First steps to python Scientific Computing Winter 2016/2017 Lecture 15 Jürgen Fuhrmann

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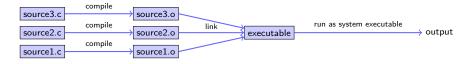


## Compiled high level languages

- 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 ⇒ 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

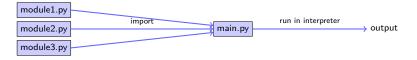


## High level scripting languages

- Algorithm description using mix of mathematical formulas and statements inspired by human language
- Need intepreter in order to be executed

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

- ► Very far away from CPU ⇒ usually significantly slower compared to compiled languages
- Matlab, Python, Lua, perl, R, Java, javascript
- Less strict type checking, often simple syntax, powerful introspection capabilities
- Immediate workflow: "just run"
  - ▶ in fact: first compiled to bytecode which can be interpreted more efficiently



# Python

- Developed since 1989, led by Guido van Rossum
- Can be seen as "open source" matlab
- Main advantage: huge ecosystem of packages for scientific computing
- Some use cases:
  - matlab replacement
  - glue language for different tools
  - system independent implementation of tools (e.g. mercurial)
  - driver language for software written in C/C++
    - quickly change parameters without recompiling etc.
    - make use of plotting capabilities
- Documentation: https://docs.python.org
  - current versions around: 2.7, 3.x
  - most python3 code works with 2.7
- Tutorial: https://docs.python.org/3/tutorial/

# Numpy / Scipy /matplotlib

- numpy: add-on of an efficient array class for numerical computations, written in C
- Python lists would be too slow
- Interfacing to lapack etc. need dense arrays
- scipy: Scientific computation package with LAPACK etc.
- matplotlib: data plotting + visualization

## Python and C++

Architecture of python

- Interpreter
- $\blacktriangleright$  Application programming interface (API) for interaction of C/C++ with python interpreter
  - register wrapper function with name
  - wrapper function knows how to fetch parameters/return values from/to python interpreter
  - wrapper function calls C++ function
- Wrapper code with code to be wrapped linked to a "shared object" (UNIX), "dylib" (Mac), "DLL" (Windows)
- Import of wrapper code makes it available in python
- Automatic tools for accessing API

# SWIG

#### Several possibilities

- Cython (python dialect with possible inclusion of C)
- pybind11 (C++11 classes for wrapping python)
- SWIG ("classical tool" for wrapping interpreter)
- Simplified Wrapper and Interface Generator:
  - ► Tool to automatically create wrapper code from C++ style description
  - Create wrapper code in C++ which is linked together with library to be wrapped