Automation and programming

Ádám T. Kocsis (adam.kocsis@fau.de)

FAU

GeoZentrum Nordbayern

2023-10-11: Computers in Geosciences

WHY? We want to ...

1. … avoid tedious manual labor (lazy)
2. ... make sure that we work correctly
3. ... be efficient: work faster, with less energy
4. … make our work reproducible

which applies both to...

- managing information, files and documents
- calculations, analyzing data

Console applications

UNIX philosophy: **Do one thing, but do it very well!**

One application = one executable file = one command!

1st example: GNU ***wget***: download the targets of URLs

2nd example: ***ImageMagick*** – image manipulation

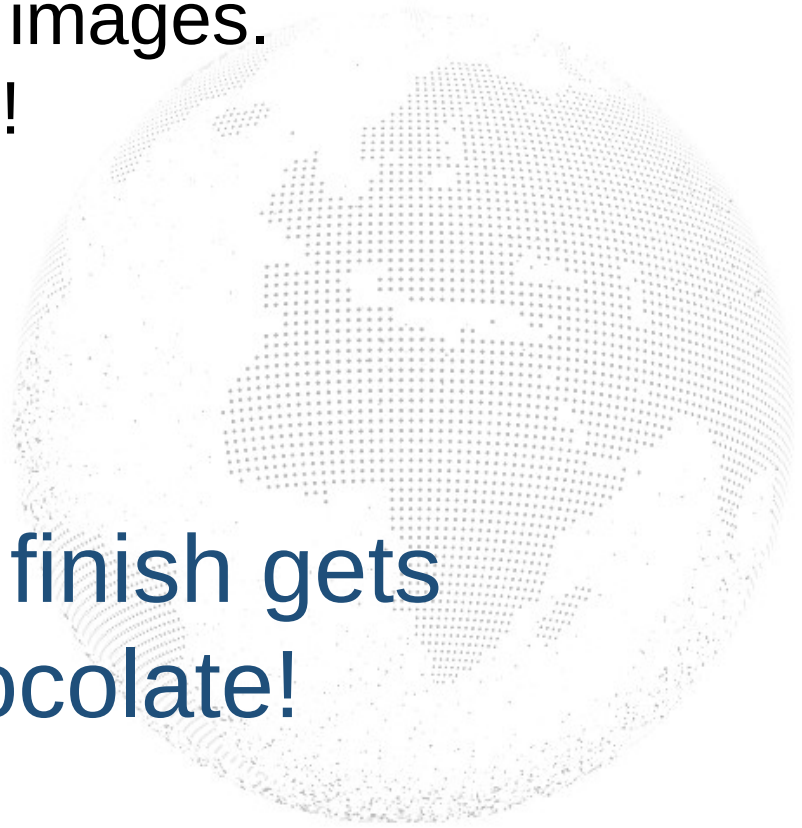
The PATH variable

- **Variable**: a named box to put information into, so you can refer to it by its name
- This is an '**Environment variable**': defines how the working environment is working
- List of directories that the shell searches for executables
- If an executable is in a directory that is 'on the path', then it can be run from any working directory

WHY? Exercise

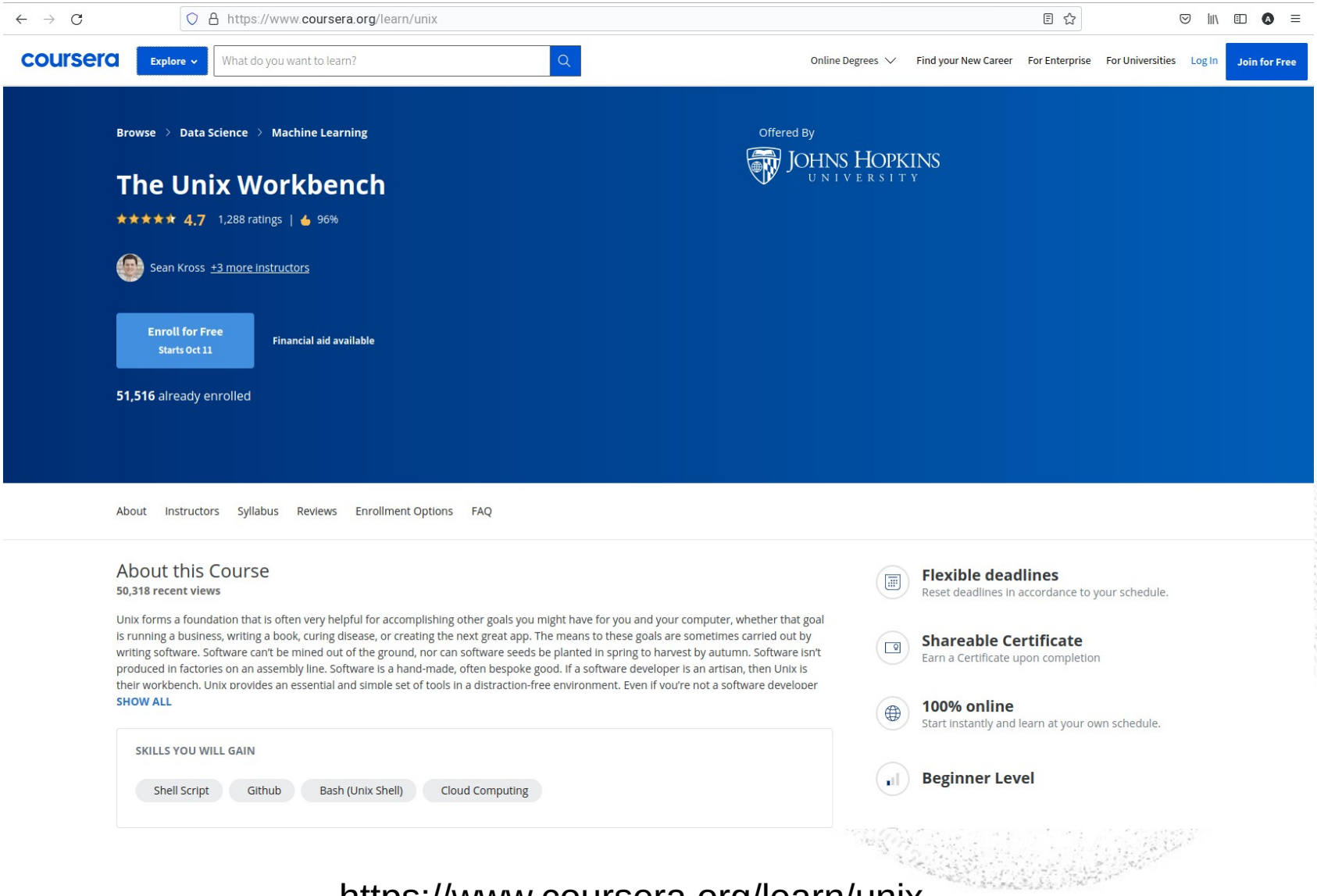
1. Go to

2. Download ‘first.txt’ file from the webpage! In the file there are URLs to images.
4. Download every image!



First person to finish gets
a bar of chocolate!

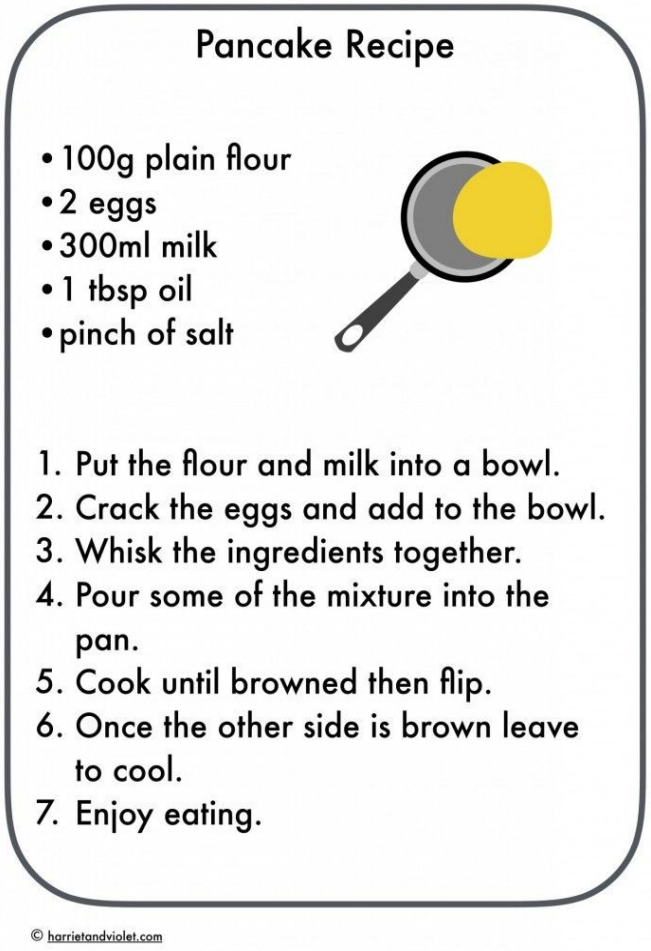
Interested? Recommendation:



https://www.coursera.org/learn/unix

Instructions?

- Statements that follow each other
- Every statement does something to change the state of the computer
- Linear sequence
- How can a computer understand what we are telling it?
- Multiple levels, exact instructions combine them

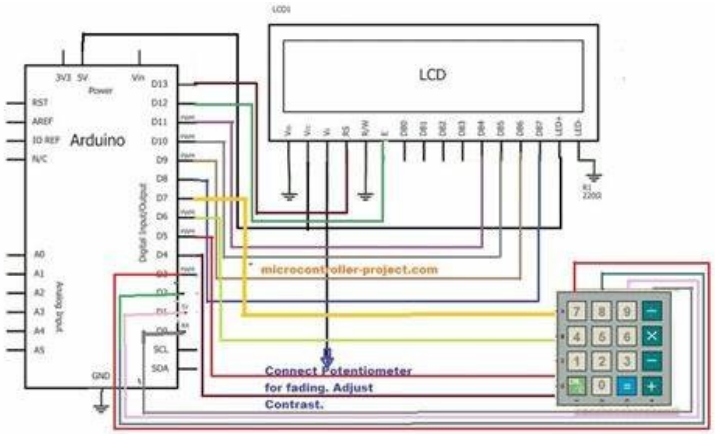


Programming, again...

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

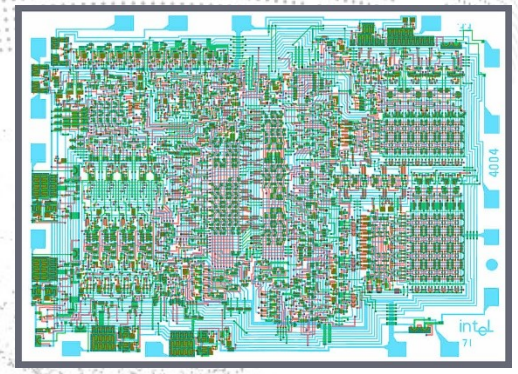
  You have 651 balls.

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



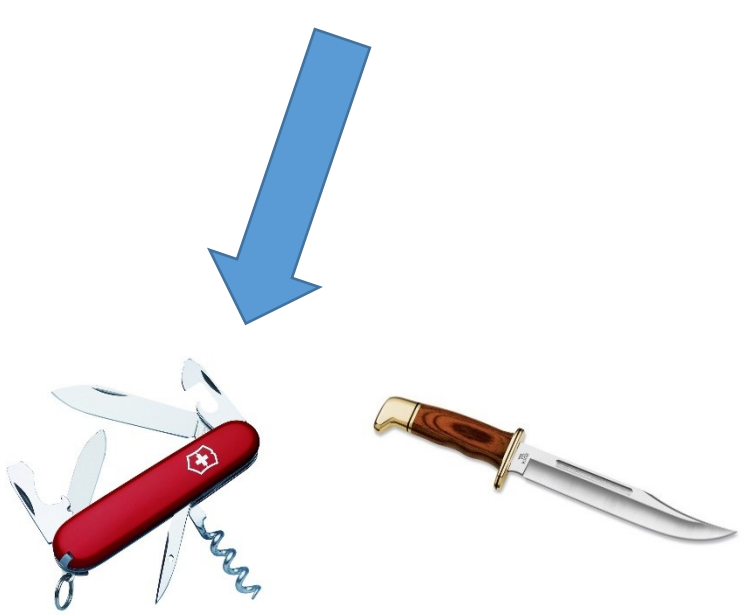
- You can do this with electricity

- You are using a machine to define a machine that calculates numbers that represent something else (programmable computer)



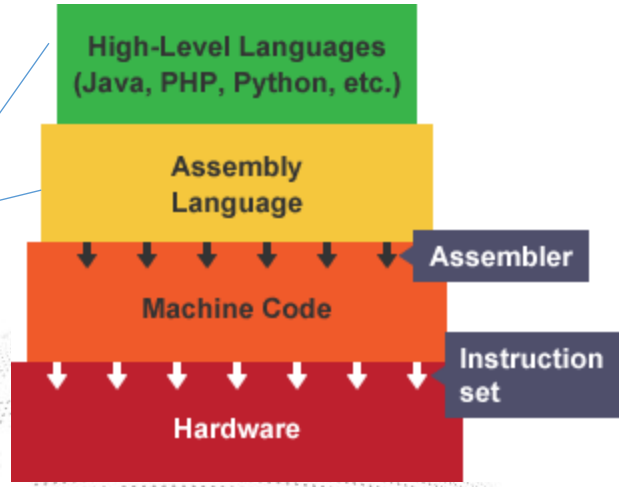
What kind of languages are there?

General purpose vs. **specialized** (e.g. domain-specific) language



What kind of languages are there?

Different **levels** of programming




```
MONITOR FOR 6802 1.4          9-14-80  TSC ASSEMBLER  PAGE    2


 C000                 ORG    ROM+$0000 BEGIN MONITOR
 C000 8E 00 70  START  LDS    #STACK

                ***************************************
                * FUNCTION: INITA - Initialize ACIA
                * INPUT: none
                * OUTPUT: none
                * CALLS: none
                * DESTROYS: acc A

 0013           RESETA  EQU    %00010011
 0011           CTLREG  EQU    %00010001

 C003 86 13     INITA   LDA A  #RESETA   RESET ACIA
 C005 B7 80 04          STA A  ACIA
 C008 86 11             LDA A  #CTLREG   SET 8 BITS AND 2 STOP
 C00A B7 80 04          STA A  ACIA

 C00D 7E C0 F1          JMP    SIGNON    GO TO START OF MONITOR

                ***************************************
                * FUNCTION: INCH - Input character
                * INPUT: none
                * OUTPUT: char in acc A
                * DESTROYS: acc A
                * CALLS: none
                * DESCRIPTION: Gets 1 character from terminal

 C010 B6 80 04  INCH    LDA A  ACIA      GET STATUS
 C013 47                ASR A            SHIFT RDRF FLAG INTO CARRY
 C014 24 FA             BCC    INCH      RECIEVE NOT READY
 C016 B6 80 05          LDA A  ACIA+1    GET CHAR
 C019 84 7F             AND A  #$7F      MASK PARITY
 C01B 7E C0 79          JMP    OUTCH     ECHO & RTS

                ***************************************
                * FUNCTION: INHEX - INPUT HEX DIGIT
                * INPUT: none
                * OUTPUT: Digit in acc A
                * CALLS: INCH
                * DESTROYS: acc A
                * Returns to monitor if not HEX input

 C01E 8D F0     INHEX   BSR    INCH      GET A CHAR
 C020 81 30             CMP A  #'0       ZERO
 C022 2B 11             BMI    HEXERR    NOT HEX
 C024 81 39             CMP A  #'9       NINE
 C026 2F 0A             BLE    HEXRTS    GOOD HEX
 C028 81 41             CMP A  #'A
 C02A 2B 09             BMI    HEXERR    NOT HEX
 C02C 81 46             CMP A  #'F
 C02E 2E 05             BGT    HEXERR
 C030 80 07             SUB A  #7        FIX A-F
 C032 84 0F     HEXRTS  AND A  #$0F      CONVERT ASCII TO DIGIT
 C034 39                RTS

 C035 7E C0 AF  HEXERR  JMP    CTRL      RETURN TO CONTROL LOOP
```

```
INPUT CELSIUS_TEMP
SET FAHRENHEIT_TEMP TO CELSIUS_TEMP * 9/5 + 32
WRITE FAHRENHEIT_TEMP
```

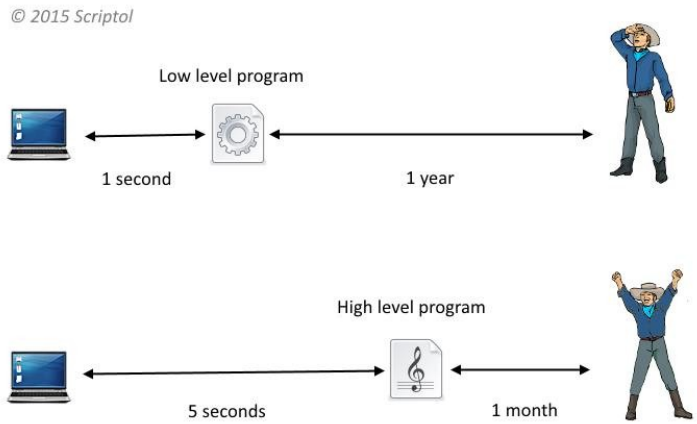
makeEggs()

getEggs()

stirEggs()

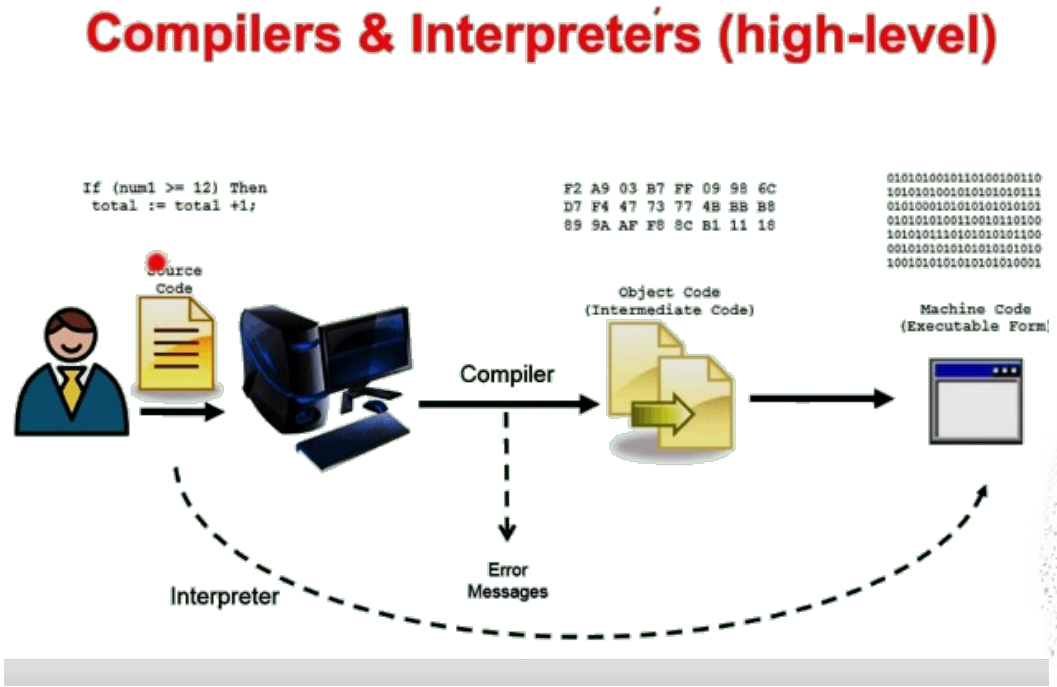
cook()

serve()

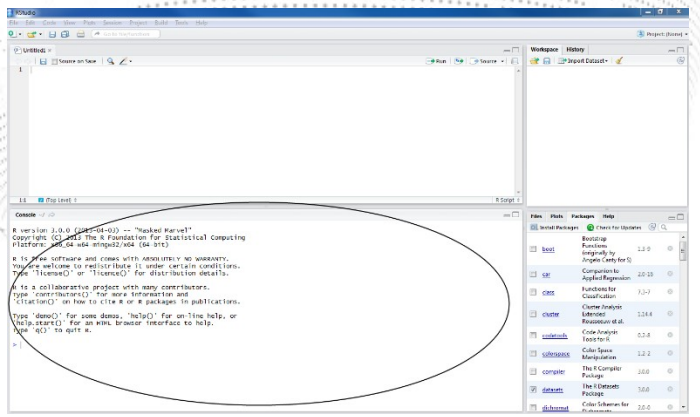


What kind of languages are there?

Interpreted vs. compiled languages

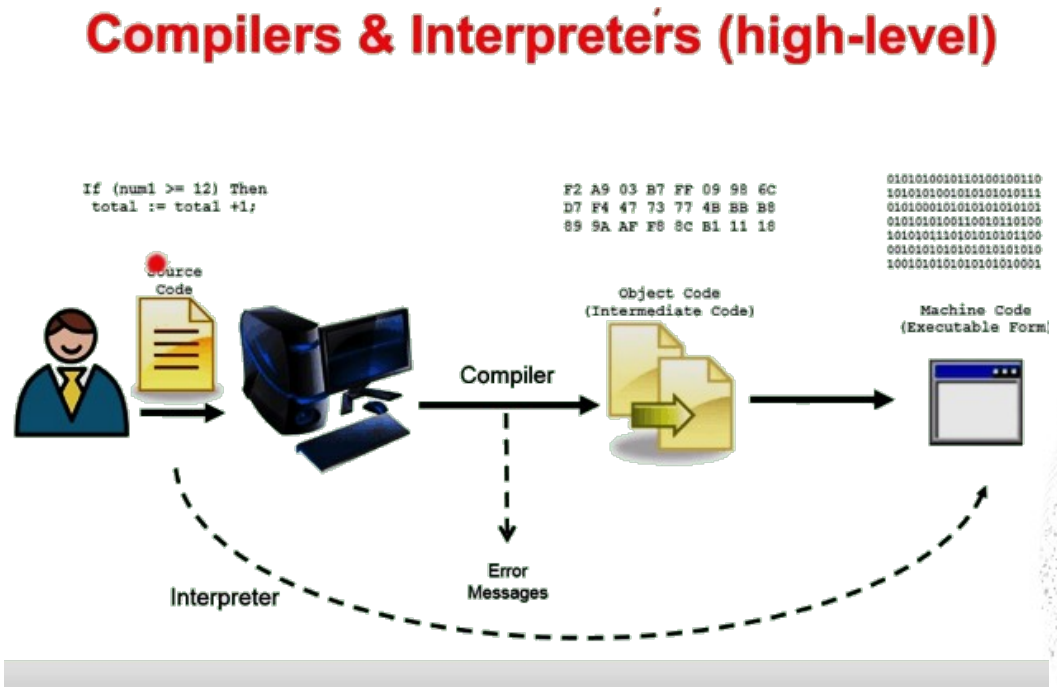


Working in a console



What kind of languages are there?

Interpreted vs. **compiled** languages




```
1  7f45 4c46 0201 0100 0000 0000 0000 0000
2  0300 3e00 0100 0000 b007 0000 0000 0000
3  4000 0000 0000 0000 981b 0000 0000 0000
4  0000 0000 4000 3800 0900 4000 1d00 1c00
5  0600 0000 0400 0000 4000 0000 0000 0000
6  4000 0000 0000 0000 4000 0000 0000 0000
7  f801 0000 0000 0000 f801 0000 0000 0000
8  0800 0000 0000 0000 0300 0000 0400 0000
9  3802 0000 0000 0000 3802 0000 0000 0000
10 3802 0000 0000 0000 1c00 0000 0000 0000
11 1c00 0000 0000 0000 0100 0000 0000 0000
12 0100 0000 0500 0000 0000 0000 0000 0000
13 0000 0000 0000 0000 0000 0000 0000 0000
14 780b 0000 0000 0000 780b 0000 0000 0000
15 0000 2000 0000 0000 0100 0000 0600 0000
16 780d 0000 0000 0000 780d 2000 0000 0000
17 780d 2000 0000 0000 9802 0000 0000 0000
18 c003 0000 0000 0000 0000 2000 0000 0000
19 0200 0000 0600 0000 900d 0000 0000 0000
20 900d 2000 0000 0000 900d 2000 0000 0000
21 0002 0000 0000 0000 0002 0000 0000 0000
22 0800 0000 0000 0000 0400 0000 0400 0000
23 5402 0000 0000 0000 5402 0000 0000 0000
24 5402 0000 0000 0000 4400 0000 0000 0000
25 4400 0000 0000 0000 0400 0000 0000 0000
26 50e5 7464 0400 0000 e409 0000 0000 0000
```

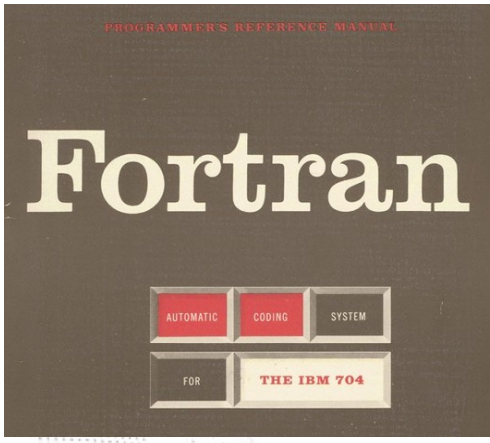
```
1  #include <iostream>
2  using namespace std;
3
4  int main()
5  {
6      cout << "Hello World!\n";
7      return 0;
8  }
9
```

```
adam@vulcanodon:~$ g++ hello.cpp -o hello_exec
```

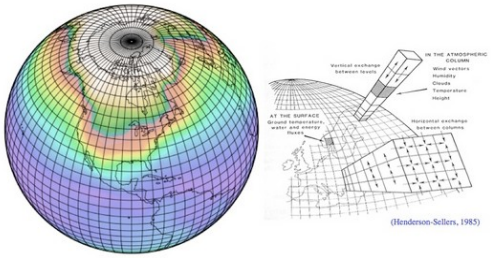
```
adam@vulcanodon:~$ chmod +x hello_exec
adam@vulcanodon:~$ ./hello_exec
Hello World!
adam@vulcanodon:~$
```

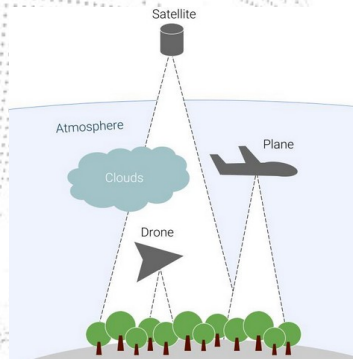
Some programming languages…

Fortran



- IBM, since 1957, first high-level language
- For mathematical computations, compiled
- One of the fastest languages, still
- climate models, remote sensing data, crystallography

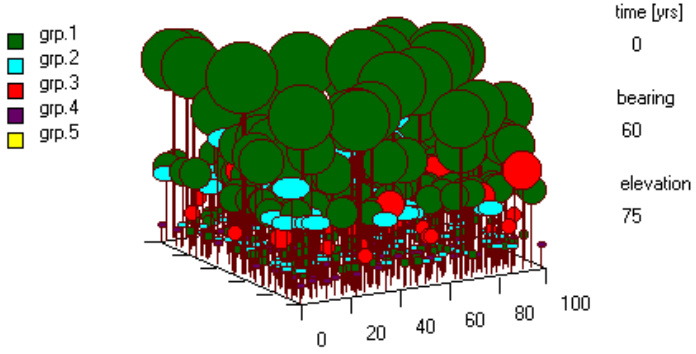




Some programming languages… **C++**

- C with extended object-oriented features
- Complex data structures, yet very fast
- Used everywhere, popular desktop applications (e.g. Adobe PS, MS Office) computer games, agent-based modelling
- Very good R integration (Rcpp package)

C++ is the new C — twice the power, twice the size, works in hostile environments, and if you try to use it without care and special training you will probably crash.



Some programming languages… **Java**

- Based on C too
- Compiled, runs in a virtual machine: code is very deployable
- Faster than either R or Python
- Some desktop applications, mesquite, imageJ

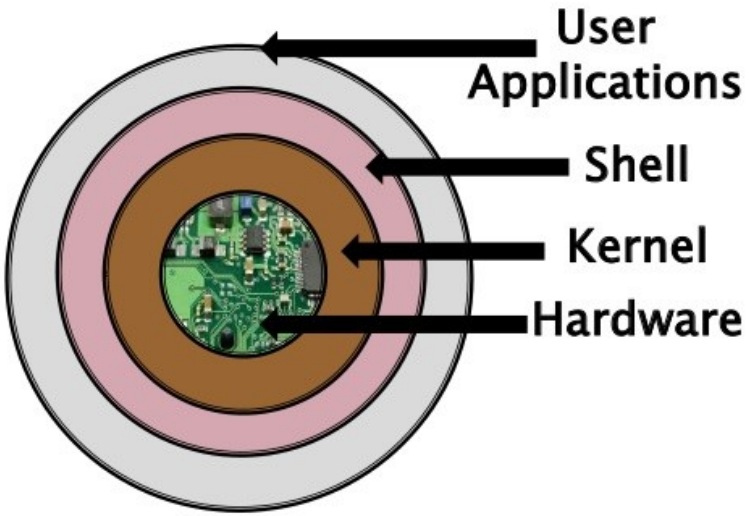
Java is another attempt to improve on C. It sort of gets the job done, but it's way slower, bulkier, spews pollution everywhere, and people will think you're a redneck.

Some programming languages **JavaScript**

- Scripting language for the World Wide Web
- Executed by the clients (the computer visiting the webpage)
- Controls animations, interactive content

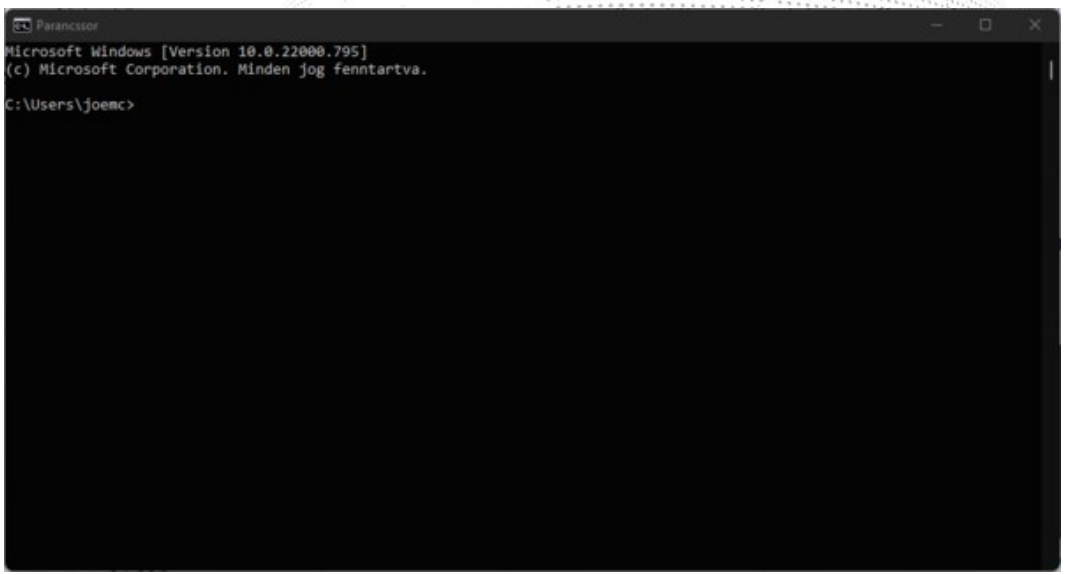
Some programming languages… **bash**

- Shell scripting language
- Current standard on unix-like operating systems (e.g. Linux)
- Useful for file management, system administration running console applications, raw data processing



Some programming languages… cmd.exe

- The command prompt
- The shell of Windows
- Very tedious to use



Some programming languages… **Python**

- Since 1991
- Higher level than C, interpreted, general purpose
- Very popular due to the clean syntax
- Two main version still in use: Python 2 and Python 3
- Tons of scientific packages, many programs have python APIs
- Some desktop applications, e.g. Gplates, debian-apt

Python is great for everyday tasks: easy to drive, versatile, comes with all the conveniences built in. It isn't fast or sexy, but neither are your errands.

Some programming languages… **Perl**

- A family of languages
- Originally for text processing, somewhat faster than python
- Used commonly in bioinformatics, e.g. DNA sequence analysis
- Sometimes for the web with databases (originally the PaleoDB website was using perl)

Perl used to serve the same purpose as Python, but now only bearded ex-hippies use it.

Paleobiology Database

THE PALEOBIOLOGY DATABASE

revealing the history of life

Some programming languages… **PHP**

- General purpose, designed for web development, interpreted
- Server-side programming
- Very good database integration
- Web-based applications, shops, content management (e.g. Wordpress)

PHP is this hand-me-down deathtrap that you only use because you're stuck with it, and when you hit a speed bump the wrong way it sets you and your passengers on fire.

Some programming languages… **SQL**

- Structured Query Language
- The language of relational databases
- Local databases: MySQL, PostgreSQL, MariaDB, Oracle Database
- Define, Manage, Query

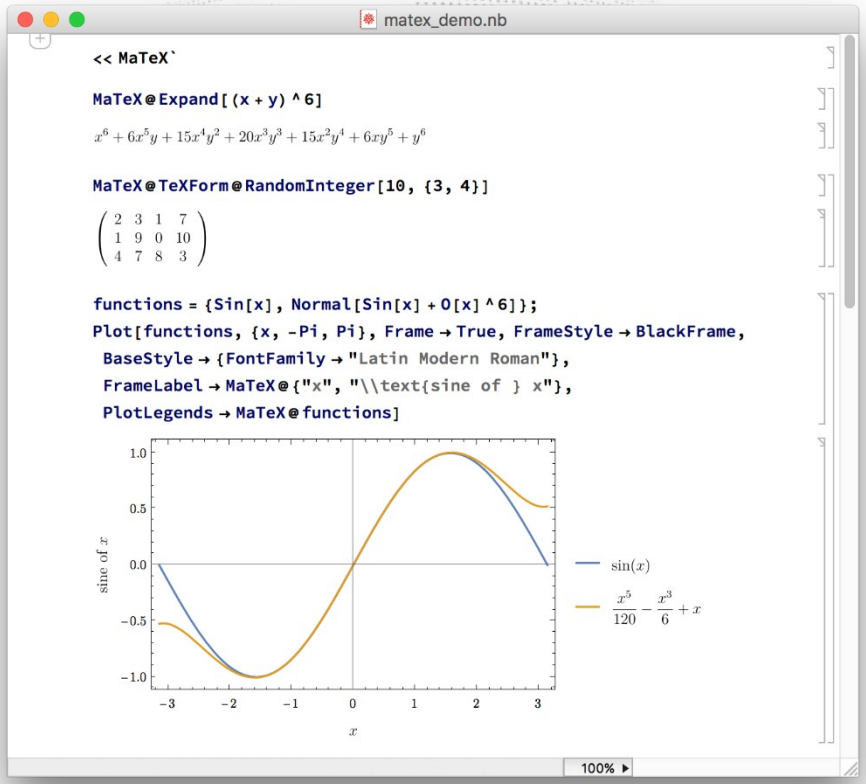
Some programming languages… **MATLAB**

- Since 1984, Mathworks
- Mathematical computations, especially linear algebra
- Proprietary – good packages
- GNU alternative: GNU Octave
- Many mathematical, engineering, scientific algorithms are only available in this language

MATLAB is what scientists use to do special scientist things.

Some programming languages… **Mathematica**

- Developed by Wolfram Research
- Symbolic language, as close to maths as possible
- Alternative to matlab (even more expensive)



Some more… Julia

- The next big thing, fastly growing
- Built for ease of use and performance at the same time
- Good choice for numerical simulations
- Only language besides Fortran and C++ to reach petaflops-level performance

R

- GNU version of **S** (1976), since 1992 (**R**oss Ihaka and **R**obert Gentleman, cf. S3, S4)
- Written mostly in C and Fortran
- Statistics-oriented
- 16th most popular language on TIOBE
- High-level language: can be very slow
- Interpreted
- CRAN packages (18719)
- Contributor to Debian

R is what scientists use when they can't afford MATLAB.

OPEN
REVOLUTION R OPEN

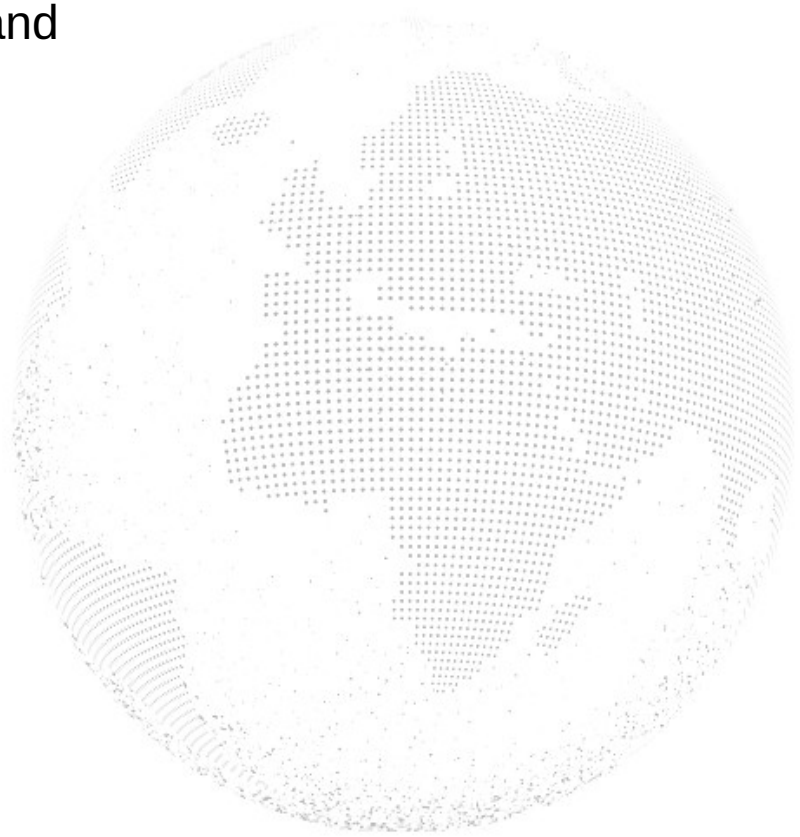
R Studio

R/Bioconductor for Genomics

	Package	Priority
boot	"boot"	"recommended"
base	"base"	"base"
boot	"boot"	"recommended"
class	"class"	"recommended"
cluster	"cluster"	"recommended"
codetools	"codetools"	"recommended"
compiler	"compiler"	"base"
datasets	"datasets"	"base"
foreign	"foreign"	"recommended"
graphics	"graphics"	"base"
grDevices	"grDevices"	"base"
grid	"grid"	"base"
KernSmooth	"KernSmooth"	"recommended"
lattice	"lattice"	"recommended"
MASS	"MASS"	"recommended"
Matrix	"Matrix"	"recommended"
methods	"methods"	"base"
mgcv	"mgcv"	"recommended"
nlme	"nlme"	"recommended"
nnet	"nnet"	"recommended"
parallel	"parallel"	"base"
rpart	"rpart"	"recommended"
spatial	"spatial"	"recommended"
splines	"splines"	"base"
stats	"stats"	"base"
stats4	"stats4"	"base"
survival	"survival"	"recommended"
tcltk	"tcltk"	"base"
tools	"tools"	"base"
utils	"utils"	"base"

Why learn / start with R?

- Isolated environment, experiment freely!
- Well-suited to statistics and scientific calculation: next step after excel
- *De facto* standard language in Ecology and Paleo
- Easy to set-up, works well on anything



R and RStudio

R: Language, tools to use it

- Terminal
- Plotting ‘devices’

Rstudio: Integrated Development Environment (IDE) for R

- Runs R
- Code editor
- Document Building