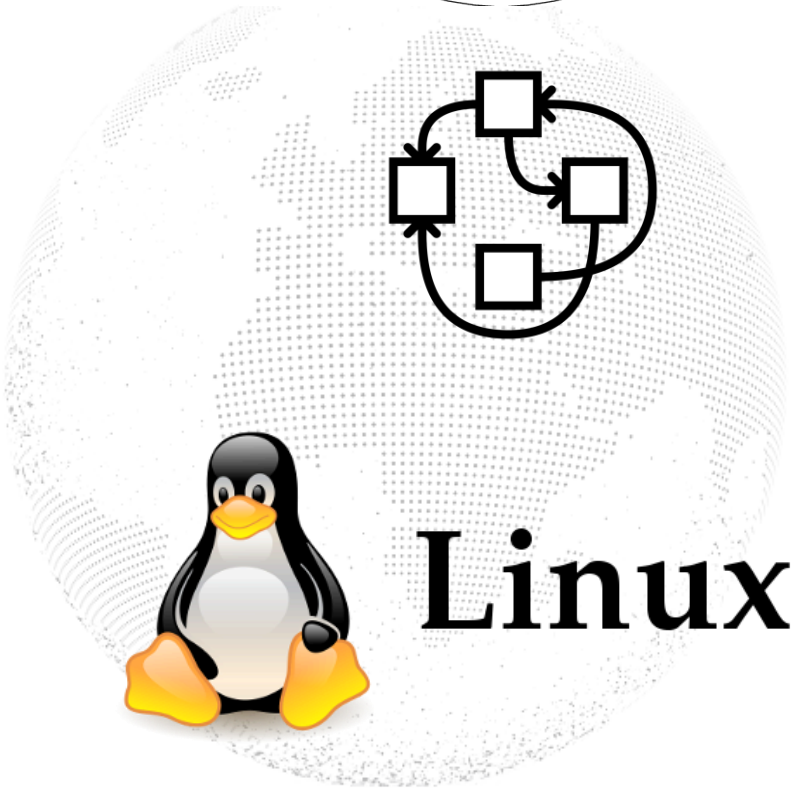
Richard Stallman

- *@MIT:* **G**NU is **N**ot **U**NIX (1983)
- Unix-like OS: Modular design
- do one thing, but very good!
- Hundreds of software (including R!!)
- Works well with other open source software

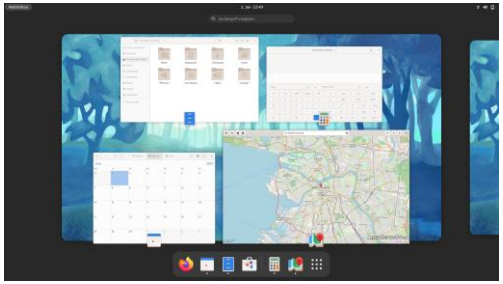
The Kernel



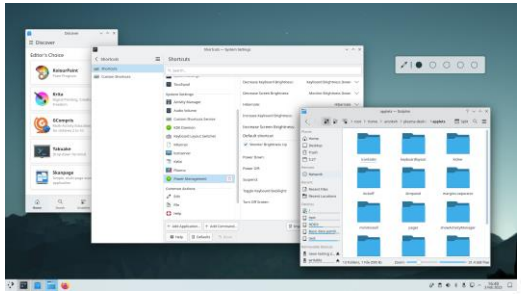
- The most important package of the OS, is built around this: Windows uses **NT,** MacOS: **Darwin**
- Handles hardware resources
- Original plans for GNU: *Hurd*
- 1991 Linux by Linus Torvalds



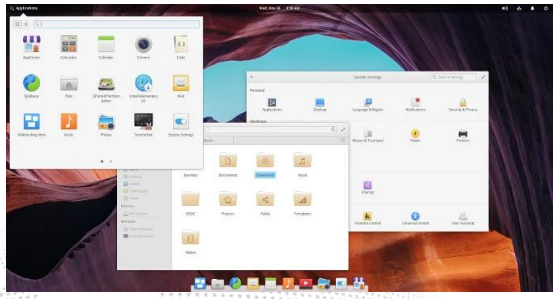
The Desktop Environment



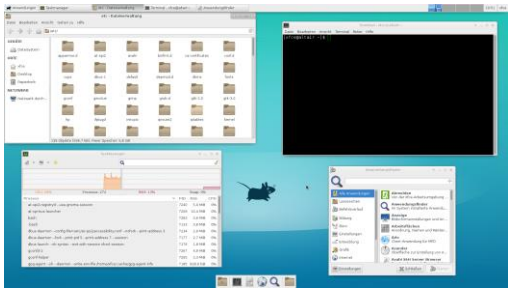
Gnome



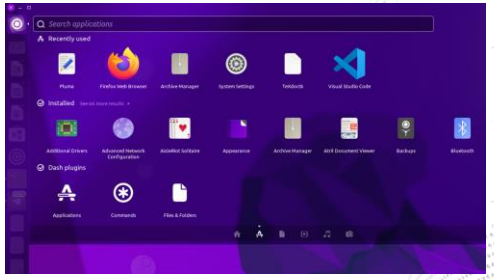
KDE



Pantheon



XFCE



Unity

Budgie

Package management

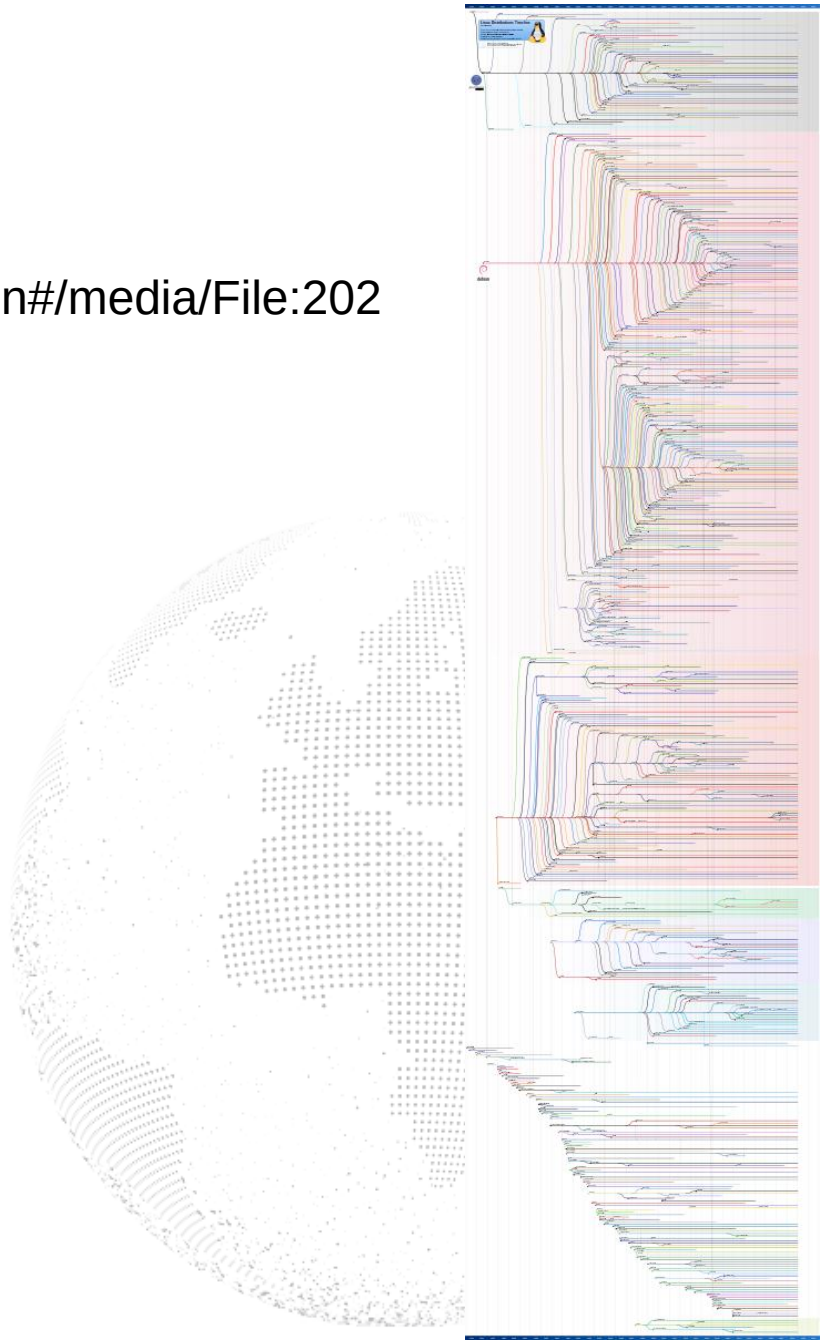
- You can build programs yourself, but it is easier to use pre-built ones
- Most important/prevalent ones



Primary Distribution	Debian	Arch	Red Hat
Manager Program	dpkg/apt	pacman	Re
Package extension	.deb	(AUR)	.rpm

The Phylogeny

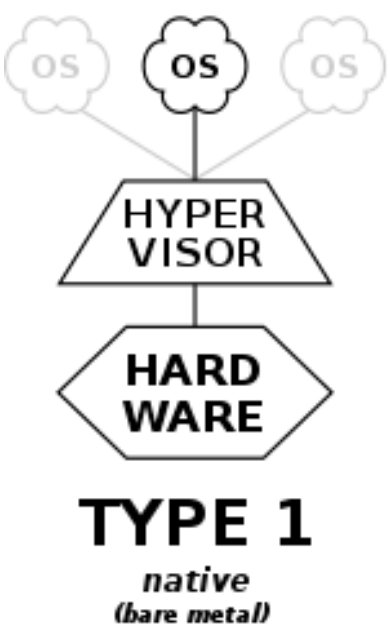
https://en.wikipedia.org/wiki/Linux_distribution#/media/File:2023_Linux_Distributions_Timeline.svg

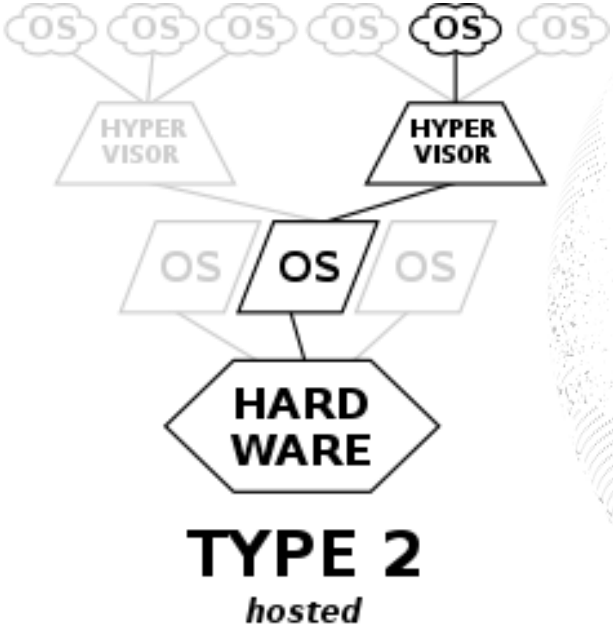


Try them!

In virtual computers...

https://www.youtube.com/watch?v=v1JVqd8M3Yc





Inkscape

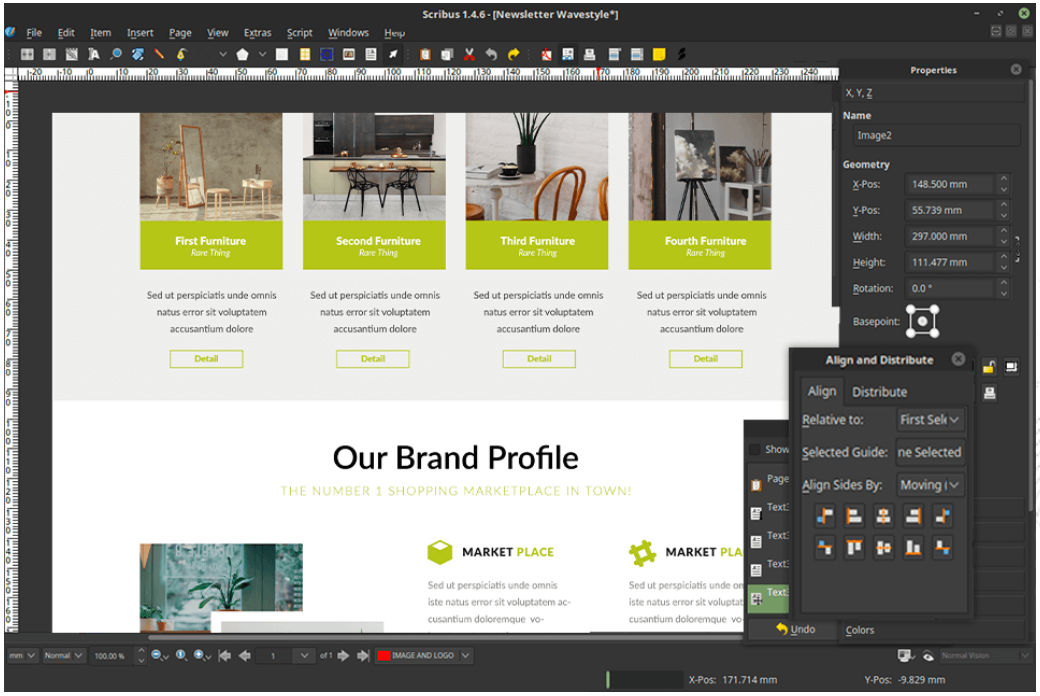
Vector graphics

GIMP

Raster graphics editor

Scribus

Publishing (InDesign)



Blender

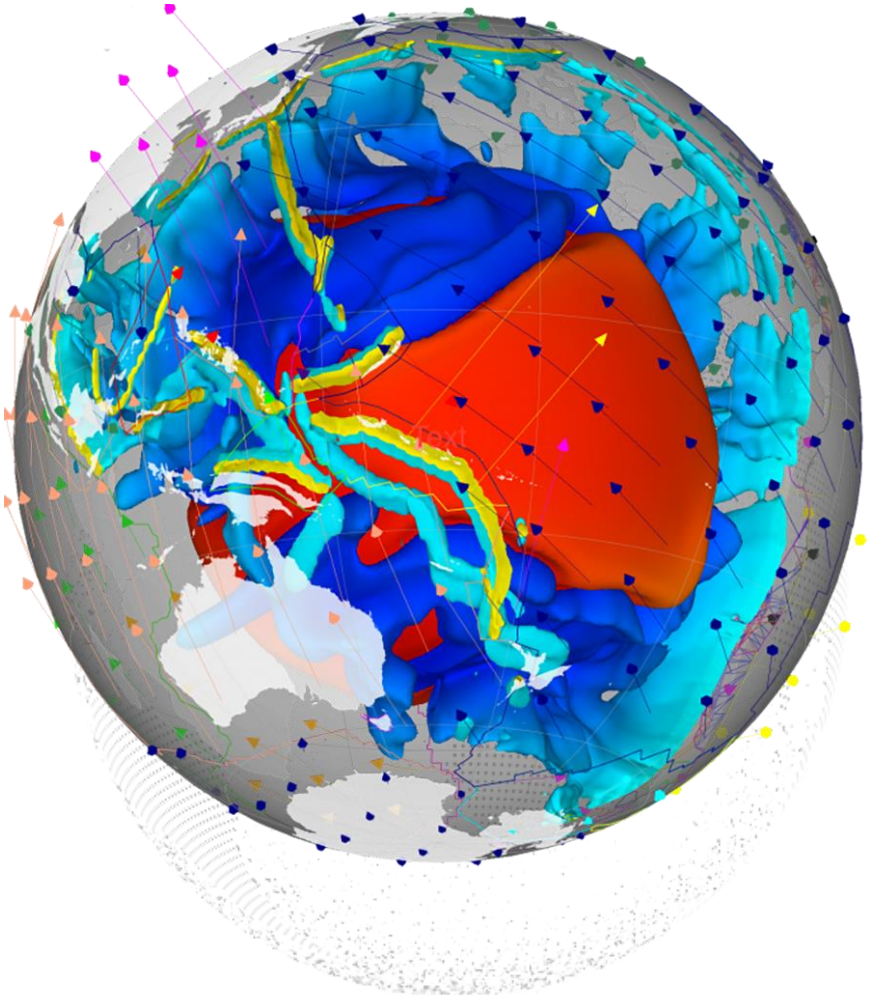
3D Graphics, Modelling, Shading, Animation, Rendering

QGIS

Open source GIS

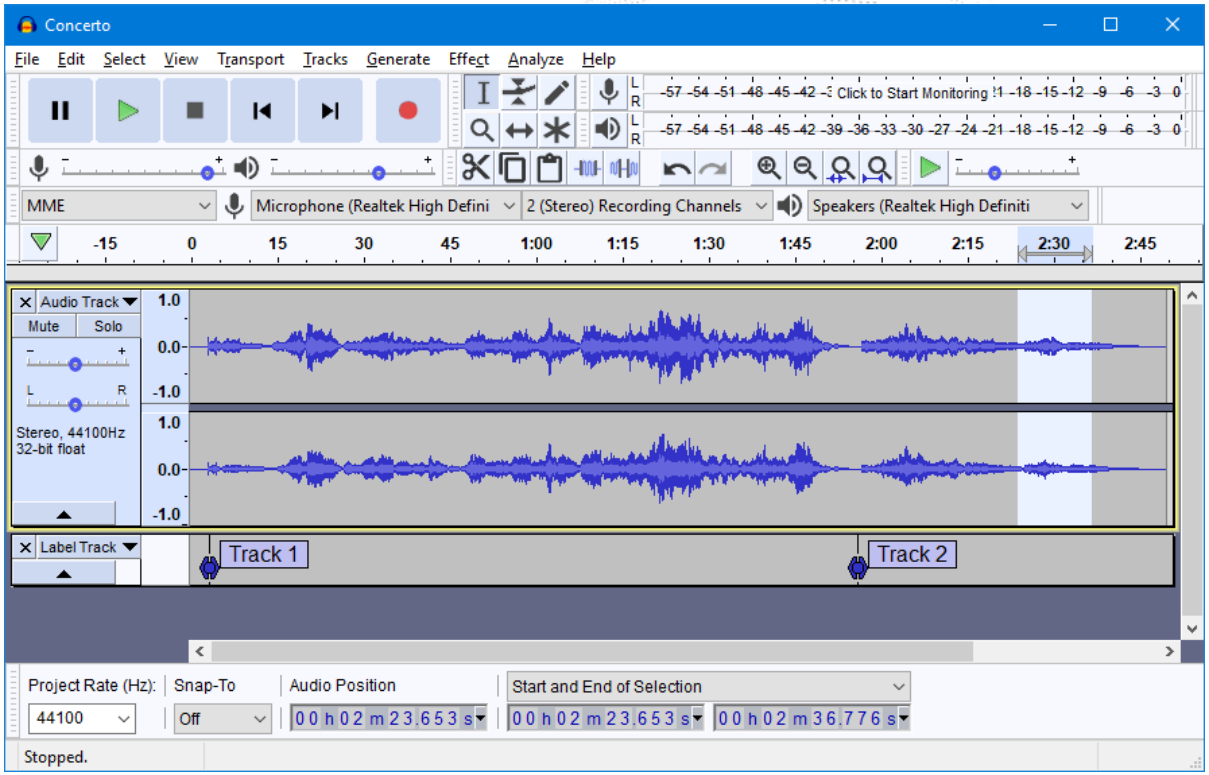
GPlates

Plate tectonic reconstructions



Audacity

Sound and music editor



Office

Open source

ONLYOFFICE

Hundreds of command line tools, e.g.

Multimedia: FFmpeg

Images: ImageMagick

Compiler: GCC

Document conversion: