Programming and Data Analysis for Scientists

Seminar – Compiled vs Interpreted code

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Compiled vs Interpreted code*

- We have been learning C/C++ for a couple of weeks now. A key feature of this language is that code is **compiled** making it **compact** and **fast.**

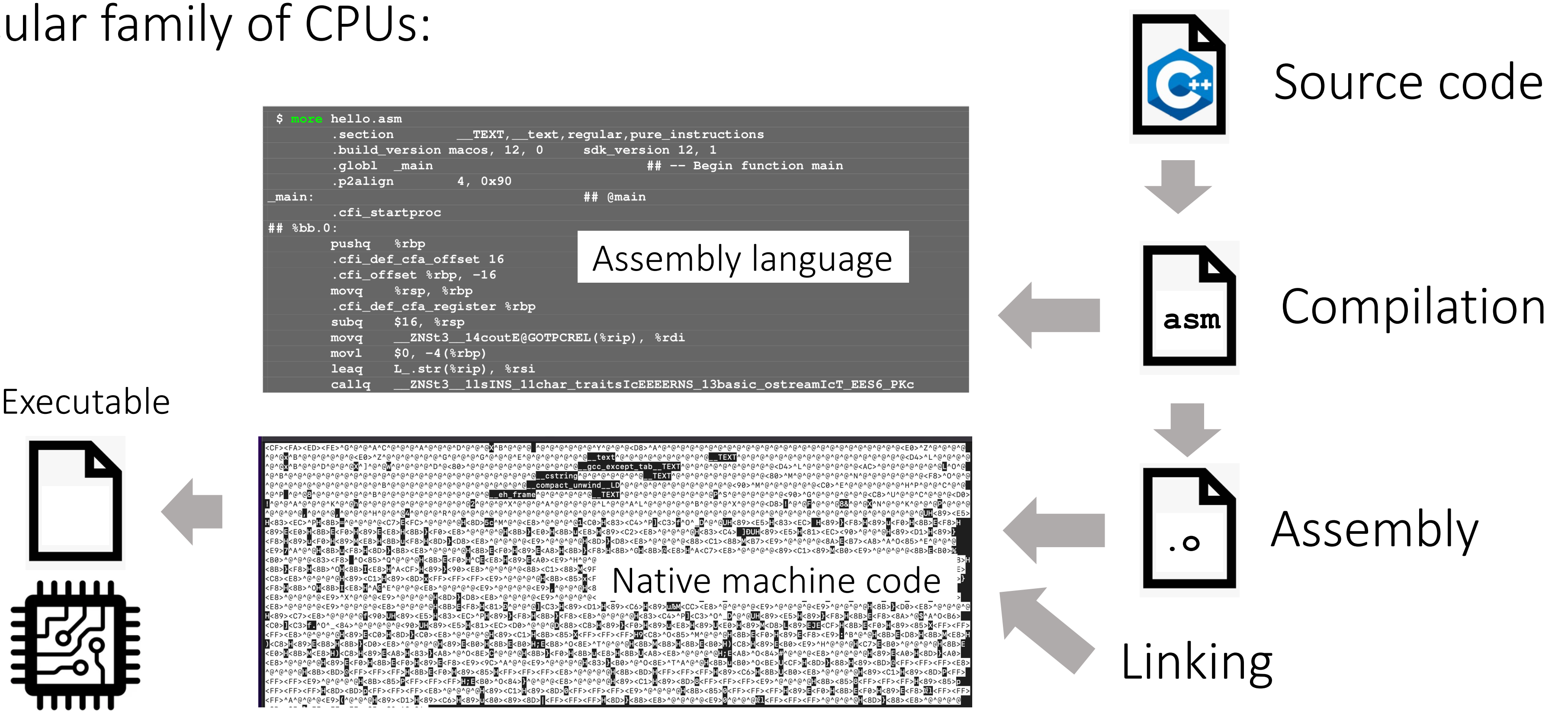
- Python is much more user-friendly than C/C++ making it extremely easy to prototype and explore new ideas and methodologies (with a big ecosystem of libraries).

- **But**, Python is slow due to being **interpreted**. In particular explicit looping is very slow due to overheads created by Python's dynamic variables type.

***Pedants**: technically whether code is compiled or interpreted is <u>not</u> a property of the *language* itself, but rather of the implementation. You could have a C/C++ interpreter and a Python compiler (although this is difficult to code).

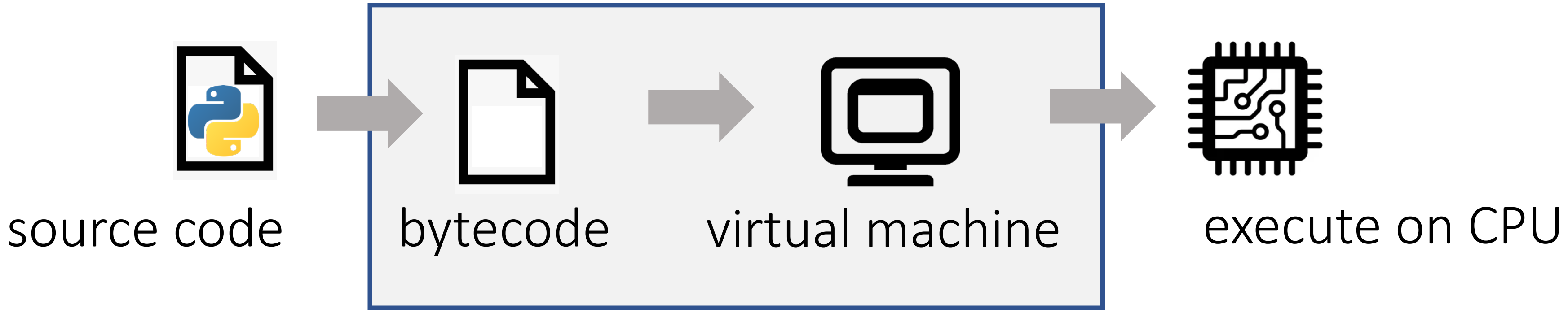
What is compilation?

Compiling takes source code and converts it into binary machine code native to a particular family of CPUs:



What is interpretation?

Interpreted source code is usually “compiled” not into binary machine code but into a bytecode – a kind of machine code for a virtual machine (hardware abstracted). The virtual machine is then a compiled executable that “runs” the bytecode instructions.



This form of virtualization approach was pioneered by Java and has become very popular because it is hardware agnostic (“write once run anywhere”).

Calling compiled C++ code from Python

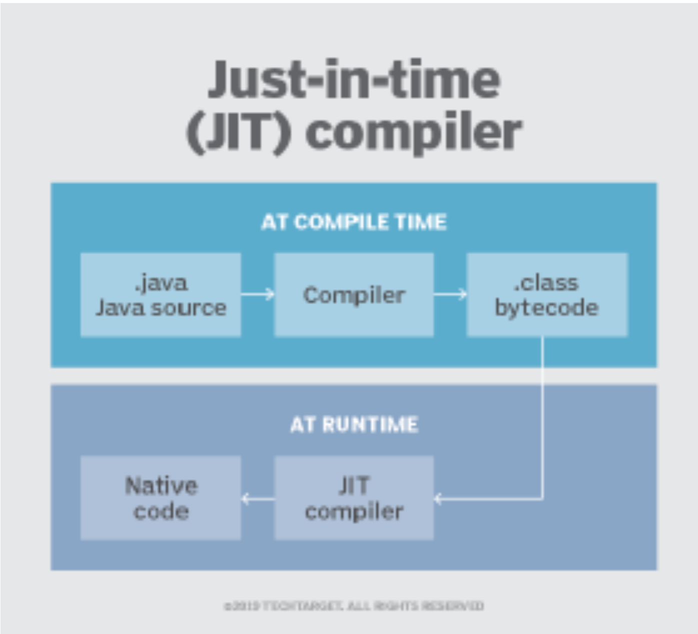
If you know which bits of your code are the bottleneck (it is usually clear) then you could write them in C++ (compile it) and then call them from Python.

This is a mixed language approach attempting to gain the best of both worlds.

We will have a look at an example using **ctypes** shortly. The issue here is that this kind of binding can be complicated to set up and tricky to debug.

Just in time compilation

An in-between possibility is so called *just in time* compilation. The virtual machine profiles your code to find the "hot-spots" and then compiles these parts during run-time into native machine code.



For numerical calculations the **Numba** package for Python basically does ctypes for you without any effort or recoding.

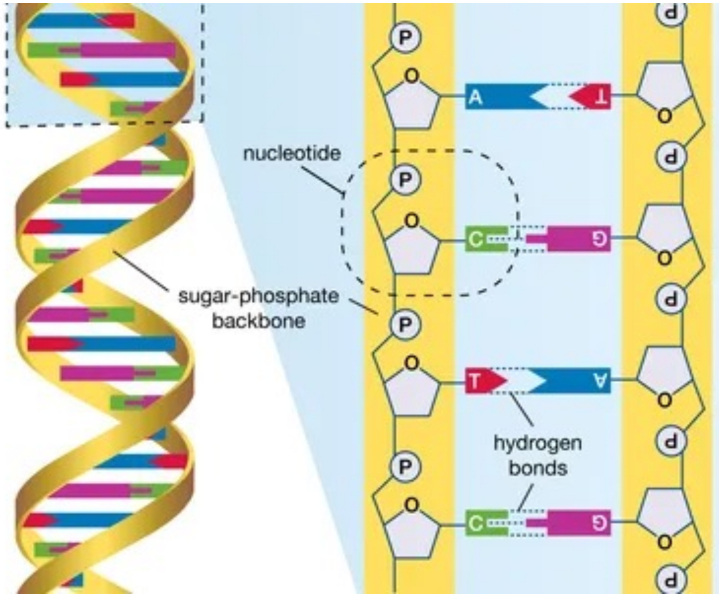
If it works you can get C/C++ similar performance from Python. Let do some tests ...

Example 1: Computing DNA K-mers

A DNA is a long chain of units called nucleotides.

There are 4 types of nucleotides labelled by A, C, G, and T. A short portion DNA could look like:

ACTAGGGATCATGAAGATAATGTTGGTGTTTG



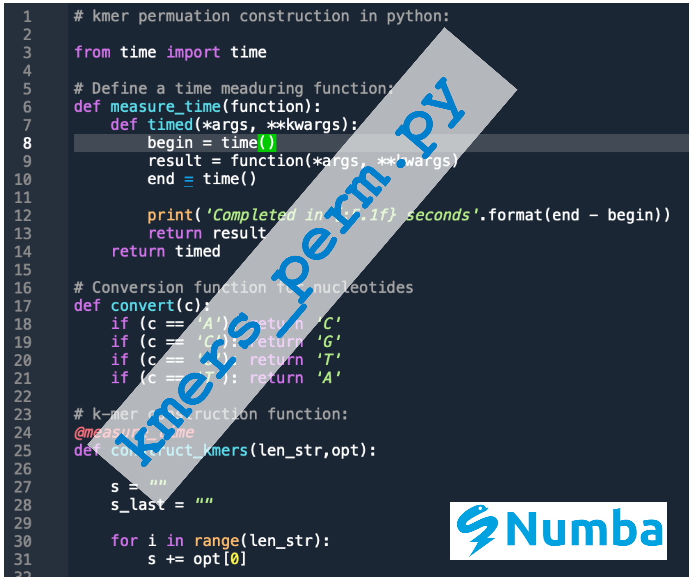
If you choose any K consecutive nucleotides (i.e. letters) from this string, it will be a K-mer. Here are some examples of 4-mers derived from the example.

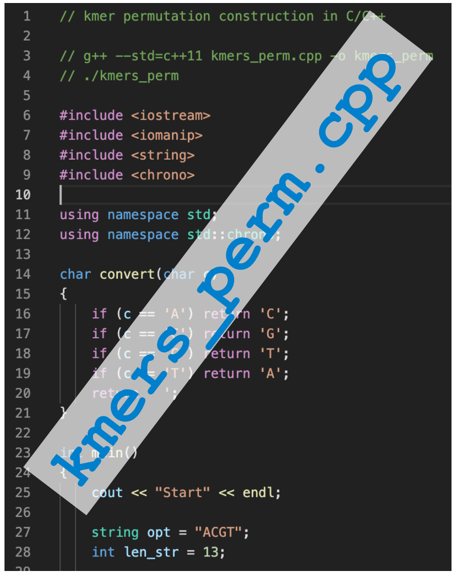
ACTA, CTAG, TAGG, AGGG, GGGA, etc.

Example 1: The challenge

Let's generate all possible 13-mers. Mathematically it is a permutation with a replacement problem. Therefore, we have 4^{13} (=67,108,864) possible 13-mers.

We will use a simple algorithm to generate results in Python and C++ paying particular attention to how long they take to run ...





=> Run the Python code

=> Compile and run the C++ code

```
g++ --std=c++11 kmers_perm.cpp -o kmers_perm
```

```
./kmers_perm
```

How do they compare?

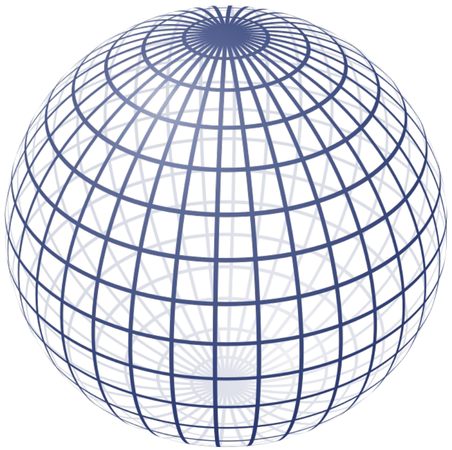
Example 2: Numerical integration in 3D

Let's try to compute the following 3D integral:

3D wave-vector

$$\mathbf{k} = \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}$$

Constant



$$\int_\Omega \frac{\mathrm{d}\mathbf{k}}{2\pi^2} \frac{e^{-\sigma^2 \mathbf{k}^\mathrm{T} \epsilon \mathbf{k}}}{\mathbf{k}^\mathrm{T} \epsilon \mathbf{k}}$$

Dielectric permittivity tensor

$$\epsilon = \begin{pmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}$$

Integrate over a sphere of radius G_{max}

Example 2: Numerical integration in 3D

There are clever methods we could use to do this integration, but let's just do brute force discretisation in Cartesian coordinates …

Use N points along each axis so the code will involve:

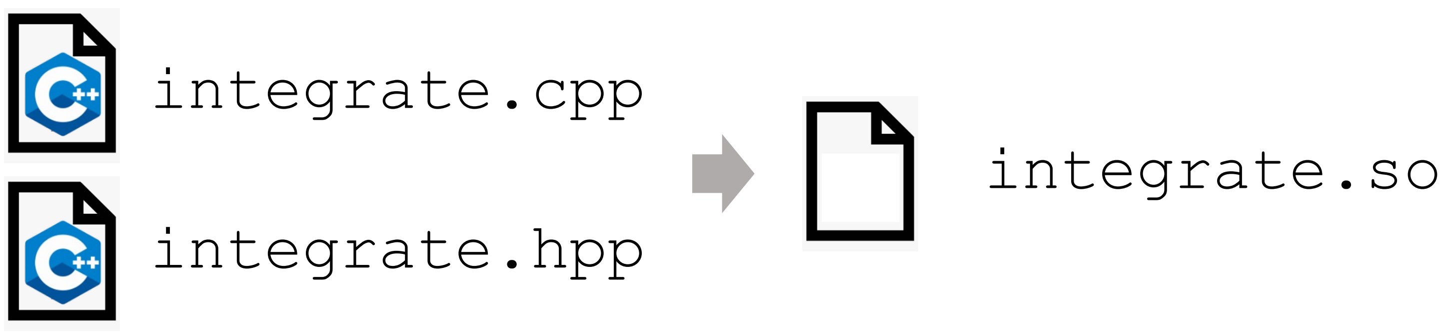
```
loop over k_x
    loop over k_y
        loop over k_z
            if inside sphere then compute
```

Effort to perform nested loops scales as N^3 … will become very slow! ☹

Example 2: Numerical integration in 3D

The code for this example illustrates 3 approaches:

- Fully Python implementation
- Python using **ctypes** binding to a compiled C++ shared library
- C++ code compiling against the C++ shared library



Compile the shared library first as: `g++ -shared integrate.cpp -o integrate.so`

Example 2: Numerical integration in 3D

Run the python script

compute_integral.py

Numba

integrate.hpp

integrate.so

and compile the standalone app:

```
g++ --std=c++11 integrate.so compute_integral.cpp -o compute_integral
```

Will need to specify the dynamic link loader path:

```
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:./
```

```
./compute_integral
```

compute_integral.cpp

compute_integral

Example 2: Numerical integration in 3D

How do the approaches compare?

We have 4 configurations to compare:

plain Python	> 1000 s got bored waiting!
Python with Numba	65.7 s
Python using integrate.so via ctypes	8.6 s
plain C++	8.5 s

To get C++ performance ultimately needs C++ compiled code to be used.