Scientific Computing WS 2019/2020

Lecture 1

Jürgen Fuhrmann

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Me

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- 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:
  `http://www.wias-berlin.de/people/fuhrmann/teach.html`
- 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: **Tue 10-12 FH 311**, **Thu 10-12 MA269**
- Consultation: **Thu 12-13 MA269**, more at WIAS on appointment
- There will be coding assignments in Julia
  - Unix pool
  - Installation possible for Linux, MacOSX, Windows
- Access to examination
  - Attend $\approx$ 80% of lectures
  - Return assignments
- Slides and code will be online, a script is being developed from the slides.
- See course homepage for literature, specific hints during course

Thursday lectures in MA269 (UNIX Pool)

https://www.math.tu-berlin.de/iuk/lehrrechnerbereich/v_menue/lehrrechnerbereich/

- Working groups of two students per account/computer
- **Please sign up to the account list provided by the admins**
- **Please check and correct the attendance list, enter your WIR account number**
- All examples during this course will be available on UNIX pool systems
- All homework can be done on UNIX pool machines as well (Room MA241 outside of course hours)
- Please find yourself in groups of two and fill in the list of accounts for the UNIX pool (on Thursday)
- Once the administrators open the accounts, you will be able to log in and enter a new password

Introduction

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.

Does this scale ?

WEATHER PREDICTION

BY

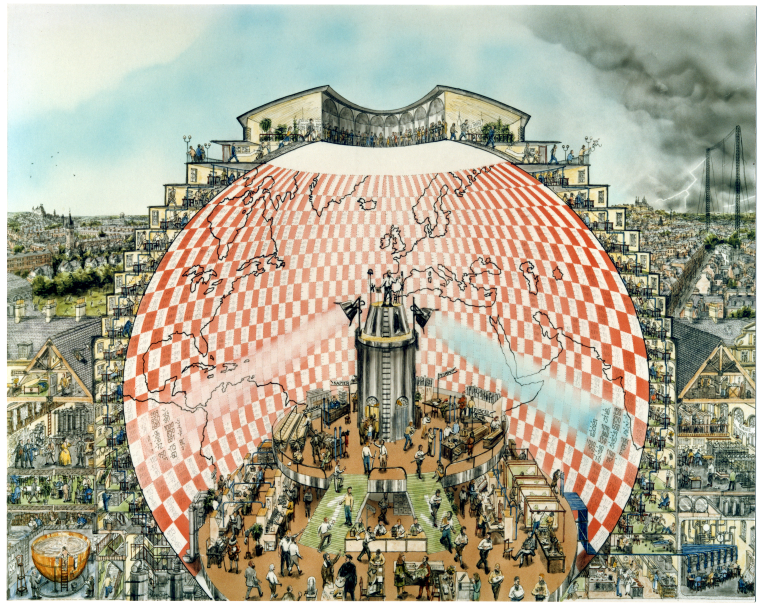
NUMERICAL PROCESS

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

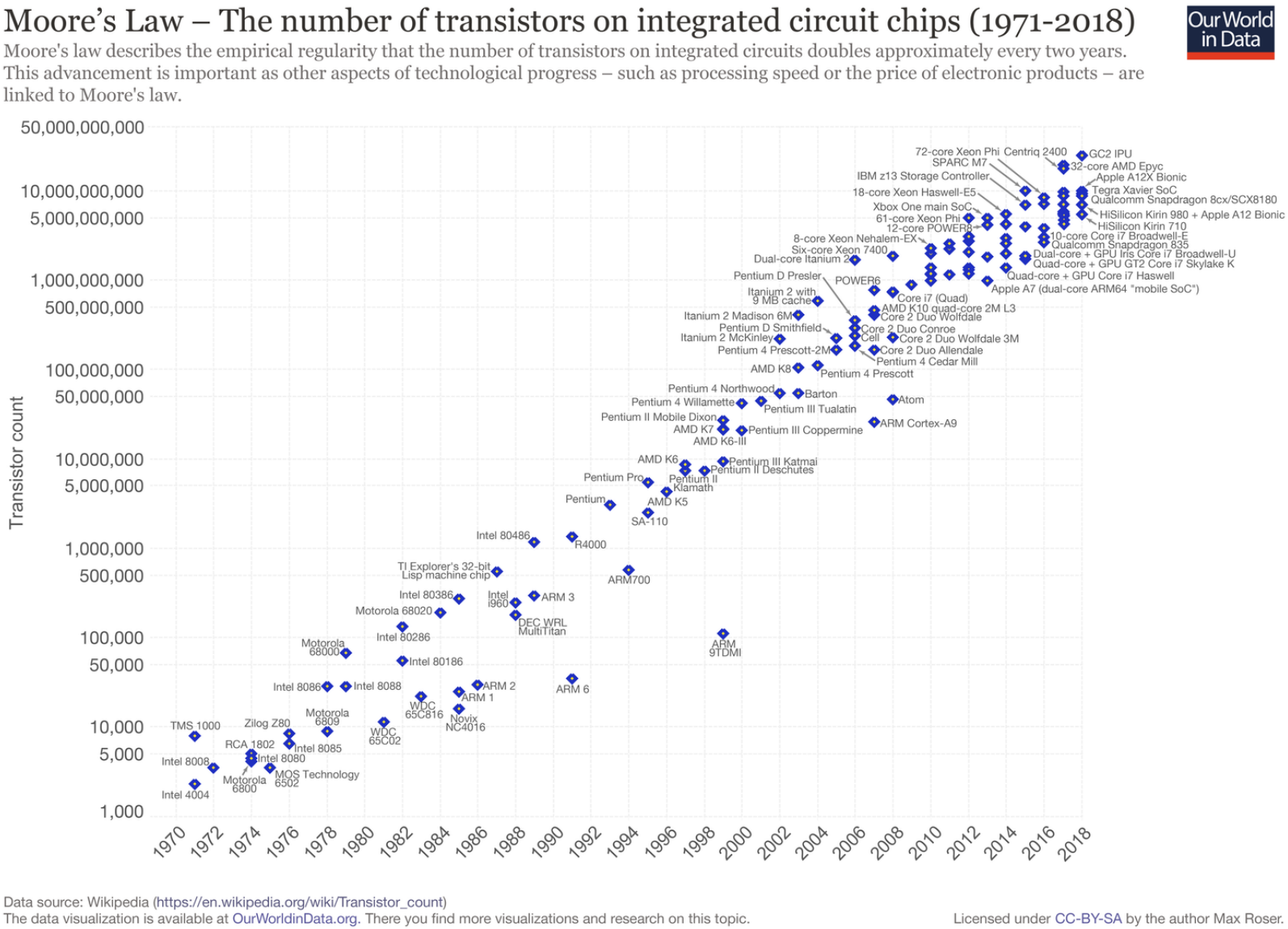


64000 computers predicting weather (1986 Illustration of L.F. Richardson's vision by S. Conlin)

L.F.Richardson 1922

- This was about weather, not science in the first place
- Science *and* Engineering need computing

Computing was taken over by machines



By Max Roser - https://ourworldindata.org/uploads/2019/05/Transistor-Count-over-time-to-2018.png, CC BY-SA 4.0,

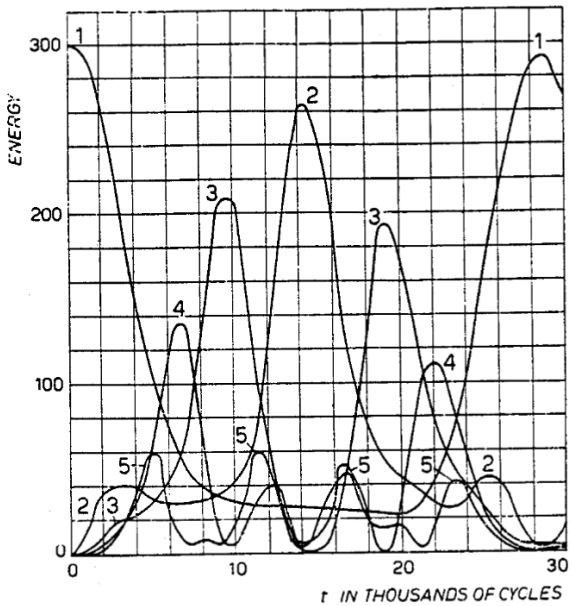
https://commons.wikimedia.org/w/index.php?curid=79751151

Computational engineering

- Starting points: Nuclear weapons + rocket design, ballistic trajectories, weather ...
- Now ubiquitous:
  - Structural engineering
  - Car industry
  - Oil recovery
  - Semiconductor design
  - ...
- Use of well established, verfied, 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.

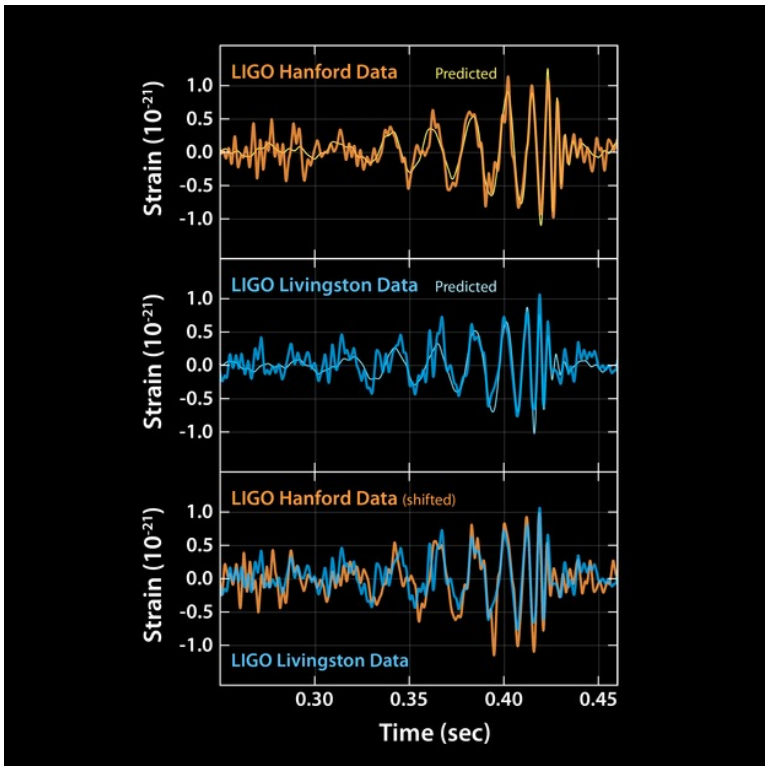
A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted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

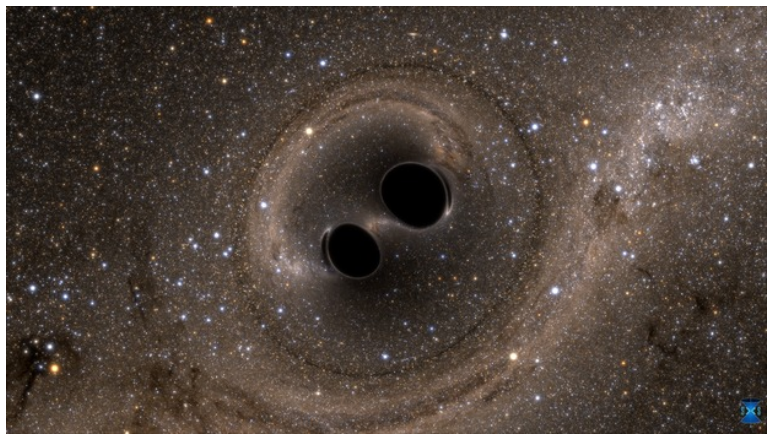
Fermi,Pasta and Ulam studied particle systems with *nonlinear* interactions

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"

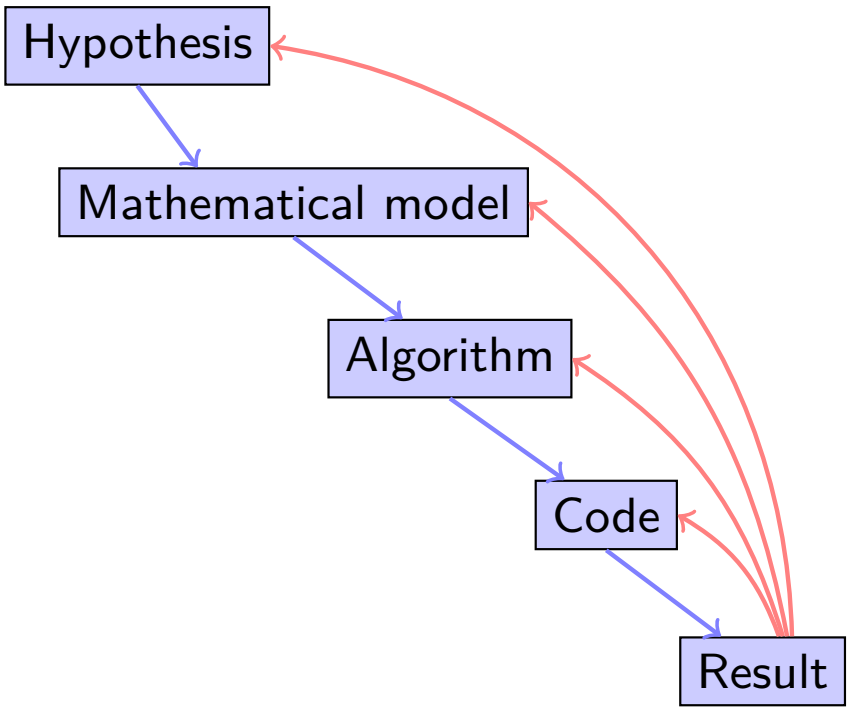
Computations significantly contributed to the 2017 Nobel prize in physics

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



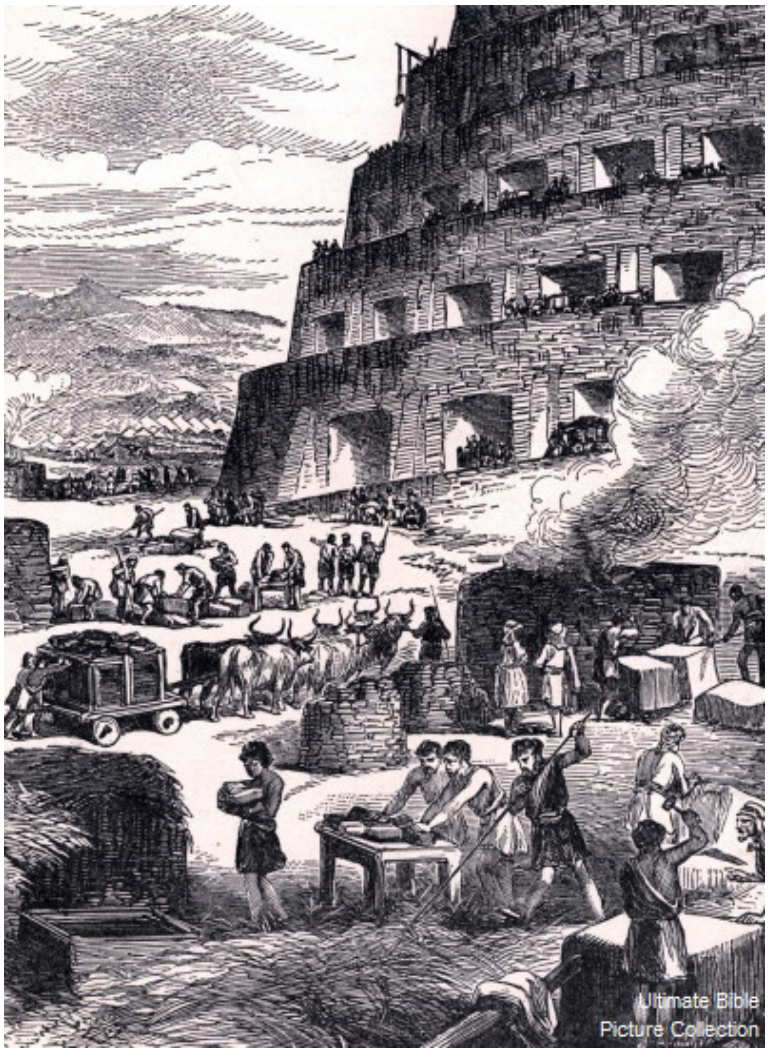
- Possible (probable) involvement of different persons, institutions
- It is important to keep interdisciplinarity in mind

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)

- 2017 this is still a problem

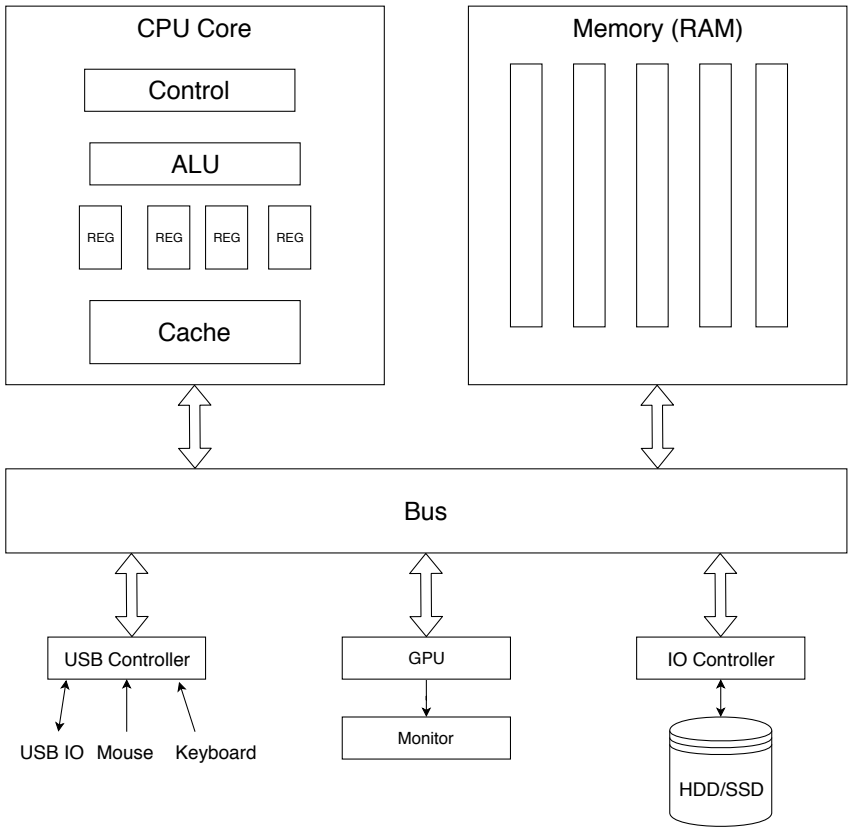
Intended aims and topics of this course

- Indicate a reasonable path within this labyrinth
- Introduction to Julia
- Software management skills (version control)
- 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)

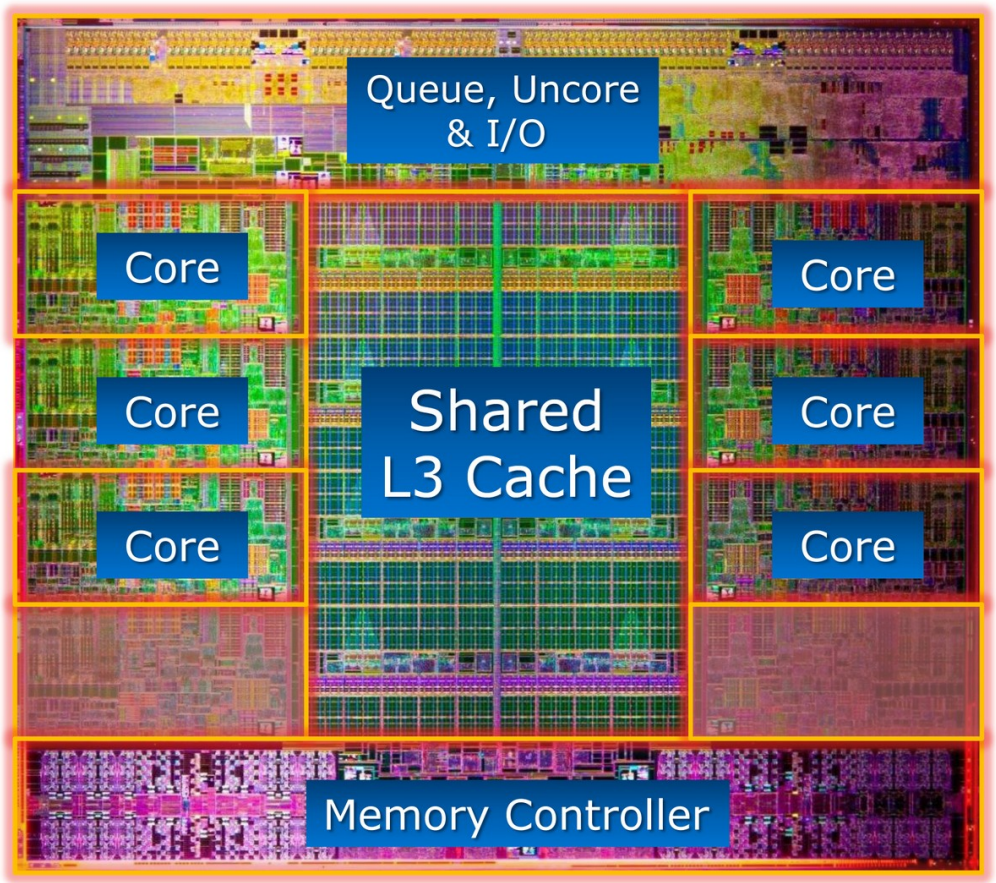
von Neumann Architecture



- Data and code stored in the same memory $\Rightarrow$ 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

Contemporary CPU Architecture

- Operations can be performed speculatively
- On-Core parallelism: multiple operations simultaneously
- Multicore parallelism
- Operands can be in memory, cache, register
- Results may need to be coordinated with other processing elements



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

Modern CPU core functionality

- Clock: "heartbeat" of CPU
- Traditionally: one instruction per clock cycle
- Modern CPUs: Multiple floating point units, complex instructions, e.g. one multiplication + one addition as single instruction
  - Peak performance is several operations /clock cycle
  - Only possible to obtain with highly optimized code
- 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

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
- 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
  - Some systems have an L3 cache, ≈10x larger than L2

Cache line

- The smallest unit of data transferred between main memory and the caches (or between levels of cache)
- N sequentially-stored, multi-byte words (usually N=8 or 16).
- If you request one word on a cache line, you get the whole line
  - make sure to use the other items, 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"
- Instructions are very hard to handle, although programming started this way ...

```
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
```

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*

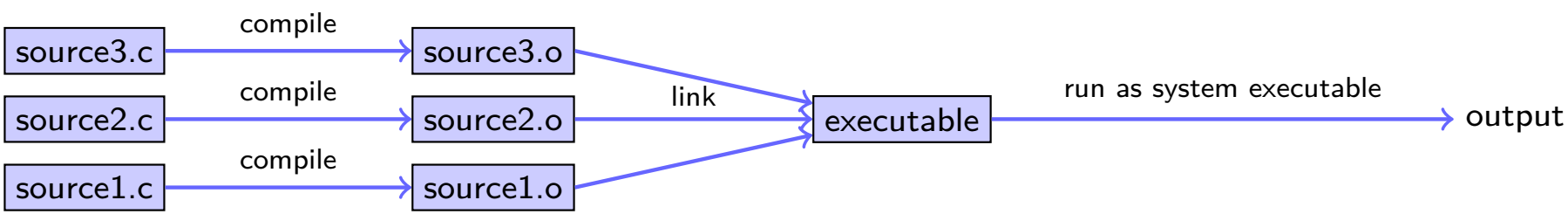
```
.file   "code.c"
.section    .rodata
.LC0:
.string "Hello world"
.text
...
pushq   %rbp
.cfi_def_cfa_offset 16
.cfi_offset 6, -16
movq    %rsp, %rbp
.cfi_def_cfa_register 6
subq    $16, %rsp
movl    %edi, -4(%rbp)
movq    %rsi, -16(%rbp)
movl    $.LC0, %edi
movl    $0, %eax
call    printf
```

Compiled high level languages

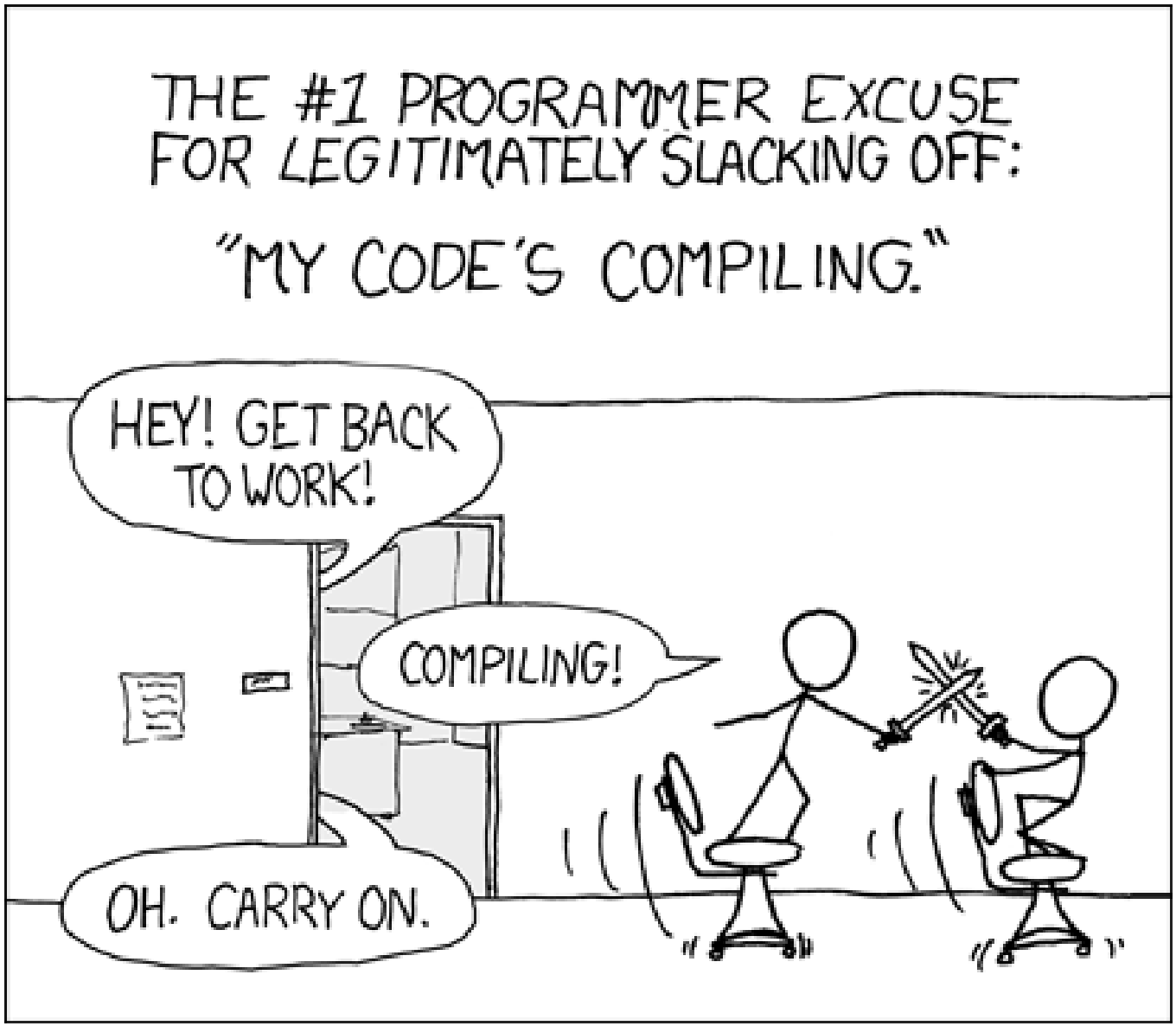
- Algorithm description using mix of mathematical formulas and statements inspired by human language
- Translated to machine code (resp. assembler) by *compiler*

```
#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

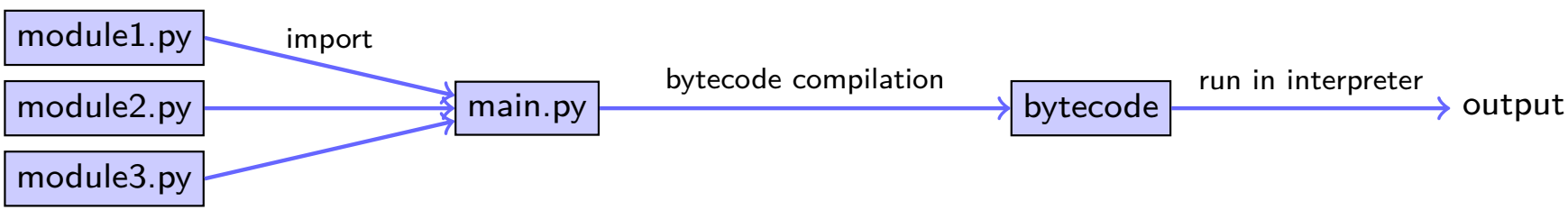
- Fortran: FORmula TRANslator (1957)
  - Fortran4: really dead
  - Fortran77: large number of legacy libs: BLAS, LAPACK, ARPACK ...
  - Fortran90, Fortran2003, Fortran 2008
    - Catch up with features of C/C++ (structures,allocation,classes,inheritance, C/C++ library calls)
    - Lost momentum among new programmers
    - Hard to integrate with C/C++
    - In many aspects very well adapted to numerical computing
    - Well designed multidimensional arrays
- 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 object oriented language
  - Superset of C (in a first approximation)
  - Classes, inheritance, overloading, templates (generic programming)
  - C++11: $\approx$ 2011 Quantum leap: smart pointers, threads, lambdas, initializer lists in standard
  - Since then: C++14, C++17, C++20
  - 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
- Simpler syntax, less "boiler plate"

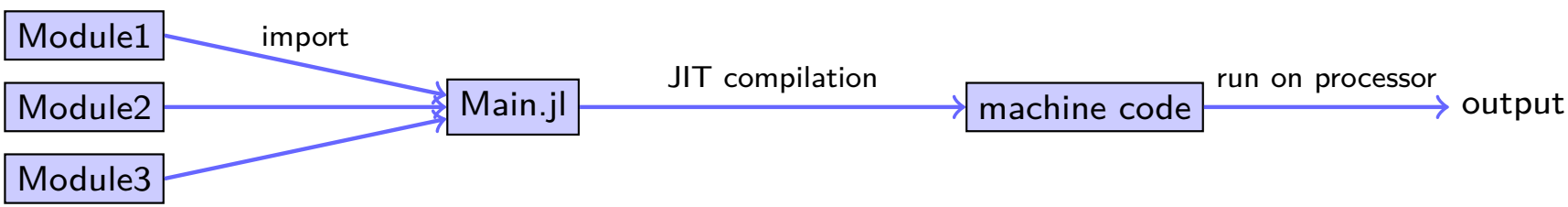
```
print("Hello world")
```

- 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



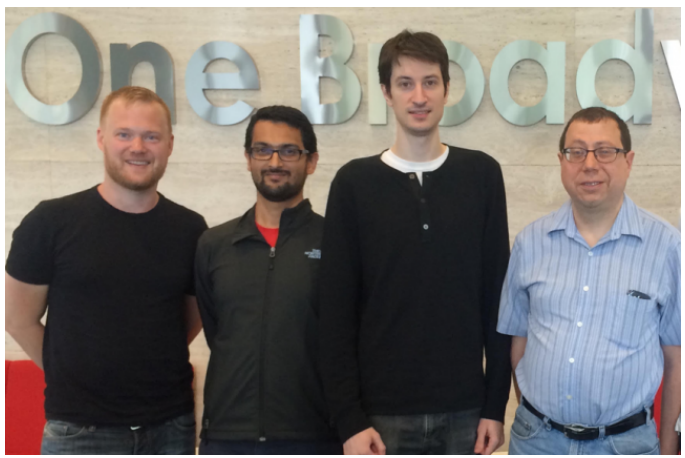
JIT based languages

- Most interpreted language first compile to bytecode wich 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"
  - V8 $\rightarrow$ javascript
  - LuaJIT, Java, Smalltalk
  - LLVM $\rightarrow$ **Julia** (v1.0 since August, 2018)
  - LLVM Compiler infrastructure $\rightarrow$ Python/NUMBA
- Drawback over compiled languages: compilation delay at every start, can be mediated by caching
- Advantage over compiled languages: simpler syntax, *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
- TU Berlin Jupyter server https://www-pool.math.tu-berlin.de/jupyter: you will be able to user your UNIX pool account

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 e.g. via atom editor (Juno)
  - Jupyter notebooks