Python in HPC
Numpy, MatPlotLib, SciPy

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• Introduction

• NumPy: Array Datastructures

• Matplotlib: Easy Visualization

• SciPy: Scientific toolkit
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• SciPy: Scientific toolkit
Instead of hello world, let’s see the MatPlotLib histogram.

From ipython --pylab or EPD on windows

In [1]: hist(randn(10000), 100)

or

From regular python

```python
>>> from numpy.random import * 
>>> from pylab import * 
>>> hist(randn(10000), 100) 
>>> show()
```
Help commands in IPython

In [2]: hist ?

In[3]: hist ??

In[4]: import pylab

In[5]: pylab ??

#Learn more about IPython
In[6]: %magic
### Help commands in Python

```python
>>> help(hist)

>>> import pylab

>>> help(pylab)
```
Timeline

- Began in 1989 at CWI as a successor of “ABC”
- Initially developed by Guido van Rossum, now Benevolent Dictator for Life
- Primarily thought of initially as a teaching language
- Early release cycle every 6 months or so, currently every 2 years
- Currently core is moving to 3.0, but most libraries only work on 2.7
Technical Specifications

• Python is a “multi-paradigm” language:
  – Imperative
  – Object Oriented
  – Dynamically Typed – Interpreted
  – Almost Functional

• This means that programmers can work in a variety of styles, freely intermixing constructs from different paradigms
Duck Typing

- If it looks like a duck, then it is a duck.
- Dynamically evaluates types
- Type (and name) errors not caught until runtime
  - Unit testing becomes more important
  - Good IDE can catch many standard errors
Speed

- Running Python code is usually 10X slower than C
- Writing Python code is usually much much much much faster than writing C
- Reading Python code is usually much much much much faster than reading C
- Write Python, profile, refine in C
- Several projects are working to speed up Python (PyPy, Cython, ...)

PyPy, Cython, ...
Gotchas

- No multithreading support
- Import problem

But who cares, let’s start hacking!
• Beautiful is better than ugly.
• Explicit is better than implicit.
• Simple is better than complex.
• Complex is better than complicated.
• Flat is better than nested.
• Sparse is better than dense.
• Readability counts.
• Special cases aren’t special enough to break the rules.
  – Although practicality beats purity.
• Errors should never pass silently.
  – Unless explicitly silenced.
• In the face of ambiguity, refuse the temptation to guess.
• There should be one— and preferably only one —obvious way to do it.
  – Although that way may not be obvious at first unless you’re Dutch.
• Now is better than never.
  – Although never is often better than right now.
• If the implementation is hard to explain, it’s a bad idea.
• If the implementation is easy to explain, it may be a good idea.
• NameSpaces are one honking great idea – let’s do more of those!
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How slow is Python? Let’s add one to a million numbers.

Using lists

In [15]: lst = range(1000000)

In [16]: %timeit [i + 1 for i in lst]
10 loops, best of 3: 65.6 ms per loop
Why is Python slow?

- Dynamic typing requires lots of metadata around variable.
- Python uses heavy frame objects during iteration

Solution:

- Make an object that has a single type and continuous storage.
- Implement common functionality into that object to iterate in C.
How slow is Python? Let’s add one to a million numbers.

**Using lists**

```python
In [15]: lst = range(1000000)

In [16]: %timeit [i + 1 for i in lst]
10 loops, best of 3: 65.6 ms per loop
```

**Using NumPy**

```python
In [18]: arr = arange(1000000)

In [19]: %timeit arr + 1
100 loops, best of 3: 2.91 ms per loop
```
History of NumPy

• Features
  – a powerful N-dimensional array object
  – sophisticated (broadcasting) functions
  – tools for integrating C/C++ and Fortran code
  – useful linear algebra, Fourier transform, and random number capabilities

• Development
  – Based originally on Numeric by Jim Hugunin
  – Also based on NumArray by Perry Greenfield
  – Written by Travis Oliphant to bring both feature sets together
What makes an array so much faster?

- **Data layout**
  - homogenous: every item takes up the same size block of memory
  - single data-type objects
  - powerful array scalar types

- **universal function (ufuncs)**
  - function that operates on ndarrays in an element-by-element fashion
  - vectorized wrapper for a function
  - built-in functions are implemented in compiled C code
Data layout

- homogenous: every item takes up the same size block of memory
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universal function (ufuncs)

- function that operates on ndarrays in an element-by-element fashion
- vectorized wrapper for a function
- built-in functions are implemented in compiled C code

```python
In [31]: %timeit [sin(i)**2 for i in arr]
1 loops, best of 3: 4.32 s per loop

In [32]: import numpy as np

In [33]: %timeit np.sin(arr)**2
10 loops, best of 3: 20.8 ms per loop
```
Creating array

In [5]: x = array([2, 3, 12]) # Create from list

# mix of tuple, lists, and types
In [6]: x = np.array([[1,2.0],[0,0],(1+1j,3.)])

In [7]: x = arange(-10, 10, 2, dtype=float)

In [8]: np.linspace(1., 4., 6)

In [9]: np.indices((3,3))

In [10]: fromfile('foo.dat')
NumPy: Array Datastructures

Array API

In [16]: x = arange(9).reshape(3,3)
In [19]: x[:, 0]
Out[19]: array([0, 3, 6])
In [20]: x.shape
Out[20]: (3, 3)
In [21]: x.strides
Out[21]: (24, 8)
In [22]: y = x[::2, ::2]
In [25]: y[0,0] = 100
In [26]: x[0, 0]
Out[26]: 100
Finite Differences

In [38]: x = np.arange(0, 20, 2)

In [40]: y = x**2

In [42]: dy_dx = ((y[1:] - y[:-1]) / (x[1:] - x[:-1]))

In [43]: dy_dx

Out[43]: array([ 2, 6, ..., 30, 34])

In [44]: dy_dx_c = ((y[2:] - y[:-2]) / (x[2:] - x[:-2]))

In [45]: dy_dx_c

Out[45]: array([ 4, 8, ..., 28, 32])
Computing a 3D grid of distances $R_{ijk} = \sqrt{i^2 + j^2 + k^2}$

With temporary matrices

In [44]: i, j, k = np.mgrid[-100:100, -100:100, -100:100]
In [45]: print(i.shape, j.shape, k.shape)
((200, 200, 200), (200, 200, 200), (200, 200, 200))

In [46]: R = np.sqrt(i**2 + j**2 + k**2)
In [47]: R.shape
Out[47]: (200, 200, 200)
Computing a 3D grid of distances $R_{ijk} = \sqrt{i^2 + j^2 + k^2}$
Computing a 3D grid of distances $R_{ijk} = \sqrt{i^2 + j^2 + k^2}$

With temporary matrices

```python
# Construct the row vector that runs from -100 to +100
In [47]: i = np.arange(-100, 100).reshape(200, 1, 1)

# Construct the column vector
In [48]: j = np.reshape(i, (1, 200, 1))

# Construct the depth vector
In [49]: k = np.reshape(i, (1, 1, 200))

In [50]: R = np.sqrt(i**2 + j**2 + k**2)
In [51]: R.shape
Out[49]: (200, 200, 200)
```
Computing a 3D grid of distances $R_{ijk} = \sqrt{i^2 + j^2 + k^2}$

With temporary matrices

```python
# Shorthand for i, j, k broadcasting
In [52]: i, j, k = ogrid[-100:100, -100:100, -100:100]

In [53]: R = np.sqrt(i**2 + j**2 + k**2)

In [53]: R.shape
Out[49]: (200, 200, 200)
```
Numpy has a sophisticated view of data.

<table>
<thead>
<tr>
<th>Type</th>
<th>Type</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>bool</td>
<td>int</td>
<td>int8</td>
</tr>
<tr>
<td>int16</td>
<td>int32</td>
<td>int64</td>
</tr>
<tr>
<td>uint8</td>
<td>uint16</td>
<td>uint32</td>
</tr>
<tr>
<td>uint64</td>
<td>float</td>
<td>float16</td>
</tr>
<tr>
<td>float32</td>
<td>float64</td>
<td>complex</td>
</tr>
<tr>
<td>complex64</td>
<td>complex128</td>
<td></td>
</tr>
</tbody>
</table>
Using NumPy types

In[55]: np.array([1, 2, 3], dtype='f')
array([ 1., 2., 3.], dtype=float32)

In[56]: z.astype(float)
array([ 0., 1., 2.])

In[57]: np.int8(z)
array([0, 1, 2], dtype=int8)

In[58]: d = np.dtype(int)
In[59]: d
dtype('int32')

In[60]: np.issubdtype(d, int)
True

In[61]: np.issubdtype(d, float)
False
Structured data

In[62]: x = np.zeros((2,), dtype=('<i4', '<f4', 'a10'))
In[63]: x[:,:] = [(1,2., 'Hello'),(2,3.,'World')]
In[64]: dt = dtype([('time', uint64),
    ...    ('pos', [
    ...    ('x', float),
    ...    ('y', float)])])
In[65]: x = np.array([100, (0, 0.5),
    ...    (200, (0, 10.3),
    ...    (300, (5.5, 15.1)],
    ...    dtype=dt)
In[66]: x['time']
In[67]: x[ x['time'] >= 200 ]
Linear Algebra

In [33]: dot(arange(10), arange(10))
Out[33]: 285

In [35]: dot(arange(9).reshape(3,3), arange(3))
Out[35]: array([[ 5, 14, 23]])

In [36]: dot(arange(9).reshape(3,3),
   ...: arange(9).reshape(3,3))
Out[36]:
array([[ 15, 18, 21],
       [ 42, 54, 66],
       [ 69, 90, 111]])
Other libraries

In [37]: fft ?

In [38]: linalg ?

In [39]: random ?
The array object has an order flag, see `array`.

1. Create a 100×100 random row and column 2D arrays.
2. Time the dot of two row arrays.
3. Time the dot of two column arrays.
4. Time the dot of the combination.

Using only slicing and indexing. Create a 2D laplacian operator. How do you handle the boundaries?
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matplotlib is a python 2D plotting library which:

- produces publication quality figures,
- interactive environments,
- generate plots, histograms, power spectra, bar charts, errorcharts, scatterplots, etc
- customize all look and feel
Matplotlib: Easy Visualization

Plotting

```
In [62]: plot([1,2,3])
In [63]: show()
```
In [69]: hold(False)

In [70]: plot([1,2,3], [.2, .3, .4], 'g+')

In [71]: plot([1,2,3], [.2, .3, .4], 'g+',
       ...: [2, 4, 6], [.2, .3, .4], 'bt')

In [72]: plot([1,2,3], [1,2,3], 'go-', label='line 1',
       ...: linewidth=2)

In [74]: hold(True)
In [75]: plot([1,2,3], [1,4,9], 'rs', label='line 2')
In [76]: axis([0, 4, 0, 10])
In [77]: legend()
In [78]: save_fig('my_file.png')
Matplotlib: Easy Visualization

Bar charts

Scores by group and gender

Scores

<table>
<thead>
<tr>
<th>Group</th>
<th>Men</th>
<th>Women</th>
</tr>
</thead>
<tbody>
<tr>
<td>G1</td>
<td>20</td>
<td>25</td>
</tr>
<tr>
<td>G2</td>
<td>35</td>
<td>32</td>
</tr>
<tr>
<td>G3</td>
<td>30</td>
<td>34</td>
</tr>
<tr>
<td>G4</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>G5</td>
<td>27</td>
<td>25</td>
</tr>
</tbody>
</table>
N = 5
menMeans = (20, 35, 30, 35, 27)
menStd = (2, 3, 4, 1, 2)

ind = np.arange(N)  # the x locations for the groups
width = 0.35        # the width of the bars

rects1 = bar(ind, menMeans, width,
             color='r',
             yerr=menStd,
             error_kw=dict(elinewidth=6, ecolor='pink'))
womenMeans = (25, 32, 34, 20, 25)
womenStd = (3, 5, 2, 3, 3)
rects2 = plt.bar(ind+width, womenMeans, width,
                color='y',
                yerr=womenStd,
                error_kw=dict(elinewidth=6, ecolor='yellow'))
# add some

```python
plt.ylabel('Scores')
plt.title('Scores by group and gender')
plt.xticks(ind+width, ('G1', 'G2', 'G3', 'G4', 'G5'))
plt.legend( (rects1[0], rects2[0]), ('Men', 'Women') )
```
Matplotlib: Easy Visualization

Bar charts

# add some
plt.ylabel('Scores')
plt.title('Scores by group and gender')
plt.xticks(ind+width, ('G1', 'G2', 'G3', 'G4', 'G5'))
plt.legend((rects1[0], rects2[0]), ('Men', 'Women'))
def autolabel(rects):
    # attach some text labels
    for rect in rects:
        height = rect.get_height()
        plt.text(rect.get_x()+rect.get_width()/2.,
                 1.05*height, '%d'%int(height),
                 ha='center', va='bottom')

autolabel(rects1)
autolabel(rects2)

plt.show()
• Using the plot command make a scatter plot (hint just use 'bo' as the format).
• Use the semilogx, semilogy, and loglog plots.
• See http://matplotlib.sourceforge.net/gallery.html and make a plot that you think is interesting.
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SciPy

- mathematical algorithms and convenience functions built on the Numpy,
- organized into subpackages covering different scientific computing domains,
- a data-processing and system-prototyping environment rivaling systems such as MATLAB, IDL, Octave, R-Lab, and SciLab
• Special functions (scipy.special)
• Integration (scipy.integrate)
• Optimization (scipy.optimize)
• Interpolation (scipy.interpolate)
• Fourier Transforms (scipy.fftpack)
• Signal Processing (scipy.signal)
• Linear Algebra (scipy.linalg)
• Sparse Eigenvalue Problems with ARPACK
• Statistics (scipy.stats)
• Multi-dimensional image processing (scipy.ndimage)
• File IO (scipy.io)
• Weave (scipy.weave)
Bessel functions

\[ x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + (x^2 - \alpha^2)y = 0 \]  (1)
```python
>>> from scipy import *
>>> from scipy.special import jn, jn_zeros
>>> def drumhead_height(n, k, distance, angle, t):
...     nth_zero = jn_zeros(n, k)
...     return cos(t)*cos(n*angle)*\n...             jn(n, distance*nth_zero)

>>> theta = r_[0:2*pi:50j]
>>> radius = r_[0:1:50j]
>>> x = array([r*cos(theta) for r in radius])
>>> y = array([r*sin(theta) for r in radius])
>>> z = array([drumhead_height(1, 1, r, theta, 0.5) \n...             for r in radius])
```
```python
>>> import pylab
>>> from mpl_toolkits.mplot3d import Axes3D
>>> from matplotlib import cm
>>> fig = pylab.figure()
>>> ax = Axes3D(fig)
>>> ax.plot_surface(x, y, z, 
... rstride=1, cstride=1, cmap=cm.jet)
>>> ax.set_xlabel('X')
>>> ax.set_ylabel('Y')
>>> ax.set_zlabel('Z')
>>> pylab.show()
```
Using quad

```python
>>> from scipy.integrate import quad
>>> def integrand(t,n,x):
...     return exp(-x*t) / t**n

>>> def expint(n,x):
...     return quad(integrand, 1, Inf, args=(n, x))[0]

>>> vec_expint = vectorize(expint)

>>> vec_expint(3,arange(1.0,4.0,0.5))
array([ 0.1097, 0.0567, 0.0301, 0.0163, 0.0089, 0.0049])

>>> special.expn(3,arange(1.0,4.0,0.5))
array([ 0.1097, 0.0567, 0.0301, 0.0163, 0.0089, 0.0049])
```
Using `quad`

```python
>>> result = quad(lambda x: expint(3, x), 0, inf)
>>> print result
(0.33333333324560266, 2.8548934485373678e-09)
```

```python
>>> I3 = 1.0/3.0
>>> print I3
0.333333333333
```

```python
>>> print I3 - result[0]
8.77306560731e-11
```
Using `dblquad`

```python
>>> from scipy.integrate import quad, dblquad
>>> def I(n):
...     return dblquad(lambda t, x: exp(-x*t)/t**n,
...                    0, Inf,
...                    lambda x: 1, lambda x: Inf)

>>> print I(4)
(0.25000000000435768, 1.0518245707751597e-09)

>>> print I(3)
(0.33333333325010883, 2.8604069919261191e-09)

>>> print I(2)
(0.49999999999857514, 1.8855523253868967e-09)
```