Numba, a JIT compiler for fast numerical code

Speaker presentation

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    - Core Python developer since 2007
    - *Not a scientist*

What is Numba?

- A just-in-time compiler based on LLVM
- Runs on CPython 2.6 to 3.4
- Opt-in
- Specialized in numerical computation
- BSD-licensed, cross-platform (Linux, OS X, Windows)

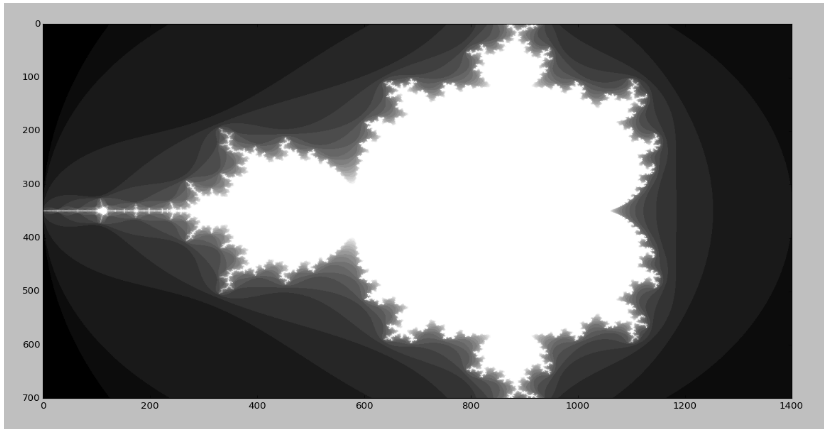
Why a just-in-time compiler?

- Pure Python is slow at number crunching
- Numpy has C accelerations, but they only apply to well-behaved problems
  - array operations are memory-heavy, can thrash CPU caches
- Many algorithms have irregular data access, per-element branching, etc.
- Want C-like speed but without writing C (or Fortran!)
- Fit for interactive use

Why a just-in-time compiler?

Mandelbrot (20 iterations):

CPython	1x
Numpy array-wide operations	13x
Numba (CPU)	120x
Numba (NVidia Tesla K20c)	2100x



LLVM

- A mature library and toolkit for writing compilers (clang)
- Multi-platform
- Supported by the industry
- Has a wide range of integrated optimizations
- Allows us to focus on *Python*

LLVM optimizations

- inlining
- loop unrolling
- SIMD vectorization
- etc.

LLVM crazy optimizations

Constant time arithmetic series

In [2]:
```
@numba.jit
def f(x):
    res = 0
    for i in range(x):
        res += i
    return res
```

In [10]:
```
%timeit -c f(10)
```

```
1000000 loops, best of 3: 211 ns per loop
```

In [15]:
```
%timeit -c f(100000)
```

```
1000000 loops, best of 3: 231 ns per loop
```

LLVM crazy optimizations

Assembler output

```
In [16]: print(f.inspect_asm((numba.int64,)))
```

```
        .text
        .file   "<string>"
        .globl  __main__.f$1.int64
        .align  16, 0x90
        .type   __main__.f$1.int64,@function
__main__.f$1.int64:
        xorl    %edx, %edx
        testq   %rcx, %rcx
        jle     .LBB0_2
        movq    %rcx, %rax
        negq    %rax
        cmpq    $-2, %rax
        movq    $-1, %rdx
        cmovgq  %rax, %rdx
        leaq    (%rdx,%rcx), %rsi
        leaq    -1(%rdx,%rcx), %rax
        mulq    %rsi
        shldq   $63, %rax, %rdx
        addq    %rsi, %rdx
.LBB0_2:
        movq    %rdx, (%rdi)
        xorl    %eax, %eax
        retq
```

Runs on CPython

- 2.6, 2.7, 3.3, 3.4, 3.5
- Can run side by side with regular Python code
- Can run side by side with all third-party C extensions and libraries
    - all the numpy / scipy / etc. ecosystem

Opt-in

- Only accelerate select functions decorated by you
- Allows us to relax *semantics* in exchange for speed
- High-level code surrounding Numba-compiled functions can be arbitrarily complex

Specialized

- Tailored for number crunching
- Tailored for Numpy arrays
- And a bunch of other things...

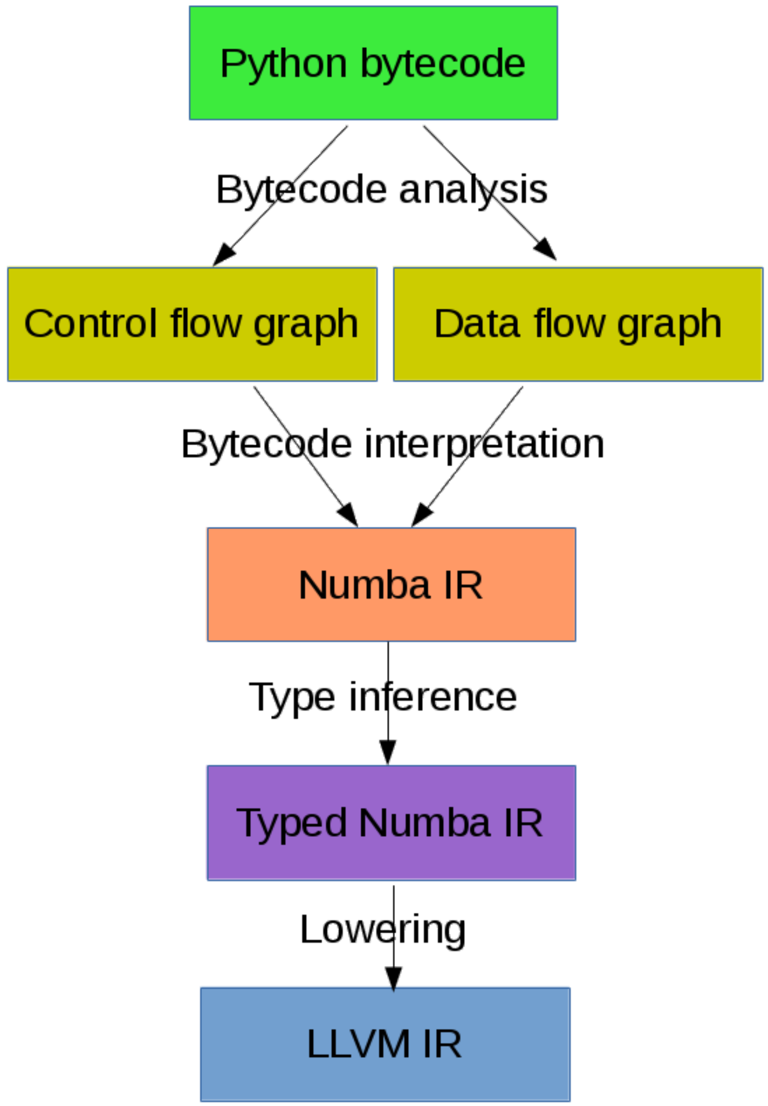
Multiple targets

- Main target is the CPU
  - officially supported: x86, x86-64
- CUDA target for NVidia GPUs with a limited feature set
- Potential support for:
  - HSA (GPU+CPU on AMD APUs)
  - ARM processors
  - ...

Numba architecture

- Straight-forward function-based JIT
- Compilation pipeline from Python bytecode to LLVM IR
- Low-level optimizations and codegen delegated to LLVM
- Python-facing wrappers

Compilation pipeline



Numba specializations

- "Lowering" pass generates LLVM code for specific types and operations
    - built-in types and operators
    - specific libraries (math, cmath, random...)
- Opens opportunities for inlining and other optimizations

Supported Python syntax

- Supported constructs:
  - if / else / for / while / break / continue
  - raising exceptions
  - calling other compiled functions
  - generators!
  - etc.

Unsupported Python syntax

- Unsupported constructs:
  - try/except/finally
  - with
  - (list, set, dict) comprehensions
  - yield from

Supported Python features

- Types:
  - int, bool, float, complex
  - tuple, None
  - bytes, bytearray, memoryview (and other buffer-like objects)
- Built-in functions:
  - abs, enumerate, len, min, max, print, range, round, zip

Supported Python modules

- Standard library:
  - cmath, math, random, ctypes...
- Third-party:
  - cffi, numpy

Supported Numpy features

- All kinds of arrays
  - scalar
  - structured
  - except when containing Python objects
- Iterating, indexing, slicing
- Reductions: argmax(), max(), prod() etc.
- Scalar types and values (including `datetime64` and `timedelta64`)

Limitations

- Recursion not supported
- Can't compile classes
- Can't allocate array data
- Type inference must be able to determine all types

Semantic changes

- Fixed-sized integers
- Global and outer variables frozen
- No frame introspection inside JIT functions:
  - tracebacks
  - debugging

Using Numba: @jit

- @jit-decorate a function to designate it for JIT compilation
- Automatic lazy compilation (recommended):

```
@numba.jit
def my_function(x, y, z):
    ...
```

- Manual specialization:

```
@numba.jit("(int32, float64, float64)")
def my_function(x, y, z):
    ...
```

GIL removal with @jit(nogil=True)

- N-core scalability by releasing the Global Interpreter Lock:

```
@numba.jit(nogil=True)
def my_function(x, y, z):
    ...
```

- No protection from race conditions!

Tip

Use `concurrent.futures.ThreadPoolExecutor` on Python 3

Using Numba: @vectorize

- Compiles a scalar function into a **Numpy universal function**
- What is a universal function?
  - Examples: np.add, np.mult, np.sqrt...
  - Apply an element-wise operation on entire arrays
  - Automatic broadcasting
  - Reduction methods: np.add.reduce(), np.add.accumulate()...
- Traditionally requires coding in C

Using Numba: @guvectorize

- Compiles a element-wise or subarray-wise function into a generalized universal function
- What is a generalized universal function?
  - like a universal function, but allows to peek at other elements
  - e.g. moving window average
  - automatic broadcasting, but not automatic reduction methods

@vectorize performance

Vectorizing optimizes the memory cost on large arrays.

In [2]:
```
@numba.vectorize(['float64(float64, float64)'])
def relative_difference(a, b):
    return abs(a - b) / (abs(a) + abs(b))
```

In [3]:
```
x = np.arange(1e8, dtype=np.float64)
y = x + 1.1
```

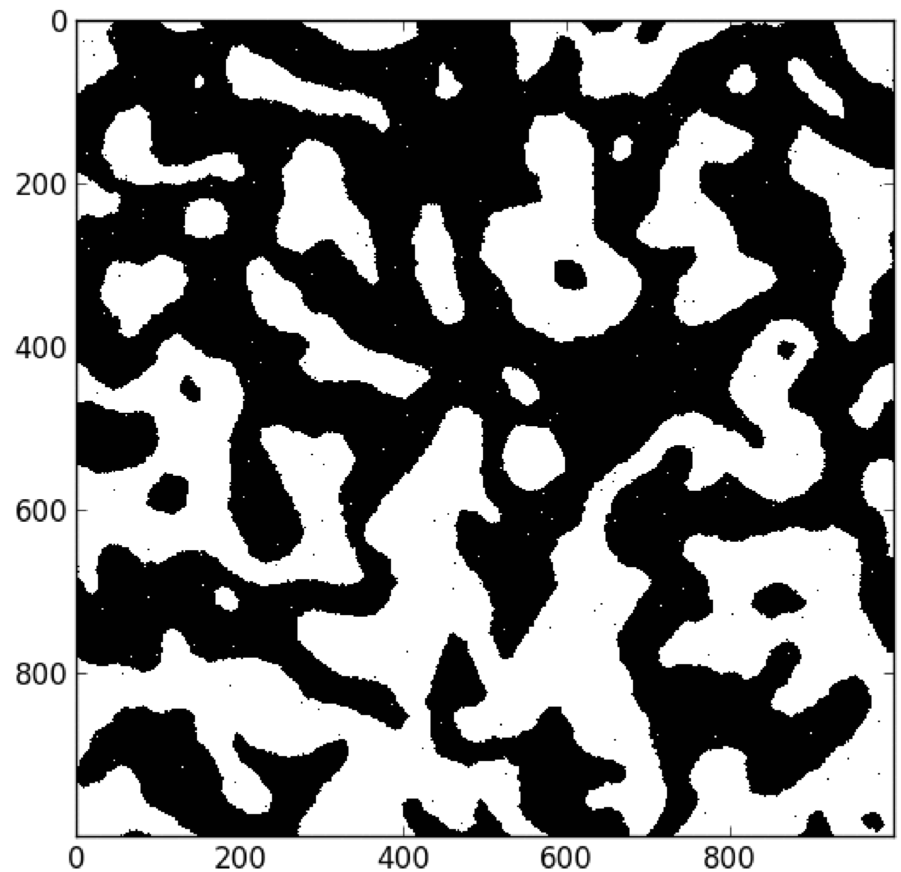
In [4]:
```
%timeit abs(x - y) / (abs(x) + abs(y))
```

```
1 loops, best of 3: 2.2 s per loop
```

In [5]:
```
%timeit relative_difference(x, y)
```

```
1 loops, best of 3: 741 ms per loop
```

@jit example: Ising models



Ising model: code

```
kT = 2 / math.log(1 + math.sqrt(2), math.e)

@numba.jit(nopython=True)
def update_one_element(x, i, j):
    n, m = x.shape
    assert n > 0
    assert m > 0
    dE = 2 * x[i, j] * (
                     x[(i-1)%n, (j-1)%m]
                   + x[(i-1)%n,  j     ]
                   + x[(i-1)%n, (j+1)%m]

                   + x[ i     , (j-1)%m]
                   + x[ i     , (j+1)%m]

                   + x[(i+1)%n, (j-1)%m]
                   + x[(i+1)%n,  j     ]
                   + x[(i+1)%n, (j+1)%m]
                   )
    if dE <= 0 or exp(-dE / kT) > np.random.random():
        x[i, j] = -x[i, j]

@numba.jit(nopython=True)
def update_one_frame(x):
    n, m = x.shape
    for i in range(n):
        for j in range(0, m, 2):  # Even columns first to avoid overlap
            update_one_element(x, j, i)
    for i in range(n):
        for j in range(1, m, 2):  # Odd columns second to avoid overlap
            update_one_element(x, j, i)
```

Ising model: performance

CPython	1x
Numba (CPU)	130x
Fortran	275x

CUDA support

- Numba provides a @cuda.jit decorator
- Exposes the CUDA programming model
- Parallel operation:
  - threads
  - blocks of threads
  - grid of blocks
- Distinguishing between:
  - kernel functions (called from CPU)
  - device functions (called from GPU)

CUDA support

- Limited array of features available
  - features requiring C helper code unavailable
- Programmer needs to make use of CUDA knowledge
- Programmer needs to take hardware capabilities into account

CUDA example

In [2]:
```
@cuda.jit
def gpu_cos(a, out):
    i = cuda.grid(1)
    if i < a.shape[0]:
        out[i] = math.cos(a[i])
```

In [3]:
```
x = np.linspace(0, 2 * math.pi, 1e7, dtype=np.float32)
cpu_out = np.zeros_like(x)
gpu_out = np.zeros_like(x)

thread_config = (len(x) // 512 + 1), 512
```

In [4]:
```
%timeit np.cos(x, cpu_out)
```

```
10 loops, best of 3: 149 ms per loop
```

In [7]:
```
%timeit gpu_cos[thread_config](x, gpu_out)
```

```
10 loops, best of 3: 27.8 ms per loop
```

The CPU is a **Core i7-4820K (3.7 GHz)**, the GPU is a **Tesla K20c**.

In [8]:
```
np.allclose(cpu_out, gpu_out)
```

Out[8]:
```
True
```

Installing Numba

- Recommended: precompiled binaries with Anaconda or Miniconda:

```
conda install numba
```

- Otherwise: install LLVM 3.5.x, compile llvmlite, install numba from source

Contact

- http://numba.pydata.org/
- Code and issue tracker at https://github.com/numba/numba/
- Numba-users mailing-list
- Numba is commercially supported (sales@continuum.io)
  - consulting
  - enhancements
  - support for new architectures
  - NumbaPro