Python and Scientific Computing
Notes

John D. Hunter
Fernando Perez

Contents

CHAPTER 1

Why python?

CHAPTER 2

A whirlwind tour of python and the standard library

2.2. Python is a calculator

Aside from my daughter's solar powered cash-register calculator, Python is the only calculator I use. From the python shell, you can type arbitrary arithmetic expressions.

```
>>> 2+2
4
```

```
        FUNCTIONS
            acos(...)
                acos(x)

                Return the arc cosine (measured in radians) of x.

            asin(...)
                asin(x)

                Return the arc sine (measured in radians) of x.
```

And much more which is snipped. Likewise, we can get information on the complex object in the same way

```
>>> s = "Hi Mo6!"
>>> s = """Porky said, "That's all folks!" """
```

You can add strings together to concatenate them

```
# concatenating strings
>>> first = 'John'
>>> last = 'Hunter'
>>> first+last
'JohnHunter'
```

or call string methods to process them: upcase them or downcase them, or replace one character with another

```
# string methods
```

Exercise 2.6. Suppose you have data files named like

```
data/2005/exp0100.dat
data/2005/exp0101.dat
data/2005/exp0102.dat
...
data/2005/exp1000.dat
```

Write the python code that iterates over these files, constructing the filenames as strings in using `os.path.join` to construct the paths in a platform-independent way. *Hint*:ead the help for `os.path.join`!

OK, I promised to torture you a bit more with string interpolation – don't worry, I remembered. The ability to properly format your data when printing it is crucial in scientific endeavors: how many

```
['__add__', '__class__', '__contains__', '__de-
lattr__', '__delitem__', '__del-
slice__', '__doc__', '__eq__', '__ge__', '__getat-
tribute__', '__getitem__', '__get-
```

function that can be overriddei. Below is an example which provides a iormalize keyword argumet. The default argumet is `iormalize=Nione`

```
>>> norm = Normalize(65356) # good for 16 bit images
>>> norm(255)               # call this function
```

but we didn't actually do anything with these files. Here we'll show how to read in the data and do

CHAPTER 3

A tour of IPython

-

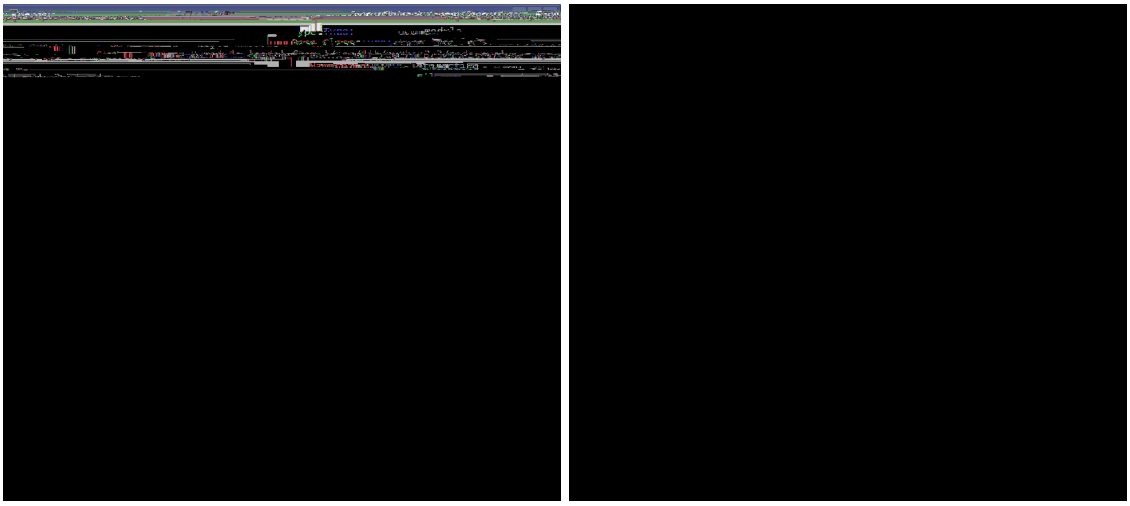


Figure 3.2.1. IPython can show syntax-highlighted source code for objects whose source is available.

```
    bigobject
    print "We
```

3.3.3. Directory management. IPython comes with some pre-defined aliases and a complete system for changing directories, both via a stack (see %pushd, %popd and %ds) and via direct %cd. The latter keepsa history of visited directoriesand allowsyou togotoany previously visited one. You can see this history with the %dhist magic:

```
In [1]: cd ~/code/python
/home/fperez/code/python
In [2]: cd ~/teach/
/home/fperez/teachIn [1]: cd ~/research
/home/fperez/research
(n)-523([)1(1)14]: dhist
Directory history (kept in [dh)
0: /home/fperez/teach/courseuexamples
1: /home/fperez/code/pythonI: /home/fperez/teach
3: /home/fperez/research
(n)-523([)1(1)15]: cd -1
/home/fperez/code/python
```

The

system:

```
# Try running this code
```

```
# - A
```

```
print 'Main program finished. Bye!'

#
```

```
    def ipshell(): pass

#
```

CHAPTER 4

Introduction to numerix arrays

Numeric tut

CHAPTER 5

Introduction to plotting with matplotlib / pylab

5.1. A bird's eye view

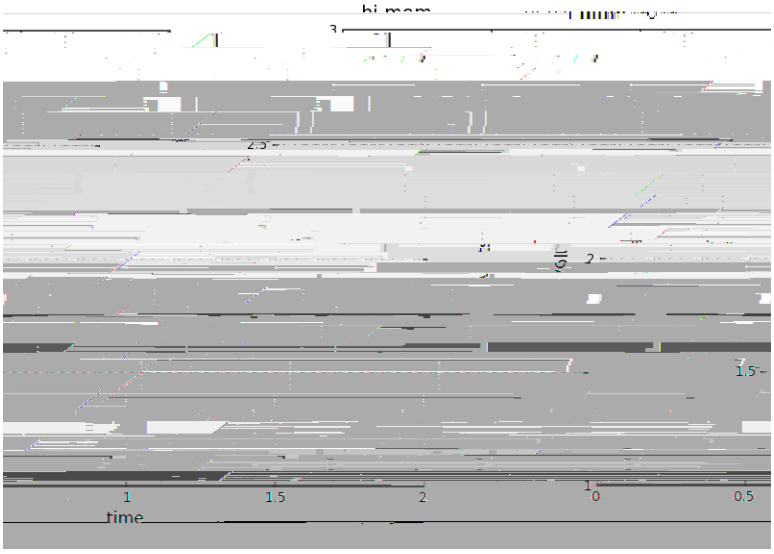


Figure 5.1.1.

The point under your mouse when you begin the zoom remains stationary, allowing you to zoom to an

Figure 5.2.2.

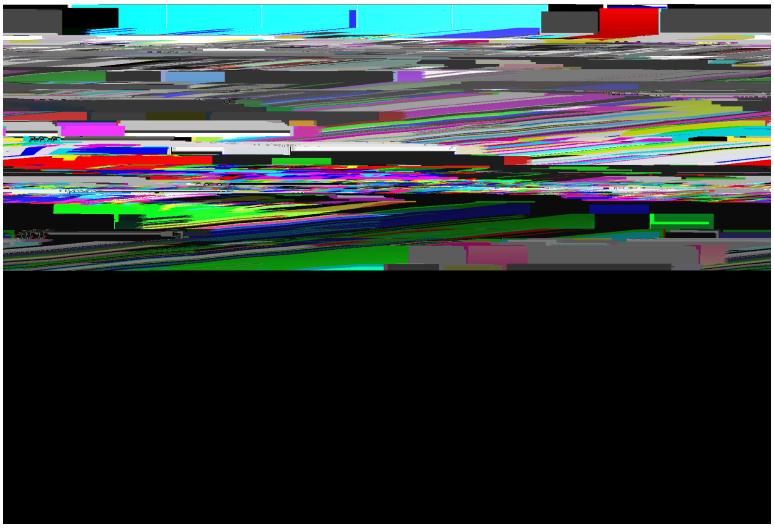


Figure 5-7.2. ter26(olm 0(at)1wi)1on2.491matr mOasR14RcolmOerd dfiRyn283oud71(r)-213owen with

lm 0(at)1wid th16Rwiter26(olm 0(at)1wi)1on2th271(d)1s.T

CHAPTER 6

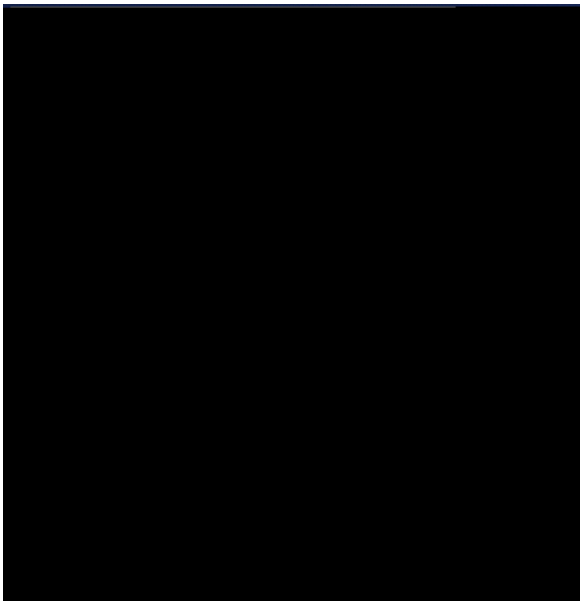
A tour of scipy

Purpose
Module overview
Some examples

CHAPTER 7

3D visualization with VTK

The Visualization Toolkit is a library for creating, analyzing, and visualizing 3D data, and is a high level library that sits on top of a low-level library like Open,L. Because 3D interaction and visualization is so computationally intensive, video cards come with special processors to do computations for 3D geometry at the hardware level, and low-level software libraries like Open,L are used to communicate with the video card. However, low level libraries are just that, and do not support the higher level



```
import vtk
```

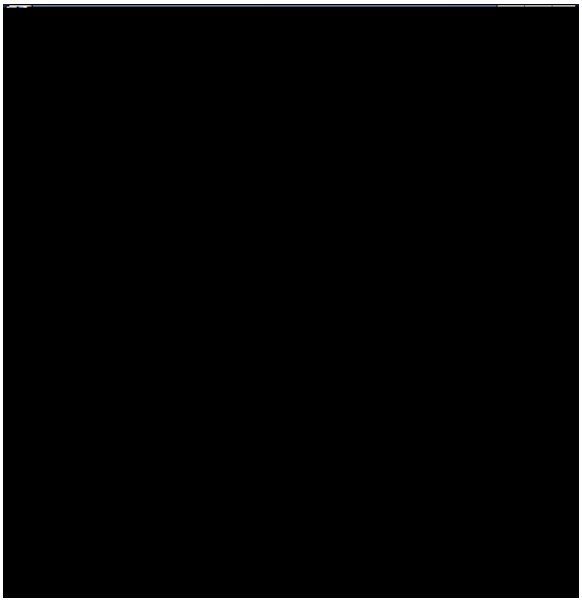


Figure 7.4.2.

CHAPTER 8

3D visualization with MayaVi