Numerical Programming in Python

Part III: Using Python for Numerics

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February 2006
Post-Processing (1)

Often need to munge output to stay sane
May need arithmetic on values in it
Python is ideal tool for this purpose

Problem occurs when output may be corrupted
Common if running multiple processes
Schedulers, NFS etc. can interleave weirdly
Or overflow causing Fortran’s ‘*********’
Post-Processing (2)

Real code from HPCF benchmarking
Replaced twice the length of *awk* script
And became a *lot* more robust, too!

(cd Examples; python streams.py)
(cd Examples; python linpack.py)
(cd Examples; cat linpack.py)
Post-Processing (3)

from re import compile
fpnum = r'\d+ \. \d+E[+-] \d \d'
fpnum_1 = fpnum + r' +'
str = r'\^ *' + fpnum_1 + fpnum_1 + \
    fpnum_1 + r'(' + fpnum + r') +' + \
    fpnum_1 + fpnum + r' * \n$

print str
pattern = compile(str)

Matches just the lines we want to use
Then use Python’s numerics to summarise
Python Output

^ \*d+\.d+E[+-]d\d +
  \d+\.d+E[+-]d\d +
  \d+\.d+E[+-]d\d +
  (\d+\.d+E[+-]d\d) +
  \d+\.d+E[+-]d\d +
  \d+\.d+E[+-]d\d *\n$
Pre-Processing (1)

Data in one format, needed in another
Can also use for data input utility
Easy to do fairly thorough checking
Could prompt for corrections, etc.

Example is using **Maple** output in **Matlab**
(cd Examples; python maple.py)
(cd Examples; cat maple.py)
(cd Examples; cat maple.out)
(cd Examples; more maple_1.py)
Pre-Processing (2)

Can both munge data and run program
(cd Examples; python matlab.py)
(cd Examples; cat matlab.py)

Or both programs (Maple is not on PWF)
(cd Examples; cat matlab_1.py)

Becomes a complete application harness
from os import popen
from sys import stdout
from maple_1 import grind

strm_1 = popen("ssh nmm1@cus.cam.ac.uk \
    maple < maple.in", "r")
strm_2 = popen("matlab -nodisplay -nojvm", "w")
grind(strm_1, strm_2)
x = strm_1.close()
if x != None : print x
x = strm_2.close()
if x != None : print x
Application Harnesses

Used on HPCF for submission script etc. Can write high-quality commands easily. Start/stop/control subprocess commands including on different systems (see above!)
If not PWF, could use SSH keys Then don’t need to provide password

Won’t go into any more detail here But strongly recommend Python for harnesses
Numpy/Scipy

Intended for efficient work in Python
Generally does what it intends
Consider as alternative to Matlab

Very limited experience here with it
So check that it does what you need

Will give VERY simple examples
And then will describe how to use it
Starting Off

Examples assume the following:

```python
from numpy import *
```

You can also use one or more of:

```python
from numpy.linalg import *
from numpy.fft import *
from numpy.random import *
```

And others . . .
Arrays

Arrays are the basic numpy data type
Matrices are specialised 2-D arrays

Come in int, float, complex forms
New arrays usually get correct type
Updating element does NOT change type

Simple use is just as you would expect
If shapes match or one argument a scalar
Simple Arrays (1)

```python
a = array([[1,2],[3,4]])
b = array([5,6])
print a
print b

print dot(a,b)
print a[0,1]*100
a[0,1] = 5
print a
```
Python Output

[[1 2]
 [3 4]]
[5 6]
[17 39]
200
[[1 5]
 [3 4]]
Simple Arrays (2)

```python
a = array([[1,2],[3,4]])
print a*a
print dot(a,a)
print a/a

b = matrix([[1,2],[3,4]])
print b*b

C = array([[[1,2],[3,4]],[[5,6],[7,8]]])
print C
```

### Python Output

```python
[[ 1 4]
 [ 9 16]]
[[ 7 10]
 [15 22]]
[[ 1 1]
 [ 1 1]]
[[ 7 10]
 [15 22]]
[[[1 2]
 [ 3 4]]
[[[5 6]
 [7 8]]]]
```
Array Types

```python
a = array([[1,2],[3.0,4]])
b = array([[5,7],[9,1]])
print a.dtype
print b.dtype

print a+b
c = array([[5,7],[9,1]],dtype=float)
print c.dtype

b[0,1] = 6.78
print b
```
Python Output

<table>
<thead>
<tr>
<th>float64</th>
<th>int64</th>
</tr>
</thead>
<tbody>
<tr>
<td>[[ 6.  9.]]</td>
<td></td>
</tr>
<tr>
<td>[ 12.  5.]]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>float64</th>
</tr>
</thead>
<tbody>
<tr>
<td>[[5 6]</td>
</tr>
<tr>
<td>[9 1]]</td>
</tr>
</tbody>
</table>
Manipulating Arrays

Various construction methods (see doc.)
Creating a zero–filled matrix is simplest

Can reshape arrays, much as in Fortran 90
Can slice arrays, just as in rest of Python
Can use stride (step), as in Fortran 90

- Both ALIAS the (sub)array, not copy it
Creation and Reshaping

```python
da = zeros((3,2,4),dtype=complex)
pint a
b = identity(5,float)
pint b

c = array([[1,2],[3,4],[5,6],[7,8]],float)
pint c
d = reshape(c,(4,2))
pint d
```
Python Output

[[ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]]

[[ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]]

[[ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  0.+0.j  0.+0.j]]
Python Output

```
[[ 1.  0.  0.  0.  0.]
 [ 0.  1.  0.  0.  0.]
 [ 0.  0.  1.  0.  0.]
 [ 0.  0.  0.  1.  0.]
 [ 0.  0.  0.  0.  1.]]
```
Python Output

[[[ 1.  2.]
  [ 3.  4.]]

[[ 5.  6.]
 [ 7.  8.]]

[[ 1.  2.]
 [ 3.  4.]
 [ 5.  6.]
 [ 7.  8.]]
Slicing

c = array([[1,2,3,4],[5,6,7,8],[9,0,1,2]])
print c
d = c[1:3,1:4]
print d

e = c[:,1:4:2]
print e

d[1,1] = 123
print c
Python Output

```
[[1 2 3 4]
 [5 6 7 8]
[9 0 1 2]]
[[6 7 8]
 [0 1 2]]
[[2 4]
 [6 8]
[0 2]]
[[ 1 2 3 4]
 [ 5 6 7 8]
 [ 9 0 123 2]]
```
Universal Functions

Ufuncs apply to each element separately
Equivalent to Fortran 90 elemental functions
Include most of the basic numeric operators
Plus the basic functions from cmath
All can also operate on mixed scalars and arrays

```python
a = array([[1,2],[3,4],[5,6],[7,8]],float)
print power(1.23,a)
print power(a,a)
print a > 5.23
```
Python Output

[[[ 1.23    1.5129 ]
  [ 1.860867  2.28886641]]
[[ 2.81530568  3.46282599]
  [ 4.25927597  5.23890944]]
[[ 1.00000000e+00  4.00000000e+00]
  [ 2.70000000e+01  2.56000000e+02]]
[[ 3.12500000e+03  4.66560000e+04]
  [ 8.23543000e+05  1.67772160e+07]]
Python Output

```
[[[False False]
  [False False]]
[[False True]
  [True True]]
```
Array Functions Proper

Large number, mainly for manipulation
Array shapes must match, as appropriate
Already mentioned reshape and dot

```python
a = array([[1,2],[3,4]])
print transpose(a)
print sort(a)
print trace(a)
```

- Some alias and some copy — watch out!
Python Output

[[1 3]
 [2 4]]
[[1 2]
 [3 4]]
5
Bare minimum features from LAPACK

from numpy.linalg import *

a = array([[1,2,3],[4,6,8],[9,6,1]])
b = array([10,11,12])
print det(a)
print inv(a)
print solve(a,b)
print eig(a)
Python Output

4.0
[[-10.5  4.  -0.5]]
[[ 17.  -6.5  1. ]]
[[ -7.5  3.  -0.5]]
[[-67.  110.5  -48. ]]
(array([ 13.28983218, -0.05752375, -5.23230844]),
 array([[ -0.26604504, -0.48835717, -0.2366787 ],
        [ -0.77502303,  0.79568926, -0.50631919],
        [ -0.57320096, -0.35830974,  0.82923101]]))
Fast Fourier Transforms

Bare minimum from FFTPACK

from numpy.fft import *

a = array([1, 2, 4, 7, 0, 3, 5, 8, 6, 9])
b = fft(a)
print b
print ifft(b)
### Python Output

```
[ 45.00000000e+00j 1.30901699 +9.90659258e+00j
  -11.28115295 +2.48989828e+00j 0.19098301 +9.64932244e+00j
  -1.21884705 +2.24513988e-01j -13.00000000e+00j
   -9.64932244e+00j
  -11.28115295 +2.48989828e+00j 1.30901699 +9.90659258e+00j
   -1.21884705 -2.24513988e-01j 0.19098301 +9.64932244e+00j
   -9.64932244e+00j
  -1.00000000e+00 -8.88178420e-17j 2.00000000e+00 +1.36026581e-15j
   -3.64153152e-15j
   4.00000000e+00 +1.36026581e-15j
   7.00000000e+00 +1.44435090e-15j
   1.06581410e-15 +5.13552392e-15j 3.00000000e+00 +1.82590004e-16j
   -1.89109605e-15j
   5.00000000e+00 +1.01999232e-15j
   8.00000000e+00 +1.82590004e-16j
```

Random Numbers

Some facilities from `ranlib`

```python
from numpy.random import *
c = array([[1, 2, 3], [4, 5, 6], [7, 8, 9]])
d = 2*c + 1
print uniform(c, d)
print normal(d, c)
```
Python Output

[[ 2.88170183  3.690092  6.39022939]
 [ 4.40842594  8.04713813 11.67611954]
 [ 9.67607436 12.55491236 11.83973885]]
[[ 4.28898176  5.57995933  6.64778541]
 [ 9.01649799 15.84265958 14.7575158 ]
 [ 17.85013703 29.66551119  3.99543002]]
f2py

f2py is a numpy command to call Fortran
Looks useful for pure Fortran90 interfaces
Unreliable and tricky for Fortran90 ones

I haven’t been able to make it work
It claims to support NAG f95, but doesn’t
Even more environment–dependent than numpy

It may be worth trying with different compilers
Please tell me if you have any success
Installation

Packages available for some systems
Installed on PWF, as you found
Also available for Microsoft Windows

Seems to compile fairly easily under Linux
• Version 0.9.6 for Python 2.4 and 1.0.1 for 2.5
Library details built into setup mechanism
• Supports only specific libraries, not ACML

Porting the build mechanism could be hard
Documentation (1)

Code is open source, documentation isn’t $40 (electronic) from http://www.tramy.us/

Numpy is close to Numeric, but with changes http://numpy.scipy.org//numpydoc/numdoc.htm

There is an online course for NumPy/SciPy: http://www.rexx.com/~dkuhlman/.../scipy_course_01.html
Can use \texttt{dir} in Python to see what’s there
\begin{verbatim}
import numpy
import numpy.linalg
print dir(numpy.linalg)
\end{verbatim}

Not always easy to work out specification
\begin{verbatim}
x = numpy.matrix([[2,0],[0,-3]])
numpy.invert(x)
numpy.linalg.inv(x)
\end{verbatim}

Extending \texttt{numpy} is for experts only
Python Output

['LinAlgError', ..., 'det', ..., 'test']

[[-3, -1]
 [-1, 2]]

[[0.5, 0.]
 [0., -0.33333333]]
Exception Handling

Simple tests indicate that it is fairly robust
Against crashing – NOT other errors
Not even Python’s standard numeric handling

```python
b = array([123456789])
print b*b*b
print b/0

c = array([1.0e200])
print c*c
```
Python Output

Warning: divide by zero encountered in divide
Warning: overflow encountered in multiply
[-2204193661661244627]
[0]
[ inf]
Many errors are diagnosed:
```
a = array([[1,2,3],[4,5,6]])
print dot(a,a)
```

Many more just do weird things:
```
print trace(a)
b = array([[1,2],[3,4],[5,6],[7,8]])
print transpose(b)
```
Traceback (most recent call last):
  File "Demos/demo_44a.py", line 3, in <module>
    print dot(a,a)
ValueError: objects are not aligned

6
[[[1 5]
  [3 7]]

[[2 6]
 [4 8]]]
What Can We Do?

Remember about complex exceptions? Exactly the same applies here!

- Put in plenty of sanity checks
  NEVER rely on automatic diagnostics

This applies WHATEVER language you use!
Similar problems apply to all of them
Some libraries (e.g. NAG) better than others