High Performance Python
EuroSciPy May 2014

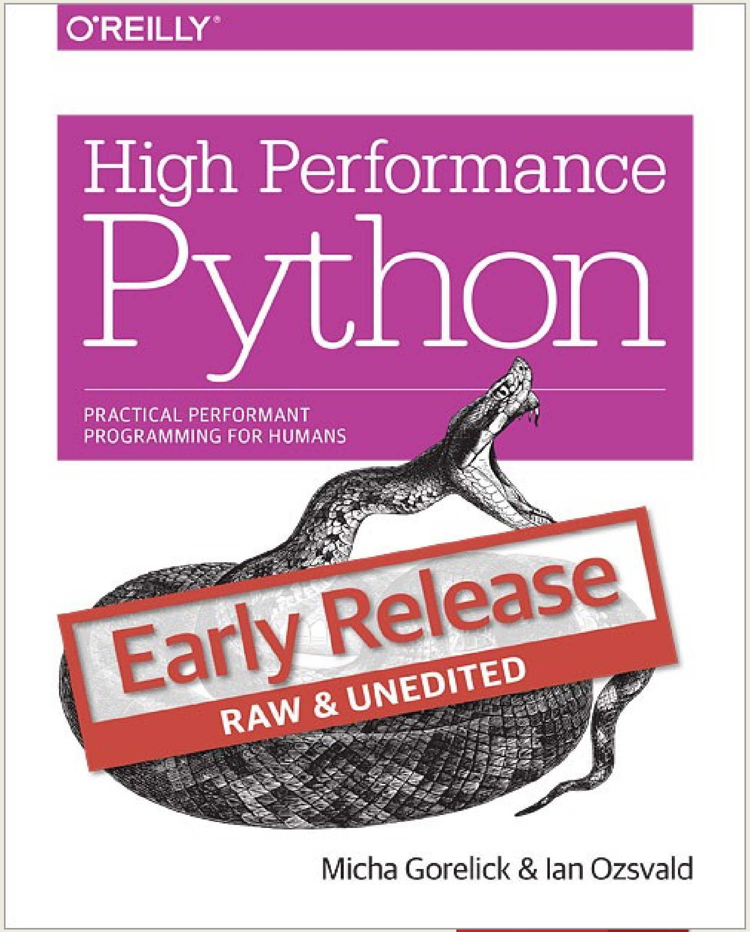
Ian Ozsvald @IanOzsvald MorConsulting.com

We'll cover

- Why we need to think about high performance
- Cython (pure Python and numpy)
- Numba
- Pythran
- PyPy

“High Performance Python”

- Published August
- Python 2.7 focused
- Lots of practical stuff



Mor Consulting

About Ian Ozsvald

- “Exploiter of Data” in ModelInsight.io
- *I teach privately (modelinsight.io)!*
- Teacher: PyCon, EuroSciPy, EuroPython
- Various ML/Parallel/Data projects
- ShowMeDo.com
- IanOzsvald.com

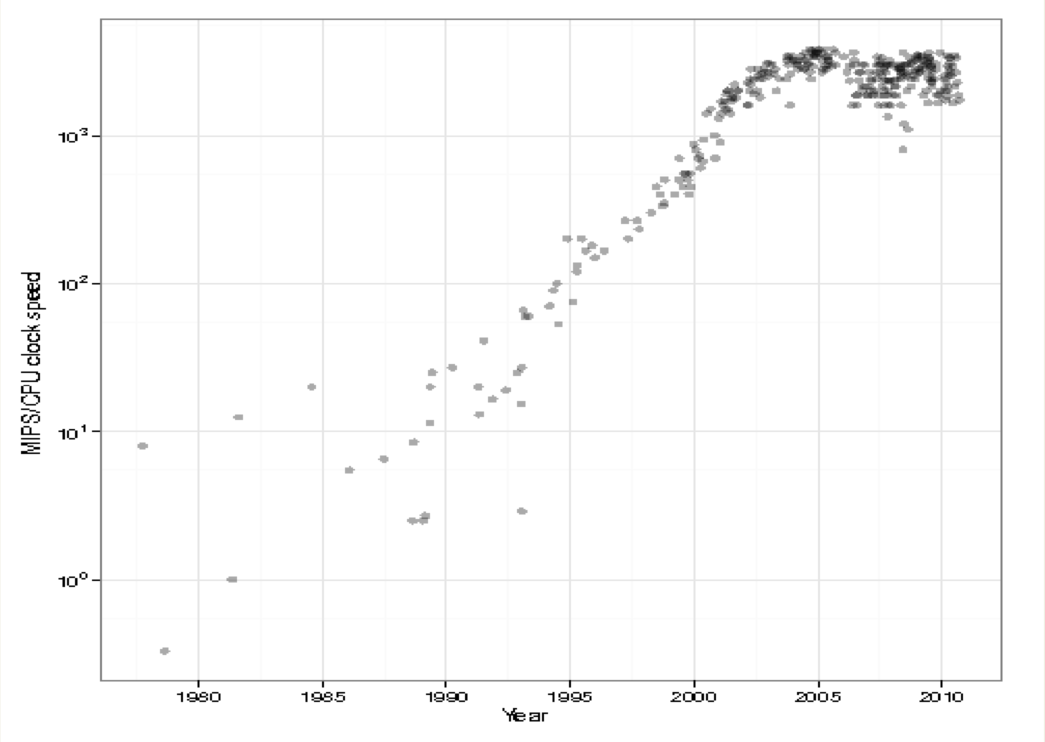
Mor Consulting

Gordon Moore's Law

- Number of transistors on an IC doubles every 18-24 months
- Self fulfilling
- Clearly doesn't mean linear speed increases...

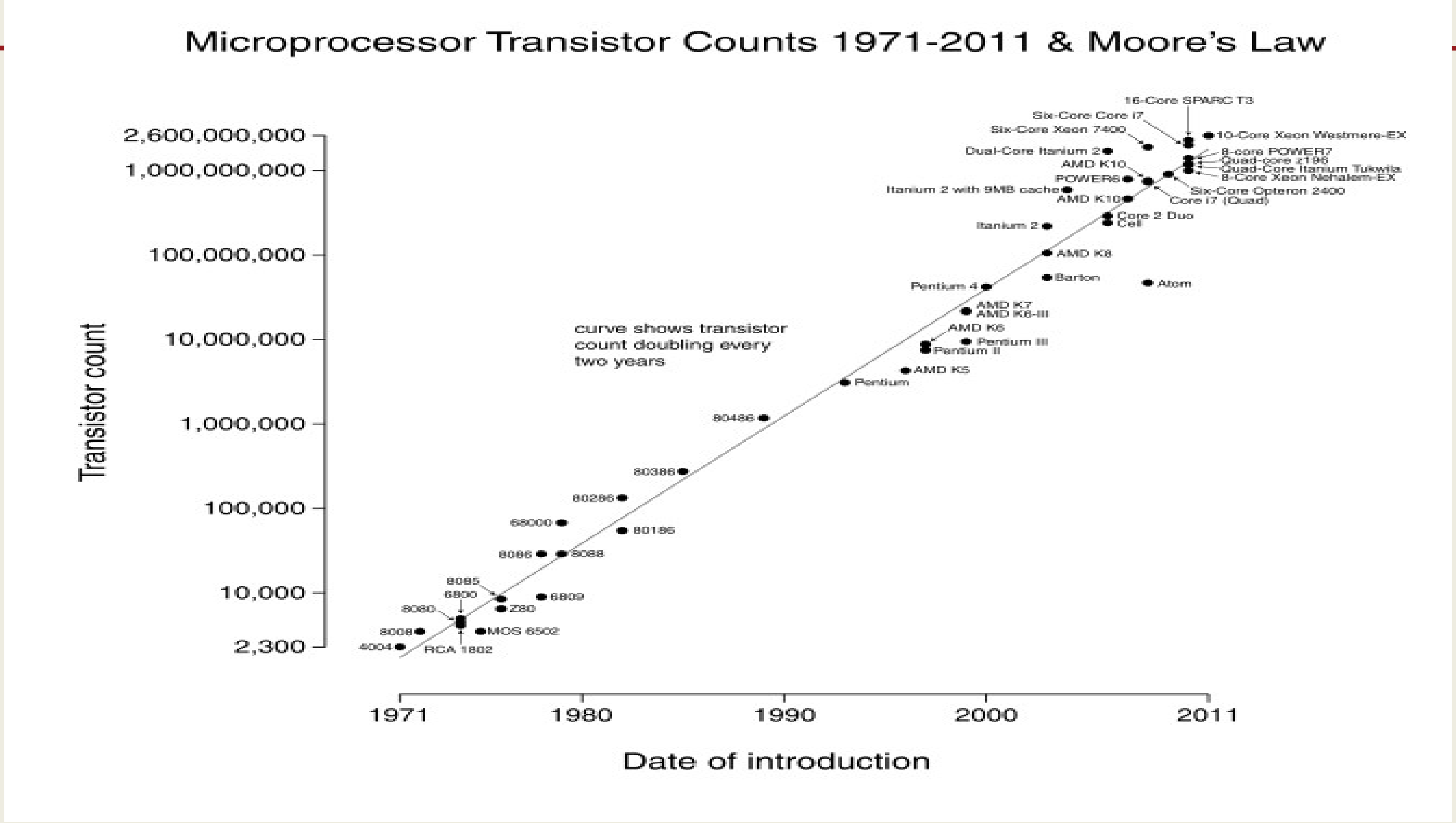
Moore's Law - limitation

- 3.4GHz – why?



- http://csgillespie.wordpress.com/2011/01/25/cpu-and-gpu-trends-over-time/

Moore's Law



http://en.wikipedia.org/wiki/Moores_law

Proebsting's Law

- *“Proebsting’s Law asserts that improvements to compiler technology double the performance of typical programs every 18 years”*
- *“Pro. has suggested that … communities should focus less on optimization and more on programmer productivity”*
- http://www.cs.virginia.edu/~techrep/CS-2001-12.pdf

Why use Python?

- Easy to use tooling
- Designed as beginner language
- Easy to keep in your head
- Large community (sci+eng)
- People are tackling *all the problems*
- Science, storage, visualisation, machine clustering, html, robustness, parsimonious coding

Mor Consulting

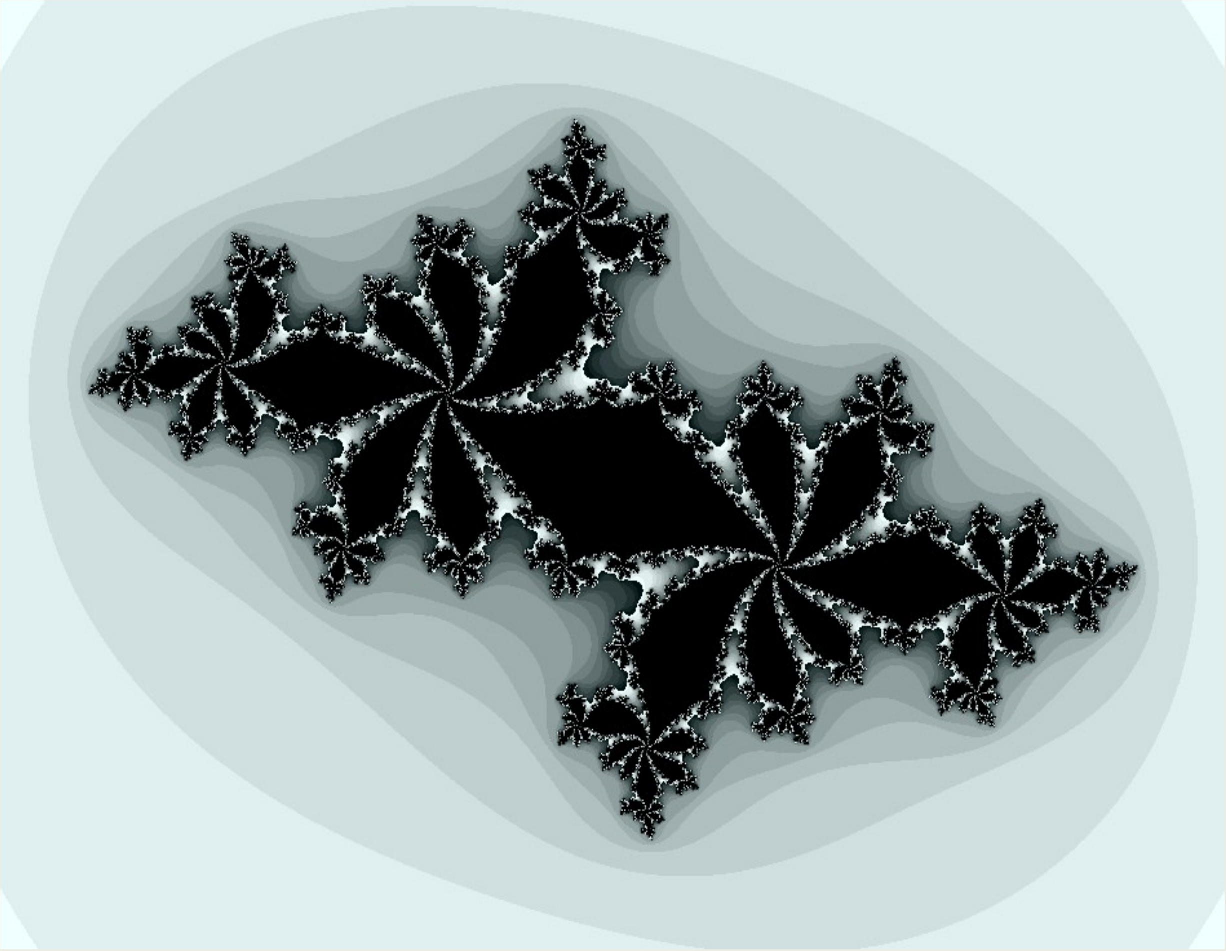
General go-fast rules

- Do as little work as possible

  You won't beat grep:
  http://lists.freebsd.org/pipermail/freebsd-current/2010-August/019310.html

- Cache to avoid re-work
- Keep everything debuggable
- Keep everything documented

The Julia Set Fractal



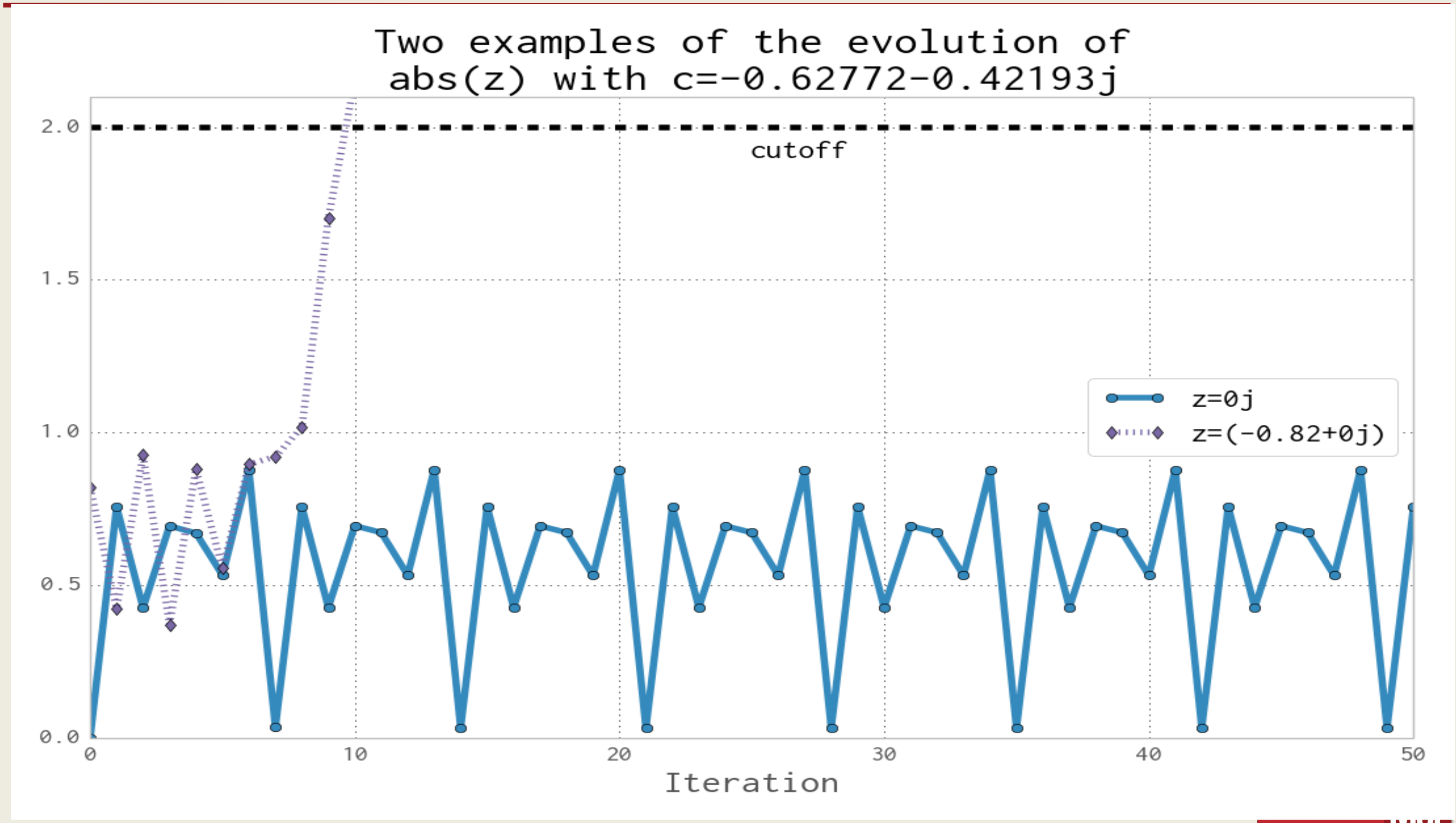
The Julia set

- Complex plane (just a co-ord set)
- Complex behaviour (what does this mean?)

$$f(z) = z^2 + c$$

- Embarrassingly parallel function
    - what does this mean?
- We're testing for bounded behaviour

The Julia set - evolution



The Julia set

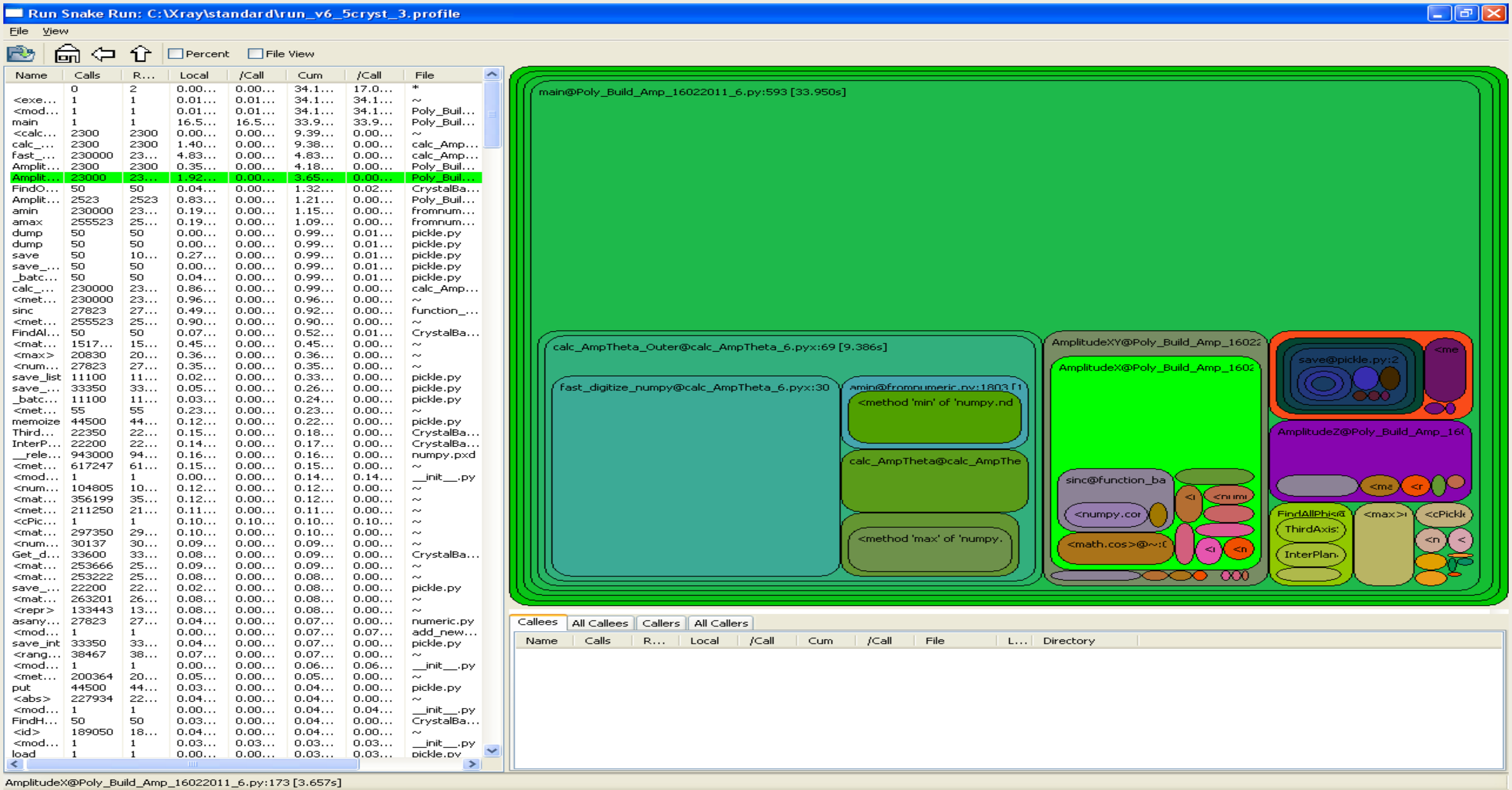
- Simple loop in code
- Let's review the code in julia.py (it is deliberately written suboptimally)
- We have a 1000 x 1000 array

```
while abs(z) < 2 and n < maxiter:
    z = z * z + c
    n += 1
output[i] = n
```

Profiling the CPU

- “We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil” - Donald Knuth
- Figure out what's slow, only optimize if it is worth it
- Optimizing takes time, costs mental cycles, introduces more complex code

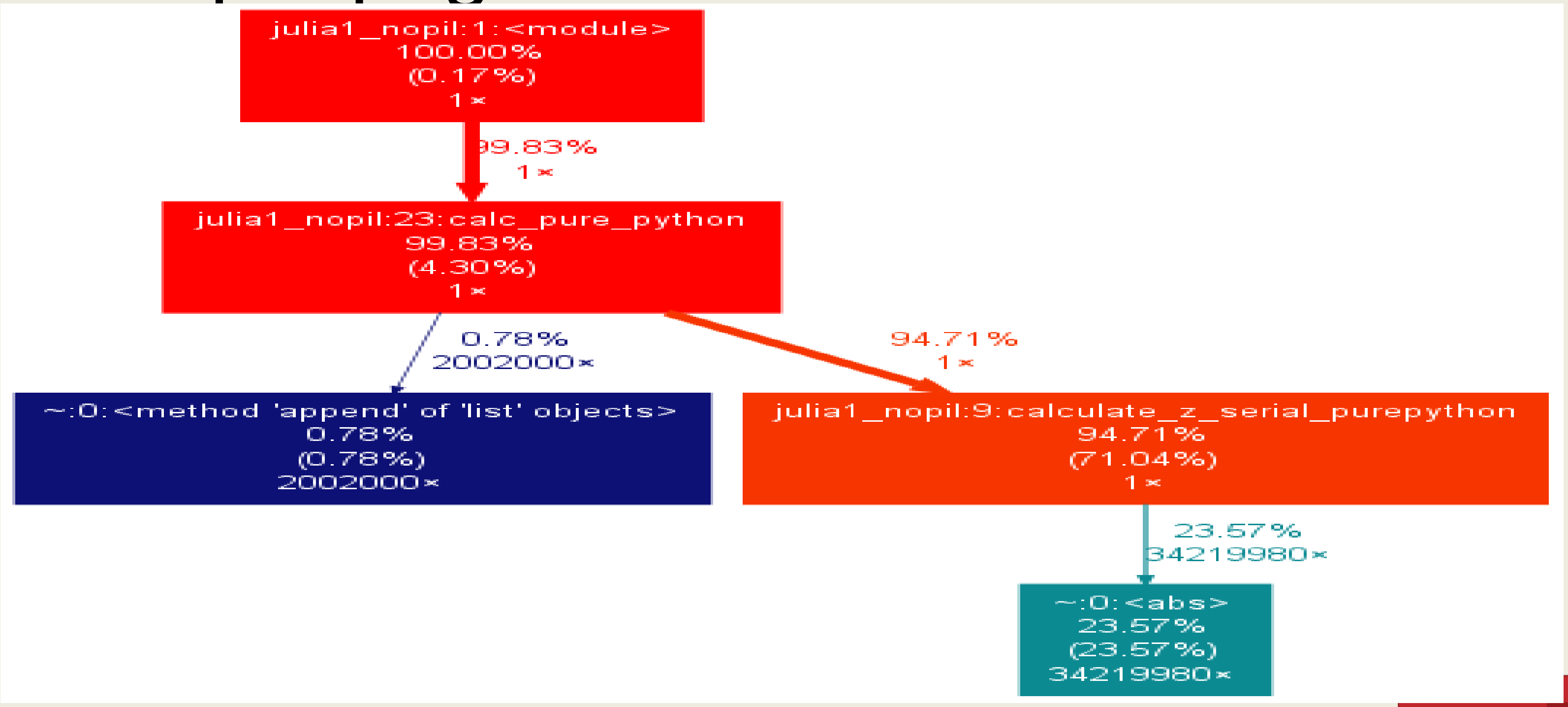
cProfile & runsnakerun



Ian@MorConsulting.com @IanOzsvald

cProfile and gprof2dot

gprof2dot -f pstats profile.stats | dot -Tpng -o output.png



line_profiler

- More informative, takes longer
- Line by line profiling
- Uses a C backend
- @profile – what is this?
- Make “julia_lineprofiler.py”, add @profile before calculate_z_serial_purepython
- !change max_iterations to 100 (from 300)
- !remove the assert

line_profiler

- kernprof.py -l -v julia_lineprofiler.py
- Run this first! It takes a while...
- *Can you explain the output to me?*
- *What is most costly?*
- We're using 100 max_iterations (not 300)
- More informative, takes longer
- Line by line profiling
- Uses a C backend

line_profiler (max 300 its.)

```
Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     9                                           @profile
    10                                           def calculate_z_serial_purepython(maxiter, zs, cs):
    11                                               """Calculate output list using Julia update rule"""
    12         1         6888   6888.0      0.0      output = [0] * len(zs)
    13   1000001       766409      0.8      0.8      for i in range(len(zs)):
    14   1000000       758497      0.8      0.8          n = 0
    15   1000000       817633      0.8      0.8          z = zs[i]
    16   1000000       757191      0.8      0.8          c = cs[i]
    17  34219980     36893641      1.1     36.7          while abs(z) < 2 and n < maxiter:
    18  33219980     31852838      1.0     31.7              z = z * z + c
    19  33219980     27775502      0.8     27.6              n += 1
    20   1000000       880494      0.9      0.9          output[i] = n
    21         1            5      5.0      0.0      return output
```

Profiling memory

- Samples system's memory report via psutil
- Can do line-by-line or graph
- What is using RAM in our Julia set? What do we expect to see? What is a surprise?

Profiling memory

- Make “julia_memoryprofiler.py”,
- add @profile before calculate_z...and calc_pure_python

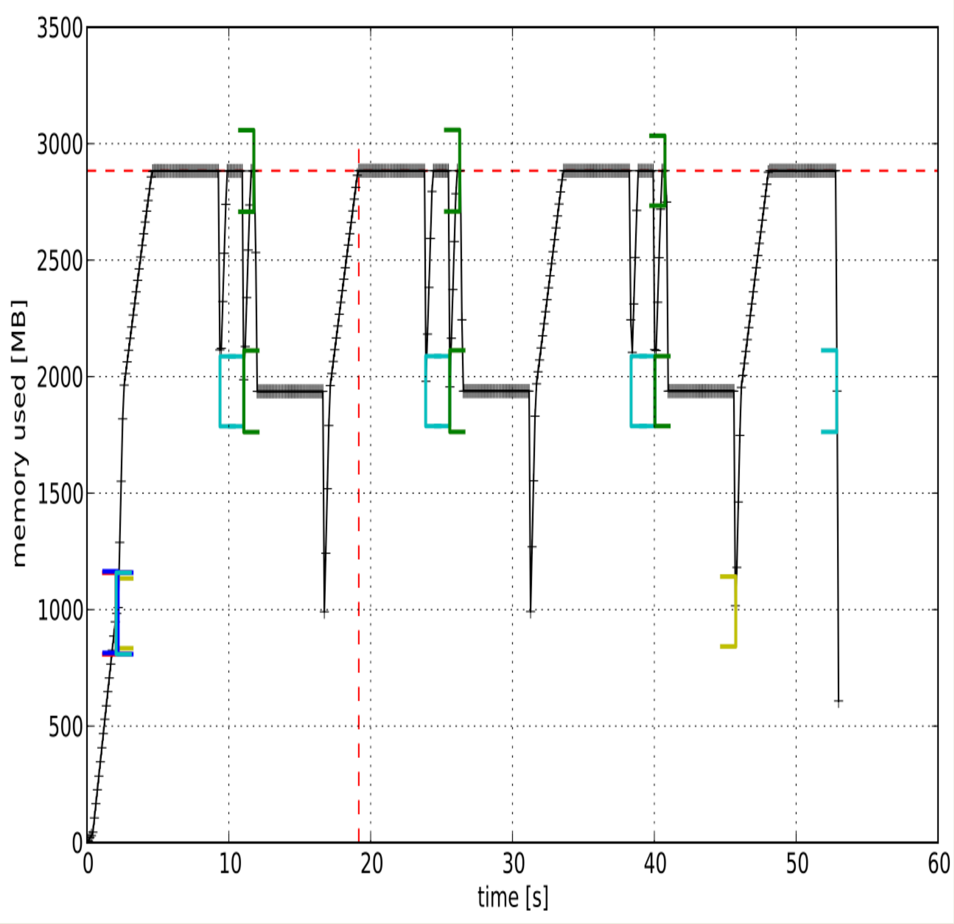
- !Set desired_width=100 (not 1000)
- !max_iterations can stay at 100
- python -m memory_profiler julia_memoryprofiler.py # from line_pr...

Mor Consulting

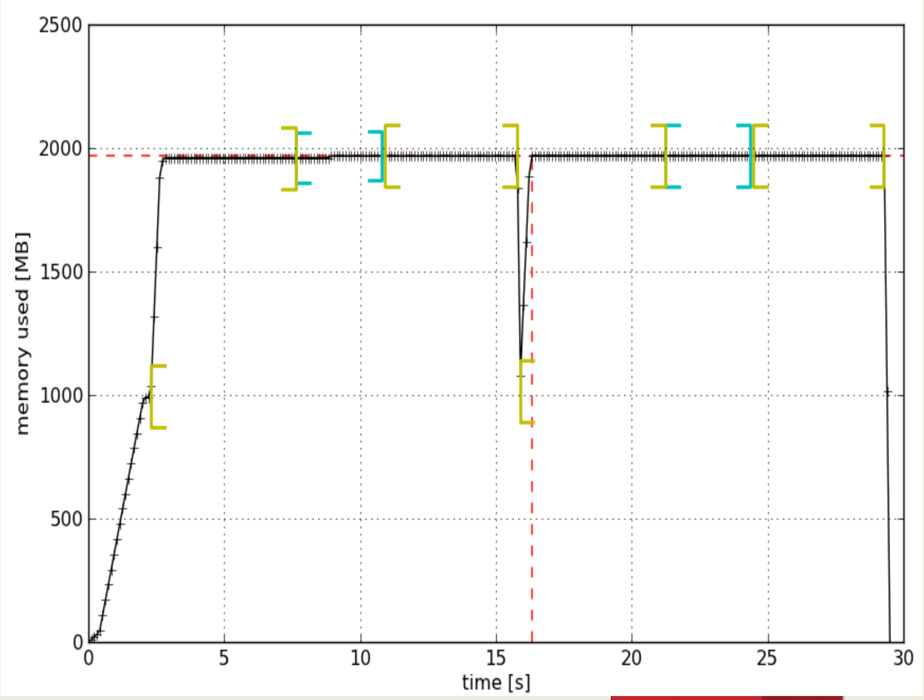
memory_profiler output

```
44   10.301 MiB    0.000 MiB       zs = []
45   10.301 MiB    0.000 MiB       cs = []
46   89.523 MiB   79.223 MiB       for ycoord in y:
47   89.523 MiB    0.000 MiB           for xcoord in x:
48   89.523 MiB    0.000 MiB               zs.append(complex(xcoord, ycoord))
49   89.523 MiB    0.000 MiB               cs.append(complex(c_real, c_imag))
50
51   89.531 MiB    0.008 MiB       print "Length of x:", len(x)
52   89.531 MiB    0.000 MiB       print "Total elements:", len(zs)
53   89.531 MiB    0.000 MiB       start_time = time.time()
54                                 output = calculate_z_serial_purepython(max_iterations, zs, cs)
55  138.000 MiB   48.469 MiB       end_time = time.time()
56  138.000 MiB    0.000 MiB       secs = end_time - start_time
57  138.004 MiB    0.004 MiB       print calculate_z_serial_purepython.func_name + " took", secs,
```

mprof (memory_profiler)



https://github.com/scikit-learn/scikit-learn/pull/2248
Before & After an improvement

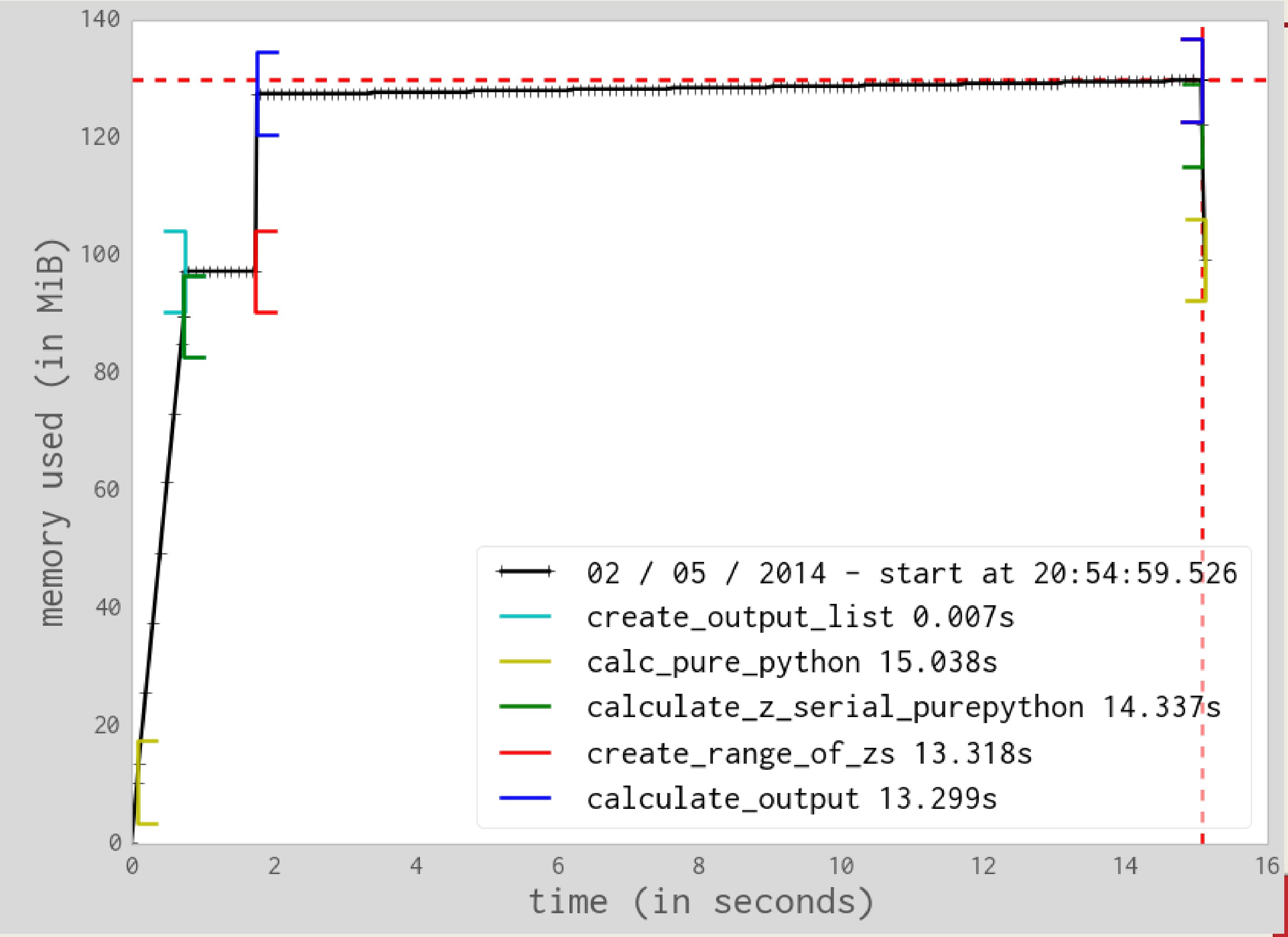


mprof – draw the mem. usage

- !desired_width=1000
- mprof run julia_memoryprofiler.py
- mprof plot # should show a graph

```
@profile
def calculate_z_serial_purepython(maxiter, zs, cs):
    """Calculate output list using Julia update rule"""
    with profile.timestamp("create_output_list"):
        output = [0] * len(zs)
    time.sleep(1)
    with profile.timestamp("create_range_of_zs"):
        iterations = range(len(zs))
        with profile.timestamp("calculate_output"):
            for i in iterations:
```

mprof



140
120
100
80
60
40
20
0
memory used (in MiB)
0
2
4
6
8
10
12
14
16
time (in seconds)
02 / 05 / 2014 - start at 20:54:59.526
create_output_list 0.007s
calc_pure_python 15.038s
calculate_z_serial_purepython 14.337s
create_range_of_zs 13.318s
calculate_output 13.299s

mprof – final tweak

- What could we change the range call to?
- Make the change – how does mprof plot change?
- We could also add annotations beyond function names

Compiling with Cython

- 2007 project (forked from Pyrex *.pyx*)
- Converts annotated Python into C
- You have to do the conversion
- We'll convert the plain Python version into C (we'll do numpy version later)
- We'll import a compiled version of the function

Cython

- Make “cython” directory, copy julia_nopil.py in there
- Make cythonfn.py (it'll become cythonfn.pyx soon)
- Move calculate_z function
- “from cythonfn import calculate_z”

Cython

- Once we know it works, rename to cythonfn.pyx (after pyrex project)
- cython -a cythonfn.pyx
- open “firefox cythonfn.html”

Cython – annotated

```
def calculate_z(maxiter, zs, cs):
    """Calculate output list using Julia update rule"""
    output = [0] * len(zs)
    for i in range(len(zs)):
        n = 0
        z = zs[i]
        c = cs[i]
        while n < maxiter and abs(z) < 2:
            z = z * z + c
            n += 1

      __pyx_t_2 = PyNumber_InPlaceAdd(__pyx_v_n, __pyx_int_1); if (unl
      __Pyx_GOTREF(__pyx_t_2);
      __Pyx_DECREF_SET(__pyx_v_n, __pyx_t_2);
      __pyx_t_2 = 0;
    }

        output[i] = n
    return output
```

Note InPlaceAdd and Reference Counting

Cython – make setup.py

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

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

Cython

- MOVE cythonfn.py → cythonfn.pyx
- To compile:

  python setup.py build_ext –inplace

  note build<under>ext dashdashinplace
- We should have a .c and a .so
- python julia_nopil.py
- This won't be much faster (and why is that?)

Ian@MorConsulting.com @IanOzsvald

Cython – add annotations

```
def calculate_z(int maxiter, zs, cs):
    """Calculate output list using Julia update rule"""
    cdef unsigned int i, n
    cdef double complex z, c
    output = [0] * len(zs)
    for i in range(len(zs)):
        n = 0
        z = zs[i]
        c = cs[i]
```

Cython

- How could we remove the abs operation?

Cython

- How could we remove the abs operation?
- abs(z) just sqrt(real^2 + imag^2)

Cython – expand the math

```
def calculate_z(int maxiter, zs, cs):
    """Calculate output list using Julia update rule"""
    cdef unsigned int i, n
    cdef double complex z, c
    output = [0] * len(zs)
    for i in range(len(zs)):
        n = 0
        z = zs[i]
        c = cs[i]
        while n < maxiter and (z.real * z.real + z.imag * z.imag) < 4:
            z = z * z + c
            n += 1
        output[i] = n
    return output
```

Cython

- Why do we expand the math?
- *Avoid doing work we don't have to do!*
- What else is abs(z) doing? We're forcing more specialisation
- We can disable bounds checking (but it doesn't change much)

Cython – tradeoffs

- Probably the fastest and most reliable solution for compiling
- You have to know some C
- You have to be happy working with C
- Removes generic behaviour, specialises your code (so less flexible)
- Use unit tests!
- Can compile with debug libs, easy enough just to use print statements

numpy serial version (slow!)

- Let's replace the Python lists with numpy arrays
- Look in src/numpy_version
- Walk through the new zs code first
- np.array is fast, right?
- Try the new demo <ouch> (>2 mins!)
- What's going on?

Cython and numpy

- We let C see the block of memory inside numpy arrays
- arr.data[0] → first byte
- __array_interface__.items() for the internal guts
- No need to manage access to Python objects any more
- What else might a C compiler do without the GIL restriction?
- Let's convert the numpy version with Cython

Cython and numpy

- Start with cythonfn.py and julia_nopil.py as before
- Check they run
- Copy setup.py from before
- “python setup.py build_ext --inplace”
- It'll take >2mins to run due to dereferencing cost

Cython and numpy

```
import numpy as np
cimport numpy as np

# to compile
# python setup.py build_ext --inplace

def calculate_z(int maxiter, double complex[:] zs,
                double complex[:] cs, long[:] output):
    """Calculate output list using Julia update rule"""
    cdef unsigned int i, length
    cdef double complex z, c
    #for i in range(len(zs)):
    length = len(zs)
    for i in xrange(length):
        z = zs[i]
        c = cs[i]
        output[i] = 0
```

Cython and numpy

- Now we're back to 4 seconds
- Can you expand the math like we did before?
- Does it run faster again? (it should be slightly faster to what we had for the lists version)
- Adding early binding, type specialisation and going to the raw low level objects means C can compile it very efficiently
- Could a non-Cython colleague understand this code?

OpenMP

- What does OMP give us?
- *shared memory multiprocessing*
- Multi-platform, multi-OS, C/C++/Fortran
- We need to make the decisions
- parallel for, parallel reduce

Cython and OpenMP

- How we do annotate the loop?
- We have to tell the compiler to use OMP
- What is *static* and *dynamic* scheduling?

Cython and OpenMP

- Add “from cython.parallel import prange”
- Change the for loop:

```
with nogil:
        for i in prange(length,
                        schedule="guided"):
```

Cython and OpenMP

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Build import cythonize
from Cython.Distutils import build_ext
ext_module = Extension("cythonfn",
    ["cythonfn.pyx"],
    extra_compile_args=['-fopenmp'],
    extra_link_args=['-fopenmp'])

setup(name = 'Cython fn',
      cmdclass = {'build_ext': build_ext},
      ext_modules = [ext_module])
```

Cython and OpenMP

- This is as fast as we can easily go!
- Fully exploits multiple cores
- Reductions are possible too

Pythran

- Somewhere between ShedSkin and Cython
- Has an annotation extension engine
- You supply the function annotation
- Works on Python and numpy variants
- Has interesting AST rebuilding and lightweight reimplemented modules
- Uses lightweight RefCounting (like CPython)
- CPython data must be copied into Pythran's memory space

Pythran

- Annotate: #pythran export calculate_z(int, complex[], complex[], int[])
- pythran fn.py → fn.so
- If you delete the .so then your original .py file will run unchanged – great for testing!

Pythran and OpenMP

- We can easily add OMP
- Add “#omp parallel for” before the for loop
- pythran -fopenmp -march=corei7-avx cython_np.py

Pythran specialisations

- Core library has been lightly reimplemented
- What if we take away a lot of the numpy machinery?
- It tries to auto-parallelise e.g. on a map

Pythran - tradeoffs

- Young project, very few users
- They're quick to respond
- Only some numpy modules supported
- Uses comments therefore does not disrupt code (unlike Cython)

Numba

- numpy-aware optimizing compiler
- Not a tracing JIT (unlike PyPy) but method-based (tracing is likely to be loop-based)
- Uses LLVM
- Requires a tiny bit of decoration
- GC handled by LLVM

Numba

- Add “from numba import jit”
- Add “@jit”, optionally add types

```
from numba import jit

@jit()
def calculate_z(maxiter, zs, cs, output):
```

- With the current version we have to pass in “output” from outside of the compiled function (but this hasn't always been the case)

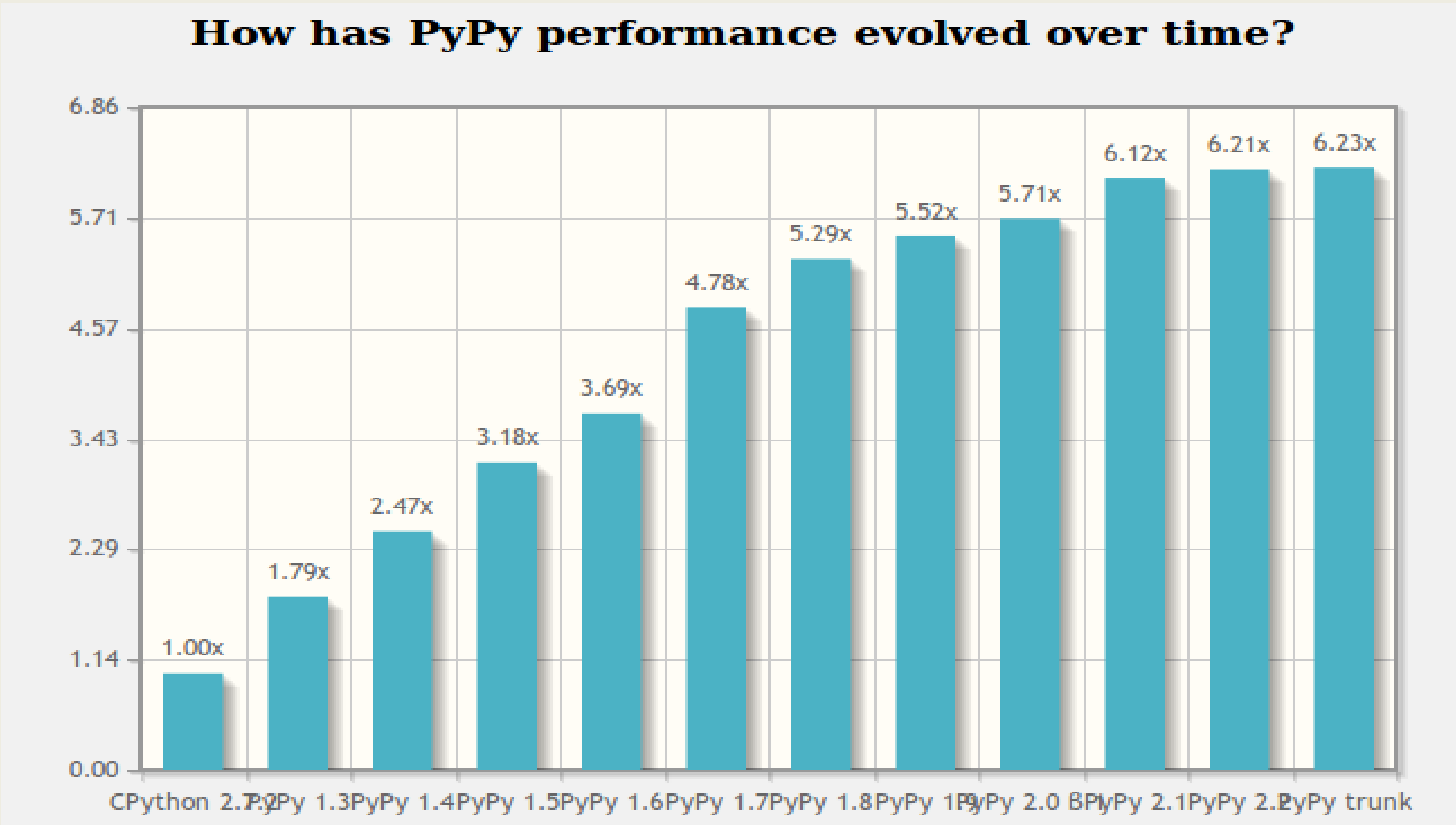
Numba - tradeoffs

- Be aware that the API changes with each release
- Really needs Anaconda
- Note run 1 has compile cost, run 2 no additional cost
- Does nothing useful for non-numpy code (but does work)
- Somewhat mixed real-world reports
- Probably has best long-term future as 'drop in replacement' for numpy speed-ups

PyPy

- “Like CPython but 6.3* faster (ish)”
- http://speed.pypy.org/
- Different implementation of Python including different GC
- Tracing JIT – considers loops and frequent code paths rather than whole functions, then compiles the hot loops
- No annotation is required
- Does have a GIL
- Python 2.7 and Python 3 (beta)
- Written in RPython (restricted Python enabling easy inference of variable's type), not written in C
- Built out of Armin's psyco (32 bit JIT)

PyPy


How has PyPy performance evolved over time?
6.86
5.71
4.57
3.43
2.29
1.14
0.00
1.00x
1.79x
2.47x
3.18x
3.69x
4.78x
5.29x
5.52x
5.71x
6.12x
6.21x
6.23x
CPython 2.7
PyPy 1.3
PyPy 1.4
PyPy 1.5
PyPy 1.6
PyPy 1.7
PyPy 1.8
PyPy 2.1
PyPy trunk

PyPy

- Run it, run with julia_nopil.py
- How much faster?
- Not bad for *no work at all*

Mor Consulting

Sidenote – ref counting GC in Python

- RefCounting to keep track of live objects
- When 0 references left – delete object
- This is a CPython implementation choice
- This is *not the only GC strategy*
- PyPy doesn't use RefCounting, it has a modifed mark-and-sweep with nursery

PyPy

- Software Transactional Memory
- Replaceable Garbage Collectors
- Has had Java backend
- PyPy.js – RPython->C->Emscripten (C to JS via LLVM))->JS – faster than CPy but slower than PyPy
- JS & LLVM receiving lots of attention in the compiler community
- If you want to write your own efficient interpreter:

  http://www.wilfred.me.uk/blog/2014/05/24/r-python-for-fun-and-profit/

PyPy tradeoffs

- There *is* numpypy support (sort of)
- CPyExt sort-of provides access to C compiled extensions (and do we really need them?) e.g. cPickle in PyPy is not written in C any more
- CFFI is the right solution for C modules with Python + PyPy compatibility

“High Performance Python”

- I think I'm signing...
- Training courses in October in London
- pyvideo.org
- PyDataLondon meetup