# Python in HPC

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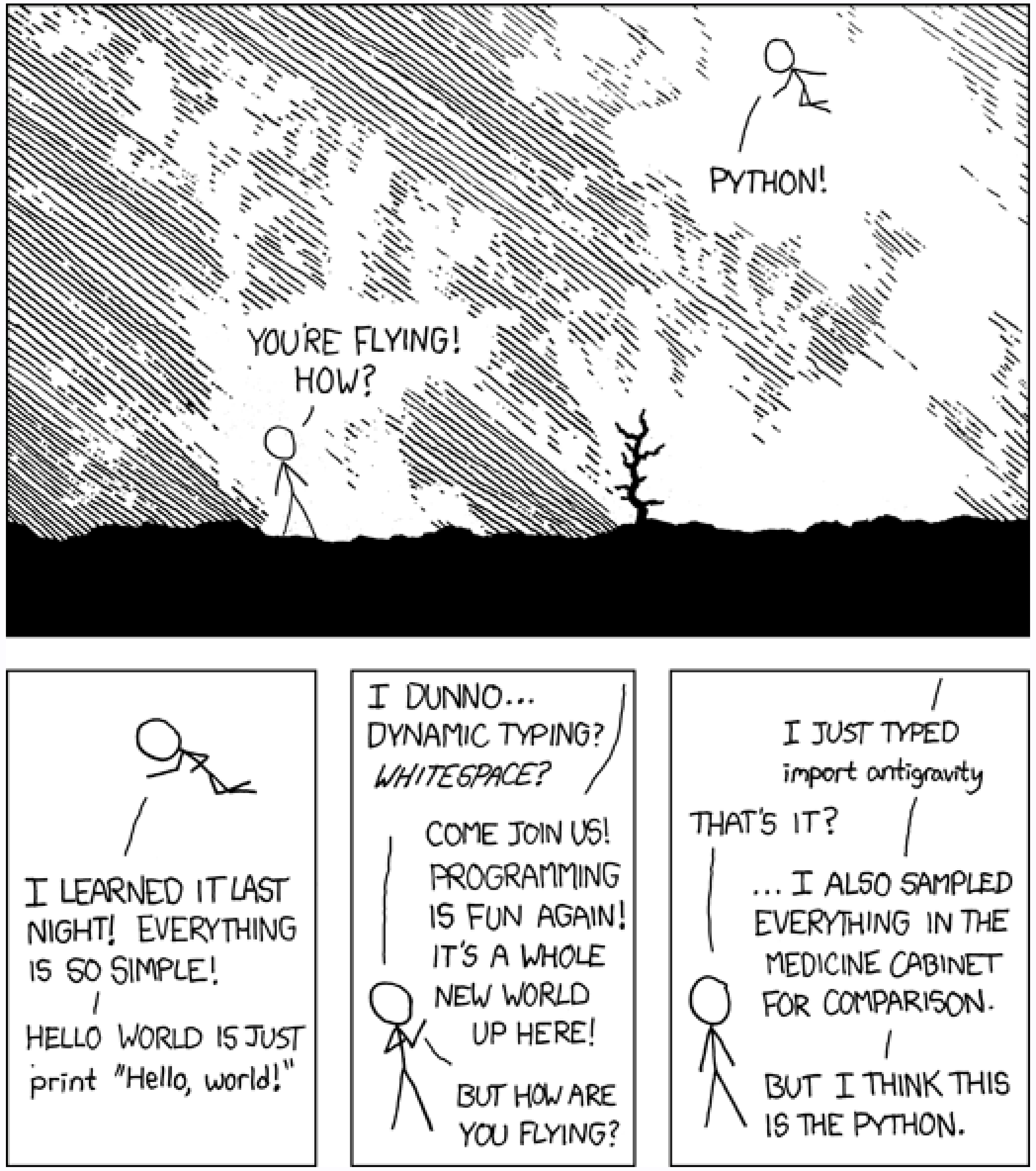
# Why python?

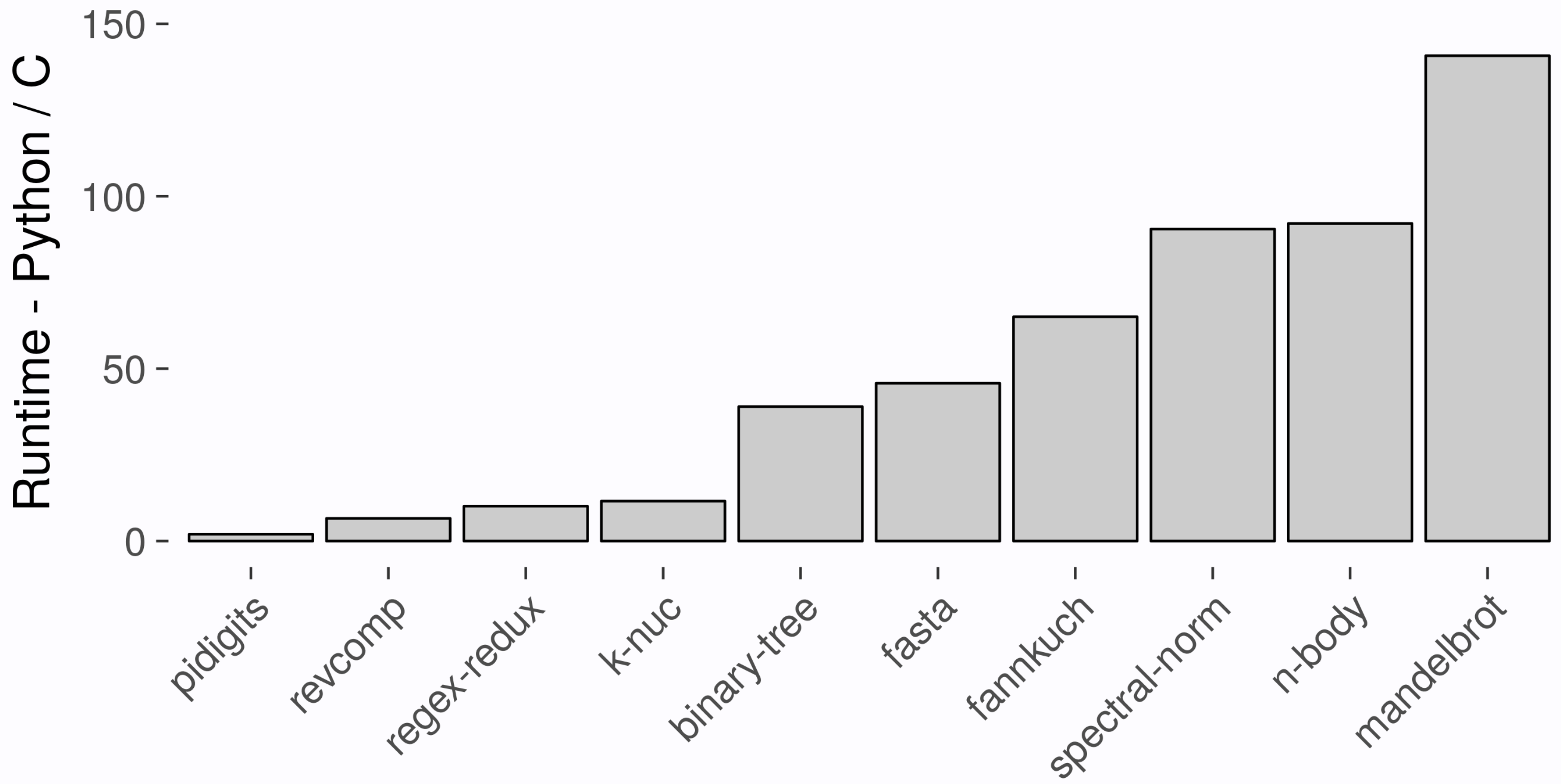
fully featured
tools
simple
readable
portable
free
ubiquitous
extensible
community
libraries


PYTHON!
YOU'RE FLYING! HOW?
I LEARNED IT LAST NIGHT! EVERYTHING IS SO SIMPLE!
HELLO WORLD IS JUST print "Hello, world!"
I DUNNO... DYNAMIC TYPING? WHITESPACE?
COME JOIN US! PROGRAMMING IS FUN AGAIN! IT'S A WHOLE NEW WORLD UP HERE!
BUT HOW ARE YOU FLYING?
I JUST TYPED import antigravity
THAT'S IT?
... I ALSO SAMPLED EVERYTHING IN THE MEDICINE CABINET FOR COMPARISON.
BUT I THINK THIS IS THE PYTHON.

https://xkcd.com/353/

## But isn't python slow?

# Well - kind of



data from http://benchmarksgame.alioth.debian.org/u64q

But for a lot of tasks it

**doesn't really matter**

## How do you decide if it matters?

- Is the code fast enough to produce results within a reasonable time?
- How many CPUh is the code going to waste over its lifetime?
  - How inefficient is it?
  - How long does it run?
  - How often will it run?
- Does it cause problems on the system it's running on?
- How much effort would it be to make it run faster?

Luckily, if it does matter

## code can often be made faster

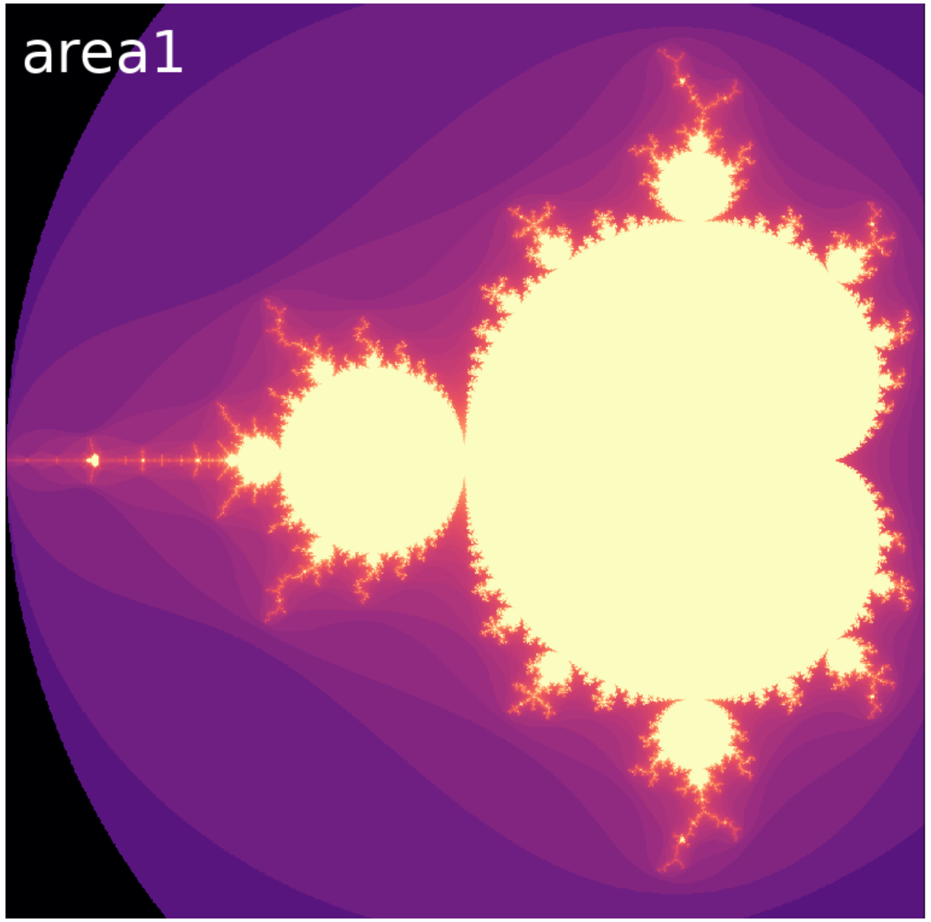
## Make it go faster

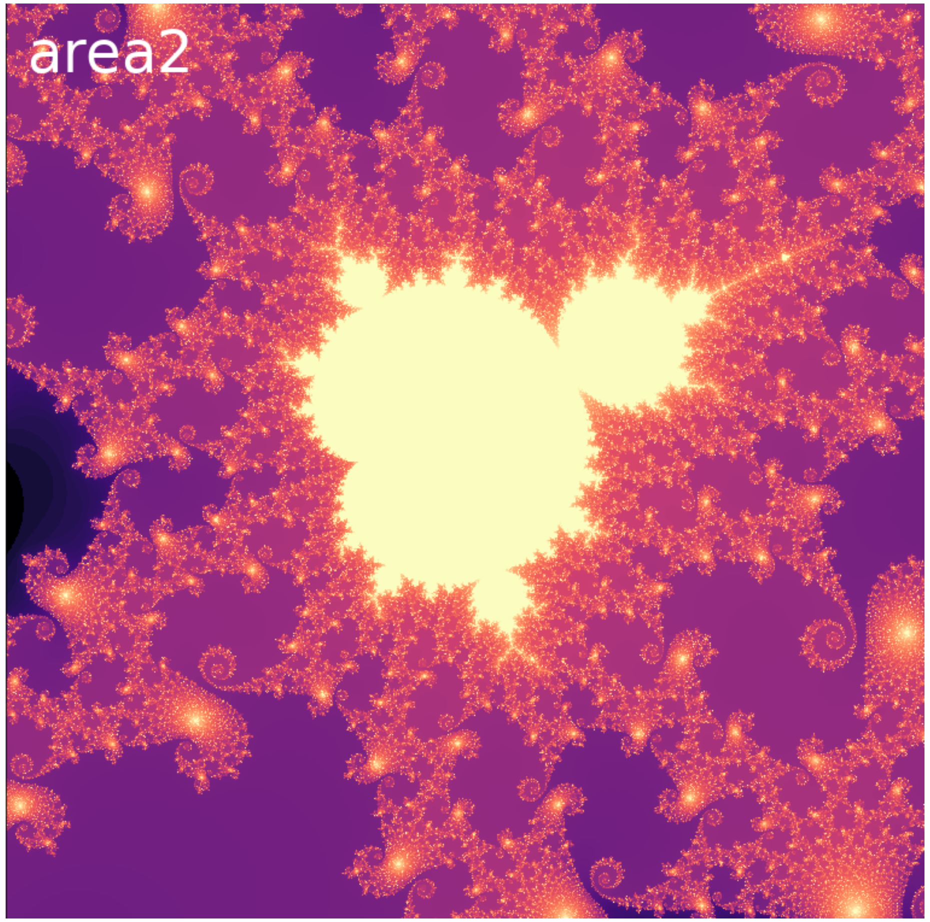
## Profiling

**It's necessary to know what sections of code are bottlenecks in order to improve performance.**

***Measure - don't guess***

## Example: Mandelbrot set





**https://github.com/NIH-HPC/python-in-hpc**

```python
def linspace(start, stop, n):
    step = float(stop - start) / (n - 1)
    return [start + i * step for i in range(n)]

def mandel1(c, maxiter):
    z = c
    for n in range(maxiter):
        if abs(z) > 2:
            return n
        z = z*z + c
    return n

def mandel_set1(xmin=-2.0, xmax=0.5, ymin=-1.25, ymax=1.25, width=1000,
                height=1000, maxiter=80):
    r = linspace(xmin, xmax, width)
    i = linspace(ymin, ymax, height)
    n = [[0]*width for _ in range(height)]
    for x in range(width):
        for y in range(height):
            n[y][x] = mandel1(complex(r[x], i[y]), maxiter)
    return n
```

## Baseline timing with `%timeit` ipython magic

```
%timeit mandel_set1()
5.93 s ± 17.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Equivalently, on the command line:

```
$ python -m timeit -s 'import mandel01' 'mandel01.mandel_set1(*a1)'
10 loops, best of 3: 7.81 sec per loop
```

~6s to calculate *area1*. ~130s for *area2*

Profiling with `%prun` ipython magic:

```
%prun -s cumulative mandel_set1()
```

or the equivalent command line below. This, however, requires an executable script.

```
$ python -m cProfile -s cumulative mandel01.py
```

## Yields something akin to

```
25214601 function calls in 12.622 seconds

   Ordered by: cumulative time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
        1    0.000    0.000   12.622   12.622 {built-in method builtins.exec}
        1    0.013    0.013   12.622   12.622 mandel01.py:1(<module>)
        1    0.941    0.941   12.609   12.609 mandel01.py:13(mandel_set1)
  1000000    9.001    0.000   11.648    0.000 mandel01.py:5(mandel1)
 24214592    2.647    0.000    2.647    0.000 {built-in method builtins.abs}
```

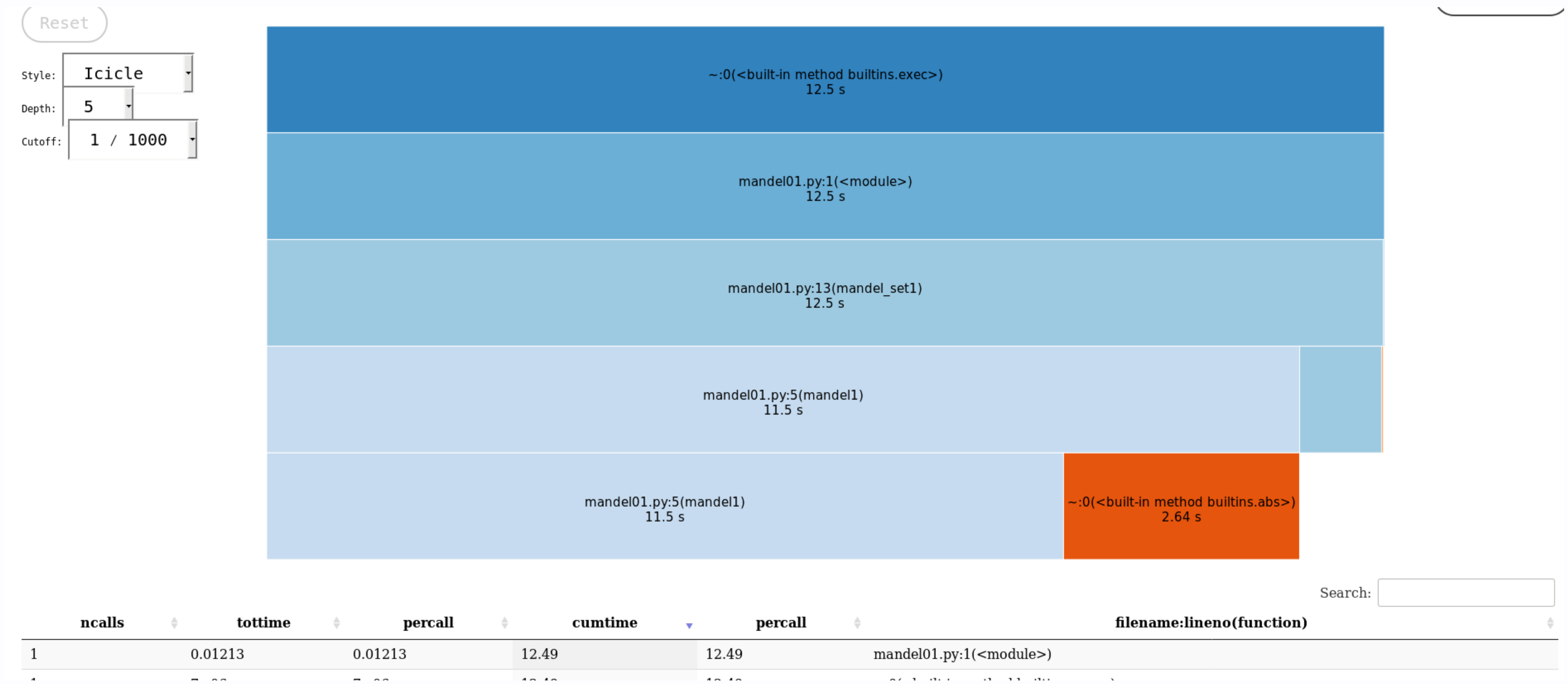
- Most time is spent in the `mandel1` function
- profiling introduces some overhead (runtime of 12s vs 8s)

Profiling results can be visualized with SnakeViz:

```
$ python -m cProfile -o mandel01.prof mandel01.py
$ snakeviz --port 6542 --hostname localhost --server mandel01.prof
```

Which starts a web server on port 6542.

## Snakeviz generates an interactive visualization and sortable table:



| ncalls | tottime | percall | cumtime | percall | filename:lineno(function) |
|---|---|---|---|---|---|
| 1 | 0.01213 | 0.01213 | 12.49 | 12.49 | mandel01.py:1(<module>) |

Most the time is spent in the `mandel1()` function. Use the `line_profiler` package to profile this function line by line with the `%lprun` ipython magic:

```
%load_ext line_profiler
%lprun -f mandel1 mandel_set1()
```

## On the command line, import the `line_profiler` package and decorate the function(s) with `@profile`

```python
import line_profiler

@profile
def mandel1(c, maxiter):
    z = c
    for n in range(maxiter):
        if abs(z) > 2:
            return n
        z = z*z + c
    return n
...
```

Then, on the command line:

```
$ kernprof -l -v mandel01.py
```

## The line-by-line profile returned by either method:

```
Total time: 33.1452 s
File: <ipython-input-10-5bd0131c44a5>
Function: mandel1 at line 5

Line #      Hits         Time Per Hit   % Time  Line Contents
==============================================================
     5                                           def mandel1(c, maxiter):
     6   1000000    362966.0      0.4      1.1      z = c
     7  24463110   9234756.0      0.4     27.9      for n in range(maxiter):
     8  24214592  12496111.0      0.5     37.7          if abs(z) > 2:
     9    751482    287491.0      0.4      0.9              return n
    10  23463110  10672517.0      0.5     32.2          z = z*z + c
    11    248518     91389.0      0.4      0.3      return n
```

There are some algorithmic improvements possible here, but let's first try the simplest thing we can do.

## Improve sequential performance

## The `numba` just in time (jit) compiler 2

```python
from numba import jit

@jit(nopython=True)
def mandel2(c, maxiter):
    z = c
    for n in range(maxiter):
        if abs(z) > 2:
            return n
        z = z*z + c
    return n
```

No changes to the code beyond a decorator on the function in the tight loop.

## Result: **~6-fold** speedup

```
%timeit mandel_set2()
986 ms ± 858 µs per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

## Using numpy arrays 3

Now mandel_set is the bottleneck. Since it uses nested lists, `numba` can't jit compile it. Can we speed it up by converting to numpy arrays?

```python
def mandel_set3(xmin=-2.0, xmax=0.5, ymin=-1.25, ymax=1.25, width=1000,
                height=1000, maxiter=80):
    r = np.linspace(xmin, xmax, width)
    i = np.linspace(ymin, ymax, height)
    n = np.empty((height, width), dtype=np.int32)
    for x in range(width):
        for y in range(height):
            n[y, x] = mandel3(complex(r[x], i[y]), maxiter)
    return n
```

## **No** - it's actually slower now.

```
%timeit mandel_set3()
1.3 s ± 10.7 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

numpy arrays have some overhead that may hurt performace with smaller array sizes. But now the function can be jit compiled with numba by decorating it with the `@jit` decorator. 4

```
%timeit mandel_set4()
387 ms ± 1.27 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

Now the speedup is **~16-fold**.

```
Total time: 42.2215 s
File: mandel01.py
Function: mandel1 at line 7

Line #      Hits         Time  Per Hit   % Time  Line Contents
==========================================================
     7                                           @profile
     8                                           def mandel1(c, maxiter):
     9   1000000       441285      0.4      1.0      z = c
    10  24463110     11668783      0.5     27.6      for n in range(maxiter):
    11  24214592     16565164      0.7     39.2          if abs(z) > 2:
    12    751482       345196      0.5      0.8              return n
    13  23463110     13081688      0.6     31.0          z = z*z + c
    14    248518       119431      0.5      0.3      return n
```

## Algorithmic improvement 5

Definitions of square, abs, and addition for complex numbers

$$(a+bi)^2 = (a+bi)(a+bi) = (a^2 - b^2) + 2abi$$

$$|a+bi| = \sqrt{a^2+b^2}$$

$$(a+bi) + (c+di) = (a+c) + (b+d)i$$

Based on the definitions of the absolute value and the square of a complex number, we can factor out some calculations in the `mandel` method:

```python
@jit(nopython=True)
def mandel5(creal, cimag, maxiter):
    real = creal
    imag = cimag
    for n in range(maxiter):
        real2 = real*real
        imag2 = imag*imag
        if real2 + imag2 > 4.0:
            return n
        imag = 2 * real*imag + cimag
        real = real2 - imag2 + creal
    return n
```

## Which gives us a respectable

```
%timeit mandel_set5()
102 ms ± 28.1 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

**~60-fold** improvement over the original pure python implementation.

## Cython

Cython is a python-like language that can be compiled to a C extension for python. In Ipython/Jupyter notebooks using cython is as simple as

```
%load_ext cython
```

## The `mandel` function in cython 6

```
%%cython
import cython
import numpy as np

cdef int mandel6(double creal, double cimag, int maxiter):
    cdef:
        double real2, imag2
        double real = creal, imag = cimag
        int n

    for n in range(maxiter):
        real2 = real*real
        imag2 = imag*imag
        if real2 + imag2 > 4.0:
            return n
        imag = 2* real*imag + cimag
        real = real2 - imag2 + creal;
    return n
```

## The `mandel_set` function in cython

```
@cython.boundscheck(False)
@cython.wraparound(False)
cpdef mandel_set6(double xmin, double xmax, double ymin, double ymax,
                  int width, int height, int maxiter):
    cdef:
        double[:] r1 = np.linspace(xmin, xmax, width)
        double[:] r2 = np.linspace(ymin, ymax, height)
        int[:,:] n = np.empty((height, width), np.int32)
        int i,j

    for i in range(width):
        for j in range(height):
            n[j,i] = mandel6(r1[i], r2[j], maxiter)
    return n
```

```
%timeit mandel_set6(-2, 0.5, -1.25, 1.25, 1000, 1000, 80)
101 ms ± 89.4 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

So cython runs about as fast as the numba version at the cost of changing code.

## GPU with pyOpenCL 7

Using `pyopencl` to implement the `mandel` function with an NVIDIA K80 backend, the following timing was measured (for code see the notebook on GitHub):

```
%timeit mandel_set7(-2, 0.5, -1.25, 1.25, 1000, 1000, 80)
16.2 ms ± 296 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

A **~370-fold** decrease in runtime compared to the pure python implementation. Much more than that for *area2*

## Fortran 8

Fortran bindings can be created with the numpy utility `f2py`. How does fortran stack up against numba and cython?

```
$ cat mandel8.f90
subroutine mandel_set8(xmin, xmax, ymin, ymax, width, height, itermax, n)
    real(8), intent(in)    :: xmin, xmax, ymin, ymax
    integer, intent(in)    :: width, height, itermax
    integer                :: niter
    integer, dimension(width, height), intent(out) :: n
    integer                :: x, y
    real(8)                :: xstep, ystep

    xstep = (xmax - xmin) / (width - 1)
$ f2py -m mb_fort -c mandel8.f90 --fcompiler=gnu95
...
```

```
from mb_fort import mandel8, mandel_set8
%timeit mandel_set8(-2, 0.5, -1.25, 1.25, 1000, 1000, 80)
107 ms ± 60.7 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

same ballpark as numba and cython

## Summary

| | Implementation | area1 time | speedup | area2 time | speedup |
|---|---|---|---|---|---|
| 1 | pure python | 6.040s | 1x | 130.20s | 1x |
| 2 | numba 1 | 0.986s | 6x | 9.71s | 13x |
| 3 | + numpy | 1.300s | 5x | 9.94s | 13x |
| 4 | + numba 2 | 0.387s | 16x | 9.14s | 14x |
| 5 | + algo | 0.102s | 60x | 2.64s | 50x |
| 8 | f2py | 0.107s | 56x | 2.62s | 50x |
| 6 | cython | 0.101s | 60x | 2.58s | 50x |
| 7 | pyopencl | 0.016s | 378x | 0.04s | 3255x |

## Was that really all sequential?

Numpy can be compiled against different backends. Some of them, like MKL and OpenBlas, implement implicit parallelism for some operations. We use Anaconda python with MKL, so some of the numpy code could have been implicitly parallel.

```
>>> import numpy
>>> numpy.show_config()
lapack_opt_info:
    define_macros = [('SCIPY_MKL_H', None), ('HAVE_CBLAS', None)]
    library_dirs = ['/usr/local/Anaconda/envs/py3.5/lib']
    include_dirs = ['/usr/local/Anaconda/envs/py3.5/include']
    libraries = ['mkl_intel_lp64', 'mkl_intel_thread', 'mkl_core', ...]
...
```

## Parallelize - within a single machine

## A word about the Python interpreter

Python only allows a singly thread to execute Python bytecode at any one time. Access to the interpreter is enforced by the **Global Interpreter Lock** (GIL).

While this is sidestepped by I/O, it does prevent true parallelism with pure Python threads.

**However**, compiled extension modules can thread and other paradigms for parallelism have developed.

## numba.vectorize 9️⃣

`numba.vectorize` and `numba.guvectorize` are convenience decorators for creating numpy ufuncs that can be single threaded, parallel, or use GPU for computation. Parallel computation uses threads.

```python
@vectorize([int32(complex64, int32)], target='parallel')
def mandel9(c, maxiter):
    nreal = 0
    real = 0
    imag = 0
    for n in range(maxiter):
        nreal = real*real - imag*imag + c.real
        imag = 2* real*imag + c.imag
        real = nreal;
        if real * real + imag * imag > 4.0:
            return n
    return n

def mandel_set9(xmin=-2.0, xmax=0.5, ymin=-1.25, ymax=1.25,
                width=1000, height=1000, maxiter=80):
    r1 = np.linspace(xmin, xmax, width, dtype=np.float32)
    r2 = np.linspace(ymin, ymax, height, dtype=np.float32)
    c = r1 + r2[:,None]*1j
    n = mandel9(c,maxiter)
    return n
```

|  | Implementation | area2 time | speedup | efficiency |
|---|---|---:|---:|---:|
| 1 | pure python | 130.20s | 1x | NA |
| 5 | numba + algo | 2.64s | 50x | NA |
| 9 | vectorize, 1 thread | 2.71s | 48x | 100% |
|  | vectorize, 2 threads | 1.36s | 96x | 99% |
|  | vectorize, 4 threads | 0.68s | 191x | 99% |
|  | vectorize, 8 threads | 0.36s | 362x | 94% |
|  | vectorize, 14 threads | 0.24s | 543x | 80% |

With one thread (set with `NUMBA_NUM_THREADS` ) it matches the best numba sequential implementation. Scaling is good up to 14 threads.

## multiprocessing

- Multiprocessing uses subprocesses rather than threads for parallelism
- Each child inherits the state of the parent
- After the fork data has to be shared explicitly via interprocess communication
- Spawning child processes and sharing data have overhead
- The multiprocessing API is similar to the threading API

# multiprocessing - things to watch out for

- If each child is also doing (implicit) threading, care has to be taken to limit $\frac{nthreads}{child} \times children$ to the number of available CPUs
- Don't use `multiprocessing.cpu_count()` - it returns all CPUs on the node
- Make children ignore `SIGINT` and parent handle it gracefully
- Script's main should to be safely importable - less important on linux

## multiprocessing example 1️⃣0️⃣

Create one to many subprocesses and execute CPU bound computations on each independently. In this example we'll see a `multiprocessing.Pool` of worker processes each processing one row of the Mandelbrot set.

```python
@jit(nopython=True)
def mandel10(creal, cimag, maxiter):
    real = creal
    imag = cimag
    for n in range(maxiter):
        real2 = real*real
        imag2 = imag*imag
        if real2 + imag2 > 4.0:
            return n
        imag = 2 * real*imag + cimag
        real = real2 - imag2 + creal
    return n

@jit(nopython=True)
def mandel10_row(args):
    y, xmin, xmax, width, maxiter = args
    r = np.linspace(xmin, xmax, width)
    res = [0] * width
    for x in range(width):
        res[x] = mandel10(r[x], y, maxiter)
    return res
```

```
def mandel_set10(ncpus=1, xmin=-2.0, xmax=0.5, ymin=-1.25,
                 ymax=1.25, width=1000, height=1000, maxiter=80):
    i = np.linspace(ymin, ymax, height)
    with mp.Pool(ncpus) as pool:
        n = pool.map(mandel10_row, ((a, xmin, xmax, width, maxiter)
            for a in i))
    return n
```

## How is the performance on *area2*?

| | **Implementation** | **area2 time** | **speedup** | **efficiency** |
|---|---|---|---|---|
| 1 | pure python | 130.20s | 1x | NA |
| 5 | numba + algo | 2.64s | 50x | NA |
| 10 | multiproc, pool(1) | 3.03s | 43x | 100% |
| | multiproc, pool(2) | 1.66s | 78x | 91% |
| | multiproc, pool(4) | 1.04s | 125x | 73% |
| | multiproc, pool(8) | 0.76s | 171x | 50% |
| | multiproc, pool(14) | 0.82s | 159x | 26% |

Slighly worse than implementation 5 with 1 CPU and not scaling well. This problem is not very suited to multiprocessing.

## Parallelize - across machines

## MPI

the **M**essage **P**assing **I**nterface is a portable, and performant standard for communication between processes (tasks) within and between compute nodes. Communication can be point-to-point or collective (broadcast, scatter, gather, ...).

`mpi4py` is a Python implementation of MPI. Documentation is available on readthedocs and at the scipy mpi4py site

## MPI - point-to-point communication

```python
#! /usr/bin/env python
from mpi4py import MPI
import numpy
import time

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

# pass data type explicitly for speed and use upper case 'Send' / 'Recv'
if rank == 0:
    data = numpy.arange(100, dtype = 'i')
    comm.Send([data, MPI.INT], dest=1)
    print("Rank 0 sent numpy array")
if rank == 1:
    data = numpy.empty(100, dtype='i')
    comm.Recv([data, MPI.INT], source=0)
    print("Rank 1 received numpy array")
```

## MPI - point-to-point communication

```bash
#! /bin/bash
#SBATCH --ntasks=4
#SBATCH --ntasks-per-core=1
#SBATCH --constraint=x2680

module load mpi4py
module load python/3.6
srun --mpi=pmix ./p2p.py
```

## MPI - Mandelbrot set 1️⃣1️⃣

Each mpi task will process a consecutive chunk of rows using the functions jit compiled with numba.

```
from mpi4py import MPI
import numpy as np
from numba import jit

comm  = MPI.COMM_WORLD
size  = comm.Get_size()
rank  = comm.Get_rank()
```

# MPI - Mandelbrot set

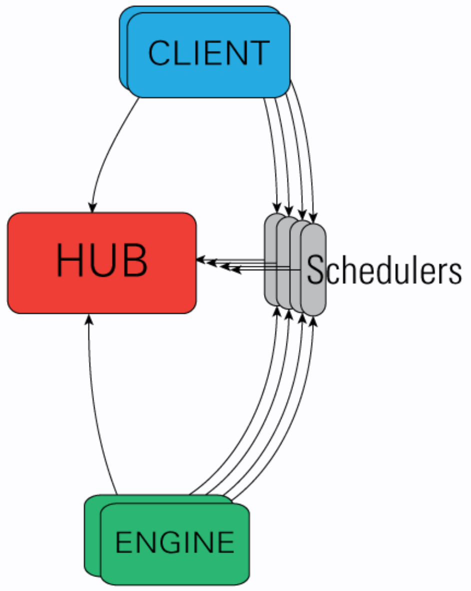
```
# how many rows to compute in this rank?
N = height // size + (height % size > rank)
N = np.array(N, dtype='i')  # so we can gather it later on

# what slice of the whole should be computed in this rank?
start_i = comm.scan(N) - N
start_y = ymin + start_i * dy
end_y   = ymin + (start_i + N - 1) * dy

# calculate the local results - using numba.jit **without parallelism**
Cl = mandel_set(xmin, xmax, start_y, end_y, width, N, maxiter)
```

## MPI - Mandelbrot set

```
rowcounts = 0
C         = None
if rank == 0:
    rowcounts = np.empty(size, dtype='i')
    C = np.zeros([height, width], dtype='i')

comm.Gather(sendbuf = [N, MPI.INT],
            recvbuf = [rowcounts, MPI.INT],
            root    = 0)

comm.Gatherv(sendbuf = [Cl, MPI.INT],
             recvbuf = [C, (rowcounts * width, None), MPI.INT],
             root    = 0)
```

## ipyparallel

> ipyparallel enables all types of parallel applications to be developed, executed, debugged and monitored interactively



Documentation - GitHub

## Spark

> Apache Spark™ is a fast and general engine for large-scale data processing.

**Key idea**: Resilient Distributed Datasets (RDDs) are collections of objects across a cluster that can be computed on via parallel transformations (map, filter, ...).

There are APIs in a number of languages: Python, R, Java, and Scala.

Home page

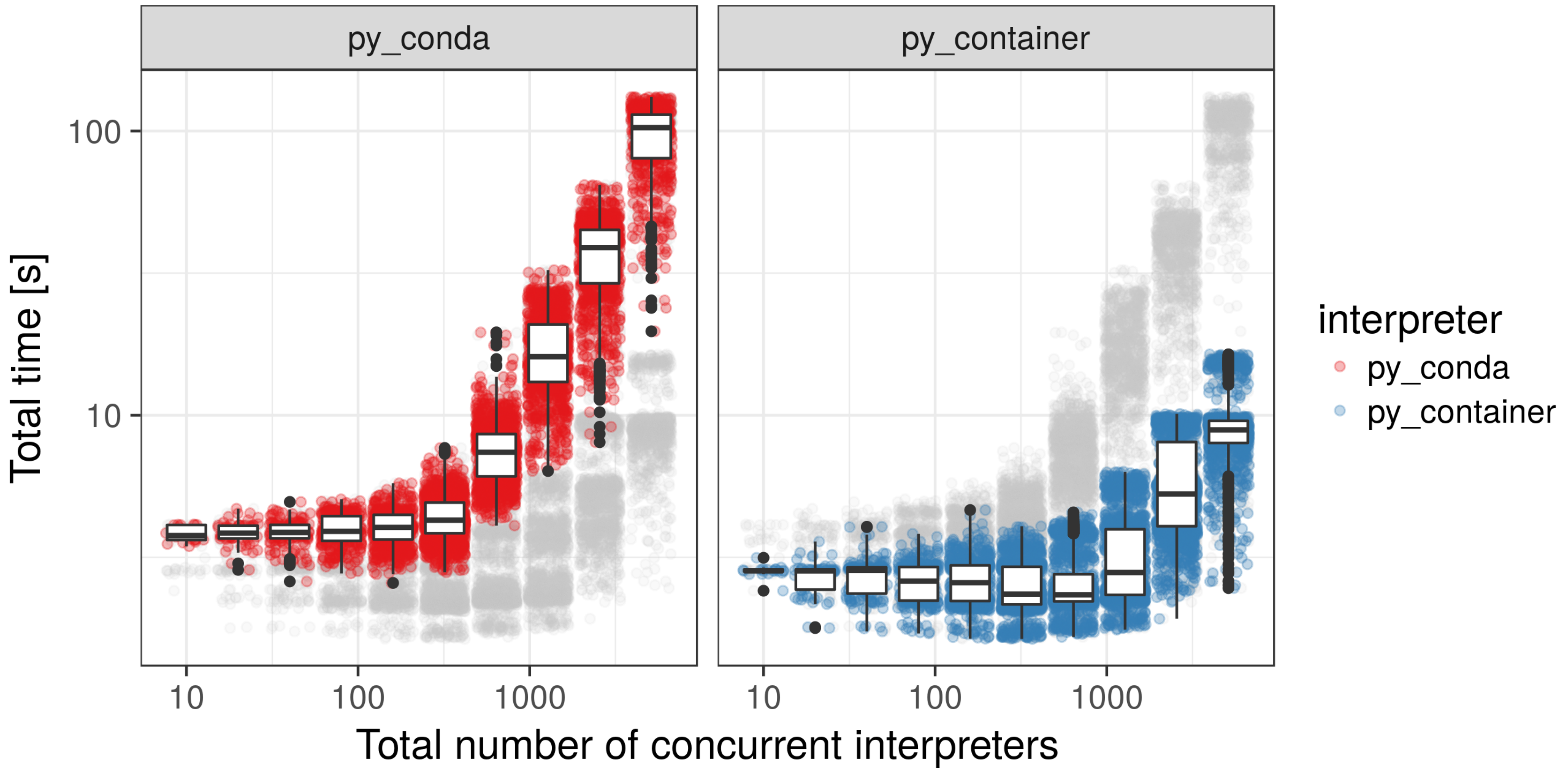
## Dask

“ Dask provides advanced parallelism for analytics, enabling performance at scale for the tools you love ”

## Python import problem

During startup python does a lot of small file operations as it locates all the files it needs. These metadata heavy operations can strain the file systems if many of them happen at the same time.

# Python import problem



## Python import problem

One solution is to containerize the python interpreter like in the example above.

### Other solutions:

- For mpi processes: import in the root process and share files via MPI
- static python builds
- cache the shared objects / python packages

NERSC talk - NERSC paper - Python MPI bcast - Static python - Scalable python

## Python on Biowulf

## Main python modules

```
$ module load python/2.7  # [D] support ended
$ module load python/3.5  #     maintenance mode
$ module load python/3.6
$ module load python/3.7
```

HPC python documentation

## Python 3

Python 3 made **backwards incompatible** changes (print, exceptions, division, unicode, comprehension variables, open(), ...).

**Support for Python 2 has ended**. All new code should be in python 3. Starting April 15 2020, python 3 will become the default module on biowulf.

## Some NIH HPC resources

- Python for matlab users
- Deep learning by example

## Private conda environments

## Set up your own conda env

```
$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
$ mkdir -p /data/$USER/conda /scratch/$USER/temp
$ export TMPDIR=/scratch/$USER/temp
$ bash Miniconda3-latest-Linux-x86_64.sh -p /data/$USER/conda -b
$ source /data/$USER/conda/etc/profile.d/conda.sh
$ conda update -n base conda
```

### Don't let it modify your `~/.bashrc`

```
$ conda create -n my_env python=3.8 numpy blas==2.14=mkl
```

## Use conda env in a batch job

```
#! /bin/bash

source /data/$USER/conda/etc/profile.d/conda.sh
conda activate my_env
...
```

or

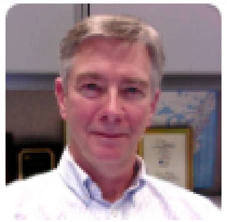
```
#! /bin/bash

PATH=/data/$USER/conda/envs/my_env/bin:$PATH
...
```

## Jupyter

Use the jupyter module and then select a kernel corresponding to one of our python installations

https://hpc.nih.gov/apps/jupyter.html

# staff@hpc.nih.gov


Steve Bailey

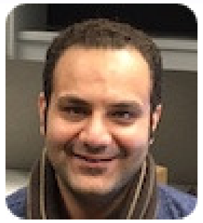
Steven Fellini, Ph.D.

Susan Chacko, Ph.D.

Gennady Denisov, Ph.D.

Picture unavailable

Afif Elghraoui


Ali Erfani

Andrew Fant, Ph.D.

David Godlove, Ph.D.

David Hoover, Ph.D.

Patsy Jones

Picture unavailable

Charles Lehr

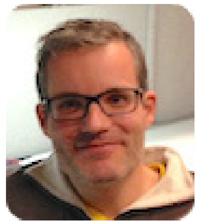
Jean Mao, Ph.D.

Tim Miller

Charlene Osborn

Mark Patkus

Dan Reisman


Wolfgang Resch, Ph.D.

Antonio Ulloa, Ph.D.