

Python and Scientific Computing

A very quick overview

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- **Interactive, high-level tools are *very* popular in science**
 - Matlab
 - IDL
 - Mathematica
 - Maple
- **'Stack'**
 - **Numpy**: fast arrays.
 - **Scipy**: algorithms for many fields.
 - **IPython**: full-time interactive use.
 - **Matplotlib**: 2d plotting (basic 3d).
 - **Mayavi**: 3d visualization.
 - **Sympy**: symbolic manipulations.
 - **Cython**: incremental optimization ('pyrex+')
 - ... lots more I won't have time to mention.

Numpy: numerical array core

- Fast, flexible and very sophisticated array object.
- Random number generation
- Basic linear algebra (no Fortran dependency)
- FFT
- f2py: support to wrap Fortran codes (Scipy needs this)
- Basic stats:

Totals grouped by language (dominant language first):

ansic: 82493 (55.19%)

python: 65694 (43.95%)

c++: 828 (0.55%)

fortran: 298 (0.20%)

f90: 97 (0.06%)

sh: 61 (0.04%)

Total Physical Source Lines of Code (SLOC) = 149,471

Development Effort Estimate, Person-Years = 38.40

Scipy: lots of libraries

- Fortran, C, C++, Cython, SWIG, Python...
- Linear algebra (full LAPACK), statistics, differential equations, optimization, numerical integration, clustering, special functions, signal processing, n-dimensional image processing, much more...
- **SciKits**: toolkits for audio, image processing, statistical modeling, time-series analysis, ...
- **Basic stats (for scipy library only):**

Totals grouped by language (dominant language first):

cpp: 217083 (49.70%)

fortran: 81717 (18.71%)

python: 77720 (17.79%)

ansic: 60225 (13.79%)

sh: 61 (0.01%)

Total Physical Source Lines of Code = 436,806

Development Effort Estimate, Person-Years = 118.39

IPython: Matlab/IDL-like interactive use

The image shows a Mac OS X desktop environment. On the left, a Terminal window titled "Terminal — Python — 71x29" displays the following IPython session:

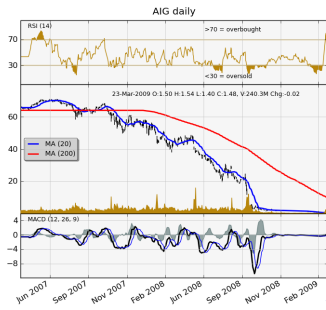
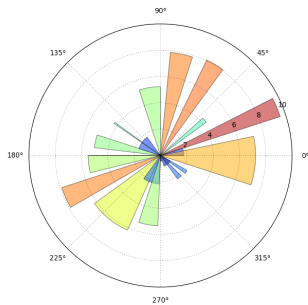
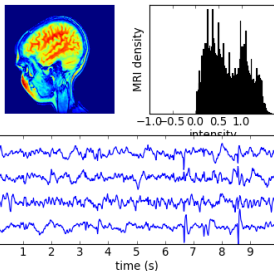
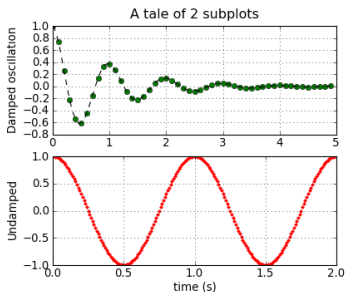
```
bgranger@pinch> ipython -wthread
Python 2.4.3 (#1, Apr 7 2006, 10:54:33)
Type "copyright", "credits" or "license" for more information.

IPython 0.7.3.svn -- An enhanced Interactive Python.
?      -> Introduction to IPython's features.
%magic -> Information about IPython's "magic" % functions.
help   -> Python's own help system.
object? -> Details about 'object'. ?object also works, ?? prints more.

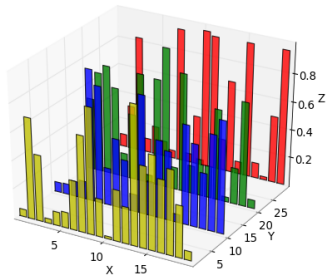
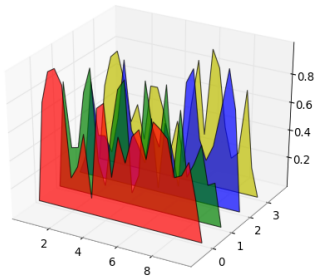
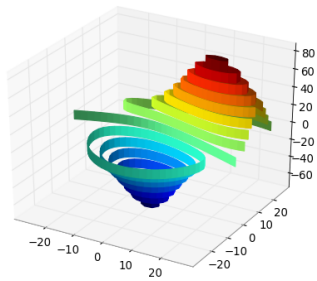
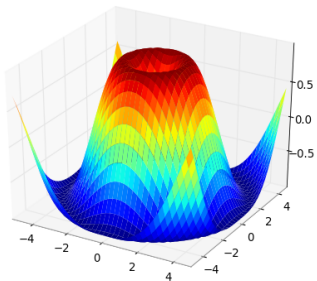
In [1]: from enthought.tvtk.tools import mlab
In [2]: from scipy import *
In [3]: def f(x, y):
...:     return sin(x+y) + sin(2*x-y) + cos(3*x+4*y)
...:
In [4]: x = linspace(-5.0, 5.0, 200)
In [5]: y = linspace(-5.0, 5.0, 200)
In [6]: fig = mlab.figure()
In [7]: surf = mlab.SurfRegularC(x, y, f)
In [8]: fig.add(surf)
In [9]:
```

On the right, a window titled "Interactive TVTK" displays a 3D surface plot. The plot shows a complex, wavy surface with a color gradient from blue (low values) to yellow (high values). The axes are labeled X, Y, and Z. The X and Y axes range from -5 to 5, and the Z axis ranges from -3 to 5. The plot is rendered in a perspective view within a 3D coordinate system.

Matplotlib: 2d plotting



Matplotlib: 3d plotting



Mayavi: 3d visualization (VTK)

The screenshot displays the Mayavi application window with the following components:

- Menu Bar:** File, Visualize, View, Tools, Help
- Scene List:** TVTK Scene 3 (expanded to show ArraySource, Colors and legends, ImagePlaneWidget, and ScalerCutPlane), TVTK Scene 4
- Mayavi object editor:**
 - Enabled:
 - Interaction:
 - Activation:
 - Volume:
 - Interpolate:
 - Visibility:
 - Use cursor:
 - Setup table:
 - X-axis: 3
 - Linear:
 - Endle size: 0.001 to 0.5
 - Ion value: 1
 - Ion action: 0 to 2
 - Ion modifier: 0 to 2
 - Origin: F0: 41.804807, F1: -0.5, F2: -0.5
 - Scale factor: 0.010 to 11.000
 - Point1: F0: 41.804807, F1: 255.5, F2: -0.5
 - Point2: F0: 41.804807, F1: -0.5, F2: 239.5
 - Priority: 0.0 to 1.0
 - Ion action: 0 to 2
 - Ion modifier: 0 to 2
 - Ion index: 42
 - Position: 41.804807008
- 3D View Window:** TVTK Scene 3, TVTK Scene 4. Shows a sagittal MRI slice of a brain with a red wireframe overlay.
- Python Console:**

```
ipython | Logger
In [6]: run brain.py
In [7]: rescale(ima,maxx255)
In [8]: imb = ima.astype(np.uint8)
In [9]: view_numpy(imb)
```

MayaVi: customizable application (CFD)

The screenshot displays the MayaVi2 application window. The top menu bar includes File, Visualize, Tools, View, and Help. The main interface is divided into several panels:

- Data Reader / Data Manager / Animation Manager:** Contains controls for frame selection (First frame: 0, Last frame: 1, Stride between frames: 1), image resolution (320x240), image format (.png), image output path (/home/psch), and image file prefix (animation_). A Render button is located at the bottom of this panel.
- TVTK Scene 1:** Displays a 3D visualization of a scalar field. The field is represented as a rectangular volume with a color gradient from blue (low values) to red (high values). The Z-axis is labeled with 0.00 and 64.0. A color bar at the bottom indicates values from 13.3 to 186. The word "scalar" is visible in the visualization area.
- MayaVi / MayaVi object editor:** Shows a tree view of the scene hierarchy, including TVTK Scene 1, ArraySource, and Modules (Outline, Axes, ImagePlaneWidget).
- Python:** A console window showing the following code and output:

```
>>> x_  
>>> dragged  
<enthought.mayavi.sources.array_source.ArraySource object at 0xb10f059c>  
>>> x_  
>>> x.scalar_data[0:5,0:5,0]  
array([[132, 132, 132, 132, 132],  
       [132, 132, 132, 132, 132],  
       [131, 132, 132, 132, 132],  
       [131, 131, 131, 132, 132],  
       [129, 130, 131, 131, 133]], dtype=uint8)  
>>>
```

The bottom taskbar shows several open applications: Shell No. 9 - Konsole, Gmail - Inbox (446) ..., Inbox for Peter.Sch..., Foo Fighters - Stair..., and MayaVi2.

Andrew Straw (Caltech)

**Virtual reality based real-time control of
fly flight**

`http://www.archive.org/details/scipy09_day1_05-Andrew_Straw`

Perry Greenfield & Michael Droetboom
**Hubble Space Telescope Science
Institute**

Enthought

Prabhu Ramachandran (IIT Bombay)

FOSSE India

Workshops and conferences

- Scipy Conference: 2001-today.
 - **SciPy 2010: Austin, TX. June27-July 4.**
- EuroScipy: since 2008.
 - **EuroScipy 2010: Paris, July 7-10.**
- **Scipy India: December 12-19 2009!**
- SIAM all-day workshops (2008, 2009)
- Sage days: 20 workshops and counting...
- **Supercomputing'09: Python sessions.**

Education

- Fossee India
- SECANT: Science Education in Computational Thinking (NSF funded)
- Sage workshops: lots of students.
- MIT 6.0X series: now in Python.

Computing in Science and Engineering (IEEE/AIP)

- Special issue in 2007: one of the most popular ever
- Special issue in 2011.

US Federal Labs

- LBL, LLNL, Los Alamos, Sandia, Oak Ridge, ...
- NASA (JPL, Hubble, ...)
- NIST
- NCAR
- NOAA

Industry

- Enthought (Austin, TX). Numpy, Scipy, Mayavi, scipy conference.
- The Python Academy: Germany, Euroscipy
- Visual Numerics: PyIMSL Studio
(IMSL+Python+ipython/numpy/scipy/matplotlib)