Efficient use of Python on the clusters

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CÉCI training

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Outline

- Analyze our code with profiling tools:
  - cpu: `cProfile`, `line_profiler`, `kernprof`
  - memory: `memory_profiler`, `mprof`
- Being a highly abstract dynamically typed language, how to make a more efficient use of hardware internals?
  - Numpy and Scipy ecosystem (mainly wrappers to C/Fortran compiled code)
  - binding to compiled code: interfaces between python and compiled modules
  - compiling: tools to compile python code
  - parallelism: modules to exploit multicores

Sieve of eratostenes

Algorithm to find all prime numbers up to any given limit.

Ex: Find all the prime numbers less than or equal to 25:

- 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

Cross out every number displaced by 2 after 2 up to the limit:

- 2 3 ~~4~~ 5 ~~6~~ 7 ~~8~~ 9 ~~10~~ 11 ~~12~~ 13 ~~14~~ 15 ~~16~~ 17 ~~18~~ 19 ~~20~~ 21 ~~22~~ 23 ~~24~~ 25

Move to next *n* non crossed, cross out each non crossed number displaced by *n*:

- 2 3 ~~4~~ 5 ~~6~~ 7 ~~8~~ ~~9~~ ~~10~~ 11 ~~12~~ 13 ~~14~~ ~~15~~ ~~16~~ 17 ~~18~~ 19 ~~20~~ ~~21~~ ~~22~~ 23 ~~24~~ 25

- 2 3 ~~4~~ 5 ~~6~~ 7 ~~8~~ ~~9~~ ~~10~~ 11 ~~12~~ 13 ~~14~~ ~~15~~ ~~16~~ 17 ~~18~~ 19 ~~20~~ ~~21~~ ~~22~~ 23 ~~24~~ ~~25~~

The remaining numbers non crossed in the list are all the primes below *limit*.
Trivial optimization: jump directly to n^2 to start crossing out.
Then, *n* must loop only up to $\sqrt{limit}$.

Simple python implementation

```
def primes_upto(limit):
    sieve = [False] * 2 + [True] * (limit - 1)
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit+1:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]


primes = primes_upto(25)
print(primes)
```

```
$ python3 sieve01_print.py

[2, 3, 5, 7, 11, 13, 17, 19, 23]
```

Measuring running time

Computing primes up to 30 000 000:

- linux `time` command

```
$ time python3 sieve01.py

real    0m10.419s
user    0m10.192s
sys     0m0.217s
```

- using `timeit` module to average several runs

```
$ python3 -m timeit -n 3 -r 3 -s "import sieve01" \
> "sieve01.primes_upto(30000000)"

3 loops, best of 3: 10.2 sec per loop
```

CPU profiling: timing functions

`cProfile`: built-in profiling tool in the standard library. It hooks into the virtual machine to measure the time taken to run every function that it sees.

```
$ python3 -m cProfile -s cumulative sieve01.py
         5 function calls in 10.859 seconds

   Ordered by: cumulative time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
        1    0.000    0.000   10.859   10.859 built-in method builtins.exec
        1    0.087    0.087   10.859   10.859 sieve01.py:3(<module>)
        1    9.447    9.447   10.772   10.772 sieve01.py:3(primes_upto)
        1    1.325    1.325    1.325    1.325 sieve01.py:11(<listcomp>)
        1    0.000    0.000    0.000    0.000 method 'disable' of '_lsprof.Profiler'
```

- Useful information but for big codes we will need extra tools to visualize the dumps

CPU profiling: line by line details of a function

`line_profiler`: profiling individual functions on a line-by-line basis, **big overhead** introduced. We must add the `@profile` decorator on the function to be analyzed.

```
@profile
def primes_upto(limit):
    sieve = [False] * 2 + [True] * (limit - 1)
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit+1:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]


primes = primes_upto(30000000)
```

Then, we run the code with the `kernprof.py` script provided by the package.

CPU profiling: line by line details of a function

```
 $ kernprof -l -v sieve01_prof.py
Wrote profile results to sieve01_prof.py.lprof
Timer unit: 1e-06 s

Total time: 101.025 s
File: sieve01_prof.py
Function: primes_upto at line 2

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     2                                           @profile
     3                                           def primes_upto(limit):
     4         1     229258.0  229258.0    0.3      sieve = [False] * 2 + [True] * (
     5      5477       2466.0       0.5    0.0      for n in range(2, int(limit**0.5
     6      5476       2578.0       0.5    0.0          if sieve[n]:
     7       723        855.0       1.2    0.0              i = n**2
     8  70634832   28295172.0       0.4   32.4              while i < limit+1:
     9  70634109   29280104.0       0.4   33.5                  sieve[i] = False
    10  70634109   26771040.0       0.4   30.7                  i += n
    11         1    2740062.0 2740062.0    3.1      return [i for i, prime in enumer
```

`% Time` is relative inside the function, not to the total running time.

Memory profiling: line by line details of a function

`memory_profiler`: module to measure memory usage on a line-by-line basis, runs will be slower than `line_profiler`. Is also required the `@profile` decorator on the function to analyze.

```
$  python3 -m memory_profiler sieve01_prof.py
Filename: sieve01_prof.py

Line #    Mem usage    Increment   Line Contents
================================================
     2   32.715 MiB    0.000 MiB   @profile
     3                             def primes_upto(limit):
     4  261.703 MiB  228.988 MiB       sieve = [False] * 2 + [True] * (limit - 1)
     5  261.703 MiB    0.000 MiB       for n in range(2, int(limit**0.5 + 1)):
     6  261.703 MiB    0.000 MiB           if sieve[n]:
     7  261.703 MiB    0.000 MiB               i = n**2
     8  261.703 MiB    0.000 MiB               while i < limit+1:
     9  261.703 MiB    0.000 MiB                   sieve[i] = False
    10  261.703 MiB    0.000 MiB                   i += n
    11                             return [i for i, prime in enumerate(sieve) if
```

Memory profiling: line by line details of a function

Why are 228 MB allocated on this line?

```
4  261.703 MiB  228.988 MiB       sieve = [False] * 2 + [True] * (limit - 1)
```

- In a Python list each boolean variable has a size of 8 bytes. The standard for a C `long int` in 64-bits.
- We are creating a list with 30000002 elements.
- Doing the math: $\frac{30000002*8}{1024*1024} = 228.881$

Remarks:

- Memory line by line analysis introduces an even bigger overhead, run can be up to 100x slower
- We can miss information due to many memory operations taking place on a single line

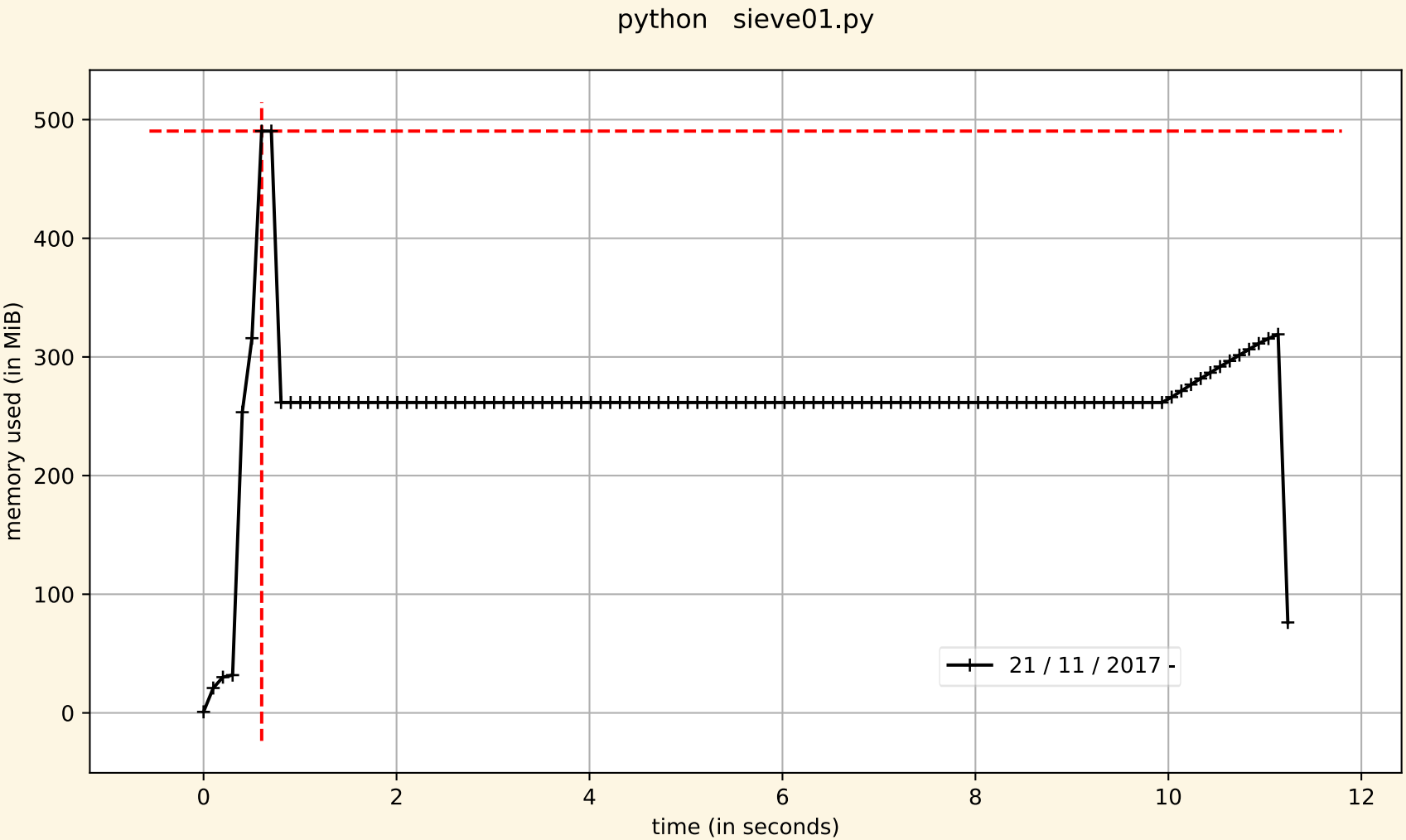
Memory profiling: analyzing the whole run vs time

- The `memory_profiler` package provides the `mprof` tool to analyze and visualize the memory usage as a function of time
- It has a very minor impact on the running time
- Usage:

```
$ mprof run --python python3 mycode.py
$ mprof plot
```

Memory profiling: analyzing the whole run vs time

```
$ mprof run --python python3 sieve01.py
$ mprof plot
```



Memory profiling: analyzing the whole run vs time

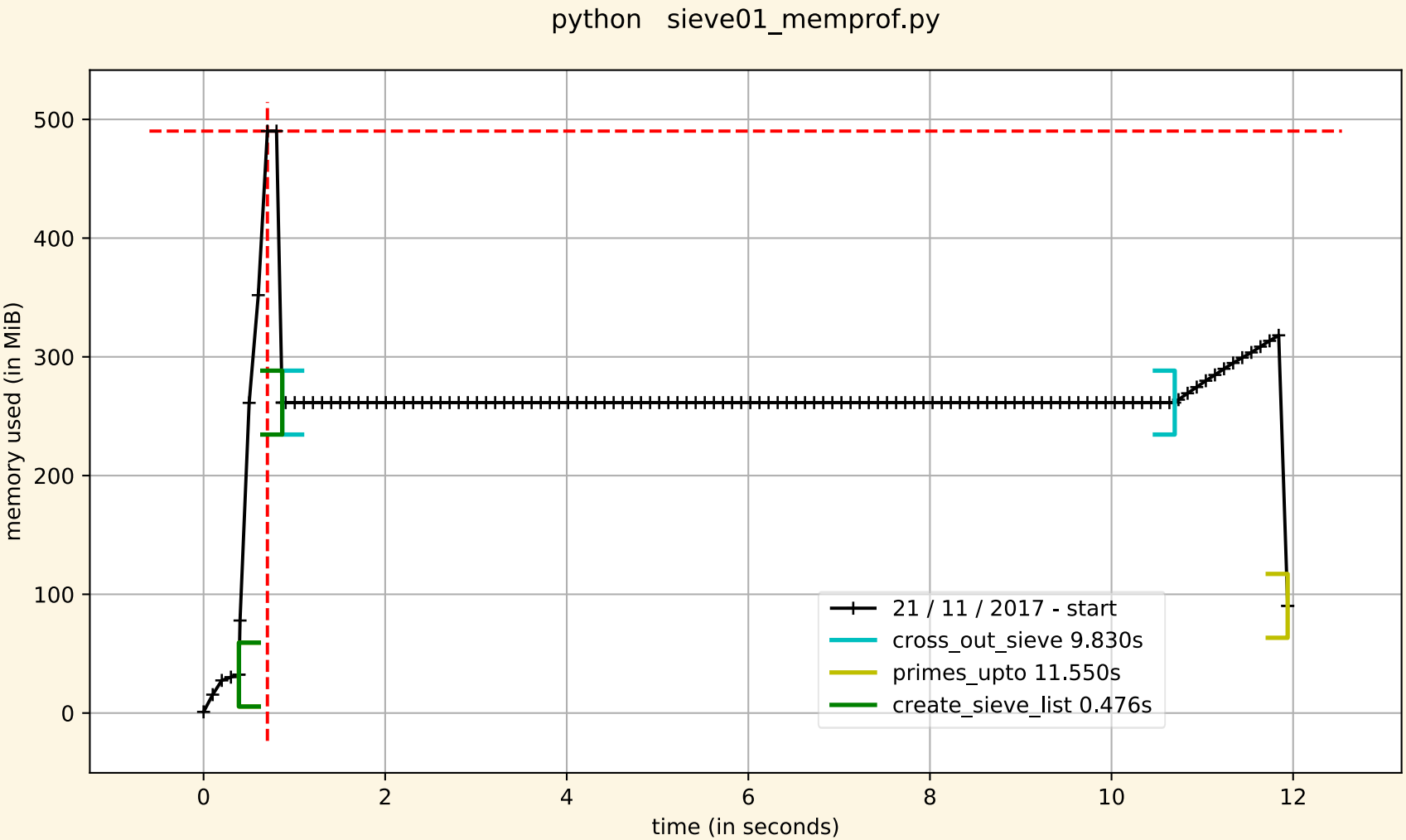
We can add a `@profile` decorator and `profile.timestamp()` labels to introduce details in the analysis

```
@profile
def primes_upto(limit):
    with profile.timestamp("create_sieve_list"):
        sieve = [False] * 2 + [True] * (limit - 1)
    with profile.timestamp("cross_out_sieve"):
        for n in range(2, int(limit**0.5 + 1)):
            if sieve[n]:
                i = n**2
                while i < limit+1:
                    sieve[i] = False
                    i += n
    return [i for i, prime in enumerate(sieve) if prime]

primes = primes_upto(30000000)
```

Memory profiling: analyzing the whole run vs time

```
$ mprof run --python python3 sieve01_memprof.py
$ mprof plot
```



Memory profiling: analyzing the whole run vs time

Why the 500 MB peak during the sieve list creation?

- Experimenting with the `mprof` tool can be verified that:

```
sieve = [False] * 2 + [True] * (limit - 1)
```

- is actually equivalent to something like:

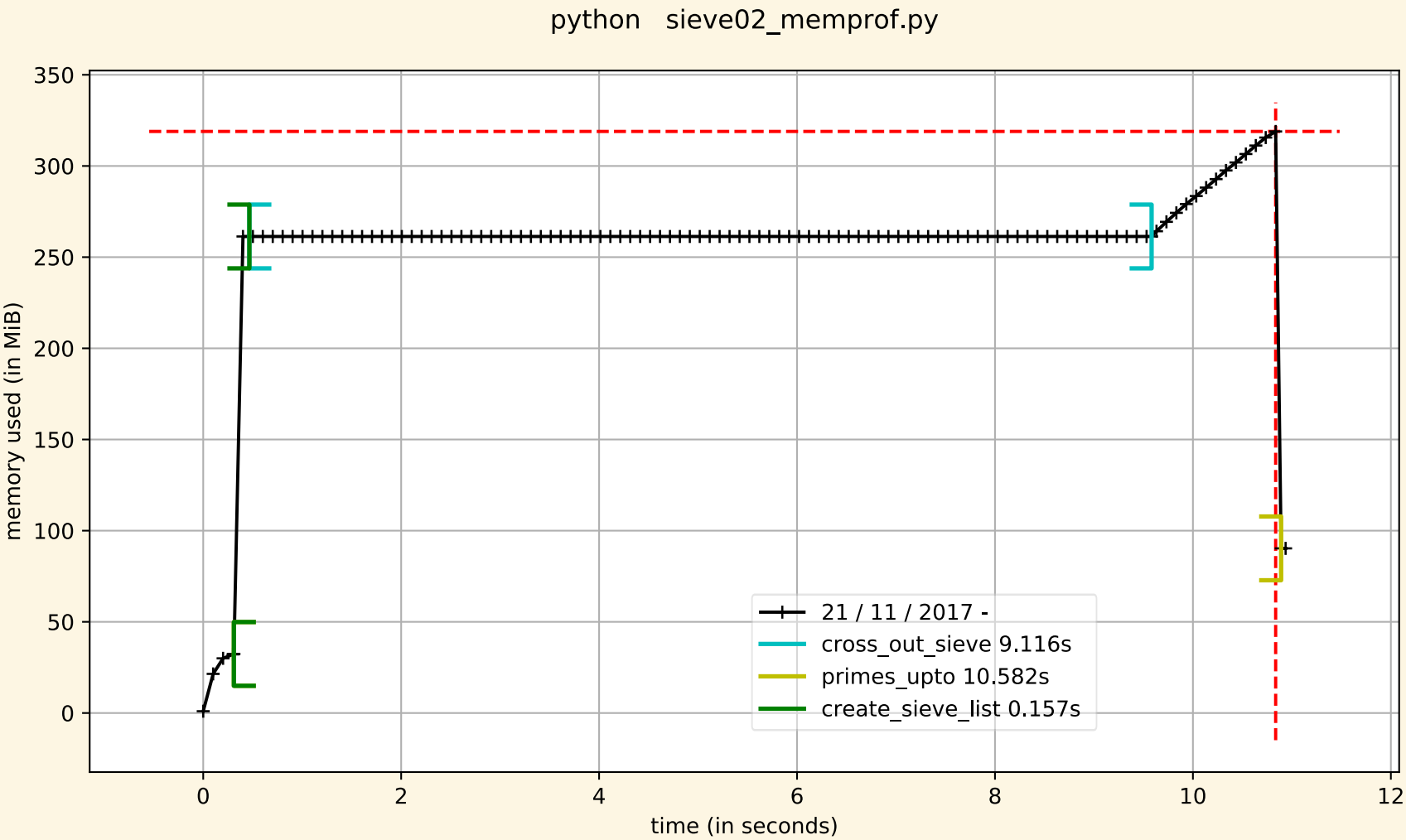
```
sieve1 = [False] * 2
sieve2 = [True] * (limit - 1)
sieve = sieve1 + sieve2
del sieve1
del sieve2
```

- is allocated temporarily an extra $\approx 30E6$ boolean list !!
- We can try to replace with:

```
sieve = [True] * (limit + 1)
sieve[0] = False
sieve[1] = False
```

Memory profiling: analyzing the whole run vs time

```
$ mprof run --python python3 sieve02_memprof.py
$ mprof plot
```



Excercise1: profile a python code

- From NIC4 or Hercules copy this folder to your home directory `/CECI/proj/training/python4hpc/examples`
- Follow the First part from `excercises/README`

Numpy library

- Provides a new kind of `array` datatype
- Contains methods for fast operations on entire arrays avoiding to define (inneficient) explicit loops
- They are basically wrappers to compiled C/Fortran/C++ code
- Their methods runs almost as quickly as C compiled code
- It is the foundation of many other higher-level numerical tools
- Compares to MATLAB in functionality

```
>>> import numpy as np
>>> a = np.array([[ 5, 1 ,3],
                  [ 1, 1 ,1],
                  [ 1, 2 ,1]])
>>> b = np.array([1, 2, 3])
>>> c = a.dot(b)
array([16, 6, 8])
```

Numpy library: sieve revisited

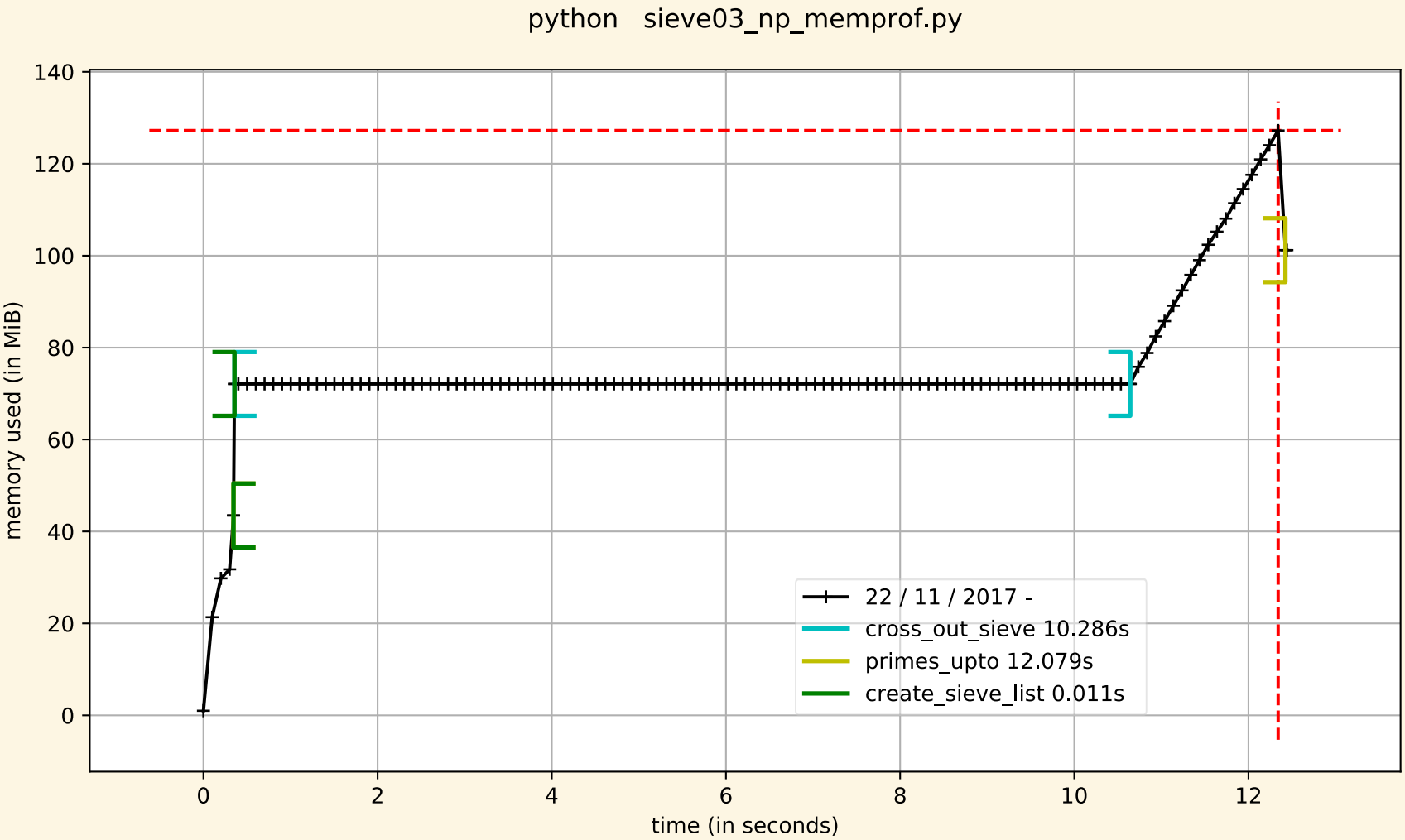
We replace the sieve list with a Numpy boolean array:

```
import numpy as np

def primes_upto(limit):
    sieve = np.ones(limit + 1, dtype=np.bool)
    sieve[0] = False
    sieve[1] = False
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit+1:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]


primes = primes_upto(30000000)
```

Numpy library: sieve revisited



- In a Numpy array each boolean has a size of 1 byte
- Math now: $\frac{30000002*1}{1024*1024} = 28.61$

Numpy library: sieve revisited

- Timing did not improve with Numpy array and same loop
- Fully Numpy solution using slice indexing to iterate:

```
import numpy as np

def primes_upto(limit):
    sieve = np.ones(limit + 1, dtype=np.bool)
    sieve[0] = False
    sieve[1] = False
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            sieve[n**2::n] = 0
    return np.nonzero(sieve)[0]
```

```
 $ time python3 sieve04_np.py
real    0m0.552s
user    0m0.518s
sys     0m0.033s
```

- 22x gain in time!!

Numpy library: sieve line by line profiling

```
 $  kernprof -l -v sieve04_np_prof.py
Wrote profile results to sieve04_np_prof.py.lprof
Timer unit: 1e-06 s

Total time: 0.482723 s
File: sieve04_np_prof.py
Function: primes_upto at line 3

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     3                                           @profile
     4                                           def primes_upto(limit):
     5         1          8785   8785.0      1.8      sieve = np.ones(limit
     6         1             5      5.0      0.0      sieve[0] = False
     7         1             0      0.0      0.0      sieve[1] = False
     8      5477          2796      0.5      0.6      for n in range(2, int(
     9      5476          3119      0.6      0.6          if sieve[n]:
    10       723        420784    582.0     87.2              sieve[n**2::n]
    11         1         47234  47234.0      9.8      return np.nonzero(siev
```

Numpy library: sieve line by line profiling

- `line_profiler` helps to understand the massive gain
- Pure python solution:

```
 6      5476       2362    0.4      0.0   if sieve[n]:
 7       723        680    0.9      0.0       i = n**2
 8  70634832   28740579    0.4     28.4       while i < limit+1:
 9  70634109   33142484    0.5     32.8           sieve[i] = False
10  70634109   26776815    0.4     26.5           i += n
```

- Full Numpy solution:

```
 9      5476       3119    0.6      0.6   if sieve[n]:
10       723     420784  582.0     87.2       sieve[n**2::n] = 0
```

- The loops to cross out the sieve are fully performed by lower level implementations in Numpy
- Time and memory usage is the same as C or Fortran compiled solutions !

CPU and Memory profiling: summary

- Line-by-line profiling introduces a huge overhead, they must be used reducing the problem size and for specific functions detected as bottlenecks
- The `mprof` tool is very dynamic, *timestammping* in a smart way can be used both as a fast CPU and Memory profiler
- The `cProfile` dumps are great to detect bottlenecks on big projects, but a visualization tool is almost mandatory. Explore the KCachegrind package, usual workflow:

```
$ python -m cProfile -o prof.out sieve02.py
$ pyprof2calltree -i prof.out -k
```

Numpy library: SciPy ecosystem

Collection of open source software for scientific computing in Python

- Core packages:
  - NumPy: the fundamental package for numerical computation
  - SciPy library: collection of numerical algorithms and domain-specific toolboxes, including signal processing, fourier transforms, clustering, optimization, statistics...
  - Matplotlib: a mature plotting package, provides publication-quality 2D plotting as well as rudimentary 3D plotting
- Data and computation:
  - pandas: providing high-performance, easy to use data structures (similar to R)
  - SymPy: symbolic mathematics and computer algebra
  - scikit-image: algorithms for image processing
  - scikit-learn: algorithms and tools for machine learning
  - h5py and PyTables: can both access data stored in the HDF5 format

Python Bindings

We saw that interfacing python with compiled code can provide huge performance gains. There are two possibilities to exploit:

- Compile python (or python-like) code
- Link python to libraries written in other languages

Compile Python

- Just in time (JIT) compilers: compile and run a python code in real time
  - Numba: jit compiler supporting numpy code
  - Pypy: jit compiler for non-numpy code
- Ahead of time (AOT) compilers: creation of a compiled static library in your machine
  - Cython: the most popular, compile a python-like C code
  - Shed skin: automatic Python-to-C++ converter (so far limited to Python 2 only)
  - Pythran: automatic Python-to-C++ converter and compiler compatible with numpy

Compiled Python: JIT

- Pypy: We can directly run the original `sieve01.py` with `pypy`
- Numba: We just need to decorate the function we wish to compile

```
from numba import jit

@jit
def primes_upto(limit):
    sieve = [False] * 2 + [True] * (limit - 1)
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit+1:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]


primes = primes_upto(30000000)
```

Compiled Python: JIT remarks

- JIT compilers offers some nice speedups with very little manual intervention
- But the more we rely on a tool to automatically optimize we are rapidly bounded on what can be improved
- Pypy is not compatible with numpy code
- Numba seems a quite promising tool and it’s numpy compatible
- You might be happy with what you obtain with very low effort, is up to your problem and how many times you are going to run your code

Compile python: Cython

You must annotate your code using a new syntax in between python and C, if you have the file `sievelib.pyx`

```
def primes_upto(int limit):
    cdef int n, i
    cdef int prime
    sieve = [True]*limit
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]
```

Then you compile it and the library can be imported in a python script

```
from sievelib import primes_upto

primes = primes_upto(30000000)
```

Compile python: Cython

It requires to create a sort of makefile, called typically `setup.py`

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Build import cythonize

setup(
    ext_modules = cythonize("sievelib.pyx")
)
```

To use the resulting module, built as a binary `.so` file, by a python script in the same directory

```
$ python setup.py build_ext --inplace
```

Compile python: Pythran

It requires annotations for the type information of the function to compile

```
#pythran export primes_upto(int)
def primes_upto(limit):
    sieve = [True]*limit
    for n in range(2, int(limit**0.5 + 1)):
        if sieve[n]:
            i = n**2
            while i < limit:
                sieve[i] = False
                i += n
    return [i for i, prime in enumerate(sieve) if prime]
```

To compile the `.so` file

```
$ pythran sievelib.py
```

Compile python: OpenMP support

- Both Cython and Pythran provide the possibility to produce OpenMP code
- This allows to use under the hood more cores in a multicore machine
- In Cython this is enabled by using special operators (i.e. `prange` instead `range`) and compiling with the `-fopenmp` flag
- In Pythran we annotate the python code to create a parallel region similar to original OpenMP usage in C

Python bindings: C libraries

- Cython allows also to wrap C libraries to provide bindings for Python
- Check the example in `compiling/fib-wrap-c` to see how wrapping works for a C function providing the n_{th} Fibonacci number.

```
 $ make
 $ make test
python test.py
The 10th Fibonacci number is: 55
```

Python Bindings: f2py example

- To wrap Fortran code the `f2py` tool provides a more straighforward approach to do so

```
subroutine foo(a)
    integer a
    print*, "Hello from Fortran!"
    print*, "a=",a
end
```

```
$ f2py -c -m hello hello.f90
```

```
import hello

hello.foo(10)
```

```
$ python call_fhello.py
 Hello from Fortran!
 a=          10
```

Compiled Python

- cython: C-Extensions for Python
  - optimising and static compiler
  - can compile Python code and Cython language
  - can compile Python with Numpy code
  - can do bindings with C code
- Pypy: Just-in-time compiler
  - sometimes less memory hungry than Cython
  - not fully compliant with Python with Numpy code
- Numba: a compiler specialized for numpy code using the LLVM compiler
- Pythran: compiler for both numpy and non-numpy code. Takes advantage of multi-cores and single instruction multiple data (SIMD) units
- All, except `pypy` requires to modify or decorate the original python code

Parallel processing

- `multiprocessing` module
  - allows to use process- and thread-based parallel processing
  - allows to share memory among processes
  - constrained to single-machine multicore parallelism
- `mpi4py`
  - Python bindings to the MPI-1/2/3 interfaces
  - if *you know* MPI on C/Fortran *you already know* mpi4py
  - can make use equivalently of multiple cores on a single-machine or distributed
  - each process has a separate address space, no possibility to share memory between them
  - we covered it in the MPI session

Excercise2: compile python code

- From NIC4 or Hercules copy this folder to your home directory `/CECI/proj/training/python4hpc/examples`
- Follow the Second part from `excercises/README`

Further information on the topic

- High Performance Python by By Micha Gorelick and Ian Ozsvald
- Python in HPC Tutorial: `https://github.com/pyHPC/pyhpc-tutorial`