Get the benefits of C without leaving Python

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Myself

- Background in Earth Sciences, Geophysics
- Using Python since 2001
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What is Cython

- Fork of Pyrex
- Easy Python C extensions
- Performance boost
- Python -> C bridge
- C -> Cython bridge

Python Demo

from https://docs.python.org/2/c-api/intro.html:

```
def incr_item(dict, key):
  try:
    item = dict[key]
  except KeyError:
    item = 0

  dict[key] = item + 1
```

Python C-API Demo

```
int
incr_item(PyObject *dict, PyObject *key)
{
    /* Objects all initialized to NULL for Py_XDECREF */
    PyObject *item = NULL,
    *const_one = NULL,
    *incremented_item = NULL;
    /* Return value initialized to -1 (failure) */
    int rv = -1;

    item = PyObject_GetItem(dict, key);
    if (item == NULL) {
        /* Handle KeyError only: */
        if (!PyErr_ExceptionMatches(PyExc_KeyError))
            goto error;
```

```
    /* Clear the error and use zero: */
    PyErr_Clear();
    item = PyInt_FromLong(0L);
    if (item == NULL)
        goto error;
}

const_one = PyInt_FromLong(1L);
if (const_one == NULL)
    goto error;

incremented_item = PyNumber_Add(item, const_one);
if (incremented_item == NULL)
    goto error;

if (PyObject_SetItem(dict, key, incremented_item) < 0)
    goto error;
rv = 0; /* Success */
/* Continue with cleanup code */
```

```
error:
    /* Cleanup code, shared by success and failure path */

    /* Use Py_XDECREF() to ignore NULL references */
    Py_XDECREF(item);
    Py_XDECREF(const_one);
    Py_XDECREF(incremented_item);

    return rv; /* -1 for error, 0 for success */
}
```

Cython Advantages

- 99% Python
- Python 2/3 compatibility
- Classes
- Garbage collection
- String handling
- Automatic reference counting
- Automatic type casting (Python->C, C->Python)
- Portable C code produced
- Stable, mature

Get the benefits of C without leaving Python

Cython Disadvantages

- Needs compilation
- Distutils
- CPython specific

Python demo counter

```
def counter(count):
  x = 0
  for i in xrange(count):  # range in Py3
    x += i
```

Cython demo counter

```
def counter(count):
  cdef int x = 0 # <- a C style data type
  for i in xrange(count):
    x += i
```

Cython cdef-ed demo counter

```
cdef int counter(int count):
  cdef int x = 0
  for i in xrange(count):
    x += i
  return x
```

Building a Cython module

- **Cython translates from .pyx to C code**

  cython inputfile.pyx

- **Or let setup.py handle it**

  python setup.py build_ext --inplace

Cython and the GIL

Bypassing the GIL with C

Modules that release the GIL:

- time.sleep()
- most of NumPy
- many C extensions

Cython nogil

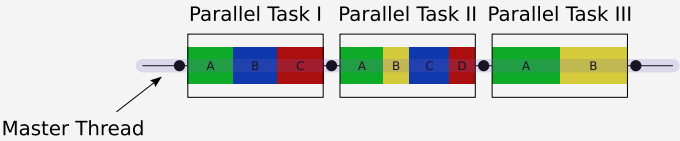
```
def cython_func():
  with nogil:
    do_something()

    if something_bad == True:
      with gil:
        raise RuntimeError('sorry...')
```

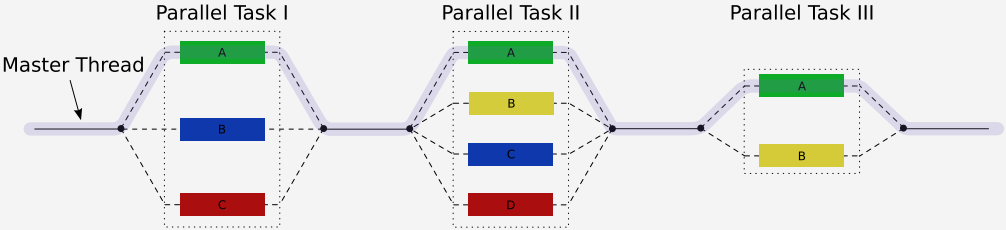
Threading headaches:

- race conditions
- deadlocks
- data corruption
- thread pools
- Yikes! Wait...

Easier multithreading... from C?!

OpenMP: Shared memory multithreading C API/spec





source: https://en.wikipedia.org/wiki/OpenMP

Classic Demo Updated

- **2D Laplace Equation benchmark by Prabhu Ramachandran in 2004:**

  http://wiki.scipy.org/PerformancePython

- **Updated in by Travis Oliphant in 2011:**

  http://technicaldiscovery.blogspot.co.nz/2011/06/speeding-up-python-numpy-cy

- **Previously compared:**

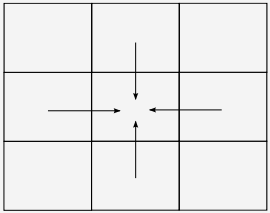
  Psyco, NumPy, Blitz, Inline, Python/Fortran, Pyrex, MatLab, Octave, Pure C++

- **We'll disucss:**

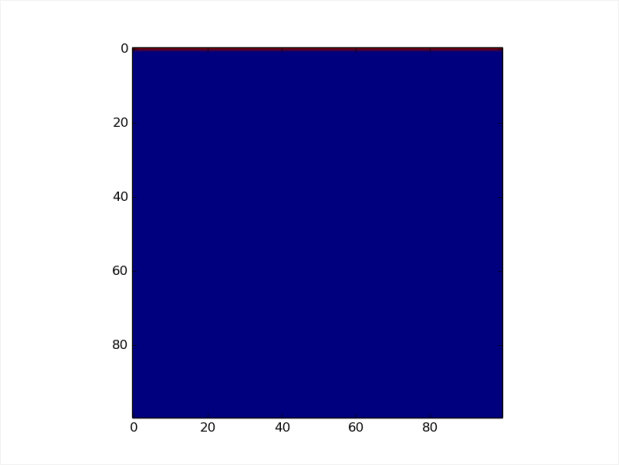
  Python, NumPy, Numba, Cython, Cython wrapping C, Cython in parallel

2D Laplace equation

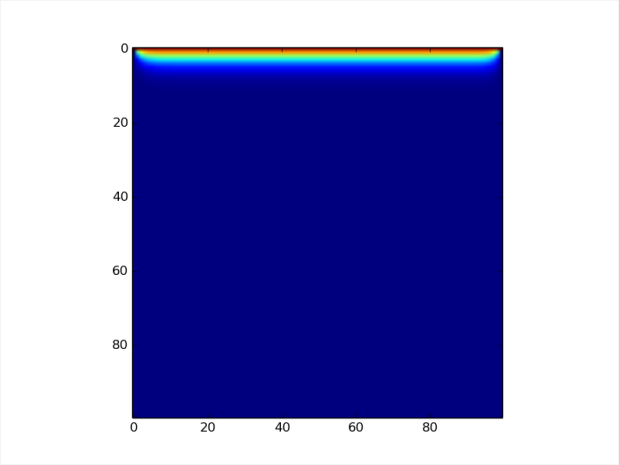
- floating point intensive
- iterative



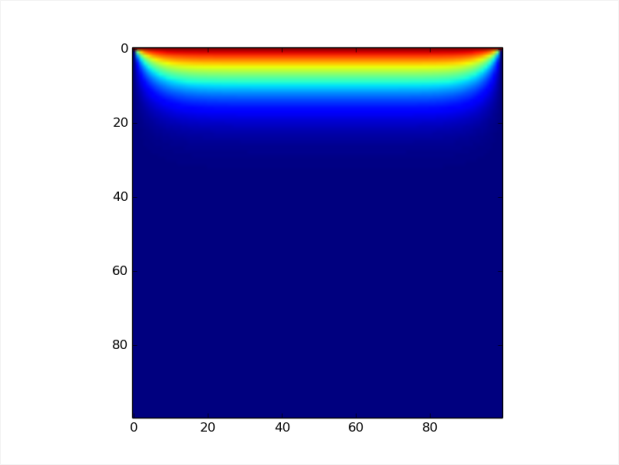
Starting state



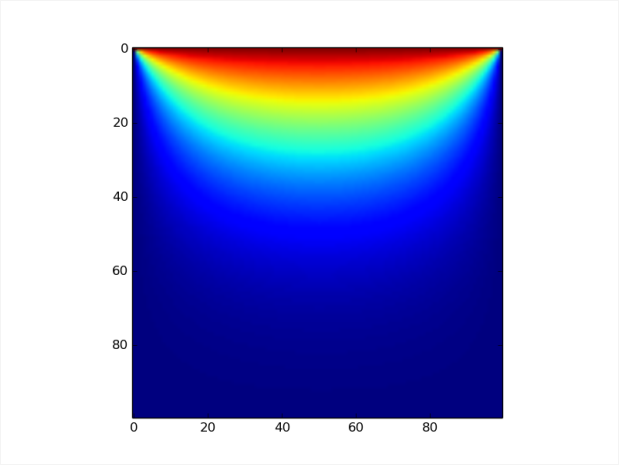
10 iterations



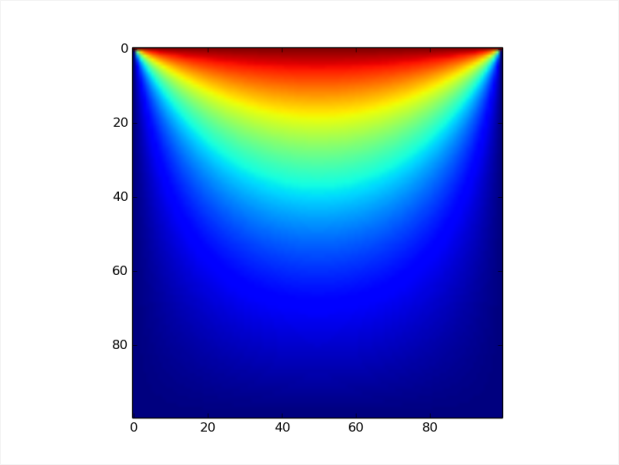
100 iterations



1000 iterations



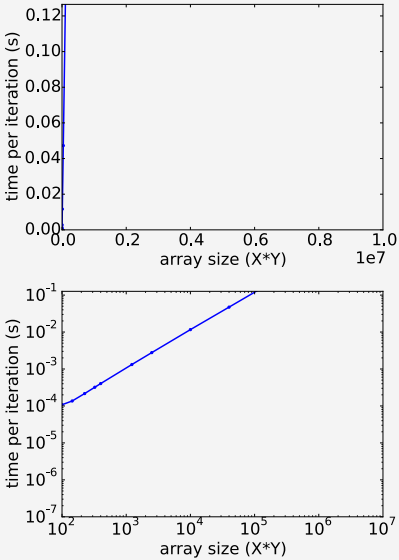
10000 iterations



Python version

```
def py_update(u, dx2, dy2):
  nx, ny = u.shape
  for i in xrange(1,nx-1):
    for j in xrange(1, ny-1):
      u[i,j] = ((u[i+1, j] + u[i-1, j]) * dy2 +
                (u[i, j+1] + u[i, j-1]) * dx2) / (2*(dx2+dy2))

work_array = np.zeros([array_shape, array_shape],
                      dtype=np.float64)
work_array[0] = 1.0

for x in range(100):
  py_update(work_array, dx2, dy2)
```

Python benchmark

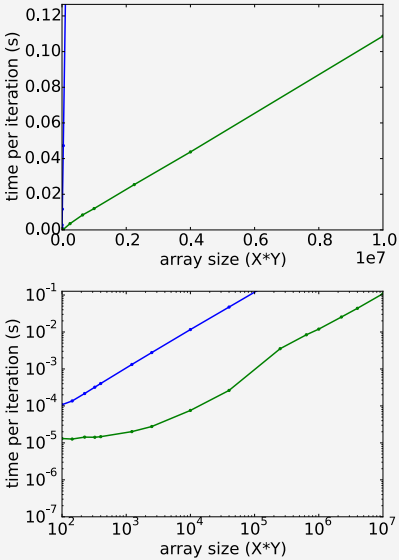


Numpy version

- Eliminates all loops
- Extensive use of NumPy vectorized operations
- Creates several temporary arrays

```
import numpy as np

def num_update(u, dx2, dy2):
  u[1:-1,1:-1] = ((u[2:,1:-1] + u[:-2,1:-1])*dy2 +
                  (u[1:-1,2:] + u[1:-1,:-2])*dx2)/(2*(dx2+dy2))
```

Numpy Benchmark

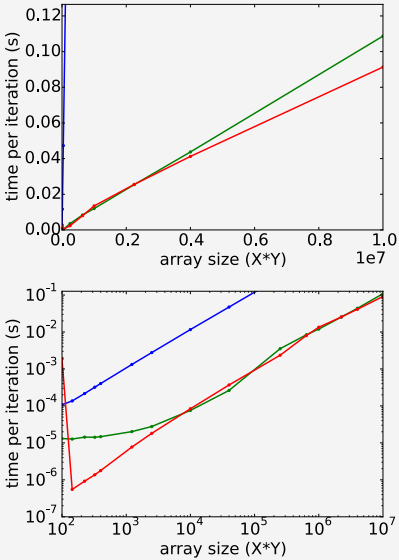


Numba version

- Identical to Python version apart from jit decorator

```
from numba import jit

@jit
def numba_update(u, dx2, dy2):
  for i in xrange(1,u.shape[0]-1):
    for j in xrange(1, u.shape[1]-1):
      u[i,j] = ((u[i+1, j] + u[i-1, j]) * dy2 +
                (u[i, j+1] + u[i, j-1]) * dx2) / (2*(dx2+dy2))
```

Numba benchmark



Cython version

- Similar to the Python and Numba versions

```
import numpy as np
cimport numpy as np
cimport cython

@cython.boundscheck(False)
@cython.wraparound(False)
def cy_update(np.ndarray[double, ndim=2] u,
              double dx2,
              double dy2):
  cdef int i, j
  for i in xrange(1,u.shape[0]-1):
    for j in xrange(1, u.shape[1]-1):
      u[i,j] = ((u[i+1, j] + u[i-1, j]) * dy2 +
                (u[i, j+1] + u[i, j-1]) * dx2) / (2*(dx2+dy2))
```

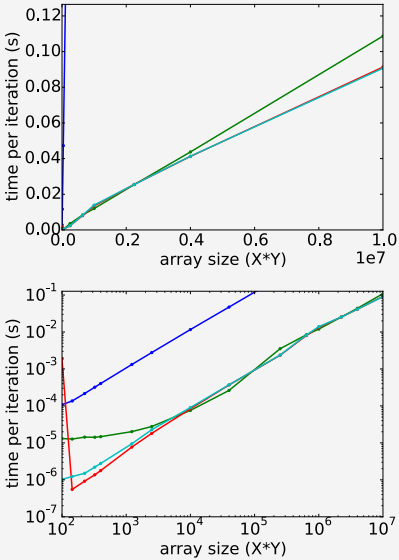
Cython version: setup.py

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

extensions = [Extension('cy_laplace', ['cy_laplace.pyx'])]

setup(name = 'Demos', ext_modules = cythonize(extensions))
```

Build module with a single command:

python setup.py build_ext --inplace

Cython benchmark



Get the benefits of C without leaving Python

Cython C wrapper

- Calls a C Laplace implementation. Similar to Ctypes or CFFI.

```
import numpy as np
cimport numpy as np

cdef extern from "claplace.h":
  void c_update(double *u, int x_len, int y_len,
                double dx2, double dy2)

def cy_update_c_wrap(np.ndarray[double, ndim=2] u, dx2, dy2):
  c_update(<double *> &u[0,0], u.shape[0], u.shape[1], dx2, dy2)
```

C implementation

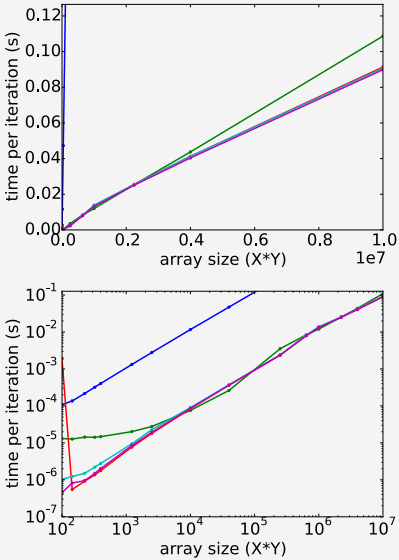
C code in a Python talk?!

```
void c_update(double *u,
              int nx,
              int ny,
              double dx2,
              double dy2) {
  int i, j, idx;
  for (i=1; i<ny-1; i++) {
    for (j=1; j<nx-1; j++) {
      idx = i*nx + j;
      u[idx] = ((u[idx+nx] + u[idx-nx]) * dy2 +
                (u[idx+1] + u[idx-1]) * dx2) / (2*(dx2+dy2));
        }
    }
}
```

Cython C wrapper: setup.py

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

extensions = [Extension('cy_wrap_claplace',
                        ['cy_wrap_claplace.pyx',
                         'claplace.c'],
                        #extra_compile_args=['-fopenmp'],
                        #extra_link_args=['-fopenmp']
                        )
              ]

setup(name = 'Demos', ext_modules = cythonize(extensions))
```

Cython C wrapper benchmark



Cython parallelism

Cython.parallel

- parallel directive: thread-local buffers
- prange: an OpenMP parallel version of xrange/range

openmp module

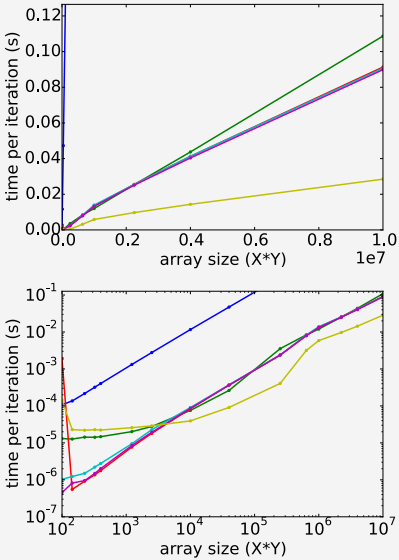
- low level C API wrappers, eg:

```
num_threads = openmp.omp_get_num_threads()
```

Cython parallel version

```
@cython.boundscheck(False)
@cython.wraparound(False)
def cy_update_parallel(np.ndarray[double, ndim=2] u,
                       double dx2,
                       double dy2):
  cdef int i, j
  for i in prange(1, u.shape[0]-1, nogil=True):
    for j in xrange(1, u.shape[1]-1):
      u[i,j] = ((u[i+1, j] + u[i-1, j]) * dy2 +
                u[i, j+1] + u[i, j-1]) * dx2) / (2*(dx2+dy2))
```

Cython parallel benchmark



Need more performance?

- Compiler flags (-O3, -ffast-math, ...)
- PyCuda/PyOpenCl
- NumbaPro
- OpenMP 4, OpenACC
- Distributed parallelism: mpi4py, ipython parallel, Spark, etc

Conclusions

- Cython make C extensions easy
- Excellent performance, especially in parallel
- Numba also impressive, but no prange

Arbitrary scores:

	Pure Python	NumPy	Cython	Cython parallel	Numba
Simplicity	***	****	**	**	***
Performance		***	****	*****	****
Distribution	*****	****	**	**	*

Thanks!

- http://cython.org
- http://numba.pydata.org
- https://github.com/crleblanc/cython_talk_2105

Questions?