Scientific Computing WS 2020/2021

Lecture 1

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de

Me

- Name: Dr. Jürgen Fuhrmann (no, not Prof.)
- Affiliation: Weierstrass Institute for Applied Analysis and Stochastics, Berlin (WIAS);
  Deputy Head, *Numerical Mathematics and Scientific Computing*
- Contact: **juergen.fuhrmann@wias-berlin.de**
- Course homepage:
  `https://www.wias-berlin.de/people/fuhrmann/SciComp-WS2021/`
- Experience/Field of work:
  - Numerical solution of partial differential equations (PDEs)
  - Development, investigation, implementation of finite volume discretizations for nonlinear systems of PDEs
  - Ph.D. on multigrid methods
  - Applications: electrochemistry, semiconductor physics, groundwater...
  - Software development:
    - WIAS code pdelib (`http://pdelib.org`)
    - Languages: C, C++, Python, Lua, Fortran, Julia
    - Visualization: OpenGL, VTK

Admin stuff

- Lectures will be recorded
- Slides + Julia notebooks will be available from the course home page `https://www.wias-berlin.de/people/fuhrmann/SciComp-WS2021/`
- Weekly material uploads by Wed night (hopefully)
- Official lecture times: Thu 16-18 and Fri 16-18 will be used for feedback sessions with zulip chat and zoom.
- Zoom links will be provided in the chat or per email.
- I will use the email address used for enrolling for all communication, zulip invitations etc. Please keep me informed about any changes.
- Please provide missing "Matrikelnummern"
- All code examples and assignments will be in Julia, either as notebooks or as Julia files. Things should work on Linux, MacOSX, Windows
- Access to examination
  - Attend $\approx$ 80% of lectures
  - Return assignments

Introduction

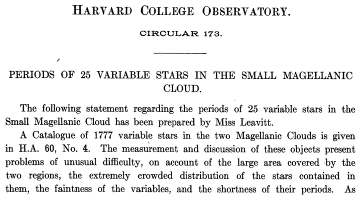
About computers and (scientific) computing

There was a time when "computers" were humans

Harvard Computers, circa 1890

By Harvard College Observatory - Public Domain

https://commons.wikimedia.org/w/index.php?curid=10392913



HARVARD COLLEGE OBSERVATORY.

CIRCULAR 173.

PERIODS OF 25 VARIABLE STARS IN THE SMALL MAGELLANIC CLOUD.

The following statement regarding the periods of 25 variable stars in the Small Magellanic Cloud has been prepared by Miss Leavitt.

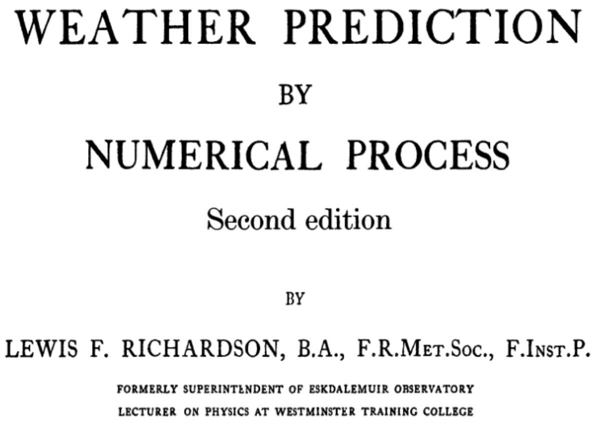
A Catalogue of 1777 variable stars in the two Magellanic Clouds is given in H.A. 60, No. 4. The measurement and discussion of these objects present problems of unusual difficulty, on account of the large area covered by the two regions, the extremely crowded distribution of the stars contained in them, the faintness of the variables, and the shortness of their periods. As

It was about science – astronomy

Computations of course have been performed since ancient times. One can trace back the termin "computer" applied to humans at least until 1613.

The "Harvard computers" became very famous in this context. Incidently, they were mostly female. They predate the NASA human computers of recent movie fame.

Weather Prediction by Numerical Process



WEATHER PREDICTION

BY

NUMERICAL PROCESS

Second edition

BY

LEWIS F. RICHARDSON, B.A., F.R.MET.SOC., F.INST.P.

FORMERLY SUPERINTENDENT OF ESKDALEMUIR OBSERVATORY

LECTURER ON PHYSICS AT WESTMINSTER TRAINING COLLEGE

L.F.Richardson 1922: 64000 human computers sit in rooms attached to a transparent cupola, they project their results which are combined by some main computers at the center

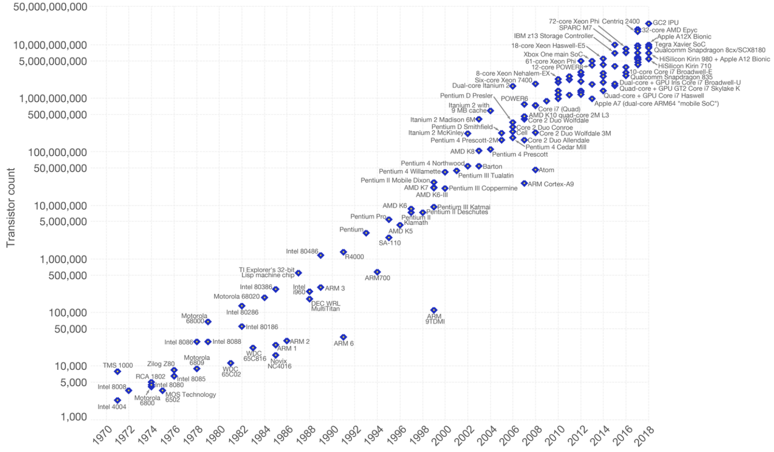
Does this scale ?

1986 Illustration of L.F. Richardson's vision by S. Conlin

Computing was taken over by machines

Moore's Law – The number of transistors on integrated circuit chips (1971-2018)

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important as other aspects of technological progress – such as processing speed or the price of electronic products – are linked to Moore's law.



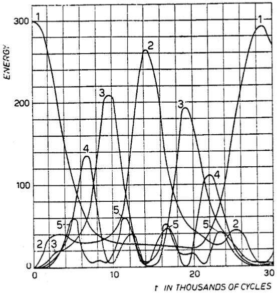
Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count)
The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

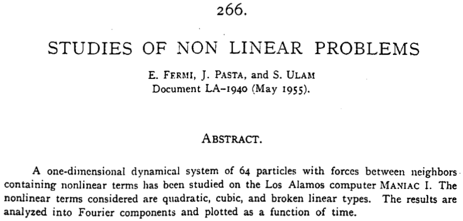
Computational engineering

- Starting points: artillery trajectories, nuclear weapons, rocket design, weather . . .
- Now ubiquitous:
  - Structural engineering
  - Car industry
  - Oil recovery
  - Semiconductor design
  - . . .
- Use of well established, verified, well supported commercial codes
  - Comsol
  - ANSYS
  - Eclipse
  - . . .

As soon as computing machines became available . . .

. . . Scientists "misused" them to satisfy their curiosity





266.

STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM

Document LA-1940 (May 1955).

ABSTRACT.

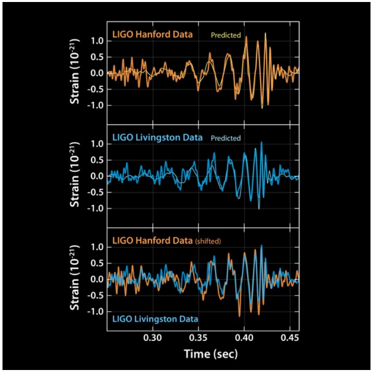
A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

". . . Fermi became interested in the development and potentialities of the electronic computing machines. He held many discussions [. . .] of the kind of future problems which could be studied through the use of such machines."

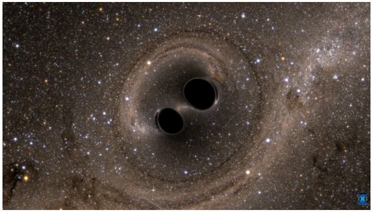
Fermi,Pasta and Ulam studied particle systems with *nonlinear* interactions

Calculations were done on the MANIAC-1 computer at Los Alamos

And they still do. . .



Caltech/MIT/LIGO Lab



SXS, the Simulating eXtreme Spacetimes (SXS) project (`http://www.black-holes.org`)

Verification of the detection of gravitational waves by numerical solution of Einstein's equations of general relativity using the "Spectral Einstein Code"

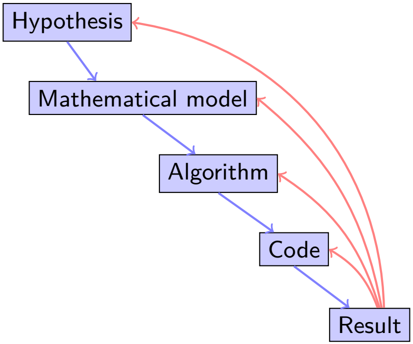
Computations significantly contributed to the 2017 Nobel prize in physics

Scientific computing

“The purpose of computing is insight, not numbers.”
(https://en.wikiquote.org/wiki/Richard_Hamming)

- Frontiers of Scientific Computing
  - Insight into complicated phenomena not accessible by other methods
  - Improvement of models to better fit reality
  - Improvment of computational methods
  - Generate testable hypothesis
  - Support experimentation in other scientific fields
  - Exploration of new computing capabilities
  - Prediction, optimization of complex systems
- Good scientifc practice
  - Reproducibility
  - Sharing of ideas and knowledge
- Interdisciplinarity
  - Numerical Analysis
  - Computer science
  - Modeling in specific fields

General approach



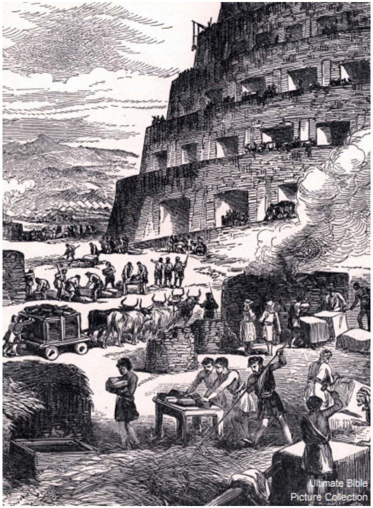
- Possible (probable) involvement of different persons, institutions
- It is important to keep interdisciplinarity in mind

Scientific computing tools

Many of them are Open Source

- General purpose environments
  - Matlab
  - COMSOL
  - Python + ecosystem
  - R + ecosystem
  - **Julia**
- "Classical" computer languages + compilers
  - Fortran
  - C, C++
- Established special purpose libraries
  - Linear algebra: LAPACK, BLAS, UMFPACK, Pardiso
  - Mesh generation: **triangle**, TetGen, NetGen
  - Eigenvalue problems: ARPACK
  - Visualization libraries: VTK
- Tools in the "background"
  - Build systems Make, CMake
  - Editors + IDEs (emacs, jedit, eclipse, atom, Visual Studio Code)
  - Debuggers
  - Version control (svn, **git**, hg)

Confusio Linguarum



"And the whole land was of one language and of one speech. ... And they said, Go to, let us build us a city and a tower whose top may reach unto heaven. ... And the Lord said, behold, the people is one, and they have all one language. ... Go to, let us go down, and there confound their language that they may not understand one another's speech. So the Lord scattered them abroad from thence upon the face of all the earth." (Daniel 1:1-7)

Once again Hamming

. . . of “Hamming code” and “Hamming distance” fame, who started his carrier programming in Los Alamos:

“Indeed, one of my major complaints about the computer field is that whereas Newton could say,”If I have seen a little farther than others, it is because I have stood on the shoulders of giants,” I am forced to say, “Today we stand on each other’s feet.” Perhaps the central problem we face in all of computer science is how we are to get to the situation where we build on top of the work of others rather than redoing so much of it in a trivially different way. Science is supposed to be cumulative, not almost endless duplication of the same kind of things.” (1968)

- 2020 this is still a problem

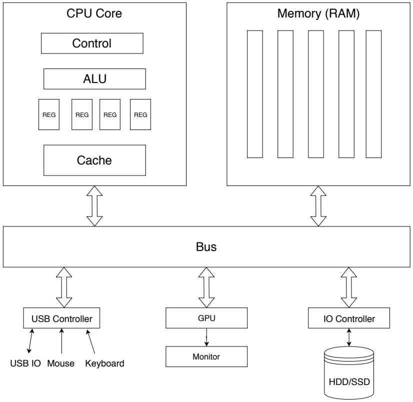
Intended aims and topics of this course

- Indicate a reasonable path within this labyrinth
- Introduction to Julia
- Relevant topics from numerical analysis
- Focus on partial differential equation (PDE) solution
  - Solution of large linear systems of equations
  - Finite elements
  - Finite volumes
  - Mesh generation
  - Linear and nonlinear solvers
  - Parallelization
  - Visualization

Hardware aspects

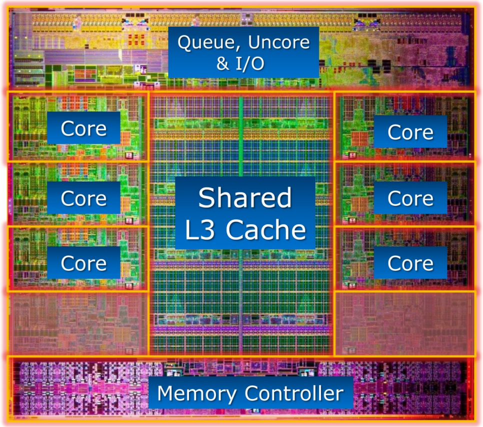
With material from “Introduction to High-Performance Scientific Computing” by Victor Eijkhout
(http://pages.tacc.utexas.edu/~eijkhout/istc/istc.html)

von Neumann Architecture



- Data and code stored in the same memory ⇒ encoded in the same way, stored as binary numbers
- Instruction cycle:
  - Instruction decode: determine operation and operands
  - Get operands from memory
  - Perform operation
  - Write results back
  - Continue with next instruction
- Controlled by clock: “heartbeat” of CPU
- Traditionally: one instruction per clock cycle

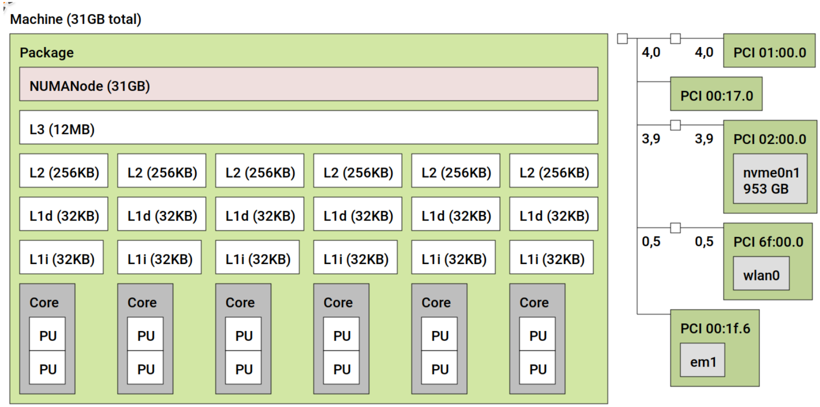
Multicore CPU



Modern CPU. From: https://www.hartware.de/review_1411_2.html

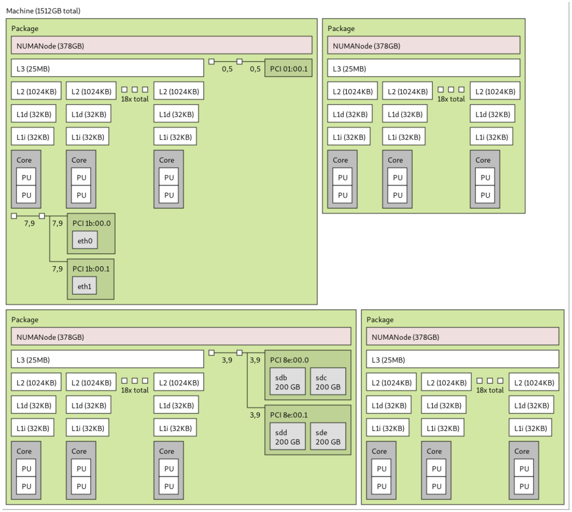
- Several computational cores on one CPU
- Cache: fast intermediate memory for often used operands

Mulicore CPU: this Laptop



- Three cache levels
- 6 Cores with similar pathways to memory

NUMA Architecture: compute server



- NUMA: Non Uniform Memory Access
- Several packages with 1 NUMA node each
- Each NUMA node has part of the system RAM attached to it.

Modern CPU workings

- Multicore parallelism
- Multiple floating point units in one core $\Rightarrow$ on-core parallelism:
- Complex instructions, e.g. one multiplication + one addition as single instruction
- Pipelining
  - A single floating point instruction takes several clock cycles to complete:
  - Subdivide an instruction:
    - Instruction decode
    - Operand exponent align
    - Actual operation
    - Normalize
  - Pipeline: separate piece of hardware for each subdivision
  - Like assembly line
- Peak performance is several operations /clock cycle for well optimized code
- Operands can be in memory, cache, register $\Rightarrow$ influence on perfomance
- Performance depends on availability of data from memory

Memory Hierachy

- Main memory access is slow compared to the processor
  - 100–1000 cycles latency before data arrive
  - Data stream maybe 1/4 floating point number/cycle;
  - processor wants 2 or 3 for full performance
- Faster memory is expensive
- *Cache* is a small piece of fast memory for intermediate storage of data
- Operands are moved to CPU *registers* immediately before operation
- Memory hierarchy:

  Registers in different cores
  Fast on-CPU cache memory (L1, L2, L3)
  Main memory

- Registers are filled with data from main memory via cache:
  - L1 Cache: Data cache closest to registers
  - L2 Cache: Secondary data cache, stores both data and instructions
  - Data from L2 has to go through L1 to registers
  - L2 is 10 to 100 times larger than L1
  - Multiple cores on one NUMA node share L3 cache , $\approx$10x larger than L2

Cache line

- Smallest unit of data transferred between main memory and the caches (or between levels of cache)
- Fixed number of sequentially stored bytes. A floating point number typically uses 8 bytes, and cache lines can be e.g. 128 bytes long (16 numbers)
- If you request one number you get several numbers at once - the whole cache line
  - For performance, make sure to use all data arrived, you've paid for them in bandwidth
  - Sequential access good, "strided" access ok, random access bad
- Cache hit: location referenced is found in the cache
- Cache miss: location referenced is not found in cache
  - Triggers access to the next higher cache or memory
- Cache thrashing
  - Two data elements can be mapped to the same cache line: loading the second "evicts" the first
  - Now what if this code is in a loop? "thrashing": really bad for performance
- Performance is limited by data transfer rate
- High performance if data items are used multiple times

Computer languages

Machine code

- Detailed instructions for the actions of the CPU
- Not human readable
- Sample types of instructions:
    - Transfer data between memory location and register
    - Perform arithmetic/logic operations with data in register
    - Check if data in register fulfills some condition
    - Conditionally change the memory address from where instructions are fetched $\equiv$ “jump” to address
    - Save all register context and take instructions from different memory location until return $\equiv$ “call”
- Programming started with hand-coding this in binary form ...

```
534c 29e5 31db 48c1 fd03 4883 ec08 e85d
feff ff48 85ed 741e 0f1f 8400 0000 0000
4c89 ea4c 89f6 4489 ff41 ff14 dc48 83c3
0148 39eb 75ea 4883 c408 5b5d 415c 415d
415e 415f c390 662e 0f1f 8400 0000 0000
f3c3 0000 4883 ec08 4883 c408 c300 0000
0100 0200 4865 6c6c 6f20 776f 726c 6400
011b 033b 3400 0000 0500 0000 20fe ffff
8000 0000 60fe ffff 5000 0000 4dff ffff
```

My first programmable computer

SER2d by VEB Elektronische Rechenmaschinen Karl-Marx-Stadt (around 1962)
My secondary school owned an exemplar around 1975

- I started programming this way
- Instructions were supplied on punched tape
- Output was printed on a typewriter
- The magnetic drum could store 127 numbers and 127 instructions

Assembler code

- Human readable representation of CPU instructions
- Some write it by hand ...
  - Code close to abilities and structure of the machine
  - Handle constrained resources (embedded systems, early computers)
- Translated to machine code by a programm called *assembler*

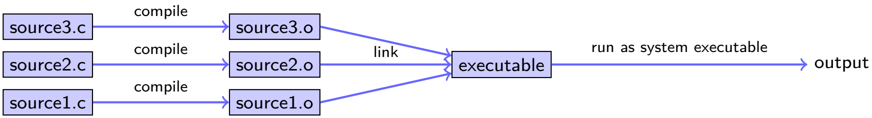
```
.file   "code.c"
.section    .rodata
.LC0:
.string "Hello world"
.text
...
pushq   %rbp
.cfi_def_cfa_offset 16
.cfi_offset 6, -16
movq    %rsp, %rbp
.cfi_def_cfa_register 6
subq    $16, %rsp
movl    %edi, -4(%rbp)
movq    %rsi, -16(%rbp)
movl    $.LC0, %edi
movl    $0, %eax
call    printf
```

Compiled high level languages

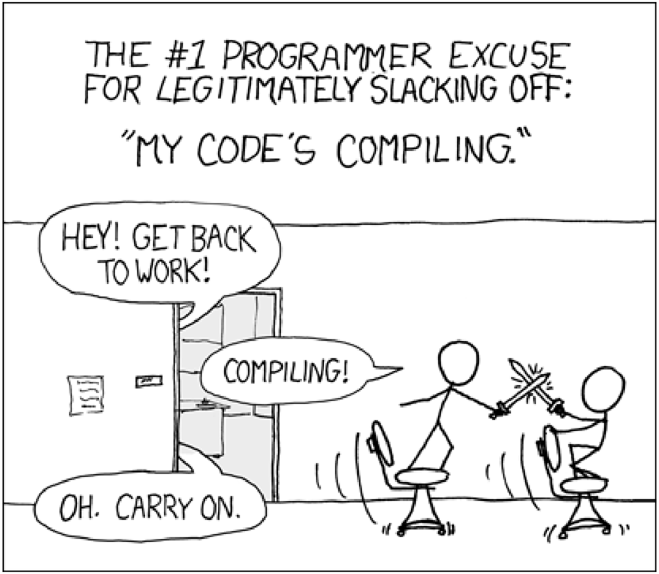
- Algorithm description using mix of mathematical formulas and statements inspired by human language
- Translated to machine code (resp. assembler) by *compiler*

```
#include <stdio.h>
int main (int argc, char *argv[])
{
  printf("Hello world");
}
```

- "Far away" from CPU $\Rightarrow$ the compiler is responsible for creation of optimized machine code
- Fortran, COBOL, C, Pascal, Ada, Modula2, C++, Go, Rust, Swift
- Strongly typed
- Tedious workflow: compile - link - run



Compiling. . .



. . . from xkcd

Compiled languages in Scientific Computing

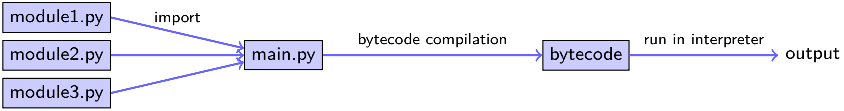
- Fortran: FORmula TRANslator (1957)
    - Fortran4: really dead
    - Fortran77: large number of legacy libs: BLAS, LAPACK, ARPACK ...
    - Fortran90, Fortran2003, Fortran 2008
        - Catch up with features of C/C++ (structures,allocation,classes,inheritance, C/C++ library calls)
        - Lost momentum among new programmers
        - Hard to integrate with C/C++
        - In many aspects very well adapted to numerical computing
        - Well designed multidimensional arrays
        - Still used in several subfields of scientific computing
- C: General purpose language
    - K&R C (1978) weak type checking
    - ANSI C (1989) strong type checking
    - Had structures and allocation early on
    - Numerical methods support via libraries
    - Fortran library calls possible
- C++: *The* powerful general purpose object oriented language used (not only) in scientific computing
    - Superset of C (in a first approximation)
    - Classes, inheritance, overloading, templates (generic programming)
    - C++11: $\approx$ 2011 Quantum leap: smart pointers, threads, lambdas, anonymous functions
    - Since then: C++14, C++17, C++20 – moving target ...
    - With great power comes the possibility of great failure...

High level scripting languages

- Algorithm description using mix of mathematical formulas and statements inspired by human language
- Often: simpler syntax, less ”boiler plate”

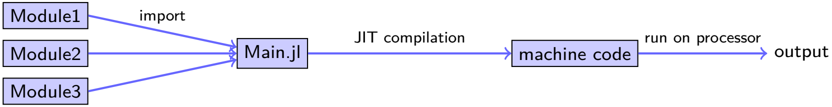
```
print("Hello world")
```

- Need intepreter in order to be executed
- Very far away from CPU $\Rightarrow$ usually significantly slower compared to compiled languages
- Matlab, Python, Lua, perl, R, Java, javascript
- Less strict type checking, powerful introspection capabilities
- Immediate workflow: “just run”
  - in fact: first compiled to *bytecode* which can be interpreted more efficiently



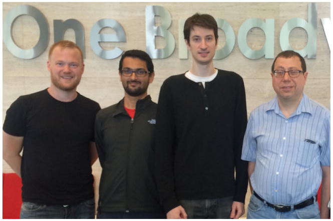
JIT based languages

- Most interpreted language first compile to bytecode which then is run in the interpreter and not on the processor $\Rightarrow$ perfomance bottleneck,
  - remedy: use compiled language for performance critical parts
  - “two language problem”, additional work for interface code
- Better: Just In Time compiler (JIT): compile to machine code “on the fly”
  - Many languages try to add JIT technology after they have been designed: javascript, Lua, Java, Smalltalk, Python/NUMBA
  - LLVM among other projects provides universal, language independent JIT infrastructure
  - **Julia** (v1.0 since August, 2018) was designed around LLVM
- Drawback over compiled languages: compilation delay at every start, can be mediated by caching
- Advantage over compiled languages: simpler syntax, option for *tracing* JIT, i.e. optimization at runtime



Julia History & Resources

- 2009-02: V0.1 Development started in 2009 at MIT (S. Bezanson, S. Karpinski, V. Shah, A. Edelman)
- 2012: V0.1
- 2016-10: V0.5 experimental threading support
- 2017-02: SIAM Review: Julia - A Fresh Approach to Numerical Computing
- 2018-08: **V1.0**
- 2018 Wilkinson Prize for numerical software



- Homepage incl. download link: `https://julialang.org/`
- Wikibook: `https://en.wikibooks.org/wiki/Introducing_Julia`

Julia - a first characterization

“**Like matlab, but faster**”

“**Like matlab, but open source**”

“**Like python + numpy, but faster and counting from 1**”

- Main purpose: performant numerics
- Multidimensional arrays as first class objects
  (like Fortran, Matlab; unlike C++, Swift, Rust, Go ...)
- Array indices counting from 1
  (like Fortran, Matlab; unlike C++, python) - but it seems this becomes more flexible
- Array slicing etc.
- Extensive library of standard functions, linear algebra operations
- Package ecosystem

. . . there is more to the picture

- Developed from scratch using modern knowledge in language development
- Strongly typed $\Rightarrow$ JIT compilation to performant code
- Multiple dispatch: all functions are essentialy templates
- Parallelization: SIMD, threading, distributed memory
- Reflexive: one can loop over struct elements
- Module system, module precompilation
- REPL (Read-Eval-Print-Loop)
- Ecosystem:
  - Package manager with github integration
  - Foreign function interface to C, Fortran, wrapper methods for C++
  - PyCall.jl: loading of python modules via reflexive proxy objects (e.g. plotting)
  - Intrinsic tools for documentation, profiling, testing
  - Code inspection of LLVM and native assembler codes
  - IDE integration with Visual Studio Code
  - Jupyter, Pluto notebooks