Numerical Python

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Intro to Python programming

Make sure you have the software

- You will need Python version 2.5
- Numerical Python (`numpy`)
- Gnuplot, gcc, g++, g77
- Tcl/Tk (for GUI programming)
- Some Python modules are needed: IPython, epydoc, Pmw, ...

Material associated with these slides

- These slides have a companion book:
  Scripting in Computational Science, 3rd edition,
  Texts in Computational Science and Engineering,
  Springer, 2008
- All examples can be downloaded as a tarfile

  ```
  http://folk.uio.no/hpl/scripting/TCSE3-3rd-examples.tar.gz
  ```
- Software associated with the book and slides: SciTools

  ```
  http://code.google.com/p/scitools/
  ```

Installing TCSE3-3rd-examples.tar.gz

- Pack `TCSE3-3rd-examples.tar.gz` out in a directory and let `scripting` be an environment variable pointing to the top directory:

  ```
  tar xvzf TCSE3-3rd-examples.tar.gz
  export scripting=‘pwd‘
  ```

  All paths in these slides are given relative to `scripting`, e.g., `src/py/intro/hw.py` is reached as

  ```
  $scripting/src/py/intro/hw.py
  ```

Scientific Hello World script

- All computer languages intros start with a program that prints "Hello, World!" to the screen
- Scientific computing extension: read a number, compute its sine value, and print out
- The script, called hw.py, should be run like this:

  ```
  python hw.py 3.4
  ```

  or just (Unix)

  ```
  ./hw.py 3.4
  ```
- Output:

  ```
  Hello, World! sin(3.4)=-0.255541102027
  ```

Purpose of this script

Demonstrate

- how to read a command-line argument
- how to call a math (sine) function
- how to work with variables
- how to print text and numbers

The code

- File hw.py:

  ```
  #!/usr/bin/env python

  # load system and math module:
  import sys, math

  # extract the 1st command-line argument:
  r = float(sys.argv[1])

  s = math.sin(r)

  print "Hello, World! sin(" + str(r) + ")=" + str(s)
  ```
- Make the file executable (on Unix):

  ```
  chmod a+rx hw.py
  ```

Comments

- The first line specifies the interpreter of the script
  (here the first python program in your path)

```
python hw.py 1.4   # first line is not treated as comment
./hw.py 1.4        # first line is used to specify an interpreter
```

- Even simple scripts must load modules:

```
import sys, math
```

- Numbers and strings are two different types:

```
r = sys.argv[1]         # r is string
s = math.sin(float(r))

# sin expects number, not string r
# s becomes a floating-point number
```

Alternative print statements

- Desired output:

```
Hello, World! sin(3.4)=-0.255541102027
```

- String concatenation:

```
print "Hello, World! sin(" + str(r) + ")=" + str(s)
```

- printf-like statement:

```
print "Hello, World! sin(%g)=%g" % (r,s)
```

- Variable interpolation:

```
print "Hello, World! sin(%(r)g)=%(s)g" % vars()
```

printf format strings

```
%d     : integer
%5d    : integer in a field of width 5 chars
%-5d   : integer in a field of width 5 chars,
         but adjusted to the left
%05d   : integer in a field of width 5 chars,
         padded with zeroes from the left
%g     : float variable in %f or %g notation
%e     : float variable in scientific notation
%11.3e : float variable in scientific notation,
         with 3 decimals, field of width 11 chars
%5.1f  : float variable in fixed decimal notation,
         with one decimal, field of width 5 chars
%.3f   : float variable in fixed decimal form,
         with three decimals, field of min. width
%s     : string
%-20s  : string in a field of width 20 chars,
         and adjusted to the left
```

Strings in Python

- Single- and double-quoted strings work in the same way

```
s1 = "some string with a number %g" % r
s2 = ’some string with a number %g’ % r  # = s1
```

- Triple-quoted strings can be multi line with embedded newlines:

```
text = """
large portions of a text
can be conveniently placed
inside triple-quoted strings
(newlines are preserved)"""
```

- Raw strings, where backslash is backslash:

```
s3 = r’\(\s+\.\d+\)’
# with ordinary string (must quote backslash):
s3 = ’\\(\\s+\\.\\d+\\)’
```

Where to find Python info

- Make a bookmark for `$scripting/doc.html`
- Follow link to *Index to Python Library Reference*
  (complete on-line Python reference)
- Click on Python keywords, modules etc.
- Online alternative: `pydoc`, e.g., `pydoc math`
- `pydoc` lists all classes and functions in a module
- Alternative: Python in a Nutshell (or Beazley’s textbook)
- Recommendation: use these slides and associated book together
  with the Python Library Reference, and learn by doing exercises

New example: reading/writing data files

Tasks:

- Read (x,y) data from a two-column file
- Transform y values to f(y)
- Write (x,f(y)) to a new file

What to learn:

- How to open, read, write and close files
- How to write and call a function
- How to work with arrays (lists)

File: `src/py/intro/datatrans1.py`

Reading input/output filenames

- Usage:

```
./datatrans1.py infilename outfilename
```

- Read the two command-line arguments:
  input and output filenames

```
infilename  = sys.argv[1]
outfilename = sys.argv[2]
```

- Command-line arguments are in `sys.argv[1:]`
- `sys.argv[0]` is the name of the script

Exception handling

- What if the user fails to provide two command-line arguments?
- Python aborts execution with an informative error message
- A good alternative is to handle the error manually inside the program code:

```
try:
    infilename  = sys.argv[1]
    outfilename = sys.argv[2]
except:
    # try block failed,
    # we miss two command-line arguments
    print ’Usage:’, sys.argv[0], ’infile outfile’
    sys.exit(1)
```

This is the common way of dealing with errors in Python, called *exception handling*

Open file and read line by line

- Open files:

```
ifile = open( infilename, ’r’)  # r for reading
ofile = open(outfilename, ’w’)  # w for writing

afile = open(appfilename, ’a’)  # a for appending
```

- Read line by line:

```
for line in ifile:
    # process line
```

- Observe: blocks are indented; no braces!

Defining a function

```
import math

def myfunc(y):
    if y >= 0.0:
        return y**5*math.exp(-y)
    else:
        return 0.0

# alternative way of calling module functions
# (gives more math-like syntax in this example):

from math import *
def myfunc(y):
    if y >= 0.0:
        return y**5*exp(-y)
    else:
        return 0.0
```

Data transformation loop

- Input file format: two columns with numbers

```
0.1   1.4397
0.2   4.325
0.5   9.0
```

- Read (x,y), transform y, write (x,f(y)):

```
for line in ifile:
    pair = line.split()
    x = float(pair[0]); y = float(pair[1])
    fy = myfunc(y)  # transform y value
    ofile.write(’%g  %12.5e\n’ % (x,fy))
```

Alternative file reading

- This construction is more flexible and traditional in Python (and a bit strange...):

```
while 1:
    line = ifile.readline()  # read a line
    if not line: break       # end of file: jump out of loop
    # process line
```

  i.e., an ’infinite’ loop with the termination criterion inside the loop

Loading data into lists

- Read input file into list of lines:

```
lines = ifile.readlines()
```

- Now the 1st line is `lines[0]`, the 2nd is `lines[1]`, etc.
- Store x and y data in lists:

```
# go through each line,
# split line into x and y columns

x = []; y = []   # store data pairs in lists x and y

for line in lines:
    xval, yval = line.split()
    x.append(float(xval))
    y.append(float(yval))
```

See `src/py/intro/datatrans2.py` for this version

Loop over list entries

- For-loop in Python:

```
for i in range(start,stop,inc):
    ...
for j in range(stop):
    ...
```

  generates

```
i = start, start+inc, start+2*inc, ..., stop-1
j = 0, 1, 2, ..., stop-1
```

- Loop over (x,y) values:

```
ofile = open(outfilename, ’w’) # open for writing

for i in range(len(x)):
    fy = myfunc(y[i])  # transform y value
    ofile.write(’%g  %12.5e\n’ % (x[i], fy))

ofile.close()
```

Running the script

- Method 1: write just the name of the scriptfile:

```
./datatrans1.py infile outfile

# or
datatrans1.py infile outfile
```

  if . (current working directory) or the directory containing datatrans1.py is in the path
- Method 2: run an interpreter explicitly:

```
python datatrans1.py infile outfile
```

  Use the first python program found in the path
- This works on Windows too (method 1 requires the right `assoc/ftype` bindings for `.py` files)

More about headers

- In method 1, the interpreter to be used is specified in the first line
- Explicit path to the interpreter:

```
#!/usr/local/bin/python
```

  or perhaps your own Python interpreter:

```
#!/home/hpl/projects/scripting/Linux/bin/python
```

- Using env to find the first Python interpreter in the path:

```
#!/usr/bin/env python
```

Are scripts compiled?

- Yes and no, depending on how you see it
- Python first compiles the script into bytecode
- The bytecode is then interpreted
- No linking with libraries; libraries are imported dynamically when needed
- It appears as there is no compilation
- Quick development: just edit the script and run!
  (no time-consuming compilation and linking)
- Extensive error checking at run time

Python and error checking

- Easy to introduce intricate bugs?
  - no declaration of variables
  - functions can "eat anything"
- No, extensive consistency checks at run time replace the need for strong typing and compile-time checks
- Example: sending a string to the sine function, `math.sin('t')`, triggers a run-time error (type incompatibility)
- Example: try to open a non-existing file

```
./datatrans1.py qqq someoutfile
Traceback (most recent call last):
  File "./datatrans1.py", line 12, in ?
    ifile = open( infilename, 'r')
IOError:[Errno 2] No such file or directory:'qqq'
```

Computing with arrays

- `x` and `y` in `datatrans2.py` are *lists*
- We can compute with lists element by element (as shown)
- However: using Numerical Python (NumPy) *arrays* instead of lists is much more efficient and convenient
- Numerical Python is an extension of Python: a new fixed-size array type and lots of functions operating on such arrays

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A first glimpse of NumPy

- Import (more on this later...):

```
from numpy import *
x = linspace(0, 1, 1001)   # 1001 values between 0 and 1
x = sin(x)                 # computes sin(x[0]), sin(x[1]) etc.
```

- `x=sin(x)` is 13 times faster than an explicit loop:

```
for i in range(len(x)):
    x[i] = sin(x[i])
```

because `sin(x)` invokes an efficient loop in C

Loading file data into NumPy arrays

- A special module loads tabular file data into NumPy arrays:

```
import scitools.filetable
f = open(infilename, 'r')
x, y = scitools.filetable.read_columns(f)
f.close()
```

- Now we can compute with the NumPy arrays `x` and `y`:

```
x = 10*x
y = 2*y + 0.1*sin(x)
```

- We can easily write `x` and `y` back to a file:

```
f = open(outfilename, 'w')
scitools.filetable.write_columns(f, x, y)
f.close()
```

More on computing with NumPy arrays

- Multi-dimensional arrays can be constructed:

```
x = zeros(n)               # array with indices 0,1,...,n-1
x = zeros((m,n))           # two-dimensional array
x[i,j] = 1.0               # indexing
x = zeros((p,q,r))         # three-dimensional array
x[i,j,k] = -2.1
x = sin(x)*cos(x)
```

- We can plot one-dimensional arrays:

```
from scitools.easyviz import *  # plotting
x = linspace(0, 2, 21)
y = x + sin(10*x)
plot(x, y)
```

- NumPy has lots of math functions and operations
- SciPy is a comprehensive extension of NumPy
- NumPy + SciPy is a kind of Matlab replacement for many people

---

Interactive Python

- Python statements can be run interactively in a *Python shell*
- The “best” shell is called IPython
- Sample session with IPython:

```
Unix/DOS> ipython
...
In [1]:3*4-1
Out[1]:11

In [2]:from math import *

In [3]:x = 1.2

In [4]:y = sin(x)

In [5]:x
Out[5]:1.2

In [6]:y
Out[6]:0.93203908596722629
```

Editing capabilities in IPython

- Up- and down-arrays: go through command history
- Emacs key bindings for editing previous commands
- The underscore variable holds the last output

```
In [6]:y
Out[6]:0.93203908596722629

In [7]:_ + 1
Out[7]:1.93203908596722629
```

TAB completion

- IPython supports TAB completion: write a part of a command or name (variable, function, module), hit the TAB key, and IPython will complete the word or show different alternatives:

  ```
  In [1]: import math

  In [2]: math.<TABKEY>
  math.__class__          math.__str__            math.frexp
  math.__delattr__        math.acos               math.hypot
  math.__dict__           math.asin               math.ldexp
  ...
  ```

  or

  ```
  In [2]: my_variable_with_a_very_long_name = True

  In [3]: my<TABKEY>
  In [3]: my_variable_with_a_very_long_name
  ```

  You can increase your typing speed with TAB completion!

More examples

```
In [1]:f = open('datafile', 'r')

IOError: [Errno 2] No such file or directory: 'datafile'

In [2]:f = open('.datatrans_infile', 'r')

In [3]:from scitools.filetable import read_columns

In [4]:x, y = read_columns(f)

In [5]:x
Out[5]:array([ 0.1,  0.2,  0.3,  0.4])

In [6]:y
Out[6]:array([ 1.1    ,  1.8    ,  2.22222,  1.8    ])
```

IPython and the Python debugger

- Scripts can be run from IPython:

  ```
  In [1]:run scriptfile arg1 arg2 ...
  ```

  e.g.,

  ```
  In [1]:run datatrans2.py .datatrans_infile tmp1
  ```

- IPython is integrated with Python's `pdb` debugger
- `pdb` can be automatically invoked when an exception occurs:

  ```
  In [29]:%pdb on  # invoke pdb automatically
  In [30]:run datatrans2.py infile tmp2
  ```

More on debugging

- This happens when the infile name is wrong:

  ```
  /home/work/scripting/src/py/intro/datatrans2.py
        7     print "Usage:",sys.argv[0], "infile outfile"; sys.exi
        8
  ----> 9 ifile = open(infilename, 'r')  # open file for reading
       10 lines = ifile.readlines()      # read file into list of l
       11 ifile.close()

  IOError: [Errno 2] No such file or directory: 'infile'
  > /home/work/scripting/src/py/intro/datatrans2.py(9)?()
  -> ifile = open(infilename, 'r')  # open file for reading
  (Pdb) print infilename
  infile
  ```

On the efficiency of scripts

Consider datatrans1.py: read 100 000 (x,y) data from file and write (x,f(y)) out again

- Pure Python: 4s
- Pure Perl: 3s
- Pure Tcl: 11s
- Pure C (fscanf/fprintf): 1s
- Pure C++ (iostream): 3.6s
- Pure C++ (buffered streams): 2.5s
- Numerical Python modules: 2.2s (!)

(Computer: IBM X30, 1.2 GHz, 512 Mb RAM, Linux, gcc 3.3)

Remarks

- The results reflect general trends:
  - Perl is up to twice as fast as Python
  - Tcl is significantly slower than Python
  - C and C++ are not *that* faster
  - Special Python modules enable the speed of C/C++
- Unfair test?
  scripts use split on each line,
  C/C++ reads numbers consecutively
- 100 000 data points would be stored in binary format in a real application, resulting in much smaller differences between the implementations

The classical script

- Simple, classical Unix shell scripts are widely used to replace sequences of operating system commands
- Typical application in numerical simulation:
  - run a simulation program
  - run a visualization program and produce graphs
- Programs are supposed to run in batch
- We want to make such a gluing script in Python

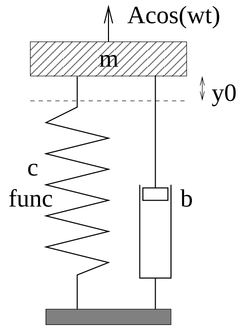
What to learn

- Parsing command-line options:

  ```
  somescript -option1 value1 -option2 value2
  ```

- Removing and creating directories
- Writing data to file
- Running applications (stand-alone programs)

Simulation example



$$m\frac{d^2y}{dt^2} + b\frac{dy}{dt} + cf(y) = A\cos\omega t$$

$$y(0) = y_0, \quad \frac{d}{dt}y(0) = 0$$

Code: `oscillator` (written in Fortran 77)

Usage of the simulation code

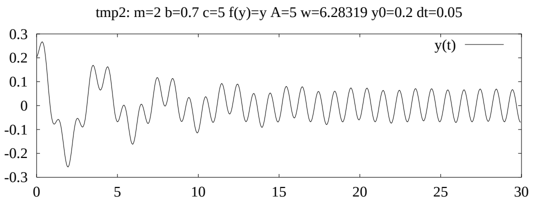
- Input: m, b, c, and so on read from standard input
- How to run the code:

  ```
  oscillator < file
  ```

  where `file` can be

  ```
  3.0
  0.04
  1.0
  ...
  (i.e., values of m, b, c, etc.)
  ```
- Results (t, y(t)) in sim.dat

A plot of the solution



Plotting graphs in Gnuplot

- Commands:

  ```
  set title ’case: m=3 b=0.7 c=1 f(y)=y A=5 ...’;

  # screen plot: (x,y) data are in the file sim.dat
  plot ’sim.dat’ title ’y(t)’ with lines;

  # hardcopies:
  set size ratio 0.3 1.5, 1.0;
  set term postscript eps mono dashed ’Times-Roman’ 28;
  set output ’case.ps’;
  plot ’sim.dat’ title ’y(t)’ with lines;

  # make a plot in PNG format as well:
  set term png small;
  set output ’case.png’;
  plot ’sim.dat’ title ’y(t)’ with lines;
  ```
- Commands can be given interactively or put in a file

Typical manual work

- Change oscillating system parameters by editing the simulator input file
- Run simulator:

  ```
  oscillator < inputfile
  ```
- Plot:

  ```
  gnuplot -persist -geometry 800x200 case.gp
  ```
- Plot annotations must be consistent with `inputfile`
- Let’s automate!

The user interface

- Usage:

  ```
  ./simviz1.py -m 3.2 -b 0.9 -dt 0.01 -case run1
  ```

  Sensible default values for all options
- Put simulation and plot files in a subdirectory (specified by `-case run1`)

File: `src/py/intro/simviz1.py`

Program tasks

- Set default values of m, b, c etc.
- Parse command-line options (-m, -b etc.) and assign new values to m, b, c etc.
- Create and move to subdirectory
- Write input file for the simulator
- Run simulator
- Write Gnuplot commands in a file
- Run Gnuplot

Parsing command-line options

- Set default values of the script’s input parameters:

  ```
  m = 1.0; b = 0.7; c = 5.0; func = ’y’; A = 5.0;
  w = 2*math.pi; y0 = 0.2; tstop = 30.0; dt = 0.05;
  case = ’tmp1’; screenplot = 1
  ```
- Examine command-line options in `sys.argv`:

  ```
  # read variables from the command line, one by one:
  while len(sys.argv) >= 2:
      option = sys.argv[1];       del sys.argv[1]
      if   option == ’-m’:
          m = float(sys.argv[1]); del sys.argv[1]
      ...
  ```

  Note: `sys.argv[1]` is text, but we may want a float for numerical operations

Modules for parsing command-line arguments

- Python offers two modules for command-line argument parsing: getopt and optparse
- These accept short options (`-m`) and long options (`-mass`)
- getopt examines the command line and returns pairs of options and values (`(-mass, 2.3)`)
- optparse is a bit more comprehensive to use and makes the command-line options available as attributes in an object
- See exercises for extending `simviz1.py` with (e.g.) getopt
- In this introductory example we rely on manual parsing since this exemplifies basic Python programming

---

Creating a subdirectory

- Python has a rich cross-platform operating system (OS) interface
- Skip Unix- or DOS-specific commands; do all OS operations in Python!
- Safe creation of a subdirectory:

```
dir = case               # subdirectory name
import os, shutil
if os.path.isdir(dir):   # does dir exist?
    shutil.rmtree(dir)   # yes, remove old files
os.mkdir(dir)            # make dir directory
os.chdir(dir)            # move to dir
```

Writing the input file to the simulator

```
f = open('%s.i' % case, 'w')
f.write("""
        %(m)g
        %(b)g
        %(c)g
        %(func)s
        %(A)g
        %(w)g
        %(y0)g
        %(tstop)g
        %(dt)g
        """ % vars())
f.close()
```

Note: triple-quoted string for multi-line output

Running the simulation

- Stand-alone programs can be run as

```
os.system(command)

# examples:
os.system('myprog < input_file')
os.system('ls *')  # bad, Unix-specific
```

- Better: get failure status and output from the command

```
cmd = 'oscillator < %s.i' % case  # command to run
import commands
failure, output = commands.getstatusoutput(cmd)
if failure:
    print 'running the oscillator code failed'
    print output
    sys.exit(1)
```

Making plots

- Make Gnuplot script:

```
f = open(case + '.gnuplot', 'w')
f.write("""
set title '%s: m=%g b=%g c=%g f(y)=%s A=%g ...';
...
""" % (case,m,b,c,func,A,w,y0,dt,case,case))
...
f.close()
```

- Run Gnuplot:

```
cmd = 'gnuplot -geometry 800x200 -persist ' \
      + case + '.gnuplot'
failure, output = commands.getstatusoutput(cmd)
if failure:
    print 'running gnuplot failed'; print output; sys.exit(1)
```

Python vs Unix shell script

- Our simviz1.py script is traditionally written as a Unix shell script
- What are the advantages of using Python here?
  - Easier command-line parsing
  - Runs on Windows and Mac as well as Unix
  - Easier extensions (loops, storing data in arrays etc)

Shell script file: src/bash/simviz1.sh

Other programs for curve plotting

- It is easy to replace Gnuplot by another plotting program
- Matlab, for instance:

```
f = open(case + '.m', 'w')  # write to Matlab M-file
# (the character % must be written as %% in printf-like strings)
f.write("""
load sim.dat                %% read sim.dat into sim matrix
plot(sim(:,1),sim(:,2))     %% plot 1st column as x, 2nd as y
legend('y(t)')
title('%s: m=%g b=%g c=%g f(y)=%s A=%g w=%g y0=%g dt=%g')
outfile = '%s.ps';  print('-dps',  outfile)  %% ps BW plot
outfile = '%s.png'; print('-dpng', outfile)  %% png color plot
""" % (case,m,b,c,func,A,w,y0,dt,case,case))
if screenplot: f.write('pause(30)\n')
f.write('exit\n'); f.close()

if screenplot:
    cmd = 'matlab -nodesktop -r ' + case + ' > /dev/null &'
else:
    cmd = 'matlab -nodisplay -nojvm -r ' + case
failure, output = commands.getstatusoutput(cmd)
```

Series of numerical experiments

- Suppose we want to run a series of experiments with different m values
- Put a script on top of simviz1.py,

```
./loop4simviz1.py m_min m_max dm \
                  [options as for simviz1.py]
```

  having a loop over m and calling simviz1.py inside the loop
- Each experiment is archived in a separate directory
- That is, loop4simviz1.py controls the -m and -case options to simviz1.py

Handling command-line args (1)

- The first three arguments define the m values:

```
try:
    m_min = float(sys.argv[1])
    m_max = float(sys.argv[2])
    dm    = float(sys.argv[3])
except:
    print ’Usage:’,sys.argv[0],\
    ’m_min m_max m_increment [ simviz1.py options ]’
    sys.exit(1)
```

- Pass the rest of the arguments, `sys.argv[4:]`, to simviz1.py
- Problem: `sys.argv[4:]` is a list, we need a string

```
[’-b’,’5’,’-c’,’1.1’] -> ’-b 5 -c 1.1’
```

Handling command-line args (2)

- `’ ’.join(list)` can make a string out of the list `list`, with a blank between each item

```
simviz1_options = ’ ’.join(sys.argv[4:])
```

- Example:

```
./loop4simviz1.py 0.5 2 0.5 -b 2.1 -A  3.6
```

results in

```
m_min:  0.5
m_max:  2.0
dm:     0.5
simviz1_options = ’-b 2.1 -A 3.6’
```

The loop over m

- Cannot use

```
for m in range(m_min, m_max, dm):
```

because `range` works with integers only

- A while-loop is appropriate:

```
m = m_min
while m <= m_max:
    case = ’tmp_m_%g’ % m
    s = ’python simviz1.py %s -m %g -case %s’ % \
        (simviz1_options,m,case)
    failure, output = commands.getstatusoutput(s)
    m += dm
```

(Note: our `-m` and `-case` will override any `-m` or `-case` option provided by the user)

Collecting plots in an HTML file

- Many runs can be handled; need a way to browse the results
- Idea: collect all plots in a common HTML file:

```
html = open(’tmp_mruns.html’, ’w’)
html.write(’<HTML><BODY BGCOLOR="white">\n’)
```

```
m = m_min
while m <= m_max:
    case = ’tmp_m_%g’ % m
    cmd = ’python simviz1.py %s -m %g -case %s’ % \
          (simviz1_options, m, case)
    failure, output = commands.getstatusoutput(cmd)
    html.write(’<H1>m=%g</H1> <IMG SRC="%s">\n’ \
         % (m,os.path.join(case,case+’.png’)))
    m += dm
html.write(’</BODY></HTML>\n’)
```

Collecting plots in a PostScript file

- For compact printing a PostScript file with small-sized versions of all the plots is useful
- `epsmerge` (Perl script) is an appropriate tool:

```
# concatenate file1.ps, file2.ps, and so on to
# one single file figs.ps, having pages with
# 3 rows with 2 plots in each row (-par preserves
# the aspect ratio of the plots)
```

```
epsmerge -o figs.ps -x 2 -y 3 -par \
         file1.ps file2.ps file3.ps ...
```

- Can use this technique to make a compact report of the generated PostScript files for easy printing

Implementation of ps-file report

```
psfiles = []  # plot files in PostScript format
...
while m <= m_max:
    case = ’tmp_m_%g’ % m
    ...
    psfiles.append(os.path.join(case,case+’.ps’))
    ...
...
s = ’epsmerge -o tmp_mruns.ps -x 2 -y 3 -par ’ + \
    ’ ’.join(psfiles)
failure, output = commands.getstatusoutput(s)
```

Animated GIF file

- When we vary m, wouldn’t it be nice to see progressive plots put together in a movie?
- Can combine the PNG files together in an animated GIF file:

```
convert -delay 50 -loop 1000 -crop 0x0 \
        plot1.png plot2.png plot3.png plot4.png ...  movie.gif
```

```
animate movie.gif  # or display movie.gif
```

(convert and animate are ImageMagick tools)

- Collect all PNG filenames in a list and join the list items (as in the generation of the ps-file report)

Some improvements

- Enable loops over an arbitrary parameter (not only m)

```
# easy:
’-m %g’ % m
# is replaced with
’-%s %s’ % (str(prm_name), str(prm_value))
# prm_value plays the role of the m variable
# prm_name (’m’, ’b’, ’c’, ...) is read as input
```

- Keep the range of the y axis fixed (for movie)
- Files:

```
simviz1.py   : run simulation and visualization
simviz2.py   : additional option for yaxis scale
```

```
loop4simviz1.py : m loop calling simviz1.py
loop4simviz2.py : loop over any parameter in
                  simviz2.py and make movie
```

Playing around with experiments

We can perform lots of different experiments:

- Study the impact of increasing the mass:

```
./loop4simviz2.py m 0.1 6.1 0.5 -yaxis -0.5 0.5 -noscreenplot
```

- Study the impact of a nonlinear spring:

```
./loop4simviz2.py c 5 30 2 -yaxis -0.7 0.7 -b 0.5 \
                  -func siny -noscreenplot
```

- Study the impact of increasing the damping:

```
./loop4simviz2.py b 0 2 0.25 -yaxis -0.5 0.5 -A 4
```

  (loop over b, from 0 to 2 in steps of 0.25)

Remarks

- Reports:

```
tmp_c.gif          # animated GIF (movie)
animate tmp_c.gif

tmp_c_runs.html    # browsable HTML document
tmp_c_runs.ps      # all plots in a ps-file
```

- All experiments are archived in a directory with a filename reflecting the varying parameter:

```
tmp_m_2.1   tmp_b_0   tmp_c_29
```

- All generated files/directories start with tmp so it is easy to clean up hundreds of experiments
- Try the listed `loop4simviz2.py` commands!!

Exercise

- Make a summary report with the equation, a picture of the system, the command-line arguments, and a movie of the solution
- Make a link to a detailed report with plots of all the individual experiments
- Demo:

```
./loop4simviz2_2html.py m 0.1 6.1 0.5 -yaxis -0.5 0.5 -noscreenpl
ls -d tmp_*
mozilla tmp_m_summary.html
```

Increased quality of scientific work

- Archiving of experiments and having a system for uniquely relating input data to visualizations or result files are fundamental for reliable scientific investigations
- The experiments can easily be reproduced
- New (large) sets of experiments can be generated
- We make tailored tools for investigating results
- All these items contribute to increased quality of numerical experimentation

---

New example: converting data file formats

- Input file with time series data:

```
some comment line
1.5
  measurements  model1 model2
     0.0          0.1    1.0
     0.1          0.1    0.188
     0.2          0.2    0.25
```

  Contents: comment line, time step, headings, time series data
- Goal: split file into two-column files, one for each time series
- Script: interpret input file, split text, extract data and write files

---

Example on an output file

- The `model1.dat` file, arising from column no 2, becomes

```
0    0.1
1.5  0.1
3    0.2
```

- The time step parameter, here 1.5, is used to generate the first column

---

Program flow

- Read inputfile name (1st command-line arg.)
- Open input file
- Read and skip the 1st (comment) line
- Extract time step from the 2nd line
- Read time series names from the 3rd line
- Make a list of file objects, one for each time series
- Read the rest of the file, line by line:
  - split lines into y values
  - write t and y value to file, for all series

File: `src/py/intro/convert1.py`

What to learn

- Reading and writing files
- Sublists
- List of file objects
- Dictionaries
- Arrays of numbers
- List comprehension
- Refactoring a flat script as functions in a module

Reading in the first 3 lines

- Open file and read comment line:

```
infilename = sys.argv[1]
ifile = open(infilename, ’r’) # open for reading
line = ifile.readline()
```

- Read time step from the next line:

```
dt = float(ifile.readline())
```

- Read next line containing the curvenames:

```
ynames = ifile.readline().split()
```

Output to many files

- Make a list of file objects for output of each time series:

```
outfiles = []
for name in ynames:
    outfiles.append(open(name + ’.dat’, ’w’))
```

Writing output

- Read each line, split into y values, write to output files:

```
t = 0.0    # t value
# read the rest of the file line by line:
while 1:
    line = ifile.readline()
    if not line: break

    yvalues = line.split()

    # skip blank lines:
    if len(yvalues) == 0: continue

    for i in range(len(outfiles)):
        outfiles[i].write(’%12g %12.5e\n’ % \
                          (t, float(yvalues[i])))
    t += dt

for file in outfiles:
    file.close()
```

Dictionaries

- Dictionary = array with a text as index
- Also called *hash* or *associative array* in other languages
- Can store ’anything’:

```
prm[’damping’] = 0.2             # number

def x3(x):
    return x*x*x
prm[’stiffness’] = x3            # function object

prm[’model1’] = [1.2, 1.5, 0.1]  # list object
```

- The text index is called *key*

Dictionaries for our application

- Could store the time series in memory as a dictionary of lists; the list items are the y values and the y names are the keys

```
y = {}           # declare empty dictionary
# ynames: names of y curves
for name in ynames:
    y[name] = [] # for each key, make empty list

lines = ifile.readlines()  # list of all lines
...
for line in lines[3:]:
    yvalues = [float(x) for x in line.split()]
    i = 0  # counter for yvalues
    for name in ynames:
        y[name].append(yvalues[i]); i += 1
```

File: `src/py/intro/convert2.py`

Dissection of the previous slide

- Specifying a sublist, e.g., the 4th line until the last line: `lines[3:]`
  Transforming all words in a line to floats:

```
yvalues = [float(x) for x in line.split()]

# same as
numbers = line.split()
yvalues = []
for s in numbers:
    yvalues.append(float(s))
```

The items in a dictionary

- The input file

```
some comment line
1.5
  measurements  model1 model2
     0.0         0.1    1.0
     0.1         0.1    0.188
     0.2         0.2    0.25
```

results in the following y dictionary:

```
’measurements’: [0.0, 0.1, 0.2],
’model1’:       [0.1, 0.1, 0.2],
’model2’:       [1.0, 0.188, 0.25]
```

(this output is plain print: `print y`)

Remarks

- Fortran/C programmers tend to think of indices as integers
- Scripters make heavy use of dictionaries and text-type indices (keys)
- Python dictionaries can use (almost) any object as key (!)
- A dictionary is also often called hash (e.g. in Perl) or associative array
- Examples will demonstrate their use

Next step: make the script reusable

- The previous script is “flat”
  (start at top, run to bottom)
- Parts of it may be reusable
- We may like to load data from file, operate on data, and then dump data
- Let’s refactor the script:
  - make a load data function
  - make a dump data function
  - collect these two functions in a reusable module

The load data function

```
def load_data(filename):
    f = open(filename, ’r’); lines = f.readlines(); f.close()
    dt = float(lines[1])
    ynames = lines[2].split()
    y = {}
    for name in ynames:  # make y a dictionary of (empty) lists
        y[name] = []

    for line in lines[3:]:
        yvalues = [float(yi) for yi in line.split()]
        if len(yvalues) == 0: continue  # skip blank lines
        for name, value in zip(ynames, yvalues):
            y[name].append(value)
    return y, dt
```

How to call the load data function

- Note: the function returns two (!) values;
  a dictionary of lists, plus a float
- It is common that output data from a Python function are returned, and multiple data structures can be returned (actually packed as a *tuple*, a kind of “constant list”)
- Here is how the function is called:

  ```
  y, dt = load_data(’somedatafile.dat’)
  print y
  ```

  Output from `print y`:

  ```
  >>> y
  {’tmp-model2’: [1.0, 0.188, 0.25],
  ’tmp-model1’: [0.10000000000000001, 0.10000000000000001,
                 0.20000000000000001],
  ’tmp-measurements’: [0.0, 0.10000000000000001, 0.2000000000000000
  ```

Iterating over several lists

- C/C++/Java/Fortran-like iteration over two arrays/lists:

  ```
  for i in range(len(list)):
      e1 = list1[i];  e2 = list2[i]
      # work with e1 and e2
  ```

- Pythonic version:

  ```
  for e1, e2 in zip(list1, list2):
      # work with element e1 from list1 and e2 from list2
  ```

  For example,

  ```
  for name, value in zip(ynames, yvalues):
      y[name].append(value)
  ```

The dump data function

```
def dump_data(y, dt):
    # write out 2-column files with t and y[name] for each name:
    for name in y.keys():
        ofile = open(name+’.dat’, ’w’)
        for k in range(len(y[name])):
            ofile.write(’%12g %12.5e\n’ % (k*dt, y[name][k]))
        ofile.close()
```

Reusing the functions

- Our goal is to reuse `load_data` and `dump_data`, possibly with some operations on `y` in between:

  ```
  from convert3 import load_data, dump_data

  y, timestep = load_data(’.convert_infile1’)

  from math import fabs
  for name in y:  # run through keys in y
      maxabsy = max([fabs(yval) for yval in y[name]])
      print ’max abs(y[%s](t)) = %g’ % (name, maxabsy)

  dump_data(y, timestep)
  ```

- Then we need to make a module `convert3`!

How to make a module

- Collect the functions in the module in a file, here the file is called `convert3.py`
- We have then made a module `convert3`
- The usage is as exemplified on the previous slide

Module with application script

- The scripts `convert1.py` and `convert2.py` load and dump data - this functionality can be reproduced by an application script using `convert3`
- The application script can be included in the module:

  ```
  if __name__ == ’__main__’:
      import sys
      try:
          infilename = sys.argv[1]
      except:
          usage = ’Usage: %s infile’ % sys.argv[0]
          print usage; sys.exit(1)
      y, dt = load_data(infilename)
      dump_data(y, dt)
  ```

- If the module file is run as a script, the `if` test is true and the application script is run
- If the module is imported in a script, the `if` test is false and no statements are executed

Usage of convert3.py

- As script:

```
unix> ./convert3.py someinputfile.dat
```

- As module:

```
import convert3
y, dt = convert3.load_data(’someinputfile.dat’)
# do more with y?
dump_data(y, dt)
```

- The application script at the end also serves as an example on how to use the module

---

How to solve exercises

- Construct an example on the functionality of the script, if that is not included in the problem description
- Write very high-level pseudo code with words
- Scan known examples for constructions and functionality that can come into use
- Look up man pages, reference manuals, FAQs, or textbooks for functionality you have minor familiarity with, or to clarify syntax details
- Search the Internet if the documentation from the latter point does not provide sufficient answers

---

Example: write a join function

- Exercise:
Write a function `myjoin` that concatenates a list of strings to a single string, with a specified delimiter between the list elements. That is, `myjoin` is supposed to be an implementation of a string’s `join` method in terms of basic string operations.
- Functionality:

```
s = myjoin([’s1’, ’s2’, ’s3’], ’*’)
# s becomes ’s1*s2*s3’
```

The next steps

- Pseudo code:

```
function myjoin(list, delimiter)
  joined = first element in list
  for element in rest of list:
    concatenate joined, delimiter and element
  return joined
```

- Known examples: string concatenation (+ operator) from hw.py, list indexing (`list[0]`) from datatrans1.py, sublist extraction (`list[1:]`) from convert1.py, function construction from datatrans1.py

---

Refined pseudo code

```
def myjoin(list, delimiter):
  joined = list[0]
  for element in list[1:]:
    joined += delimiter + element
  return joined
```

That’s it!

How to present the answer to an exercise

- Use comments to explain *ideas*
- Use descriptive variable names to reduce the need for more comments
- Find generic solutions (unless the code size explodes)
- Strive at compact code, but not too compact
- Invoke the Python interpreter and run `import this`
- Always construct a demonstrating running example and include in it the source code file inside triple-quoted strings:

```
"""
unix> python hw.py 3.1459
Hello, World! sin(3.1459)=-0.00430733309102
"""
```

How to print exercises with a2ps

- Here is a suitable command for printing exercises for a week:

```
unix> a2ps --line-numbers=1 -4 -o outputfile.ps *.py
```

  This prints all `*.py` files, with 4 (because of `-4`) pages per sheet
- See man a2ps for more info about this command
- In every exercise you also need examples on how a script is run and what the output is – one recommendation is to put all this info (cut from the terminal window and pasted in your editor) in a triple double quoted Python string (such a string can be viewed as example/documentation/comment as it does not affect the behavior of the script)

Python as a Matlab-like computing environment

Contents

- Efficient array computing in Python
- Creating arrays
- Indexing/slicing arrays
- Random numbers
- Linear algebra
- Plotting

More info

- Ch. 4 in the course book
- www.scipy.org
- The NumPy manual
- The SciPy tutorial

Numerical Python (NumPy)

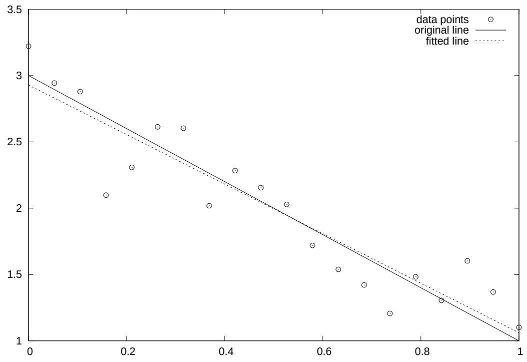
- NumPy enables efficient numerical computing in Python
- NumPy is a package of modules, which offers efficient arrays (contiguous storage) with associated array operations coded in C or Fortran
- There are three implementations of Numerical Python
  - Numeric from the mid 90s (still widely used)
  - numarray from about 2000
  - numpy from 2006
- We recommend to use numpy (by Travis Oliphant)

  ```
  from numpy import *
  ```

A taste of NumPy: a least-squares procedure

```
x = linspace(0.0, 1.0, n)               # coordinates
y_line = -2*x + 3
y = y_line + random.normal(0, 0.25, n)  # line with noise

# goal: fit a line to the data points x, y

# create and solve least squares system:
A = array([x, ones(n)])
A = A.transpose()
result = linalg.lstsq(A, y)
# result is a 4-tuple, the solution (a,b) is the 1st entry:
a, b = result[0]
plot(x, y, ’o’,         # data points w/noise
     x, y_line, ’r’,    # original line
     x, a*x + b, ’b’)  # fitted lines
legend(’data points’, ’original line’, ’fitted line’)
hardcopy(’myplot.png’)
```

Resulting plot



NumPy: making arrays

```
>>> from numpy import *
>>> n = 4
>>> a = zeros(n)      # one-dim. array of length n
>>> print a
[ 0.  0.  0.  0.]
>>> a
array([ 0.,  0.,  0.,  0.])
>>> p = q = 2
>>> a = zeros((p,q,3))     # p*q*3 three-dim. array
>>> print a
[[[ 0.  0.  0.]
  [ 0.  0.  0.]]

 [[ 0.  0.  0.]
  [ 0.  0.  0.]]]
>>> a.shape                # a’s dimension
(2, 2, 3)
```

NumPy: making float, int, complex arrays

```
>>> a = zeros(3)
>>> print a.dtype # a’s data type
float64
>>> a = zeros(3, int)
>>> print a
[0 0 0]
>>> print a.dtype
int32
>>> a = zeros(3, float32)   # single precision
>>> print a
[ 0.  0.  0.]
>>> print a.dtype
float32
>>> a = zeros(3, complex)
>>> a
array([ 0.+0.j,  0.+0.j,  0.+0.j])
>>> a.dtype
dtype(’complex128’)

>>> given an array a, make a new array of same dimension
>>> and data type:
>>> x = zeros(a.shape, a.dtype)
```

Array with a sequence of numbers

- `linspace(a, b, n)` generates n uniformly spaced coordinates, starting with a and ending with b

  ```
  >>> x = linspace(-5, 5, 11)
  >>> print x
  [-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
  ```

- A special compact syntax is also available:

  ```
  >>> a = r_[-5:5:11j]  # same as linspace(-1, 1, 11)
  >>> print a
  [-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
  ```

- `arange` works like `range` (`xrange`)

  ```
  >>> x = arange(-5, 5, 1, float)
  >>> print x  # upper limit 5 is not included!!
  [-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.]
  ```

Warning: arange is dangerous

- `arange`’s upper limit may or may not be included (due to round-off errors)
- Better to use a safer method:

```
>>> from scitools.numpyutils import seq
>>> x = seq(-5, 5, 1)
>>> print x   # upper limit always included
[-5. -4. -3. -2. -1.  0.  1.  2.  3.  4.  5.]
```

Array construction from a Python list

- `array(list, [datatype])` generates an array from a list:

```
>>> pl = [0, 1.2, 4, -9.1, 5, 8]
>>> a = array(pl)
```

- The array elements are of the simplest possible type:

```
>>> z = array([1, 2, 3])
>>> print z                     # array of integers
[1 2 3]
>>> z = array([1, 2, 3], float)
>>> print z
[ 1.  2.  3.]
```

- A two-dim. array from two one-dim. lists:

```
>>> x = [0, 0.5, 1]; y = [-6.1, -2, 1.2]  # Python lists
>>> a = array([x, y])  # form array with x and y as rows
```

- From array to list: `alist = a.tolist()`

From “anything” to a NumPy array

- Given an object a,

  ```
  a = asarray(a)
  ```

  converts a to a NumPy array (if possible/necessary)
- Arrays can be ordered as in C (default) or Fortran:

```
a = asarray(a, order=’Fortran’)
isfortran(a)  # returns True if a’s order is Fortran
```

- Use `asarray` to, e.g., allow flexible arguments in functions:

```
def myfunc(some_sequence):
    a = asarray(some_sequence)
    return 3*a - 5

myfunc([1,2,3])       # list argument
myfunc((-1,1))        # tuple argument
myfunc(zeros(10))     # array argument
myfunc(-4.5)          # float argument
myfunc(6)             # int argument
```

Changing array dimensions

```
>>> a = array([0, 1.2, 4, -9.1, 5, 8])
>>> a.shape = (2,3)       # turn a into a 2x3 matrix
>>> print a
[[ 0.   1.2  4. ]
 [-9.1  5.   8. ]]
>>> a.size
6
>>> a.shape = (a.size,)   # turn a into a vector of length 6 again
>>> a.shape
(6,)
>>> print a
[ 0.   1.2  4.  -9.1  5.   8. ]
>>> a = a.reshape(2,3)    # same effect as setting a.shape
>>> a.shape
(2, 3)
```

Array initialization from a Python function

```
>>> def myfunc(i, j):
...     return (i+1)*(j+4-i)
...
>>> # make 3x6 array where a[i,j] = myfunc(i,j):
>>> a = fromfunction(myfunc, (3,6))
>>> a
array([[  4.,   5.,   6.,   7.,   8.,   9.],
       [  6.,   8.,  10.,  12.,  14.,  16.],
       [  6.,   9.,  12.,  15.,  18.,  21.]])
```

Basic array indexing

```
a = linspace(-1, 1, 6)
a[2:4] = -1      # set a[2] and a[3] equal to -1
a[-1]  = a[0]    # set last element equal to first one
a[:]   = 0       # set all elements of a equal to 0
a.fill(0)        # set all elements of a equal to 0

a.shape = (2,3)  # turn a into a 2x3 matrix
print a[0,1]     # print element (0,1)
a[i,j] = 10      # assignment to element (i,j)
a[i][j] = 10     # equivalent syntax (slower)
print a[:,k]     # print column with index k
print a[1,:]     # print second row
a[:,:] = 0       # set all elements of a equal to 0
```

More advanced array indexing

```
>>> a = linspace(0, 29, 30)
>>> a.shape = (5,6)
>>> a
array([[  0.,  1.,  2.,  3.,  4.,  5.,]
       [  6.,  7.,  8.,  9., 10., 11.,]
       [ 12., 13., 14., 15., 16., 17.,]
       [ 18., 19., 20., 21., 22., 23.,]
       [ 24., 25., 26., 27., 28., 29.,]])
>>> a[1:3,:-1:2]   # a[i,j] for i=1,2 and j=0,2,4
array([[  6.,   8.,  10.],
       [ 12.,  14.,  16.]])
>>> a[::3,2:-1:2]   # a[i,j] for i=0,3 and j=2,4
array([[  2.,   4.],
       [ 20.,  22.]])
>>> i = slice(None, None, 3);  j = slice(2, -1, 2)
>>> a[i,j]
array([[  2.,   4.],
       [ 20.,  22.]])
```

Slices refer the array data

- With a as list, `a[:]` makes a copy of the data
- With a as array, `a[:]` is a reference to the data

```
>>> b = a[1,:]      # extract 2nd column of a
>>> print a[1,1]
12.0
>>> b[1] = 2
>>> print a[1,1]
2.0                 # change in b is reflected in a!
```

- Take a copy to avoid referencing via slices:

```
>>> b = a[1,:].copy()
>>> print a[1,1]
12.0
>>> b[1] = 2     # b and a are two different arrays now
>>> print a[1,1]
12.0             # a is not affected by change in b
```

Integer arrays as indices

- An integer array or list can be used as (vectorized) index

```
>>> a = linspace(1, 8, 8)
>>> a
array([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.])
>>> a[[1,6,7]] = 10
>>> a
array([  1.,  10.,   3.,   4.,   5.,   6.,  10.,  10.])
>>> a[range(2,8,3)] = -2
>>> a
array([  1.,  10.,  -2.,   4.,   5.,  -2.,  10.,  10.])
>>> a[a < 0]            # pick out the negative elements of a
array([-2., -2.])
>>> a[a < 0] = a.max()
>>> a
array([  1.,  10.,  10.,   4.,   5.,  10.,  10.,  10.])
```

- Such array indices are important for efficient vectorized code

Loops over arrays (1)

- Standard loop over each element:

```
for i in xrange(a.shape[0]):
    for j in xrange(a.shape[1]):
        a[i,j] = (i+1)*(j+1)*(j+2)
        print 'a[%d,%d]=%g ' % (i,j,a[i,j]),
    print  # newline after each row
```

- A standard for loop iterates over the first index:

```
>>> print a
[[  2.   6.  12.]
 [  4.  12.  24.]]
>>> for e in a:
...     print e
...
[  2.   6.  12.]
[  4.  12.  24.]
```

Loops over arrays (2)

- View array as one-dimensional and iterate over all elements:

```
for e in a.flat:
    print e
```

- For loop over all index tuples and values:

```
>>> for index, value in ndenumerate(a):
...     print index, value
...
(0, 0) 2.0
(0, 1) 6.0
(0, 2) 12.0
(1, 0) 4.0
(1, 1) 12.0
(1, 2) 24.0
```

Array computations

- Arithmetic operations can be used with arrays:

```
b = 3*a - 1    # a is array, b becomes array
```

1) compute `t1 = 3*a`, 2) compute `t2= t1 - 1`, 3) set `b = t2`

- Array operations are much faster than element-wise operations:

```
>>> import time  # module for measuring CPU time
>>> a = linspace(0, 1, 1E+07)  # create some array
>>> t0 = time.clock()
>>> b = 3*a -1
>>> t1 = time.clock()   # t1-t0 is the CPU time of 3*a-1

>>> for i in xrange(a.size): b[i] = 3*a[i] - 1
>>> t2 = time.clock()
>>> print '3*a-1: %g sec, loop: %g sec' % (t1-t0, t2-t1)
3*a-1: 2.09 sec, loop: 31.27 sec
```

In-place array arithmetics

- Expressions like `3*a-1` generates temporary arrays
- With in-place modifications of arrays, we can avoid temporary arrays (to some extent)

```
b = a
b *= 3  # or multiply(b, 3, b)
b -= 1  # or subtract(b, 1, b)
```

Note: a is changed, use `b = a.copy()`

- In-place operations:

```
a *= 3.0     # multiply a's elements by 3
a -= 1.0     # subtract 1 from each element
a /= 3.0     # divide each element by 3
a += 1.0     # add 1 to each element
a **= 2.0    # square all elements
```

- Assign values to all elements of an existing array:

```
a[:] = 3*c - 1
```

Standard math functions can take array arguments

```
# let b be an array

c = sin(b)
c = arcsin(c)
c = sinh(b)
# same functions for the cos and tan families
c = b**2.5  # power function
c = log(b)
c = exp(b)
c = sqrt(b)
```

Other useful array operations

```
# a is an array

a.clip(min=3, max=12)  # clip elements
a.mean(); mean(a)      # mean value
a.var();  var(a)       # variance
a.std();  std(a)       # standard deviation
median(a)
cov(x,y)               # covariance
trapz(a)               # Trapezoidal integration
diff(a)                # finite differences (da/dx)

# more Matlab-like functions:
corrcoeff, cumprod, diag, eig, eye, fliplr, flipud, max, min,
prod, ptp, rot90, squeeze, sum, svd, tri, tril, triu
```

Temporary arrays

- Let us evaluate `f1(x)` for a vector `x`:

```
def f1(x):
    return exp(-x*x)*log(1+x*sin(x))
```

- `temp1 = -x`
- `temp2 = temp1*x`
- `temp3 = exp(temp2)`
- `temp4 = sin(x)`
- `temp5 = x*temp4`
- `temp6 = 1 + temp4`
- `temp7 = log(temp5)`
- `result = temp3*temp7`

More useful array methods and attributes

```
>>> a = zeros(4) + 3
>>> a
array([ 3.,  3.,  3.,  3.])  # float data
>>> a.item(2)                # more efficient than a[2]
3.0
>>> a.itemset(3,-4.5)        # more efficient than a[3]=-4.5
>>> a
array([ 3. ,  3. ,  3. , -4.5])
>>> a.shape = (2,2)
>>> a
array([[ 3. ,  3. ],
       [ 3. , -4.5]])
>>> a.ravel()                # from multi-dim to one-dim
array([ 3. ,  3. ,  3. , -4.5])
>>> a.ndim                   # no of dimensions
2
>>> len(a.shape)             # no of dimensions
2
>>> rank(a)                  # no of dimensions
2
>>> a.size                   # total no of elements
4
>>> b = a.astype(int)        # change data type
>>> b
array([3, 3, 3, 3])
```

Complex number computing

```
>>> from math import sqrt
>>> sqrt(-1)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: math domain error

>>> from numpy import sqrt
>>> sqrt(-1)
Warning: invalid value encountered in sqrt
nan

>>> from cmath import sqrt   # complex math functions
>>> sqrt(-1)
1j
>>> sqrt(4)   # cmath functions always return complex...
(2+0j)

>>> from numpy.lib.scimath import sqrt
>>> sqrt(4)
2.0                # real when possible
>>> sqrt(-1)
1j                 # otherwise complex
```

A root function

```
# Goal: compute roots of a parabola, return real when possible,
# otherwise complex

def roots(a, b, c):
    # compute roots of a*x^2 + b*x + c = 0
    from numpy.lib.scimath import sqrt
    q = sqrt(b**2 - 4*a*c)  # q is real or complex
    r1 = (-b + q)/(2*a)
    r2 = (-b - q)/(2*a)
    return r1, r2

>>> a = 1; b = 2; c = 100
>>> roots(a, b, c)                           # complex roots
((-1+9.94987437107j), (-1-9.94987437107j))

>>> a = 1; b = 4; c = 1
>>> roots(a, b, c)                           # real roots
(-0.267949192431, -3.73205080757)
```

Array type and data type

```
>>> import numpy
>>> a = numpy.zeros(5)

>>> type(a)
<type 'numpy.ndarray'>
>>> isinstance(a, ndarray)    # is a of type ndarray?
True

>>> a.dtype                   # data (element) type object
dtype('float64')
>>> a.dtype.name
'float64'
>>> a.dtype.char              # character code
'd'
>>> a.dtype.itemsize          # no of bytes per array element
8
>>> b = zeros(6, float32)
>>> a.dtype == b.dtype  # do a and b have the same data type?
False
>>> c = zeros(2, float)
>>> a.dtype == c.dtype
True
```

Matrix objects (1)

- NumPy has an array type, matrix, much like Matlab's array type

```
>>> x1 = array([1, 2, 3], float)
>>> x2 = matrix(x)               # or just mat(x)
>>> x2                           # row vector
matrix([[ 1.,  2.,  3.]])
>>> x3 = mat(x).transpose()      # column vector
>>> x3
matrix([[ 1.],
        [ 2.],
        [ 3.]])

>>> type(x3)
<class 'numpy.core.defmatrix.matrix'>
>>> isinstance(x3, matrix)
True
```

- Only 1- and 2-dimensional arrays can be `matrix`

Matrix objects (2)

- For `matrix` objects, the `*` operator means matrix-matrix or matrix-vector multiplication (not elementwise multiplication)

```
>>> A = eye(3)                    # identity matrix
>>> A = mat(A)                    # turn array to matrix
>>> A
matrix([[ 1.,  0.,  0.],
        [ 0.,  1.,  0.],
        [ 0.,  0.,  1.]])
>>> y2 = x2*A                     # vector-matrix product
>>> y2
matrix([[ 1.,  2.,  3.]])
>>> y3 = A*x3                     # matrix-vector product
>>> y3
matrix([[ 1.],
        [ 2.],
        [ 3.]])
```

Vectorization (1)

- Loops over an array run slowly
- Vectorization = replace explicit loops by functions calls such that the whole loop is implemented in C (or Fortran)
- Explicit loops:

```
r = zeros(x.shape, x.dtype)
for i in xrange(x.size):
    r[i] = sin(x[i])
```

- Vectorized version:

```
r = sin(x)
```

- Arithmetic expressions work for both scalars and arrays
- Many fundamental functions work for scalars and arrays
- Ex: `x**2 + abs(x)` works for x scalar or array

Vectorization (2)

A mathematical function written for scalar arguments can (normally) take a array arguments:

```
>>> def f(x):
...     return x**2 + sinh(x)*exp(-x) + 1
...
>>> # scalar argument:
>>> x = 2
>>> f(x)
5.4908421805556333

>>> # array argument:
>>> y = array([2, -1, 0, 1.5])
>>> f(y)
array([ 5.49084218, -1.19452805,  1.        ,  3.72510647])
```

Vectorization of functions with if tests; problem

- Consider a function with an if test:

```
def somefunc(x):
    if x < 0:
        return 0
    else:
        return sin(x)

# or
def somefunc(x): return 0 if x < 0 else sin(x)
```

- This function works with a scalar `x` but not an array
- Problem: `x<0` results in a boolean array, not a boolean *value* that can be used in the if test

```
>>> x = linspace(-1, 1, 3); print x
[-1.  0.  1.]
>>> y = x < 0
>>> y
array([ True, False, False], dtype=bool)
>>> bool(y)  # turn object into a scalar boolean value
...
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

Vectorization of functions with if tests; solutions

- Simplest remedy: use NumPy's `vectorize` class to allow array arguments to a function:

```
>>> somefuncv = vectorize(somefunc, otypes=’d’)

>>> # test:
>>> x = linspace(-1, 1, 3); print x
[-1.  0.  1.]
>>> somefuncv(x)
array([ 0.        ,  0.        ,  0.84147098])
```

  Note: The data type must be specified as a character (`’d’` for double)

- The speed of `somefuncv` is unfortunately quite slow
- A better solution, using `where`:

```
def somefuncv2(x):
    x1 = zeros(x.size, float)
    x2 = sin(x)
    return where(x < 0, x1, x2)
```

General vectorization of if-else tests

```
def f(x):                     # scalar x
    if condition:
        x = <expression1>
    else:
        x = <expression2>
    return x

def f_vectorized(x):          # scalar or array x
    x1 = <expression1>
    x2 = <expression2>
    return where(condition, x1, x2)
```

Vectorization via slicing

- Consider a recursion scheme like

$$u_i^{\ell+1} = \beta u_{i-1}^{\ell} + (1-2\beta)u_i^{\ell} + \beta u_{i+1}^{\ell}, \quad i = 1,\ldots,n-1,$$

  (which arises from a one-dimensional diffusion equation)

- Straightforward (slow) Python implementation:

```
n = size(u)-1
for i in xrange(1,n,1):
    u_new[i] = beta*u[i-1] + (1-2*beta)*u[i] + beta*u[i+1]
```

- Slices enable us to vectorize the expression:

```
u[1:n] = beta*u[0:n-1] + (1-2*beta)*u[1:n] + beta*u[2:n+1]
```

Random numbers

- Drawing scalar random numbers:

```
import random
random.seed(2198)  # control the seed
print ’uniform random number on (0,1):’,  random.random()
print ’uniform random number on (-1,1):’, random.uniform(-1,1)
print ’Normal(0,1) random number:’,       random.gauss(0,1)
```

- Vectorized drawing of random numbers (arrays):

```
from numpy import random

random.seed(12)                # set seed
u = random.random(n)           # n uniform numbers on (0,1)
u = random.uniform(-1, 1, n)   # n uniform numbers on (-1,1)
u = random.normal(m, s, n)     # n numbers from N(m,s)
```

- Note that both modules have the name `random`! A remedy:

```
import random as random_number   # rename random for scalars
from numpy import *              # random is now numpy.random
```

Basic linear algebra

NumPy contains the `linalg` module for

- solving linear systems
- computing the determinant of a matrix
- computing the inverse of a matrix
- computing eigenvalues and eigenvectors of a matrix
- solving least-squares problems
- computing the singular value decomposition of a matrix
- computing the Cholesky decomposition of a matrix

A linear algebra session

```
from numpy import *   # includes import of linalg

# fill matrix A and vectors x and b
b = dot(A, x)             # matrix-vector product
y = linalg.solve(A, b)    # solve A*y = b

if allclose(x, y, atol=1.0E-12, rtol=1.0E-12):
    print ’correct solution!’

d = linalg.det(A)
B = linalg.inv(A)

# check result:
R = dot(A, B) - eye(n)   # residual
R_norm = linalg.norm(R)  # Frobenius norm of matrix R
print ’Residual R = A*A-inverse - I:’, R_norm

A_eigenvalues = linalg.eigvals(A)  # eigenvalues only
A_eigenvalues, A_eigenvectors = linalg.eig(A)

for e, v in zip(A_eigenvalues, A_eigenvectors):
    print ’eigenvalue %g has corresponding vector\n%s’ % (e, v)
```

Modules for curve plotting and 2D/3D visualization

- Matplotlib (curve plotting, 2D scalar and vector fields)
- PyX (PostScript/TeX-like drawing)
- Interface to Gnuplot
- Interface to Vtk
- Interface to OpenDX
- Interface to IDL
- Interface to Grace
- Interface to Matlab
- Interface to R
- Interface to Blender

Curve plotting with Easyviz

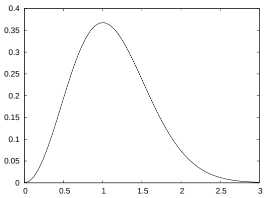
- Easyviz is a light-weight interface to many plotting packages, using a Matlab-like syntax
- Goal: write your program using Easyviz (“Matlab”) syntax and postpone your choice of plotting package
- Note: some powerful plotting packages (Vtk, R, matplotlib, ...) may be troublesome to install, while Gnuplot is easily installed on all platforms
- Easyviz supports (only) the most common plotting commands
- Easyviz is part of SciTools (Simula development)

  ```
  from scitools.all import *
  ```

  (imports all of `numpy`, all of `easyviz`, plus `scitools`)

Basic Easyviz example

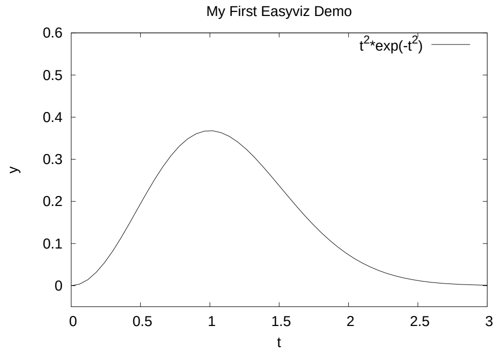
```
from scitools.all import *  # import numpy and plotting
t = linspace(0, 3, 51)      # 51 points between 0 and 3
y = t**2*exp(-t**2)         # vectorized expression
plot(t, y)
hardcopy(’tmp1.eps’)  # make PostScript image for reports
hardcopy(’tmp1.png’)  # make PNG image for web pages
```



Decorating the plot

```
plot(t, y)

xlabel(’t’)
ylabel(’y’)
legend(’t^2*exp(-t^2)’)
axis([0, 3, -0.05, 0.6])   # [tmin, tmax, ymin, ymax]
title(’My First Easyviz Demo’)

# or
plot(t, y, xlabel=’t’, ylabel=’y’,
     legend=’t^2*exp(-t^2)’,
     axis=[0, 3, -0.05, 0.6],
     title=’My First Easyviz Demo’,
     hardcopy=’tmp1.eps’,
     show=True)   # display on the screen (default)
```

The resulting plot

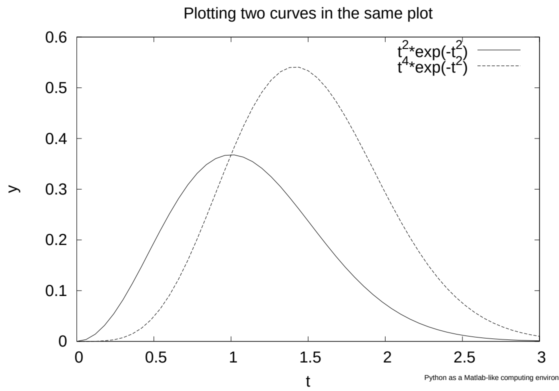


Plotting several curves in one plot

Compare $f_1(t) = t^2 e^{-t^2}$ and $f_2(t) = t^4 e^{-t^2}$ for $t \in [0, 3]$

```
from scitools.all import *   # for curve plotting

def f1(t):
    return t**2*exp(-t**2)

def f2(t):
    return t**2*f1(t)

t = linspace(0, 3, 51)
y1 = f1(t)
y2 = f2(t)

plot(t, y1)
hold(’on’)   # continue plotting in the same plot
plot(t, y2)

xlabel(’t’)
ylabel(’y’)
legend(’t^2*exp(-t^2)’, ’t^4*exp(-t^2)’)
title(’Plotting two curves in the same plot’)
hardcopy(’tmp2.eps’)
```

The resulting plot



Example: plot a function given on the command line

- Task: plot (e.g.) $f(x) = e^{-0.2x} \sin(2\pi x)$ for $x \in [0, 4\pi]$
- Specify $f(x)$ and x interval as text on the command line:

  ```
  Unix/DOS> python plotf.py "exp(-0.2*x)*sin(2*pi*x)" 0 4*pi
  ```

- Program:

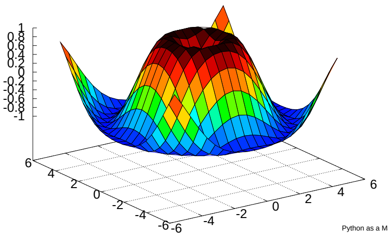
  ```
  from scitools.all import *
  formula = sys.argv[1]
  xmin = eval(sys.argv[2])
  xmax = eval(sys.argv[3])

  x = linspace(xmin, xmax, 101)
  y = eval(formula)
  plot(x, y, title=formula)
  ```

- Thanks to `eval`, input (text) with correct Python syntax can be turned to running code on the fly

---

Plotting 2D scalar fields

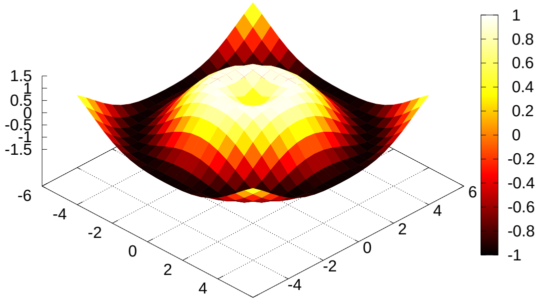
```
from scitools.all import *

x = y = linspace(-5, 5, 21)
xv, yv = ndgrid(x, y)
values = sin(sqrt(xv**2 + yv**2))
surf(xv, yv, values)
```



Adding plot features

```
# Matlab style commands:
setp(interactive=False)
surf(xv, yv, values)
shading('flat')
colorbar()
colormap(hot())
axis([-6,6,-6,6,-1.5,1.5])
view(35,45)
show()

# Optional Easyviz (Pythonic) short cut:
surf(xv, yv, values,
     shading='flat',
     colorbar='on',
     colormap=hot(),
     axis=[-6,6,-6,6,-1.5,1.5],
     view=[35,45])
```

The resulting plot



Other commands for visualizing 2D scalar fields

- `contour` (standard contours)), `contourf` (filled contours), `contour3` (elevated contours)
- `mesh` (elevated mesh), `meshc` (elevated mesh with contours in the xy plane)
- `surf` (colored surface), `surfc` (colored surface with contours in the xy plane)
- `pcolor` (colored cells in a 2D mesh)

Commands for visualizing 3D fields

Scalar fields:

- `isosurface`
- `slice_` (colors in slice plane), `contourslice` (contours in slice plane)

Vector fields:

- `quiver3` (arrows), (`quiver` for 2D vector fields)
- `streamline`, `streamtube`, `streamribbon` (flow sheets)

More info about Easyviz

- A plain text version of the Easyviz manual:

  ```
  pydoc scitools.easyviz
  ```

- The HTML version:

  `http://folk.uio.no/hpl/easyviz/`

- Download SciTools (incl. Easyviz):

  `http://code.google.com/p/scitools/`

File I/O with arrays; plain ASCII format

- Plain text output to file (just dump `repr(array)`):

  ```
  a = linspace(1, 21, 21); a.shape = (2,10)

  file = open('tmp.dat', 'w')
  file.write('Here is an array a:\n')
  file.write(repr(a))   # dump string representation of a
  file.close()
  ```

- Plain text input (just take `eval` on input line):

  ```
  file = open('tmp.dat', 'r')
  file.readline()  # load the first line (a comment)
  b = eval(file.read())
  file.close()
  ```

File I/O with arrays; binary pickling

- Dump arrays with `cPickle`:

  ```
  # a1 and a2 are two arrays

  import cPickle
  file = open('tmp.dat', 'wb')
  file.write('This is the array a1:\n')
  cPickle.dump(a1, file)
  file.write('Here is another array a2:\n')
  cPickle.dump(a2, file)
  file.close()
  ```

- Read in the arrays again (in correct order):

  ```
  file = open('tmp.dat', 'rb')
  file.readline()  # swallow the initial comment line
  b1 = cPickle.load(file)
  file.readline()  # swallow next comment line
  b2 = cPickle.load(file)
  file.close()
  ```

ScientificPython

- ScientificPython (by Konrad Hinsen)
- Modules for automatic differentiation, interpolation, data fitting via nonlinear least-squares, root finding, numerical integration, basic statistics, histogram computation, visualization, parallel computing (via MPI or BSP), physical quantities with dimension (units), 3D vectors/tensors, polynomials, I/O support for Fortran files and netCDF
- Very easy to install

ScientificPython: numbers with units

```
>>> from Scientific.Physics.PhysicalQuantities \
         import PhysicalQuantity as PQ
>>> m = PQ(12, ’kg’)        # number, dimension
>>> a = PQ(’0.88 km/s**2’)  # alternative syntax (string)
>>> F = m*a
>>> F
PhysicalQuantity(10.56,’kg*km/s**2’)
>>> F = F.inBaseUnits()
>>> F
PhysicalQuantity(10560.0,’m*kg/s**2’)
>>> F.convertToUnit(’MN’)  # convert to Mega Newton
>>> F
PhysicalQuantity(0.01056,’MN’)
>>> F = F + PQ(0.1, ’kPa*m**2’)  # kilo Pascal m^2
>>> F
PhysicalQuantity(0.010759999999999999,’MN’)
>>> F.getValue()
0.010759999999999999
```

SciPy

- SciPy is a comprehensive package (by Eric Jones, Travis Oliphant, Pearu Peterson) for scientific computing with Python
- Much overlap with ScientificPython
- SciPy interfaces many classical Fortran packages from Netlib (QUADPACK, ODEPACK, MINPACK, ...)
- Functionality: special functions, linear algebra, numerical integration, ODEs, random variables and statistics, optimization, root finding, interpolation, ...
- May require some installation efforts (applies ATLAS)
- See www.scipy.org

SymPy: symbolic computing in Python

- SymPy is a Python package for symbolic computing
- Easy to install, easy to extend
- Easy to use:

```
>>> from sympy import *
>>> x = Symbol(’x’)
>>> f = cos(acos(x))
>>> f
cos(acos(x))
>>> sin(x).series(x, 4)       # 4 terms of the Taylor series
x - 1/6*x**3 + O(x**4)
>>> dcos = diff(cos(2*x), x)
>>> dcos
-2*sin(2*x)
>>> dcos.subs(x, pi).evalf()  # x=pi, float evaluation
0
>>> I = integrate(log(x), x)
>>> print I
-x + x*log(x)
```

Python + Matlab = true

- A Python module, pymat, enables communication with Matlab:

```
from numpy import *
import pymat

x = linspace(0, 4*math.pi, 11)
m = pymat.open()
# can send numpy arrays to Matlab:
pymat.put(m, ’x’, x);
pymat.eval(m, ’y = sin(x)’)
pymat.eval(m, ’plot(x,y)’)
# get a new numpy array back:
y = pymat.get(m, ’y’)
```

Mixed language programming

Contents

- Why Python and C are two different worlds
- Wrapper code
- Wrapper tools
- F2PY: wrapping Fortran (and C) code
- SWIG: wrapping C and C++ code

More info

- Ch. 5 in the course book
- F2PY manual
- SWIG manual
- Examples coming with the SWIG source code
- Ch. 9 and 10 in the course book

Optimizing slow Python code

- Identify bottlenecks (via profiling)
- Migrate slow functions to Fortran, C, or C++
- Tools make it easy to combine Python with Fortran, C, or C++

Getting started: Scientific Hello World

- Python-F77 via F2PY
- Python-C via SWIG
- Python-C++ via SWIG

Later: Python interface to `oscillator` code for interactive computational steering of simulations (using F2PY)

The nature of Python vs. C

- A Python variable can hold different objects:

```
d = 3.2    # d holds a float
d = 'txt'  # d holds a string
d = Button(frame, text='push')  # instance of class Button
```

- In C, C++ and Fortran, a variable is declared of a specific type:

```
double d; d = 4.2;
d = "some string";  /* illegal, compiler error */
```

- This difference makes it quite complicated to call C, C++ or Fortran from Python

---

Calling C from Python

- Suppose we have a C function

```
extern double hw1(double r1, double r2);
```

- We want to call this from Python as

```
from hw import hw1
r1 = 1.2; r2 = -1.2
s = hw1(r1, r2)
```

- The Python variables `r1` and `r2` hold numbers (`float`), we need to extract these in the C code, convert to `double` variables, then call `hw1`, and finally convert the `double` result to a Python `float`
- All this conversion is done in *wrapper code*

Wrapper code

- Every object in Python is represented by C struct `PyObject`
- Wrapper code converts between `PyObject` variables and plain C variables (from `PyObject r1` and `r2` to `double`, and `double` result to `PyObject`):

```
static PyObject *_wrap_hw1(PyObject *self, PyObject *args) {
    PyObject *resultobj;
    double arg1, arg2, result;

    PyArg_ParseTuple(args,(char *)"dd:hw1",&arg1,&arg2))

    result = hw1(arg1,arg2);

    resultobj = PyFloat_FromDouble(result);
    return resultobj;
}
```

Extension modules

- The wrapper function and `hw1` must be compiled and linked to a shared library file
- This file can be loaded in Python as module
- Such modules written in other languages are called *extension modules*

Writing wrapper code

- A wrapper function is needed for each C function we want to call from Python
- Wrapper codes are tedious to write
- There are tools for automating wrapper code development
- We shall use SWIG (for C/C++) and F2PY (for Fortran)

Integration issues

- Direct calls through wrapper code enables efficient data transfer; large arrays can be sent by pointers
- COM, CORBA, ILU, .NET are different technologies; more complex, less efficient, but safer (data are copied)
- Jython provides a seamless integration of Python and Java

Scientific Hello World example

- Consider this Scientific Hello World module (hw):

```
import math, sys

def hw1(r1, r2):
    s = math.sin(r1 + r2)
    return s

def hw2(r1, r2):
    s = math.sin(r1 + r2)
    print 'Hello, World! sin(%g+%g)=%g' % (r1,r2,s)
```

  Usage:

```
from hw import hw1, hw2
print hw1(1.0, 0)
hw2(1.0, 0)
```

- We want to implement the module in Fortran 77, C and C++, and use it as if it were a pure Python module

Fortran 77 implementation

- We start with Fortran (F77);
  Python-F77 is simpler than Python-C (because F2PY almost automates Py-F77 integration)
- F77 code:

```
      real*8 function hw1(r1, r2)
      real*8 r1, r2
      hw1 = sin(r1 + r2)
      return
      end

      subroutine hw2(r1, r2)
      real*8 r1, r2, s
      s = sin(r1 + r2)
      write(*,1000) 'Hello, World! sin(',r1+r2,')=',s
 1000 format(A,F6.3,A,F8.6)
      return
      end
```

One-slide F77 course

- Fortran is case insensitive (`reAL` is as good as `real`)
- One statement per line, must start in column 7 or later
- Comma on separate lines
- All function arguments are input and output
  (as pointers in C, or references in C++)
- A function returning one value is called `function`
- A function returning no value is called `subroutine`
- Types: `real`, `double precision`, `real*4`, `real*8`, `integer`, `character` (array)
- Arrays: just add dimension, as in
  `real*8 a(0:m, 0:n)`
- Format control of output requires `FORMAT` statements

Using F2PY

- F2PY automates integration of Python and Fortran
- Say the F77 code is in the file `hw.f`
- Make a subdirectory for wrapping code:

```
mkdir f2py-hw; cd f2py-hw
```

- Run F2PY:

```
f2py -m hw -c ../hw.f
```

- Load module into Python and test:

```
from hw import hw1, hw2
print hw1(1.0, 0)
hw2(1.0, 0)
```

- It cannot be simpler!

Call by reference issues

- In Fortran (and C/C++) functions often modify arguments; here the result `s` is an output *argument*:

```
      subroutine hw3(r1, r2, s)
      real*8 r1, r2, s
      s = sin(r1 + r2)
      return
      end
```

- Running F2PY results in a module with wrong behavior:

```
>>> from hw import hw3
>>> r1 = 1;  r2 = -1;  s = 10
>>> hw3(r1, r2, s)
>>> print s
10   # should be 0
```

- Why? F2PY assumes that all arguments are input arguments

Check F2PY-generated doc strings

- F2PY generates doc strings that document the interface:

```
>>> import hw
>>> print hw.__doc__
Functions:
  hw1 = hw1(r1,r2)
  hw2(r1,r2)
  hw3(r1,r2,s)

>>> print hw.hw3.__doc__
hw3 - Function signature:
  hw3(r1,r2,s)
Required arguments:
  r1 : input float
  r2 : input float
  s : input float
```

- `hw3` assumes `s` is *input* argument!

Interface files

- We can tailor the interface by editing an F2PY-generated *interface file*
- Run F2PY in two steps: (i) generate interface file, (ii) generate wrapper code, compile and link
- Generate interface file `hw.pyf` (`-h` option):

```
f2py -m hw -h hw.pyf ../hw.f
```

Outline of the interface file

- The interface applies a Fortran 90 module (class) syntax
- Each function/subroutine, its arguments and its return value is specified:

```
python module hw ! in
    interface  ! in :hw
        ...
        subroutine hw3(r1,r2,s) ! in :hw:../hw.f
            real*8 :: r1
            real*8 :: r2
            real*8 :: s
        end subroutine hw3
    end interface
end python module hw
```

(Fortran 90 syntax)

Adjustment of the interface

- We may edit `hw.pyf` and specify `s` in `hw3` as an output argument, using F90's `intent(out)` keyword:

```
python module hw ! in
    interface  ! in :hw
        ...
        subroutine hw3(r1,r2,s) ! in :hw:../hw.f
            real*8 :: r1
            real*8 :: r2
            real*8, intent(out) :: s
        end subroutine hw3
    end interface
end python module hw
```

- Next step: run F2PY with the edited interface file:

```
f2py -c hw.pyf ../hw.f
```

Output arguments are returned

- Load the module and print its doc string:

```
>>> import hw
>>> print hw.__doc__
Functions:
  hw1 = hw1(r1,r2)
  hw2(r1,r2)
  s = hw3(r1,r2)
```

  Oops! `hw3` takes only two arguments and *returns* `s`!
- This is the “Pythonic” function style; input data are arguments, output data are returned
- By default, F2PY treats all arguments as input
- F2PY generates Pythonic interfaces, different from the original Fortran interfaces, so check out the module’s doc string!

General adjustment of interfaces

- Function with multiple input and output variables

```
subroutine somef(i1, i2, o1, o2, o3, o4, io1)
```

- input: `i1`, `i2`
- output: `o1`, ..., `o4`
- input *and* output: `io1`
- Pythonic interface:

```
o1, o2, o3, o4, io1 = somef(i1, i2, io1)
```

Specification of input/output arguments

- In the interface file:

```
python module somemodule
    interface
        ...
        subroutine somef(i1, i2, o1, o2, o3, o4, io1)
            real*8, intent(in) :: i1
            real*8, intent(in) :: i2
            real*8, intent(out) :: o1
            real*8, intent(out) :: o2
            real*8, intent(out) :: o3
            real*8, intent(out) :: o4
            real*8, intent(in,out) :: io1
        end subroutine somef
        ...
    end interface
end python module somemodule
```

- Note: no `intent` implies `intent(in)`

Specification of input/output arguments

- Instead of editing the interface file, we can add special F2PY comments in the Fortran source code:

```
       subroutine somef(i1, i2, o1, o2, o3, o4, io1)
       real*8 i1, i2, o1, o2, o3, o4, io1
Cf2py  intent(in) i1
Cf2py  intent(in) i2
Cf2py  intent(out) o1
Cf2py  intent(out) o2
Cf2py  intent(out) o3
Cf2py  intent(out) o4
Cf2py  intent(in,out) io1
```

- Now a single F2PY command generates correct interface:

```
f2py -m hw -c ../hw.f
```

Integration of Python and C

- Let us implement the `hw` module in C:

```
#include <stdio.h>
#include <math.h>
#include <stdlib.h>

double hw1(double r1, double r2)
{
  double s;  s = sin(r1 + r2);  return s;
}

void hw2(double r1, double r2)
{
  double s;  s = sin(r1 + r2);
  printf("Hello, World! sin(%g+%g)=%g\n", r1, r2, s);
}

/* special version of hw1 where the result is an argument: */
void hw3(double r1, double r2, double *s)
{
  *s = sin(r1 + r2);
}
```

Using F2PY

- F2PY can also wrap C code if we specify the function signatures as Fortran 90 modules
- My procedure:
    - write the C functions as empty Fortran 77 functions or subroutines
    - run F2PY on the Fortran specification to generate an interface file
    - run F2PY with the interface file and the C source code

Step 1: Write Fortran 77 signatures

```
C file signatures.f

      real*8 function hw1(r1, r2)
Cf2py intent(c) hw1
      real*8 r1, r2
Cf2py intent(c) r1, r2
      end

      subroutine hw2(r1, r2)
Cf2py intent(c)  hw2
      real*8 r1, r2
Cf2py intent(c) r1, r2
      end

      subroutine hw3(r1, r2, s)
Cf2py intent(c) hw3
      real*8 r1, r2, s
Cf2py intent(c) r1, r2
Cf2py intent(out) s
      end
```

Step 2: Generate interface file

- Run

```
Unix/DOS> f2py -m hw -h hw.pyf signatures.f
```

- Result: `hw.pyf`

```
python module hw ! in
    interface  ! in :hw
        function hw1(r1,r2) ! in :hw:signatures.f
            intent(c) hw1
            real*8 intent(c) :: r1
            real*8 intent(c) :: r2
            real*8 intent(c) :: hw1
        end function hw1
        ...
        subroutine hw3(r1,r2,s) ! in :hw:signatures.f
            intent(c) hw3
            real*8 intent(c) :: r1
            real*8 intent(c) :: r2
            real*8 intent(out) :: s
        end subroutine hw3
    end interface
end python module hw
```

Step 3: compile C code into extension module

- Run

```
Unix/DOS> f2py -c hw.pyf hw.c
```

- Test:

```
import hw
print hw.hw3(1.0,-1.0)
print hw.__doc__
```

- One can either write the interface file by hand or write F77 code to generate, but for every C function the Fortran signature must be specified

---

Using SWIG

- Wrappers to C and C++ codes can be automatically generated by SWIG
- SWIG is more complicated to use than F2PY
- First make a SWIG interface file
- Then run SWIG to generate wrapper code
- Then compile and link the C code and the wrapper code

SWIG interface file

- The interface file contains C preprocessor directives and special SWIG directives:

```
/* file: hw.i */
%module hw
%{
/* include C header files necessary to compile the interface */
#include "hw.h"
%}

/* list functions to be interfaced: */
double hw1(double r1, double r2);
void   hw2(double r1, double r2);
void   hw3(double r1, double r2, double *s);
# or
%include "hw.h"  /* make interface to all funcs in hw.h */
```

Making the module

- Run SWIG (preferably in a subdirectory):

```
swig -python -I.. hw.i
```

- SWIG generates wrapper code in

```
hw_wrap.c
```

- Compile and link a shared library module:

```
gcc -I.. -O -I/some/path/include/python2.3 \
    -c ../hw.c hw_wrap.c
gcc -shared -o _hw.so hw.o hw_wrap.o
```

Note the underscore prefix in `_hw.so`

A build script

- Can automate the compile+link process
- Can use Python to extract where `Python.h` resides (needed by any wrapper code)

```
swig -python -I.. hw.i

root=‘python -c ’import sys; print sys.prefix’‘
ver=‘python -c ’import sys; print sys.version[:3]’‘
gcc -O -I.. -I$root/include/python$ver -c ../hw.c hw_wrap.c
gcc -shared -o _hw.so hw.o hw_wrap.o

python -c "import hw" # test
```

(these statements are found in `make_module_1.sh`)

- The module consists of two files: `hw.py` (which loads) `_hw.so`

Building modules with Distutils (1)

- Python has a tool, Distutils, for compiling and linking extension modules
- First write a script `setup.py`:

```
import os
from distutils.core import setup, Extension

name = ’hw’           # name of the module
version = 1.0         # the module’s version number

swig_cmd = ’swig -python -I.. %s.i’ % name
print ’running SWIG:’, swig_cmd
os.system(swig_cmd)

sources = [’../hw.c’, ’hw_wrap.c’]

setup(name = name, version = version,
      ext_modules = [Extension(’_’ + name,  # SWIG requires _
                               sources,
                               include_dirs=[os.pardir])
                     ])
```

Building modules with Distutils (2)

- Now run

```
python setup.py build_ext
python setup.py install --install-platlib=.
python -c ’import hw’  # test
```

- Can install resulting module files in any directory
- Use Distutils for professional distribution!

Testing the hw3 function

- Recall hw3:

```
void hw3(double r1, double r2, double *s)
{
  *s = sin(r1 + r2);
}
```

- Test:

```
>>> from hw import hw3
>>> r1 = 1;  r2 = -1;  s = 10
>>> hw3(r1, r2, s)
>>> print s
10   # should be 0 (sin(1-1)=0)
```

Major problem - as in the Fortran case

Specifying input/output arguments

- We need to adjust the SWIG interface file:

```
/* typemaps.i allows input and output pointer arguments to be
   specified using the names INPUT, OUTPUT, or INOUT */
%include "typemaps.i"

void   hw3(double r1, double r2, double *OUTPUT);
```

- Now the usage from Python is

```
s = hw3(r1, r2)
```

- Unfortunately, SWIG does not document this in doc strings

Other tools

- Pyfort for Python-Fortran integration
  (does not handle F90/F95, not as simple as F2PY)
- SIP: tool for wrapping C++ libraries
- Boost.Python: tool for wrapping C++ libraries
- CXX: C++ interface to Python (Boost is a replacement)
- Note: SWIG can generate interfaces to most scripting languages
  (Perl, Ruby, Tcl, Java, Guile, Mzscheme, ...)

Integrating Python with C++

- SWIG supports C++
- The only difference is when we run SWIG (`-c++` option):

```
swig -python -c++ -I.. hw.i
# generates wrapper code in hw_wrap.cxx
```

- Use a C++ compiler to compile and link:

```
root=‘python -c ’import sys; print sys.prefix’‘
ver=‘python -c ’import sys; print sys.version[:3]’‘
g++ -O -I.. -I$root/include/python$ver \
    -c ../hw.cpp hw_wrap.cxx
g++ -shared -o _hw.so hw.o hw_wrap.o
```

Interfacing C++ functions (1)

- This is like interfacing C functions, except that pointers are usual replaced by references

```
void hw3(double r1, double r2, double *s)  // C style
{ *s = sin(r1 + r2); }

void hw4(double r1, double r2, double& s)  // C++ style
{ s = sin(r1 + r2); }
```

Interfacing C++ functions (2)

- Interface file (`hw.i`):

```
%module hw
%{
#include "hw.h"
%}
%include "typemaps.i"
%apply double *OUTPUT { double* s }
%apply double *OUTPUT { double& s }
%include "hw.h"
```

- That's it!

Interfacing C++ classes

- C++ classes add more to the SWIG-C story
- Consider a class version of our Hello World module:

```
class HelloWorld
{
 protected:
  double r1, r2, s;
  void compute();    // compute s=sin(r1+r2)
 public:
  HelloWorld();
  ~HelloWorld();

  void set(double r1, double r2);
  double get() const { return s; }
  void message(std::ostream& out) const;
};
```

- Goal: use this class as a Python class

Function bodies and usage

- Function bodies:

```
void HelloWorld:: set(double r1_, double r2_)
{
  r1 = r1_;  r2 = r2_;
  compute();  // compute s
}
void HelloWorld:: compute()
{ s = sin(r1 + r2); }
```

  etc.
- Usage:

```
HelloWorld hw;
hw.set(r1, r2);
hw.message(std::cout);  // write "Hello, World!" message
```

- Files: `HelloWorld.h`, `HelloWorld.cpp`

Adding a subclass

- To illustrate how to handle class hierarchies, we add a subclass:

```
class HelloWorld2 : public HelloWorld
{
 public:
  void gets(double& s_) const;
};

void HelloWorld2:: gets(double& s_) const { s_ = s; }
```

  i.e., we have a function with an output argument
- Note: `gets` should return the value when called from Python
- Files: `HelloWorld2.h`, `HelloWorld2.cpp`

SWIG interface file

```
/* file: hw.i */
%module hw
%{
/* include C++ header files necessary to compile the interface */
#include "HelloWorld.h"
#include "HelloWorld2.h"
%}

%include "HelloWorld.h"

%include "typemaps.i"
%apply double* OUTPUT { double& s }
%include "HelloWorld2.h"
```

Adding a class method

- SWIG allows us to add class methods
- Calling `message` with standard output (`std::cout`) is tricky from Python so we add a `print` method for printing to std.output
- `print` coincides with Python's keyword `print` so we follow the convention of adding an underscore:

  ```
  %extend HelloWorld {
      void print_() { self->message(std::cout); }
  }
  ```

- This is basically C++ syntax, but `self` is used instead of `this` and `%extend HelloWorld` is a SWIG directive
- Make extension module:

  ```
  swig -python -c++ -I.. hw.i
  # compile HelloWorld.cpp HelloWorld2.cpp hw_wrap.cxx
  # link HelloWorld.o HelloWorld2.o hw_wrap.o to _hw.so
  ```

Using the module

```
from hw import HelloWorld

hw = HelloWorld()  # make class instance
r1 = float(sys.argv[1]);  r2 = float(sys.argv[2])
hw.set(r1, r2)     # call instance method
s = hw.get()
print "Hello, World! sin(%g + %g)=%g" % (r1, r2, s)
hw.print_()

hw2 = HelloWorld2()  # make subclass instance
hw2.set(r1, r2)
s = hw.gets()        # original output arg. is now return value
print "Hello, World2! sin(%g + %g)=%g" % (r1, r2, s)
```

Remark

- It looks that the C++ class hierarchy is mirrored in Python
- Actually, SWIG wraps a *function* interface to any class:

  ```
  import _hw   # use _hw.so directly
  _hw.HelloWorld_set(r1, r2)
  ```

- SWIG also makes a proxy class in `hw.py`, mirroring the original C++ class:

  ```
  import hw    # use hw.py interface to _hw.so
  c = hw.HelloWorld()
  c.set(r1, r2)   # calls _hw.HelloWorld_set(r1, r2)
  ```

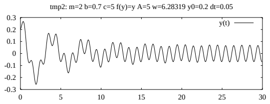
- The proxy class introduces overhead

Computational steering

- Consider a simulator written in F77, C or C++
- Aim: write the administering code and run-time visualization in Python
- Use a Python interface to Gnuplot
- Use NumPy arrays in Python
- F77/C and NumPy arrays share the same data
- Result:
  - steer simulations through scripts
  - do low-level numerics efficiently in C/F77
  - send simulation data to plotting a program

  The best of all worlds?

Example on computational steering



Consider the `oscillator` code. The following interactive features would be nice:

- set parameter values
- run the simulator for a number of steps and visualize
- change a parameter
- option: rewind a number of steps
- continue simulation and visualization

Realization (1)

- Here is an interactive session:

  ```
  >>> from simviz_f77 import *
  >>> A=1; w=4*math.pi  # change parameters
  >>> setprm()   # send parameters to oscillator code
  >>> run(60)    # run 60 steps and plot solution
  >>> w=math.pi  # change frequency
  >>> setprm()   # update prms in oscillator code
  >>> rewind(30) # rewind 30 steps
  >>> run(120)   # run 120 steps and plot
  >>> A=10; setprm()
  >>> rewind()   # rewind to t=0
  >>> run(400)
  ```

Realization (2)

- The F77 code performs the numerics
- Python is used for the interface (`setprm`, `run`, `rewind`, plotting)
- F2PY was used to make an interface to the F77 code (fully automated process)
- Arrays (NumPy) are created in Python and transferred to/from the F77 code
- Python communicates with both the simulator and the plotting program ("sends pointers around")

About the F77 code

- Physical and numerical parameters are in a common block
- `scan2` sets parameters in this common block:

  ```
  subroutine scan2(m_, b_, c_, A_, w_, y0_, tstop_, dt_, func_)
  real*8 m_, b_, c_, A_, w_, y0_, tstop_, dt_
  character func_*(*)
  ```

  can use `scan2` to send parameters from Python to F77
- `timeloop2` performs `nsteps` time steps:

  ```
  subroutine timeloop2(y, n, maxsteps, step, time, nsteps)

  integer n, step, nsteps, maxsteps
  real*8 time, y(n,0:maxsteps-1)
  ```

  solution available in `y`

Creating a Python interface w/F2PY

- `scan2`: trivial (only input arguments)
- `timestep2`: need to be careful with
  - output and input/output arguments
  - multi-dimensional arrays (`y`)
- Note: multi-dimensional arrays are stored differently in Python (i.e. C) and Fortran!

Using timeloop2 from Python

- This is how we would like to write the Python code:

  ```
  maxsteps = 10000; n = 2
  y = zeros((n,maxsteps), Float)
  step = 0; time = 0.0

  def run(nsteps):
      global step, time, y

      y, step, time = \
         oscillator.timeloop2(y, step, time, nsteps)

      y1 = y[0,0:step+1]
      g.plot(Gnuplot.Data(t, y1, with='lines'))
  ```

Arguments to timeloop2

- Subroutine signature:

  ```
  subroutine timeloop2(y, n, maxsteps, step, time, nsteps)

  integer n, step, nsteps, maxsteps
  real*8 time, y(n,0:maxsteps-1)
  ```
- Arguments:

  ```
  y  : solution (all time steps), input and output
  n  : no of solution components (2 in our example), input
  maxsteps : max no of time steps, input
  step   : no of current time step, input and output
  time   : current value of time, input and output
  nsteps : no of time steps to advance the solution
  ```

Interfacing the timeloop2 routine

- Use `Cf2py` comments to specify argument type:

  ```
  Cf2py intent(in,out) step
  Cf2py intent(in,out) time
  Cf2py intent(in,out) y
  Cf2py intent(in)     nsteps
  ```
- Run F2PY:

  ```
  f2py -m oscillator -c --build-dir tmp1 --fcompiler='Gnu' \
     ../timeloop2.f \
     $scripting/src/app/oscillator/F77/oscillator.f \
     only: scan2 timeloop2 :
  ```

Testing the extension module

- Import and print documentation:

  ```
  >>> import oscillator
  >>> print oscillator.__doc__
  This module 'oscillator' is auto-generated with f2py
  Functions:
    y,step,time = timeloop2(y,step,time,nsteps,
                            n=shape(y,0),maxsteps=shape(y,1))
    scan2(m_,b_,c_,a_,w_,y0_,tstop_,dt_,func_)
  COMMON blocks:
    /data/ m,b,c,a,w,y0,tstop,dt,func(20)
  ```
- Note: array dimensions (`n`, `maxsteps`) are moved to the end of the argument list and given default values!
- Rule: always print and study the doc string since F2PY perturbs the argument list

More info on the current example

- Directory with Python interface to the oscillator code:

  ```
  src/py/mixed/simviz/f2py/
  ```
- Files:

  ```
  simviz_steering.py    :  complete script running oscillator
                           from Python by calling F77 routines
  simvizGUI_steering.py :  as simviz_steering.py, but with a GUI
  make_module.sh        :  build extension module
  ```

Comparison with Matlab

- The demonstrated functionality can be coded in Matlab
- Why Python + F77?
- We can define our own interface in a much more powerful language (Python) than Matlab
- We can much more easily transfer data to and from or own F77 or C or C++ libraries
- We can use any appropriate visualization tool
- We can call up Matlab if we want
- Python + F77 gives tailored interfaces and maximum flexibility

Contents

- Migrating slow for loops over NumPy arrays to Fortran, C and C++
- F2PY handling of arrays
- Handwritten C and C++ modules
- C++ class for wrapping NumPy arrays
- C++ modules using SCXX
- Pointer communication and SWIG
- Efficiency considerations

More info

- Ch. 5, 9 and 10 in the course book
- F2PY manual
- SWIG manual
- Examples coming with the SWIG source code
- Electronic Python documentation:
  Extending and Embedding..., Python/C API
- Python in a Nutshell
- Python Essential Reference (Beazley)

Is Python slow for numerical computing?

- Fill a NumPy array with function values:

```
n = 2000
a = zeros((n,n))
xcoor = arange(0,1,1/float(n))
ycoor = arange(0,1,1/float(n))

for i in range(n):
    for j in range(n):
        a[i,j] = f(xcoor[i], ycoor[j])  # f(x,y) = sin(x*y) + 8*x
```

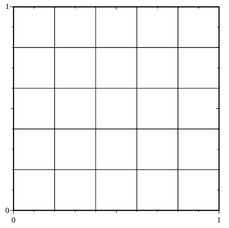
- Fortran/C/C++ version: (normalized) time 1.0
- NumPy vectorized evaluation of `f`: time 3.0
- Python loop version (version): time 140 (`math.sin`)
- Python loop version (version): time 350 (`numarray.sin`)

Comments

- Python loops over arrays are extremely slow
- NumPy vectorization may be sufficient
- However, NumPy vectorization may be inconvenient
  - plain loops in Fortran/C/C++ are much easier
- Write administering code in Python
- Identify bottlenecks (via profiling)
- Migrate slow Python code to Fortran, C, or C++
- Python-Fortran w/NumPy arrays via F2PY: easy
- Python-C/C++ w/NumPy arrays via SWIG: not that easy,
  handwritten wrapper code is most common

Case: filling a grid with point values

- Consider a rectangular 2D grid



- A NumPy array `a[i,j]` holds values at the grid points

Python object for grid data

- Python class:

```
class Grid2D:
    def __init__(self,
                 xmin=0, xmax=1, dx=0.5,
                 ymin=0, ymax=1, dy=0.5):
        self.xcoor = sequence(xmin, xmax, dx)
        self.ycoor = sequence(ymin, ymax, dy)

        # make two-dim. versions of these arrays:
        # (needed for vectorization in __call__)
        self.xcoorv = self.xcoor[:,NewAxis]
        self.ycoorv = self.ycoor[NewAxis,:]

    def __call__(self, f):
        # vectorized code:
        return f(self.xcoorv, self.ycoorv)
```

Slow loop

- Include a straight Python loop also:

```
class Grid2D:
    ....
    def gridloop(self, f):
        lx = size(self.xcoor); ly = size(self.ycoor)
        a = zeros((lx,ly))
        for i in range(lx):
            x = self.xcoor[i]
            for j in range(ly):
                y = self.ycoor[j]
                a[i,j] = f(x, y)
        return a
```

- Usage:

```
g = Grid2D(dx=0.01, dy=0.2)
def myfunc(x, y):
    return sin(x*y) + y
a = g(myfunc)
i=4; j=10;
print 'value at (%g,%g) is %g' % (g.xcoor[i],g.ycoor[j],a[i,j])
```

Migrate gridloop to F77

```
class Grid2Deff(Grid2D):
    def __init__(self,
                 xmin=0, xmax=1, dx=0.5,
                 ymin=0, ymax=1, dy=0.5):
        Grid2D.__init__(self, xmin, xmax, dx, ymin, ymax, dy)

    def ext_gridloop1(self, f):
        """compute a[i,j] = f(xi,yj) in an external routine."""
        lx = size(self.xcoor);  ly = size(self.ycoor)
        a = zeros((lx,ly))
        ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, f)
        return a
```

We can also migrate to C and C++ (done later)

F77 function

- First try (typical attempt by a Fortran/C programmer):

```
      subroutine gridloop1(a, xcoor, ycoor, nx, ny, func1)
      integer nx, ny
      real*8 a(0:nx-1,0:ny-1), xcoor(0:nx-1), ycoor(0:ny-1)
      real*8 func1
      external func1

      integer i,j
      real*8 x, y
      do j = 0, ny-1
         y = ycoor(j)
         do i = 0, nx-1
            x = xcoor(i)
            a(i,j) = func1(x, y)
         end do
      end do
      return
      end
```

- Note: `float` type in NumPy array *must* match `real*8` or `double precision` in Fortran! (Otherwise F2PY will take a copy of the array a so the type matches that in the F77 code)

Making the extension module

- Run F2PY:

```
f2py -m ext_gridloop -c gridloop.f
```

- Try it from Python:

```
import ext_gridloop
ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, myfunc,
                       size(self.xcoor), size(self.ycoor))
```

  wrong results; a is not modified!

- Reason: the `gridloop1` function works on a copy a (because higher-dimensional arrays are stored differently in C/Python and Fortran)

Array storage in Fortran and C/C++

- C and C++ has row-major storage
  (two-dimensional arrays are stored row by row)
- Fortran has column-major storage
  (two-dimensional arrays are stored column by column)
- Multi-dimensional arrays: first index has fastest variation in Fortran, last index has fastest variation in C and C++

Example: storing a 2x3 array

1	2	3	4	5	6	C storage
1	4	2	5	3	6	Fortran storage

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

F2PY and multi-dimensional arrays

- F2PY-generated modules treat storage schemes transparently
- If input array has C storage, a copy is taken, calculated with, and returned as output
- F2PY needs to know whether arguments are input, output or both
- To monitor (hidden) array copying, turn on the flag

```
f2py ... -DF2PY_REPORT_ON_ARRAY_COPY=1
```

- In-place operations on NumPy arrays are possible in Fortran, but the default is to work on a copy, that is why our `gridloop1` function does not work

---

Always specify input/output data

- Insert Cf2py comments to tell that a is an output variable:

```
      subroutine gridloop2(a, xcoor, ycoor, nx, ny, func1)
      integer nx, ny
      real*8 a(0:nx-1,ny-1), xcoor(0:nx-1), ycoor(0:ny-1), func1
      external func1
Cf2py intent(out) a
Cf2py intent(in) xcoor
Cf2py intent(in) ycoor
Cf2py depend(nx,ny) a
```

---

gridloop2 seen from Python

- F2PY generates this Python interface:

```
>>> import ext_gridloop
>>> print ext_gridloop.gridloop2.__doc__

gridloop2 - Function signature:
  a = gridloop2(xcoor,ycoor,func1,[nx,ny,func1_extra_args])
Required arguments:
  xcoor : input rank-1 array('d') with bounds (nx)
  ycoor : input rank-1 array('d') with bounds (ny)
  func1 : call-back function
Optional arguments:
  nx := len(xcoor) input int
  ny := len(ycoor) input int
  func1_extra_args := () input tuple
Return objects:
  a : rank-2 array('d') with bounds (nx,ny)
```

- `nx` and `ny` are optional (!)

Handling of arrays with F2PY

- Output arrays are returned and are not part of the argument list, as seen from Python
- Need `depend(nx,ny)` a to specify that a is to be created with size `nx`, `ny` in the wrapper
- Array dimensions are optional arguments (!)

```
class Grid2Deff(Grid2D):
    ...
    def ext_gridloop2(self, f):
        a = ext_gridloop.gridloop2(self.xcoor, self.ycoor, f)
        return a
```

- The modified interface is well documented in the doc strings generated by F2PY

Input/output arrays (1)

- What if we really want to send a as argument and let F77 modify it?

```
def ext_gridloop1(self, f):
    lx = size(self.xcoor);  ly = size(self.ycoor)
    a = zeros((lx,ly))
    ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, f)
    return a
```

- This is not Pythonic code, but it can be realized
- 1. the array must have Fortran storage
- 2. the array argument must be `intent(inout)` (in general not recommended)

Input/output arrays (2)

- F2PY generated modules has a function for checking if an array has column major storage (i.e., Fortran storage):

```
>>> a = zeros((n,n), order='Fortran')
>>> isfortran(a)
True
>>> a = asarray(a, order='C')  # back to C storage
>>> isfortran(a)
False
```

Input/output arrays (3)

- Fortran function:

```
      subroutine gridloop1(a, xcoor, ycoor, nx, ny, func1)
      integer nx, ny
      real*8 a(0:nx-1,ny-1), xcoor(0:nx-1), ycoor(0:ny-1), func1
C     call this function with an array a that has
C     column major storage!
Cf2py intent(inout) a
Cf2py intent(in) xcoor
Cf2py intent(in) ycoor
Cf2py depend(nx, ny) a
```

- Python call:

```
def ext_gridloop1(self, f):
    lx = size(self.xcoor);  ly = size(self.ycoor)
    a = asarray(a, order='Fortran')
    ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, f)
    return a
```

Storage compatibility requirements

- Only when a has Fortran (column major) storage, the Fortran function works on a itself
- If we provide a plain NumPy array, it has C (row major) storage, and the wrapper sends a copy to the Fortran function and transparently transposes the result
- Hence, F2PY is very user-friendly, at a cost of some extra memory
- The array returned from F2PY has Fortran (column major) storage

F2PY and storage issues

- `intent(out)` a is the right specification; a should not be an argument in the Python call
- F2PY wrappers will work on copies, if needed, and hide problems with different storage scheme in Fortran and C/Python
- Python call:

```
a = ext_gridloop.gridloop2(self.xcoor, self.ycoor, f)
```

Caution

- Find problems with this code (`comp` is a Fortran function in the extension module `pde`):

```
x = arange(0, 1, 0.01)
b = myfunc1(x)  # compute b array of size (n,n)
u = myfunc2(x)  # compute u array of size (n,n)
c = myfunc3(x)  # compute c array of size (n,n)

dt = 0.05
for i in range(n)
    u = pde.comp(u, b, c, i*dt)
```

About Python callbacks

- It is convenient to specify the `myfunc` in Python
- However, a callback to Python is costly, especially when done a large number of times (for every grid point)
- Avoid such callbacks; vectorize callbacks
- The Fortran routine should actually direct a back to Python (i.e., do nothing...) for a vectorized operation
- Let's do this for illustration

Vectorized callback seen from Python

```
class Grid2Deff(Grid2D):
    ...
    def ext_gridloop_vec(self, f):
        """Call extension, then do a vectorized callback to Python."""
        lx = size(self.xcoor);  ly = size(self.ycoor)
        a = zeros((lx,ly))
        a = ext_gridloop.gridloop_vec(a, self.xcoor, self.ycoor, f)
        return a

def myfunc(x, y):
    return sin(x*y) + 8*x

def myfuncf77(a, xcoor, ycoor, nx, ny):
    """Vectorized function to be called from extension module."""
    x = xcoor[:,NewAxis];  y = ycoor[NewAxis,:]
    a[:,:] = myfunc(x, y)  # in-place modification of a

g = Grid2Deff(dx=0.2, dy=0.1)
a = g.ext_gridloop_vec(myfuncf77)
```

Vectorized callback from Fortran

```
      subroutine gridloop_vec(a, xcoor, ycoor, nx, ny, func1)
      integer nx, ny
      real*8 a(0:nx-1,ny-1), xcoor(0:nx-1), ycoor(0:ny-1)
Cf2py intent(in,out) a
Cf2py intent(in) xcoor
Cf2py intent(in) ycoor
      external func1

C     fill array a with values taken from a Python function,
C     do that without loop and point-wise callback, do a
C     vectorized callback instead:
      call func1(a, xcoor, ycoor, nx, ny)

C     could work further with array a here...

      return
      end
```

Caution

- What about this Python callback:

```
def myfuncf77(a, xcoor, ycoor, nx, ny):
    """Vectorized function to be called from extension module."""
    x = xcoor[:,NewAxis];  y = ycoor[NewAxis,:]
    a = myfunc(x, y)
```

- a now refers to a new NumPy array; no in-place modification of the input argument

Avoiding callback by string-based if-else wrapper

- Callbacks are expensive
- Even vectorized callback functions degrades performace a bit
- Alternative: implement “callback” in F77
- Flexibility from the Python side: use a string to switch between the “callback” (F77) functions

```
a = ext_gridloop.gridloop2_str(self.xcoor, self.ycoor, ’myfunc’)
```

F77 wrapper:

```
       subroutine gridloop2_str(xcoor, ycoor, func_str)
       character*(*) func_str
       ...
      if (func_str .eq. ’myfunc’) then
         call gridloop2(a, xcoor, ycoor, nx, ny, myfunc)
      else if (func_str .eq. ’f2’) then
         call gridloop2(a, xcoor, ycoor, nx, ny, f2)
      ...
```

Compiled callback function

- Idea: if callback formula is a string, we could embed it in a Fortran function and call Fortran instead of Python
- F2PY has a module for “inline” Fortran code specification and building

```
source = """
      real*8 function fcb(x, y)
      real*8 x, y
      fcb = %s
      return
      end
""" % fstr
import f2py2e
f2py_args = "--fcompiler=’Gnu’ --build-dir tmp2 etc..."
f2py2e.compile(source, modulename=’callback’,
               extra_args=f2py_args, verbose=True,
               source_fn=’sourcecodefile.f’)
import callback
<work with the new extension module>
```

gridloop2 wrapper

- To glue F77 `gridloop2` and the F77 callback function, we make a `gridloop2` wrapper:

```
      subroutine gridloop2_fcb(a, xcoor, ycoor, nx, ny)
      integer nx, ny
      real*8 a(0:nx-1,ny-1), xcoor(0:nx-1), ycoor(0:ny-1)
Cf2py intent(out) a
Cf2py depend(nx,ny) a
      real*8 fcb
      external fcb

      call gridloop2(a, xcoor, ycoor, nx, ny, fcb)
      return
      end
```

- This wrapper and the callback function `fc` constitute the F77 source code, stored in `source`
- The source calls `gridloop2` so the module must be linked with the module containing `gridloop2` (`ext_gridloop.so`)

Building the module on the fly

```
source = """
      real*8 function fcb(x, y)
      ...
      subroutine gridloop2_fcb(a, xcoor, ycoor, nx, ny)
      ...
""" % fstr

f2py_args = "--fcompiler=’Gnu’ --build-dir tmp2"\
            " -DF2PY_REPORT_ON_ARRAY_COPY=1 "\
            " ./ext_gridloop.so"
f2py2e.compile(source, modulename=’callback’,
               extra_args=f2py_args, verbose=True,
               source_fn=’_cb.f’)

import callback
a = callback.gridloop2_fcb(self.xcoor, self.ycoor)
```

gridloop2 could be generated on the fly

```
def ext_gridloop2_compile(self, fstr):
    if not isinstance(fstr, str):
        <error>
    # generate Fortran source for gridloop2:
    import f2py2e
    source = """
      subroutine gridloop2(a, xcoor, ycoor, nx, ny)
      ...
      do j = 0, ny-1
         y = ycoor(j)
         do i = 0, nx-1
            x = xcoor(i)
            a(i,j) = %s
      ...
""" % fstr  # no callback, the expression is hardcoded
    f2py2e.compile(source, modulename=’ext_gridloop2’, ...)

def ext_gridloop2_v2(self):
    import ext_gridloop2
    return ext_gridloop2.gridloop2(self.xcoor, self.ycoor)
```

Extracting a pointer to the callback function

- We can implement the callback function in Fortran, grab an F2PY-generated pointer to this function and feed that as the `func1` argument such that Fortran calls Fortran and not Python
- For a module `m`, the pointer to a function/subroutine `f` is reached as `m.f._cpointer`

```
def ext_gridloop2_fcb_ptr(self):
    from callback import fcb
    a = ext_gridloop.gridloop2(self.xcoor, self.ycoor,
                               fcb._cpointer)
    return a
```

`fcb` is a Fortran implementation of the callback in an F2PY-generated extension module `callback`

C implementation of the loop

- Let us write the `gridloop1` and `gridloop2` functions in C
- Typical C code:

```
void gridloop1(double** a, double* xcoor, double* ycoor,
               int nx, int ny, Fxy func1)
{
  int i, j;
  for (i=0; i<nx; i++) {
    for (j=0; j<ny; j++) {
       a[i][j] = func1(xcoor[i], ycoor[j])
}
```

- Problem: NumPy arrays use single pointers to data
- The above function represents a as a double pointer (common in C for two-dimensional arrays)

Using F2PY to wrap the C function

- Use single-pointer arrays
- Write C function signature with Fortran 77 syntax
- Use F2PY to generate an interface file
- Use F2PY to compile the interface file and the C code

Step 0: The modified C function

```
ypedef double (*Fxy)(double x, double y);

#define index(a, i, j) a[j*ny + i]

void gridloop2(double *a, double *xcoor, double *ycoor,
               int nx, int ny, Fxy func1)
{
  int i, j;
  for (i=0; i<nx; i++) {
    for (j=0; j<ny; j++) {
      index(a, i, j) = func1(xcoor[i], ycoor[j]);
    }
  }
}
```

Step 1: Fortran 77 signatures

```
C file: signatures.f

      subroutine gridloop2(a, xcoor, ycoor, nx, ny, func1)
Cf2py intent(c) gridloop2
      integer nx, ny
Cf2py intent(c) nx,ny
      real*8 a(0:nx-1,0:ny-1), xcoor(0:nx-1), ycoor(0:ny-1), func1
      external func1
Cf2py intent(c, out) a
Cf2py intent(in) xcoor, ycoor
Cf2py depend(nx,ny) a

C sample call of callback function:
      real*8 x, y, r
      real*8 func1
Cf2py intent(c) x, y, r, func1
      r = func1(x, y)
      end
```

Step 3 and 4: Generate interface file and compile module

- 3: Run

```
Unix/DOS> f2py -m ext_gridloop -h ext_gridloop.pyf signatures.f
```

- 4: Run

```
Unix/DOS> f2py -c --fcompiler=Gnu --build-dir tmp1 \
     -DF2PY_REPORT_ON_ARRAY_COPY=1 ext_gridloop.pyf gridloop.c
```

- See

  `src/py/mixed/Grid2D/C/f2py`

  for all the involved files

Manual writing of extension modules

- SWIG needs some non-trivial tweaking to handle NumPy arrays (i.e., the use of SWIG is much more complicated for array arguments than running F2PY)
- We shall write a complete extension module by hand
- We will need documentation of the Python C API (from Python's electronic doc.) and the NumPy C API (from the NumPy book)
- Source code files in

  `src/mixed/py/Grid2D/C/plain`

NumPy objects as seen from C

NumPy objects are C structs with attributes:

- `int nd`: no of indices (dimensions)
- `int dimensions[nd]`: length of each dimension
- `char *data`: pointer to data
- `int strides[nd]`: no of bytes between two successive data elements for a fixed index
- Access element (i,j) by

  `a->data + i*a->strides[0] + j*a->strides[1]`

Creating new NumPy array in C

- Allocate a new array:

```
PyObject * PyArray_FromDims(int n_dimensions,
                            int dimensions[n_dimensions],
                            int type_num);

int dims[2]; dims[0] = nx; dims[2] = ny;
PyArrayObject *a;  int dims[2];
dims[0] = 10;  dims[1] = 21;
a = (PyArrayObject *) PyArray_FromDims(2, dims, PyArray_DOUBLE);
```

Wrapping data in a NumPy array

- Wrap an existing memory segment (with array data) in a NumPy array object:

```
PyObject * PyArray_FromDimsAndData(int n_dimensions,
           int dimensions[n_dimensions],
           int item_type,
           char *data);
```

```
/* vec is a double* with 10*21 double entries */
PyArrayObject *a;  int dims[2];
dims[0] = 10;  dims[1] = 21;
a = (PyArrayObject *) PyArray_FromDimsAndData(2, dims,
    PyArray_DOUBLE, (char *) vec);
```

Note: `vec` is a stream of numbers, now interpreted as a two-dimensional array, stored row by row

---

From Python sequence to NumPy array

- Turn any relevant Python sequence type (list, type, array) into a NumPy array:

```
PyObject * PyArray_ContiguousFromObject(PyObject *object,
                                        int item_type,
                                        int min_dim,
                                        int max_dim);
```

Use `min_dim` and `max_dim` as 0 to preserve the original dimensions of `object`

- Application: ensure that an object is a NumPy array,

```
/* a_ is a PyObject pointer, representing a sequence
   (NumPy array or list or tuple) */
PyArrayObject a;
a = (PyArrayObject *) PyArray_ContiguousFromObject(a_,
                      PyArray_DOUBLE, 0, 0);
```

a list, tuple or NumPy array a is now a NumPy array

Python interface

```
class Grid2Deff(Grid2D):
    def __init__(self,
                 xmin=0, xmax=1, dx=0.5,
                 ymin=0, ymax=1, dy=0.5):
        Grid2D.__init__(self, xmin, xmax, dx, ymin, ymax, dy)

    def ext_gridloop1(self, f):
        lx = size(self.xcoor);  ly = size(self.ycoor)
        a = zeros((lx,ly))

        ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, f)

        return a

    def ext_gridloop2(self, f):

        a = ext_gridloop.gridloop2(self.xcoor, self.ycoor, f)

        return a
```

---

gridloop1 in C; header

- Transform `PyObject` argument tuple to NumPy arrays:

```
static PyObject *gridloop1(PyObject *self, PyObject *args)
{
  PyArrayObject *a, *xcoor, *ycoor;
  PyObject *func1, *arglist, *result;
  int nx, ny, i, j;
  double *a_ij, *x_i, *y_j;

  /* arguments: a, xcoor, ycoor */
  if (!PyArg_ParseTuple(args, "O!O!O!O:gridloop1",
                        &PyArray_Type, &a,
                        &PyArray_Type, &xcoor,
                        &PyArray_Type, &ycoor,
                        &func1)) {
    return NULL; /* PyArg_ParseTuple has raised an exception */
  }
```

---

gridloop1 in C; safety checks

```
  if (a->nd != 2 || a->descr->type_num != PyArray_DOUBLE) {
    PyErr_Format(PyExc_ValueError,
    "a array is %d-dimensional or not of type float", a->nd);
    return NULL;
  }
  nx = a->dimensions[0];  ny = a->dimensions[1];
  if (xcoor->nd != 1 || xcoor->descr->type_num != PyArray_DOUBLE ||
      xcoor->dimensions[0] != nx) {
    PyErr_Format(PyExc_ValueError,
    "xcoor array has wrong dimension (%d), type or length (%d)",
                 xcoor->nd,xcoor->dimensions[0]);
    return NULL;
  }
  if (ycoor->nd != 1 || ycoor->descr->type_num != PyArray_DOUBLE ||
      ycoor->dimensions[0] != ny) {
    PyErr_Format(PyExc_ValueError,
    "ycoor array has wrong dimension (%d), type or length (%d)",
                 ycoor->nd,ycoor->dimensions[0]);
    return NULL;
  }
  if (!PyCallable_Check(func1)) {
    PyErr_Format(PyExc_TypeError,
    "func1 is not a callable function");
    return NULL;
  }
```

Callback to Python from C

- Python functions can be called from C
- Step 1: for each argument, convert C data to Python objects and collect these in a tuple

```
PyObject *arglist; double x, y;
/* double x,y -> tuple with two Python float objects: */
arglist = Py_BuildValue("(dd)", x, y);
```

- Step 2: call the Python function

```
PyObject *result;  /* return value from Python function */
PyObject *func1;   /* Python function object */
result = PyEval_CallObject(func1, arglist);
```

- Step 3: convert result to C data

```
double r;  /* result is a Python float object */
r = PyFloat_AS_DOUBLE(result);
```

---

gridloop1 in C; the loop

```
  for (i = 0; i < nx; i++) {
    for (j = 0; j < ny; j++) {
      a_ij = (double *)(a->data+i*a->strides[0]+j*a->strides[1]);
      x_i = (double *)(xcoor->data + i*xcoor->strides[0]);
      y_j = (double *)(ycoor->data + j*ycoor->strides[0]);

      /* call Python function pointed to by func1: */
      arglist = Py_BuildValue("(dd)", *x_i, *y_j);
      result = PyEval_CallObject(func1, arglist);
      *a_ij = PyFloat_AS_DOUBLE(result);
    }
  }
  return Py_BuildValue("");  /* return None: */
}
```

Memory management

- There is a major problem with our loop:

```
      arglist = Py_BuildValue("(dd)", *x_i, *y_j);
      result = PyEval_CallObject(func1, arglist);
      *a_ij = PyFloat_AS_DOUBLE(result);
```

- For each pass, `arglist` and `result` are dynamically allocated, but not destroyed
- From the Python side, memory management is automatic
- From the C side, we must do it ourself
- Python applies reference counting
- Each object has a number of references, one for each usage
- The object is destroyed when there are no references

Reference counting

- Increase the reference count:

  `Py_INCREF(myobj);`

  (i.e., I need this object, it cannot be deleted elsewhere)
- Decrease the reference count:

  `Py_DECREF(myobj);`

  (i.e., I don't need this object, it can be deleted)

---

gridloop1; loop with memory management

```
for (i = 0; i < nx; i++) {
  for (j = 0; j < ny; j++) {
    a_ij = (double *)(a->data + i*a->strides[0] + j*a->strides[1]);
    x_i = (double *)(xcoor->data + i*xcoor->strides[0]);
    y_j = (double *)(ycoor->data + j*ycoor->strides[0]);

    /* call Python function pointed to by func1: */
    arglist = Py_BuildValue("(dd)", *x_i, *y_j);
    result = PyEval_CallObject(func1, arglist);
    Py_DECREF(arglist);
    if (result == NULL) return NULL; /* exception in func1 */
    *a_ij = PyFloat_AS_DOUBLE(result);
    Py_DECREF(result);
  }
}
```

---

gridloop1; more testing in the loop

- We should check that allocations work fine:

```
arglist = Py_BuildValue("(dd)", *x_i, *y_j);
if (arglist == NULL) {  /* out of memory */
   PyErr_Format(PyExc_MemoryError,
                "out of memory for 2-tuple);
```

- The C code becomes quite comprehensive; much more testing than "active" statements

---

gridloop2 in C; header

gridloop2: as gridloop1, but array a is returned

```
static PyObject *gridloop2(PyObject *self, PyObject *args)
{
  PyArrayObject *a, *xcoor, *ycoor;
  int a_dims[2];
  PyObject *func1, *arglist, *result;
  int nx, ny, i, j;
  double *a_ij, *x_i, *y_j;

  /* arguments: xcoor, ycoor, func1 */
  if (!PyArg_ParseTuple(args, "O!O!O:gridloop2",
                        &PyArray_Type, &xcoor,
                        &PyArray_Type, &ycoor,
                        &func1)) {
    return NULL; /* PyArg_ParseTuple has raised an exception */
  }
  nx = xcoor->dimensions[0];  ny = ycoor->dimensions[0];
```

---

gridloop2 in C; macros

- NumPy array code in C can be simplified using macros
- First, a smart macro wrapping an argument in quotes:

```
#define QUOTE(s) # s   /* turn s into string "s" */
```

- Check the type of the array data:

```
#define TYPECHECK(a, tp) \
  if (a->descr->type_num != tp) { \
    PyErr_Format(PyExc_TypeError, \
    "%s array is not of correct type (%d)", QUOTE(a), tp); \
    return NULL; \
  }
```

- `PyErr_Format` is a flexible way of raising exceptions in C (must return `NULL` afterwards!)

---

gridloop2 in C; another macro

- Check the length of a specified dimension:

```
#define DIMCHECK(a, dim, expected_length) \
  if (a->dimensions[dim] != expected_length) { \
    PyErr_Format(PyExc_ValueError, \
    "%s array has wrong %d-dimension=%d (expected %d)", \
              QUOTE(a),dim,a->dimensions[dim],expected_length); \
    return NULL; \
  }
```

---

gridloop2 in C; more macros

- Check the dimensions of a NumPy array:

```
#define NDIMCHECK(a, expected_ndim) \
  if (a->nd != expected_ndim) { \
    PyErr_Format(PyExc_ValueError, \
    "%s array is %d-dimensional, expected to be %d-dimensional",\
                 QUOTE(a), a->nd, expected_ndim); \
    return NULL; \
  }
```

- Application:

```
NDIMCHECK(xcoor, 1); TYPECHECK(xcoor, PyArray_DOUBLE);
```

  If `xcoor` is 2-dimensional, an exceptions is raised by `NDIMCHECK`:

```
exceptions.ValueError
xcoor array is 2-dimensional, but expected to be 1-dimensional
```

---

gridloop2 in C; indexing macros

- Macros can greatly simplify indexing:

```
#define IND1(a, i) *((double *)(a->data + i*a->strides[0]))
#define IND2(a, i, j) \
 *((double *)(a->data + i*a->strides[0] + j*a->strides[1]))
```

- Application:

```
for (i = 0; i < nx; i++) {
  for (j = 0; j < ny; j++) {
    arglist = Py_BuildValue("(dd)", IND1(xcoor,i), IND1(ycoor,j))
    result = PyEval_CallObject(func1, arglist);
    Py_DECREF(arglist);
    if (result == NULL) return NULL; /* exception in func1 */
    IND2(a,i,j) = PyFloat_AS_DOUBLE(result);
    Py_DECREF(result);
  }
}
```

gridloop2 in C; the return array

- Create return array:

```
a_dims[0] = nx; a_dims[1] = ny;
a = (PyArrayObject *) PyArray_FromDims(2, a_dims,
                                       PyArray_DOUBLE);
if (a == NULL) {
  printf("creating a failed, dims=(%d,%d)\n",
         a_dims[0],a_dims[1]);
  return NULL; /* PyArray_FromDims raises an exception */
}
```

- After the loop, return a:

```
return PyArray_Return(a);
```

Registering module functions

- The method table must always be present - it lists the functions that should be callable from Python:

```
static PyMethodDef ext_gridloop_methods[] = {
  {"gridloop1",    /* name of func when called from Python */
   gridloop1,      /* corresponding C function */
   METH_VARARGS,   /* ordinary (not keyword) arguments */
   gridloop1_doc}, /* doc string for gridloop1 function */
  {"gridloop2",    /* name of func when called from Python */
   gridloop2,      /* corresponding C function */
   METH_VARARGS,   /* ordinary (not keyword) arguments */
   gridloop2_doc}, /* doc string for gridloop1 function */
  {NULL, NULL}
};
```

- `METH_KEYWORDS` (instead of `METH_VARARGS`) implies that the function takes 3 arguments (`self`, `args`, `kw`)

Doc strings

```
static char gridloop1_doc[] = \
  "gridloop1(a, xcoor, ycoor, pyfunc)";

static char gridloop2_doc[] = \
  "a = gridloop2(xcoor, ycoor, pyfunc)";

static char module_doc[] = \
  "module ext_gridloop:\n\
   gridloop1(a, xcoor, ycoor, pyfunc)\n\
   a = gridloop2(xcoor, ycoor, pyfunc)";
```

The required init function

```
PyMODINIT_FUNC initext_gridloop()
{
  /* Assign the name of the module and the name of the
     method table and (optionally) a module doc string:
  */
  Py_InitModule3("ext_gridloop", ext_gridloop_methods, module_doc);
  /* without module doc string:
  Py_InitModule ("ext_gridloop", ext_gridloop_methods); */

  import_array();   /* required NumPy initialization */
}
```

Building the module

```
root=‘python -c ’import sys; print sys.prefix’‘
ver=‘python -c ’import sys; print sys.version[:3]’‘
gcc -O3 -g -I$root/include/python$ver \
    -I$scripting/src/C \
    -c gridloop.c -o gridloop.o
gcc -shared -o ext_gridloop.so gridloop.o

# test the module:
python -c ’import ext_gridloop; print dir(ext_gridloop)’
```

A setup.py script

- The script:

```
from distutils.core import setup, Extension
import os

name = ’ext_gridloop’
setup(name=name,
      include_dirs=[os.path.join(os.environ[’scripting’],
                                 ’src’, ’C’)],
      ext_modules=[Extension(name, [’gridloop.c’])])
```

- Usage:

```
python setup.py build_ext
python setup.py install --install-platlib=.
# test module:
python -c ’import ext_gridloop; print ext_gridloop.__doc__’
```

Using the module

- The usage is the same as in Fortran, when viewed from Python
- No problems with storage formats and unintended copying of a in `gridloop1`, or optional arguments; here we have full control of all details
- `gridloop2` is the “right” way to do it
- It is much simpler to use Fortran and F2PY

Debugging

- Things usually go wrong when you program...
- Errors in C normally shows up as “segmentation faults” or “bus error” - no nice exception with traceback
- Simple trick: run `python` under a debugger

```
unix> gdb ‘which python‘
(gdb) run test.py
```

- When the script crashes, issue the gdb command `where` for a traceback (if the extension module is compiled with -g you can see the line number of the line that triggered the error)
- You can only see the traceback, no breakpoints, prints etc., but a tool, PyDebug, allows you to do this

Debugging example (1)

- In src/py/mixed/Grid2D/C/plain/debugdemo there are some C files with errors
- Try

  ```
  ./make_module_1.sh gridloop1
  ```

  This scripts runs

  ```
  ../../../Grid2Deff.py verify1
  ```

  which leads to a segmentation fault, implying that something is wrong in the C code (errors in the Python script shows up as exceptions with traceback)

1st debugging example (1)

- Check that the extension module was compiled with debug mode on (usually the -g option to the C compiler)
- Run `python` under a debugger:

  ```
  unix> gdb ‘which python‘
  GNU gdb 6.0-debian
  ...
  (gdb) run ../../../Grid2Deff.py verify1
  Starting program: /usr/bin/python ../../../Grid2Deff.py verify1
  ...
  Program received signal SIGSEGV, Segmentation fault.
  0x40cdfab3 in gridloop1 (self=0x0, args=0x1) at gridloop1.c:20
  20        if (!PyArg_ParseTuple(args, "O!O!O!O:gridloop1",
  ```

  This is the line where something goes wrong...

1st debugging example (3)

```
(gdb) where
#0  0x40cdfab3 in gridloop1 (self=0x0, args=0x1) at gridloop1.c:20
#1  0x080fde1a in PyCFunction_Call ()
#2  0x080ab824 in PyEval_CallObjectWithKeywords ()
#3  0x080a9bde in Py_MakePendingCalls ()
#4  0x080aa76c in PyEval_EvalCodeEx ()
#5  0x080ab8d9 in PyEval_CallObjectWithKeywords ()
#6  0x080ab71c in PyEval_CallObjectWithKeywords ()
#7  0x080a9bde in Py_MakePendingCalls ()
#8  0x080ab95d in PyEval_CallObjectWithKeywords ()
#9  0x080ab71c in PyEval_CallObjectWithKeywords ()
#10 0x080a9bde in Py_MakePendingCalls ()
#11 0x080aa76c in PyEval_EvalCodeEx ()
#12 0x080acf69 in PyEval_EvalCode ()
#13 0x080d90db in PyRun_FileExFlags ()
#14 0x080d9d1f in PyRun_String ()
#15 0x08100c20 in _IO_stdin_used ()
#16 0x401ee79c in ?? ()
#17 0x41096bdc in ?? ()
```

1st debugging example (3)

- What is wrong?
- The `import_array()` call was removed, but the segmentation fault happended in the first call to a Python C function

2nd debugging example

- Try

  ```
  ./make_module_1.sh gridloop2
  ```

  and experience that

  ```
  python -c ’import ext_gridloop; print dir(ext_gridloop); \
             print ext_gridloop.__doc__’
  ```

  ends with an exception

  ```
  Traceback (most recent call last):
    File "<string>", line 1, in ?
  SystemError: dynamic module not initialized properly
  ```

- This signifies that the module misses initialization
- Reason: no `Py_InitModule3` call

3rd debugging example (1)

- Try

  ```
  ./make_module_1.sh gridloop3
  ```

- Most of the program seems to work, but a segmentation fault occurs (according to gdb):

  ```
  (gdb) where
  (gdb) #0  0x40115d1e in mallopt () from /lib/libc.so.6
  #1  0x40114d33 in malloc () from /lib/libc.so.6
  #2  0x40449fb9 in PyArray_FromDimsAndDataAndDescr ()
     from /usr/lib/python2.3/site-packages/Numeric/_numpy.so
  ...
  #42 0x080d90db in PyRun_FileExFlags ()
  #43 0x080d9d1f in PyRun_String ()
  #44 0x08100c20 in _IO_stdin_used ()
  #45 0x401ee79c in ?? ()
  #46 0x41096bdc in ?? ()
  ```

  Hmmm...no sign of where in `gridloop3.c` the error occurs, except that the `Grid2Deff.py` script successfully calls both `gridloop1` and `gridloop2`, it fails when printing the returned array

3rd debugging example (2)

- Next step: print out information

  ```
    for (i = 0; i <= nx; i++) {
      for (j = 0; j <= ny; j++) {
        arglist = Py_BuildValue("(dd)", IND1(xcoor,i), IND1(ycoor,j
        result = PyEval_CallObject(func1, arglist);
        IND2(a,i,j) = PyFloat_AS_DOUBLE(result);

  #ifdef DEBUG
        printf("a[%d,%d]=func1(%g,%g)=%g\n",i,j,
               IND1(xcoor,i),IND1(ycoor,j),IND2(a,i,j));
  #endif
      }
    }
  ```

- Run

  ```
  ./make_module_1.sh gridloop3 -DDEBUG
  ```

3rd debugging example (3)

- Loop debug output:

  ```
  a[2,0]=func1(1,0)=1
  f1...x-y= 3.0
  a[2,1]=func1(1,1)=3
  f1...x-y= 1.0
  a[2,2]=func1(1,7.15113e-312)=1
  f1...x-y= 7.66040480538e-312
  a[3,0]=func1(7.6604e-312,0)=7.6604e-312
  f1...x-y= 2.0
  a[3,1]=func1(7.6604e-312,1)=2
  f1...x-y= 2.19626564365e-311
  a[3,2]=func1(7.6604e-312,7.15113e-312)=2.19627e-311
  ```

- Ridiculous values (coordinates) and wrong indices reveal the problem: wrong upper loop limits

4th debugging example

- Try

  ```
  ./make_module_1.sh gridloop4
  ```

  and experience

  ```
  python -c import ext_gridloop; print dir(ext_gridloop); \
             print ext_gridloop.__doc__
  Traceback (most recent call last):
    File "<string>", line 1, in ?
  ImportError: dynamic module does not define init function (initex
  ```

- Eventuall we got a precise error message (the `initext_gridloop` was not implemented)

5th debugging example

- Try

  ```
  ./make_module_1.sh gridloop5
  ```

  and experience

  ```
  python -c import ext_gridloop; print dir(ext_gridloop); \
             print ext_gridloop.__doc__
  Traceback (most recent call last):
    File "<string>", line 1, in ?
  ImportError: ./ext_gridloop.so: undefined symbol: mydebug
  ```

- `gridloop2` in `gridloop5.c` calls a function `mydebug`, but the function is not implemented (or linked)
- Again, a precise ImportError helps detecting the problem

Summary of the debugging examples

- Check that `import_array()` is called if the NumPy C API is in use!
- ImportError suggests wrong module initialization or missing required/user functions
- You need experience to track down errors in the C code
- An error in one place often shows up as an error in another place (especially indexing out of bounds or wrong memory handling)
- Use a debugger (gdb) and print statements in the C code and the calling script
- C++ modules are (almost) as error-prone as C modules

Next example

- Implement the computational loop in a traditional C function
- Aim: pretend that we have this loop already in a C library
- Need to write a wrapper between this C function and Python
- Could think of SWIG for generating the wrapper, but SWIG with NumPy arrays is a bit tricky - it is in fact simpler to write the wrapper by hand

---

Two-dim. C array as double pointer

- C functions taking a two-dimensional array as argument will normally represent the array as a double pointer:

  ```
  void gridloop1_C(double **a, double *xcoor, double *ycoor,
                   int nx, int ny, Fxy func1)
  {
    int i, j;
    for (i=0; i<nx; i++) {
      for (j=0; j<ny; j++) {
         a[i][j] = func1(xcoor[i], ycoor[j]);
      }
    }
  }
  ```

- `Fxy` is a function pointer:

  ```
  typedef double (*Fxy)(double x, double y);
  ```

- An existing C library would typically work with multi-dim. arrays and callback functions this way

---

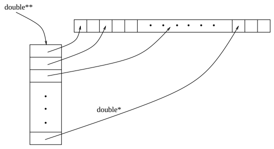
Problems

- How can we write wrapper code that sends NumPy array data to a C function as a double pointer?
- How can we make callbacks to Python when the C function expects callbacks to standard C functions, represented as function pointers?
- We need to cope with these problems to interface (numerical) C libraries!

src/mixed/py/Grid2D/C/clibcall

From NumPy array to double pointer

- 2-dim. C arrays stored as a double pointer:



- The wrapper code must allocate extra data:

  ```
  double **app;  double *ap;
  ap = (double *) a->data;   /* a is a PyArrayObject* pointer */
  app = (double **) malloc(nx*sizeof(double*));
  for (i = 0; i < nx; i++) {
    app[i] = &(ap[i*ny]);    /* point row no. i in a->data */
  }
  /* clean up when app is no longer needed: */ free(app);
  ```

Callback via a function pointer (1)

- `gridloop1_C` calls a function like

  ```
  double somefunc(double x, double y)
  ```

  but our function is a Python object...

- Trick: store the Python function in

  ```
  PyObject* _pyfunc_ptr;  /* global variable */
  ```

  and make a “wrapper” for the call:

  ```
  double _pycall(double x, double y)
  {
    /* perform call to Python function object in _pyfunc_ptr */
  }
  ```

Callback via a function pointer (2)

- Complete function wrapper:

```
double _pycall(double x, double y)
{
  PyObject *arglist, *result;
  arglist = Py_BuildValue("(dd)", x, y);
  result = PyEval_CallObject(_pyfunc_ptr, arglist);
  return PyFloat_AS_DOUBLE(result);
}
```

- Initialize `_pyfunc_ptr` with the `func1` argument supplied to the `gridloop1` wrapper function

```
_pyfunc_ptr = func1;  /* func1 is PyObject* pointer */
```

The alternative gridloop1 code (1)

```
static PyObject *gridloop1(PyObject *self, PyObject *args)
{
  PyArrayObject *a, *xcoor, *ycoor;
  PyObject *func1, *arglist, *result;
  int nx, ny, i;
  double **app;
  double *ap, *xp, *yp;

  /* arguments: a, xcoor, ycoor, func1 */
  /* parsing without checking the pointer types: */
  if (!PyArg_ParseTuple(args, "OOOO", &a, &xcoor, &ycoor, &func1))
    { return NULL; }
  NDIMCHECK(a,     2); TYPECHECK(a,     PyArray_DOUBLE);
  nx = a->dimensions[0];  ny = a->dimensions[1];
  NDIMCHECK(xcoor, 1); DIMCHECK(xcoor, 0, nx);
  TYPECHECK(xcoor, PyArray_DOUBLE);
  NDIMCHECK(ycoor, 1); DIMCHECK(ycoor, 0, ny);
  TYPECHECK(ycoor, PyArray_DOUBLE);
  CALLABLECHECK(func1);
```

The alternative gridloop1 code (2)

```
  _pyfunc_ptr = func1;  /* store func1 for use in _pycall */

  /* allocate help array for creating a double pointer: */
  app = (double **) malloc(nx*sizeof(double*));
  ap = (double *) a->data;
  for (i = 0; i < nx; i++) { app[i] = &(ap[i*ny]); }
  xp = (double *) xcoor->data;
  yp = (double *) ycoor->data;
  gridloop1_C(app, xp, yp, nx, ny, _pycall);
  free(app);
  return Py_BuildValue("");  /* return None */
}
```

---

gridloop1 with C++ array object

- Programming with NumPy arrays in C is much less convenient than programming with C++ array objects

```
SomeArrayClass a(10, 21);
a(1,2) = 3;       // indexing
```

- Idea: wrap NumPy arrays in a C++ class
- Goal: use this class wrapper to simplify the `gridloop1` wrapper

src/py/mixed/Grid2D/C++/plain

The C++ class wrapper (1)

```
class NumPyArray_Float
{
 private:
  PyArrayObject* a;

 public:
  NumPyArray_Float () { a=NULL; }
  NumPyArray_Float (int n1, int n2)  { create(n1, n2); }
  NumPyArray_Float (double* data, int n1, int n2)
    { wrap(data, n1, n2); }
  NumPyArray_Float (PyArrayObject* array) { a = array; }
```

The C++ class wrapper (2)

```
  // redimension (reallocate) an array:
  int create (int n1, int n2) {
    int dim2[2]; dim2[0] = n1; dim2[1] = n2;
    a = (PyArrayObject*) PyArray_FromDims(2, dim2, PyArray_DOUBLE);
    if (a == NULL) { return 0; } else { return 1; } }

  // wrap existing data in a NumPy array:
  void wrap (double* data, int n1, int n2) {
    int dim2[2]; dim2[0] = n1; dim2[1] = n2;
    a = (PyArrayObject*) PyArray_FromDimsAndData(\
        2, dim2, PyArray_DOUBLE, (char*) data);
  }

  // for consistency checks:
  int checktype () const;
  int checkdim  (int expected_ndim) const;
  int checksize (int expected_size1, int expected_size2=0,
                 int expected_size3=0) const;
```

The C++ class wrapper (3)

```
  // indexing functions (inline!):
  double  operator() (int i, int j) const
  { return *((double*) (a->data +
                        i*a->strides[0] + j*a->strides[1])); }
  double& operator() (int i, int j)
  { return *((double*) (a->data +
                        i*a->strides[0] + j*a->strides[1])); }

  // extract dimensions:
  int dim() const { return a->nd; }  // no of dimensions
  int size1() const { return a->dimensions[0]; }
  int size2() const { return a->dimensions[1]; }
  int size3() const { return a->dimensions[2]; }
  PyArrayObject* getPtr () { return a; }
};
```

Using the wrapper class

```
static PyObject* gridloop2(PyObject* self, PyObject* args)
{
  PyArrayObject *xcoor_, *ycoor_;
  PyObject *func1, *arglist, *result;
  /* arguments: xcoor, ycoor, func1 */
  if (!PyArg_ParseTuple(args, "O!O!O:gridloop2",
                        &PyArray_Type, &xcoor_,
                        &PyArray_Type, &ycoor_,
                        &func1)) {
    return NULL; /* PyArg_ParseTuple has raised an exception */
  }
  NumPyArray_Float xcoor (xcoor_); int nx = xcoor.size1();
  if (!xcoor.checktype()) { return NULL; }
  if (!xcoor.checkdim(1)) { return NULL; }
  NumPyArray_Float ycoor (ycoor_); int ny = ycoor.size1();
  // check ycoor dimensions, check that func1 is callable...
  NumPyArray_Float a(nx, ny);  // return array
```

The loop is straightforward

```
int i,j;
for (i = 0; i < nx; i++) {
  for (j = 0; j < ny; j++) {
    arglist = Py_BuildValue("(dd)", xcoor(i), ycoor(j));
    result = PyEval_CallObject(func1, arglist);
    a(i,j) = PyFloat_AS_DOUBLE(result);
  }
}

return PyArray_Return(a.getPtr());
```

Reference counting

- We have omitted a very important topic in Python-C programming: reference counting
- Python has a garbage collection system based on reference counting
- Each object counts the no of references to itself
- When there are no more references, the object is automatically deallocated
- Nice when used from Python, but in C we must program the reference counting manually

```
PyObject *obj;
...
Py_XINCREF(obj);   /* new reference created */
...
Py_DECREF(obj);    /* a reference is destroyed */
```

SCXX: basic ideas

- Thin C++ layer on top of the Python C API
- Each Python type (number, tuple, list, ...) is represented as a C++ class
- The resulting code is quite close to Python
- SCXX objects performs reference counting automatically

Example

```
#include <PWONumber.h>     // class for numbers
#include <PWOSequence.h>   // class for tuples
#include <PWOMSequence.h>  // class for lists (immutable sequences)

void test_scxx()
{
  double a_ = 3.4;
  PWONumber a = a_; PWONumber b = 7;
  PWONumber c; c = a + b;
  PWOList list; list.append(a).append(c).append(b);
  PWOTuple tp(list);
  for (int i=0; i<tp.len(); i++) {
    std::cout << "tp["<<i<<"]="<<double(PWONumber(tp[i]))<<" ";
  }
  std::cout << std::endl;
  PyObject* py_a = (PyObject*) a;  // convert to Python C struct
}
```

The similar code with Python C API

```
void test_PythonAPI()
{
  double a_ = 3.4;
  PyObject* a = PyFloat_FromDouble(a_);
  PyObject* b = PyFloat_FromDouble(7);
  PyObject* c = PyNumber_Add(a, b);
  PyObject* list = PyList_New(0);
  PyList_Append(list, a);
  PyList_Append(list, c);
  PyList_Append(list, b);
  PyObject* tp = PyList_AsTuple(list);
  int tp_len = PySequence_Length(tp);
  for (int i=0; i<tp_len; i++) {
    PyObject* qp = PySequence_GetItem(tp, i);
    double q = PyFloat_AS_DOUBLE(qp);
    std::cout << "tp[" << i << "]=" << q << " ";
  }
  std::cout << std::endl;
}
```

Note: reference counting is omitted

gridloop1 with SCXX

```
static PyObject* gridloop1(PyObject* self, PyObject* args_)
{
  /* arguments: a, xcoor, ycoor */
  try {
    PWOSequence args (args_);
    NumPyArray_Float a ((PyArrayObject*) ((PyObject*) args[0]));
    NumPyArray_Float xcoor ((PyArrayObject*) ((PyObject*) args[1]));
    NumPyArray_Float ycoor ((PyArrayObject*) ((PyObject*) args[2]));
    PWOCallable func1 (args[3]);

    // work with a, xcoor, ycoor, and func1
    ...

    return PWONone();
  }
  catch (PWException e) { return e; }
}
```

Error checking

- `NumPyArray_Float` objects are checked using their member functions (`checkdim`, etc.)
- SCXX objects also have some checks:

```
if (!func1.isCallable()) {
  PyErr_Format(PyExc_TypeError,
               "func1 is not a callable function");
  return NULL;
}
```

The loop over grid points

```
int i,j;
for (i = 0; i < nx; i++) {
  for (j = 0; j < ny; j++) {
    PWOTuple arglist(Py_BuildValue("(dd)", xcoor(i), ycoor(j)));
    PWONumber result(func1.call(arglist));
    a(i,j) = double(result);
  }
}
```

The Weave tool (1)

- Weave is an easy-to-use tool for inlining C++ snippets in Python codes
- A quick demo shows its potential

```
class Grid2Deff:
    ...
    def ext_gridloop1_weave(self, fstr):
        """Migrate loop to C++ with aid of Weave."""

        from scipy import weave

        # the callback function is now coded in C++
        # (fstr must be valid C++ code):

        extra_code = r"""
double cppcb(double x, double y) {
  return %s;
}
""" % fstr
```

The Weave tool (2)

- The loops: inline C++ with Blitz++ array syntax:

```
        code = r"""
int i,j;
for (i=0; i<nx; i++) {
  for (j=0; j<ny; j++) {
    a(i,j) = cppcb(xcoor(i), ycoor(j));
  }
}
"""
```

The Weave tool (3)

- Compile and link the extra code `extra_code` and the main code (loop) `code`:

```
nx = size(self.xcoor);  ny = size(self.ycoor)
a = zeros((nx,ny))
xcoor = self.xcoor;  ycoor = self.ycoor
err = weave.inline(code, [’a’, ’nx’, ’ny’, ’xcoor’, ’ycoor’],
         type_converters=weave.converters.blitz,
         support_code=extra_code, compiler=’gcc’)
return a
```

- Note that we pass the names of the Python objects we want to access in the C++ code
- Weave is smart enough to avoid recompiling the code if it has not changed since last compilation

Exchanging pointers in Python code

- When interfacing many libraries, data must be grabbed from one code and fed into another
- Example: NumPy array to/from some C++ data class
- Idea: make filters, converting one data to another
- Data objects are represented by pointers
- SWIG can send pointers back and forth without needing to wrap the whole underlying data object
- Let’s illustrate with an example!

MyArray: some favorite C++ array class

- Say our favorite C++ array class is `MyArray`

```
template< typename T >
class MyArray
{
 public:
  T* A;                   // the data
  int ndim;               // no of dimensions (axis)
  int size[MAXDIM];       // size/length of each dimension
  int length;             // total no of array entries
  ...
};
```

- We can work with this class from Python without needing to SWIG the class (!)
- We make a filter class converting a NumPy array (pointer) to/from a `MyArray` object (pointer)

src/py/mixed/Grid2D/C++/convertptr

Filter between NumPy array and C++ class

```
class Convert_MyArray
{
 public:
  Convert_MyArray();

  // borrow data:
  PyObject*         my2py (MyArray<double>& a);
  MyArray<double>*  py2my (PyObject* a);

  // copy data:
  PyObject*         my2py_copy (MyArray<double>& a);
  MyArray<double>*  py2my_copy (PyObject* a);

  // print array:
  void              dump(MyArray<double>& a);

  // convert Py function to C/C++ function calling Py:
  Fxy               set_pyfunc (PyObject* f);
 protected:
  static PyObject* _pyfunc_ptr;  // used in _pycall
  static double    _pycall (double x, double y);
};
```

Typical conversion function

```
PyObject* Convert_MyArray:: my2py(MyArray<double>& a)
{
  PyArrayObject* array =  (PyArrayObject*) \
          PyArray_FromDimsAndData(a.ndim, a.size, PyArray_DOUBLE,
                                  (char*) a.A);
  if (array == NULL) {
    return NULL; /* PyArray_FromDimsAndData raised exception */
  }
  return PyArray_Return(array);
}
```

Version with data copying

```
PyObject* Convert_MyArray:: my2py_copy(MyArray<double>& a)
{
  PyArrayObject* array =  (PyArrayObject*) \
          PyArray_FromDims(a.ndim, a.size, PyArray_DOUBLE);
  if (array == NULL) {
    return NULL; /* PyArray_FromDims raised exception */
  }
  double* ad = (double*) array->data;
  for (int i = 0; i < a.length; i++) {
    ad[i] = a.A[i];
  }
  return PyArray_Return(array);
}
```

Ideas

- SWIG `Convert_MyArray`
- Do not SWIG `MyArray`
- Write numerical C++ code using `MyArray`
  (or use a library that already makes use of `MyArray`)
- Convert pointers (data) explicitly in the Python code

gridloop1 in C++

```
void gridloop1(MyArray<double>& a,
               const MyArray<double>& xcoor,
               const MyArray<double>& ycoor,
               Fxy func1)
{
  int nx = a.shape(1), ny = a.shape(2);
  int i, j;
  for (i = 0; i < nx; i++) {
    for (j = 0; j < ny; j++) {
      a(i,j) = func1(xcoor(i), ycoor(j));
    }
  }
}
```

Calling C++ from Python (1)

- Instead of just calling

  ```
  ext_gridloop.gridloop1(a, self.xcoor, self.ycoor, func)
  return a
  ```

  as before, we need some explicit conversions:

  ```
  # a is a NumPy array
  # self.c is the conversion module (class Convert_MyArray)
  a_p = self.c.py2my(a)
  x_p = self.c.py2my(self.xcoor)
  y_p = self.c.py2my(self.ycoor)
  f_p = self.c.set_pyfunc(func)
  ext_gridloop.gridloop1(a_p, x_p, y_p, f_p)
  return a  # a_p and a share data!
  ```

Calling C++ from Python (2)

- In case we work with copied data, we must copy both ways:

  ```
  a_p = self.c.py2my_copy(a)
  x_p = self.c.py2my_copy(self.xcoor)
  y_p = self.c.py2my_copy(self.ycoor)
  f_p = self.c.set_pyfunc(func)
  ext_gridloop.gridloop1(a_p, x_p, y_p, f_p)
  a = self.c.my2py_copy(a_p)
  return a
  ```

- Note: final `a` is not the same `a` object as we started with

SWIG’ing the filter class

- C++ code: `convert.h/.cpp` + `gridloop.h/.cpp`
- SWIG interface file:

  ```
  /* file: ext_gridloop.i */
  %module ext_gridloop
  %{
  /* include C++ header files needed to compile the interface */
  #include "convert.h"
  #include "gridloop.h"
  %}

  %include "convert.h"
  %include "gridloop.h"
  ```

- Important: call NumPy’s `import_array` (here in `Convert_MyArray` constructor)
- Run SWIG:

  ```
  swig -python -c++ -I. ext_gridloop.i
  ```

- Compile and link shared library module

setup.py

```
import os
from distutils.core import setup, Extension
name = ’ext_gridloop’

swig_cmd = ’swig -python -c++ -I. %s.i’ % name
os.system(swig_cmd)

sources = [’gridloop.cpp’,’convert.cpp’,’ext_gridloop_wrap.cxx’]
setup(name=name,
      ext_modules=[Extension(’_’ + name,  # SWIG requires _
                             sources=sources,
                             include_dirs=[os.curdir])])
```

Manual alternative

```
swig -python -c++ -I. ext_gridloop.i

root=‘python -c ’import sys; print sys.prefix’‘
ver=‘python -c ’import sys; print sys.version[:3]’‘
g++ -I. -O3 -g -I$root/include/python$ver \
    -c convert.cpp gridloop.cpp ext_gridloop_wrap.cxx
g++ -shared -o _ext_gridloop.so \
     convert.o gridloop.o ext_gridloop_wrap.o
```

Summary

We have implemented several versions of `gridloop1` and `gridloop2`:

- Fortran subroutines, working on Fortran arrays, automatically wrapped by F2PY
- Hand-written C extension module, working directly on NumPy array structs in C
- Hand-written C wrapper to a C function, working on standard C arrays (incl. double pointer)
- Hand-written C++ wrapper, working on a C++ class wrapper for NumPy arrays
- As last point, but simplified wrapper utilizing SCXX
- C++ functions based on `MyArray`, plus C++ filter for pointer conversion, wrapped by SWIG

Comparison

- What is the most convenient approach in this case?
  Fortran!
- If we cannot use Fortran, which solution is attractive?
  C++, with classes allowing higher-level programming
- To interface a large existing library, the filter idea and exchanging pointers is attractive (no need to SWIG the whole library)
- When using the Python C API extensively, SCXX simplifies life

Efficiency

- Which alternative is computationally most efficient?
  Fortran, but C/C++ is quite close – no significant difference between all the C/C++ versions
- Too bad: the (point-wise) callback to Python destroys the efficiency of the extension module!
- Pure Python script w/NumPy is much more efficient...
- Nevertheless: this is a pedagogical case teaching you how to migrate/interface numerical code

Efficiency test: 1100x1100 grid

```
language  function         func1 argument             CPU time
F77       gridloop1        F77 function with formula    1.0
C++       gridloop1        C++ function with formula    1.07

Python    Grid2D.__call__  vectorized numpy myfunc      1.5
Python    Grid2D.gridloop  myfunc w/math.sin          120
Python    Grid2D.gridloop  myfunc w/numpy.sin         220

F77       gridloop1        myfunc w/math.sin           40
F77       gridloop1        myfunc w/numpy.sin         180
F77       gridloop2        myfunc w/math.sin           40
F77       gridloop_vec2    vectorized myfunc            2.7
F77       gridloop2_str    F77 myfunc                   1.1
F77       gridloop_noalloc (no alloc. as in pure C++)   1.0

C         gridloop1        myfunc w/math.sin           38
C         gridloop2        myfunc w/math.sin           38
C++ (with class NumPyArray) had the same numbers as C
```

Conclusions about efficiency

- `math.sin` is much faster than `numpy.sin` for scalar expressions
- Callbacks to Python are extremely expensive
- Python+NumPy is 1.5 times slower than pure Fortran
- C and C++ run equally fast
- C++ w/`MyArray` was only 7% slower than pure F77

Minimize the no of callbacks to Python!

More F2PY features

- Hide work arrays (i.e., allocate in wrapper):

```
      subroutine myroutine(a, b, m, n, w1, w2)
      integer m, n
      real*8 a(m), b(n), w1(3*n), w2(m)
Cf2py intent(in,hide) w1
Cf2py intent(in,hide) w2
Cf2py intent(in,out) a
```

  Python interface:

```
a = myroutine(a, b)
```

- Reuse work arrays in subsequent calls (`cache`):

```
      subroutine myroutine(a, b, m, n, w1, w2)
      integer m, n
      real*8 a(m), b(n), w1(3*n), w2(m)
Cf2py intent(in,hide,cache) w1
Cf2py intent(in,hide,cache) w2
```

Other tools

- Pyfort for Python-Fortran integration
  (does not handle F90/F95, not as simple as F2PY)
- SIP: tool for wrapping C++ libraries
- Boost.Python: tool for wrapping C++ libraries
- CXX: C++ interface to Python (Boost is a replacement)
- Note: SWIG can generate interfaces to most scripting languages
  (Perl, Ruby, Tcl, Java, Guile, Mzscheme, ...)

Class programming in Python

Contents

- Intro to the class syntax
- Special attributes
- Special methods
- Classic classes, new-style classes
- Static data, static functions
- Properties
- About scope

More info

- Ch. 8.6 in the course book
- Python Tutorial
- Python Reference Manual (special methods in 3.3)
- Python in a Nutshell (OOP chapter - recommended!)

Classes in Python

- Similar class concept as in Java and C++
- All functions are virtual
- No private/protected variables
  (the effect can be "simulated")
- Single and multiple inheritance
- Everything in Python is a class and works with classes
- Class programming is easier and faster than in C++ and Java (?)

The basics of Python classes

- Declare a base class `MyBase`:

```
class MyBase:

    def __init__(self,i,j):  # constructor
        self.i = i; self.j = j

    def write(self):         # member function
        print ’MyBase: i=’,self.i,’j=’,self.j
```

- `self` is a reference to this object
- Data members are prefixed by self:
  `self.i`, `self.j`
- All functions take `self` as first argument in the declaration, but not in the call

```
inst1 = MyBase(6,9); inst1.write()
```

Implementing a subclass

- Class `MySub` is a subclass of `MyBase`:

```
class MySub(MyBase):

    def __init__(self,i,j,k):  # constructor
        MyBase.__init__(self,i,j)
        self.k = k;

   def write(self):
        print ’MySub: i=’,self.i,’j=’,self.j,’k=’,self.k
```

- Example:

```
# this function works with any object that has a write func:
def write(v): v.write()

# make a MySub instance
i = MySub(7,8,9)

write(i)   # will call MySub’s write
```

Comment on object-orientation

- Consider

```
def write(v):
    v.write()

write(i)   # i is MySub instance
```

- In C++/Java we would declare `v` as a `MyBase` reference and rely on `i.write()` as calling the virtual function `write` in `MySub`
- The same works in Python, but we do not need inheritance and virtual functions here: `v.write()` will work for *any* object `v` that has a callable attribute `write` that takes no arguments
- Object-orientation in C++/Java for parameterizing types is not needed in Python since variables are not declared with types

---

Private/non-public data

- There is no technical way of preventing users from manipulating data and methods in an object
- Convention: attributes and methods starting with an underscore are treated as non-public (“protected”)
- Names starting with a double underscore are considered strictly private (Python mangles class name with method name in this case: `obj.__some` has actually the name `_obj__some`)

```
class MyClass:
    def __init__(self):
        self._a = False     # non-public
        self.b = 0          # public
        self.__c = 0        # private
```

Special attributes

`i1` is `MyBase`, `i2` is `MySub`

- Dictionary of user-defined attributes:

```
>>> i1.__dict__  # dictionary of user-defined attributes
{’i’: 5, ’j’: 7}
>>> i2.__dict__
{’i’: 7, ’k’: 9, ’j’: 8}
```

- Name of class, name of method:

```
>>> i2.__class__.__name__ # name of class
’MySub’
>>> i2.write.__name__     # name of method
’write’
```

- List names of all methods and attributes:

```
>>> dir(i2)
[’__doc__’, ’__init__’, ’__module__’, ’i’, ’j’, ’k’, ’write’]
```

Testing on the class type

- Use `isinstance` for testing class type:

```
if isinstance(i2, MySub):
    # treat i2 as a MySub instance
```

- Can test if a class is a subclass of another:

```
if issubclass(MySub, MyBase):
    ...
```

- Can test if two objects are of the same class:

```
if inst1.__class__ is inst2.__class__
```

  (`is` checks object identity, `==` checks for equal contents)
- `a.__class__` refers the class object of instance a

Creating attributes on the fly

- Attributes can be added at run time (!)

```
>>> class G: pass

>>> g = G()
>>> dir(g)
[’__doc__’, ’__module__’]  # no user-defined attributes

>>> # add instance attributes:
>>> g.xmin=0; g.xmax=4; g.ymin=0; g.ymax=1
>>> dir(g)
[’__doc__’, ’__module__’, ’xmax’, ’xmin’, ’ymax’, ’ymin’]
>>> g.xmin, g.xmax, g.ymin, g.ymax
(0, 4, 0, 1)

>>> # add static variables:
>>> G.xmin=0; G.xmax=2; G.ymin=-1; G.ymax=1
>>> g2 = G()
>>> g2.xmin, g2.xmax, g2.ymin, g2.ymax  # static variables
(0, 2, -1, 1)
```

Another way of adding new attributes

- Can work with `__dict__` directly:

```
>>> i2.__dict__[’q’] = ’some string’
>>> i2.q
’some string’
>>> dir(i2)
[’__doc__’, ’__init__’, ’__module__’,
 ’i’, ’j’, ’k’, ’q’, ’write’]
```

Special methods

- Special methods have leading and trailing double underscores (e.g. `__str__`)
- Here are some operations defined by special methods:

```
len(a)             # a.__len__()
c = a*b            # c = a.__mul__(b)
a = a+b            # a = a.__add__(b)
a += c             # a.__iadd__(c)
d = a[3]           # d = a.__getitem__(3)
a[3] = 0           # a.__setitem__(3, 0)
f = a(1.2, True)   # f = a.__call__(1.2, True)
if a:              # if a.__len__()>0: or if a.__nonzero():
```

Example: functions with extra parameters

- Suppose we need a function of `x` and `y` with three additional parameters `a`, `b`, and `c`:

```
def f(x, y, a, b, c):
    return a + b*x + c*y*y
```

- Suppose we need to send this function to another function

```
def gridvalues(func, xcoor, ycoor, file):
    for i in range(len(xcoor)):
        for j in range(len(ycoor)):
            f = func(xcoor[i], ycoor[j])
            file.write(’%g %g %g\n’ % (xcoor[i], ycoor[j], f)
```

  `func` is expected to be a function of `x` and `y` only (many libraries need to make such assumptions!)

- How can we send our `f` function to `gridvalues`?

Possible (inferior) solutions

- Solution 1: global parameters

```
global a, b, c
...
def f(x, y):
    return a + b*x + c*y*y

...
a = 0.5;  b = 1;  c = 0.01
gridvalues(f, xcoor, ycoor, somefile)
```

  Global variables are usually considered evil

- Solution 2: keyword arguments for parameters

```
def f(x, y, a=0.5, b=1, c=0.01):
    return a + b*x + c*y*y

...
gridvalues(f, xcoor, ycoor, somefile)
```

  useless for other values of `a`, `b`, `c`

Solution: class with call operator

- Make a class with function behavior instead of a pure function
- The parameters are class attributes
- Class instances can be called as ordinary functions, now with `x` and `y` as the only formal arguments

```
class F:
    def __init__(self, a=1, b=1, c=1):
        self.a = a;  self.b = b;  self.c = c

    def __call__(self, x, y):    # special method!
        return self.a + self.b*x + self.c*y*y

f = F(a=0.5, c=0.01)
# can now call f as
v = f(0.1, 2)
...
gridvalues(f, xcoor, ycoor, somefile)
```

Some special methods

- `__init__(self [, args])`: constructor
- `__del__(self)`: destructor (seldom needed since Python offers automatic garbage collection)
- `__str__(self)`: string representation for pretty printing of the object (called by `print` or `str`)
- `__repr__(self)`: string representation for initialization (`a==eval(repr(a))` is true)

Comparison, length, call

- `__eq__(self, x)`: for equality (a==b), should return `True` or `False`
- `__cmp__(self, x)`: for comparison (`<, <=, >, >=, ==, !=`); return negative integer, zero or positive integer if `self` is less than, equal or greater than `x` (resp.)
- `__len__(self)`: length of object (called by `len(x)`)
- `__call__(self [, args])`: calls like `a(x,y)` implies `a.__call__(x,y)`

Indexing and slicing

- `__getitem__(self, i)`: used for subscripting:
  `b = a[i]`
- `__setitem__(self, i, v)`: used for subscripting: `a[i] = v`
- `__delitem__(self, i)`: used for deleting: `del a[i]`
- These three functions are also used for slices:
  `a[p:q:r]` implies that `i` is a `slice object` with attributes `start` (`p`), `stop` (`q`) and `step` (`r`)

```
b = a[:-1]
# implies
b = a.__getitem__(i)
isinstance(i, slice) is True
i.start is None
i.stop  is -1
i.step  is None
```

Arithmetic operations

- `__add__(self, b)`: used for `self+b`, i.e., `x+y` implies `x.__add__(y)`
- `__sub__(self, b)`: `self-b`
- `__mul__(self, b)`: `self*b`
- `__div__(self, b)`: `self/b`
- `__pow__(self, b)`: `self**b` or `pow(self,b)`

In-place arithmetic operations

- `__iadd__(self, b)`: `self += b`
- `__isub__(self, b)`: `self -= b`
- `__imul__(self, b)`: `self *= b`
- `__idiv__(self, b)`: `self /= b`

Right-operand arithmetics

- `__radd__(self, b)`: This method defines `b+self`, while `__add__(self, b)` defines `self+b`. If `a+b` is encountered and `a` does not have an `__add__` method, `b.__radd__(a)` is called if it exists (otherwise `a+b` is not defined).
- Similar methods: `__rsub__`, `__rmul__`, `__rdiv__`

Type conversions

- `__int__(self)`: conversion to integer
  (`int(a)` makes an `a.__int__()` call)
- `__float__(self)`: conversion to float
- `__hex__(self)`: conversion to hexadecimal number

Documentation of special methods: see the *Python Reference Manual* (not the Python Library Reference!), follow link from index “overloading - operator”

Boolean evaluations

- `if a`:
  when is `a` evaluated as true?
- If `a` has `__len__` or `__nonzero__` and the return value is 0 or `False`, `a` evaluates to false
- Otherwise: `a` evaluates to true
- Implication: no implementation of `__len__` or `__nonzero__` implies that `a` evaluates to true!!
- `while a` follows (naturally) the same set-up

Example on call operator: StringFunction

- Matlab has a nice feature: mathematical formulas, written as text, can be turned into callable functions
- A similar feature in Python would be like

```
f = StringFunction_v1(’1+sin(2*x)’)
print f(1.2)  # evaluates f(x) for x=1.2
```

- `f(x)` implies `f.__call__(x)`
- Implementation of class `StringFunction_v1` is compact! (see next slide)

Implementation of StringFunction classes

- Simple implementation:

```
class StringFunction_v1:
    def __init__(self, expression):
        self._f = expression

    def __call__(self, x):
        return eval(self._f)  # evaluate function expression
```

- Problem: `eval(string)` is slow; should pre-compile expression

```
class StringFunction_v2:
    def __init__(self, expression):
        self._f_compiled = compile(expression,
                                   ’<string>’, ’eval’)

    def __call__(self, x):
        return eval(self._f_compiled)
```

New-style classes

- The class concept was redesigned in Python v2.2
- We have *new-style* (v2.2) and *classic* classes
- New-style classes add some convenient functionality to classic classes
- New-style classes must be derived from the `object` base class:

```
class MyBase(object):
    # the rest of MyBase is as before
```

Static data

- Static data (or class variables) are common to all instances

```
>>> class Point:
        counter = 0 # static variable, counts no of instances
        def __init__(self, x, y):
                self.x = x;  self.y = y;
                Point.counter += 1

>>> for i in range(1000):
        p = Point(i*0.01, i*0.001)

>>> Point.counter     # access without instance
1000
>>> p.counter         # access through instance
1000
```

Static methods

- New-style classes allow static methods
(methods that can be called without having an instance)

```
class Point(object):
    _counter = 0
    def __init__(self, x, y):
        self.x = x;  self.y = y;  Point._counter += 1
    def ncopies(): return Point._counter
    ncopies = staticmethod(ncopies)
```

- Calls:

```
>>> Point.ncopies()
0
>>> p = Point(0, 0)
>>> p.ncopies()
1
>>> Point.ncopies()
1
```

- Cannot access `self` or class attributes in static methods

Properties

- Python 2.3 introduced “intelligent” assignment operators, known as *properties*
- That is, assignment may imply a function call:

```
x.data = mydata;     yourdata = x.data
# can be made equivalent to
x.set_data(mydata);  yourdata = x.get_data()
```

- Construction:

```
class MyClass(object):   # new-style class required!
    ...
    def set_data(self, d):
        self._data = d
        <update other data structures if necessary...>

    def get_data(self):
        <perform actions if necessary...>
        return self._data

    data = property(fget=get_data, fset=set_data)
```

Attribute access; traditional

- Direct access:

```
my_object.attr1 = True
a = my_object.attr1
```

- get/set functions:

```
class A:
    def set_attr1(attr1):
        self._attr1 = attr # underscore => non-public variable
        self._update(self._attr1)  # update internal data too
    ...

my_object.set_attr1(True)

a = my_object.get_attr1()
```

Tedious to write! Properties are simpler...

Attribute access; recommended style

- Use direct access if user is allowed to read *and* assign values to the attribute
- Use properties to restrict access, with a corresponding underlying non-public class attribute
- Use properties when assignment or reading requires a set of associated operations
- Never use get/set functions explicitly
- Attributes and functions are somewhat interchanged in this scheme
⇒ that’s why we use the same naming convention

```
myobj.compute_something()
myobj.my_special_variable = yourobj.find_values(x,y)
```

More about scope

- Example: a is global, local, and class attribute

```
a = 1                 # global variable

def f(x):
    a = 2             # local variable

class B:
    def __init__(self):
        self.a = 3    # class attribute

    def scopes(self):
        a = 4         # local (method) variable
```

- Dictionaries with variable names as keys and variables as values:

```
locals()    : local variables
globals()   : global variables
vars()      : local variables
vars(self)  : class attributes
```

Demonstration of scopes (1)

- Function scope:

```
>>> a = 1
>>> def f(x):
        a = 2          # local variable
        print ’locals:’, locals(), ’local a:’, a
        print ’global a:’, globals()[’a’]

>>> f(10)
locals: {’a’: 2, ’x’: 10} local a: 2
global a: 1
```

a refers to local variable

Demonstration of scopes (2)

- Class:

```
class B:
    def __init__(self):
        self.a = 3    # class attribute

    def scopes(self):
        a = 4         # local (method) variable
        print ’locals:’, locals()
        print ’vars(self):’, vars(self)
        print ’self.a:’, self.a
        print ’local a:’, a, ’global a:’, globals()[’a’]
```

- Interactive test:

```
>>> b=B()
>>> b.scopes()
locals: {’a’: 4, ’self’: <scope.B instance at 0x4076fb4c>}
vars(self): {’a’: 3}
self.a: 3
local a: 4 global a: 1
```

Demonstration of scopes (3)

- Variable interpolation with `vars`:

```
class C(B):
    def write(self):
        local_var = -1
        s = ’%(local_var)d %(global_var)d %(a)s’ % vars()
```

- Problem: `vars()` returns dict with local variables and the string needs global, local, and class variables
- Primary solution: use printf-like formatting:

```
s = ’%d %d %d’ % (local_var, global_var, self.a)
```

- More exotic solution:

```
all = {}
for scope in (locals(), globals(), vars(self)):
    all.update(scope)
s = ’%(local_var)d %(global_var)d %(a)s’ % all
```

(but now we overwrite a...)

Namespaces for exec and eval

- `exec` and `eval` may take dictionaries for the global and local namespace:

```
exec code in globals, locals
eval(expr, globals, locals)
```

- Example:

```
a = 8;  b = 9
d = {’a’:1, ’b’:2}
eval(’a + b’, d)  # yields 3
```

and

```
from math import *
d[’b’] = pi
eval(’a+sin(b)’, globals(), d)  # yields 1
```

- Creating such dictionaries can be handy

Generalized StringFunction class (1)

- Recall the StringFunction-classes for turning string formulas into callable objects

```
f = StringFunction(’1+sin(2*x)’)
print f(1.2)
```

- We would like:
  - an arbitrary name of the independent variable
  - parameters in the formula

```
f = StringFunction_v3(’1+A*sin(w*t)’,
                      independent_variable=’t’,
                      set_parameters=’A=0.1; w=3.14159’)
print f(1.2)
f.set_parameters(’A=0.2; w=3.14159’)
print f(1.2)
```

First implementation

- Idea: hold independent variable and “set parameters” code as strings
- Exec these strings (to bring the variables into play) right before the formula is evaluated

```
class StringFunction_v3:
    def __init__(self, expression, independent_variable=’x’,
                 set_parameters=’’):
        self._f_compiled = compile(expression,
                                   ’<string>’, ’eval’)
        self._var = independent_variable  # ’x’, ’t’ etc.
        self._code = set_parameters

    def set_parameters(self, code):
        self._code = code

    def __call__(self, x):
        exec ’%s = %g’ % (self._var, x)  # assign indep. var.
        if self._code:  exec(self._code) # parameters?
        return eval(self._f_compiled)
```

Efficiency tests

- The exec used in the `__call__` method is slow!
- Think of a hardcoded function,

```
def f1(x):
    return sin(x) + x**3 + 2*x
```

and the corresponding `StringFunction`-like objects

- Efficiency test (time units to the right):

```
f1               :  1
StringFunction_v1: 13
StringFunction_v2:  2.3
StringFunction_v3: 22
```

Why?

- eval w/compile is important; exec is very slow

A more efficient StringFunction (1)

- Ideas: hold parameters in a dictionary, set the independent variable into this dictionary, run eval with this dictionary as local namespace
- Usage:

```
f = StringFunction_v4(’1+A*sin(w*t)’, A=0.1, w=3.14159)
f.set_parameters(A=2)   # can be done later
```

A more efficient StringFunction (2)

- Code:

```
class StringFunction_v4:
    def __init__(self, expression, **kwargs):
        self._f_compiled = compile(expression,
                                   ’<string>’, ’eval’)
        self._var = kwargs.get(’independent_variable’, ’x’)
        self._prms = kwargs
        try:    del self._prms[’independent_variable’]
        except: pass

    def set_parameters(self, **kwargs):
        self._prms.update(kwargs)

    def __call__(self, x):
        self._prms[self._var] = x
        return eval(self._f_compiled, globals(), self._prms)
```

Extension to many independent variables

- We would like arbitrary functions of arbitrary parameters and independent variables:

```
f = StringFunction_v5('A*sin(x)*exp(-b*t)', A=0.1, b=1,
                      independent_variables=('x','t'))
print f(1.5, 0.01)  # x=1.5, t=0.01
```

- Idea: add functionality in subclass

```
class StringFunction_v5(StringFunction_v4):
    def __init__(self, expression, **kwargs):
        StringFunction_v4.__init__(self, expression, **kwargs)
        self._var = tuple(kwargs.get('independent_variables',
                                     'x'))
        try:    del self._prms['independent_variables']
        except: pass

    def __call__(self, *args):
        for name, value in zip(self._var, args):
            self._prms[name] = value  # add indep. variable
        return eval(self._f_compiled,
                    self._globals, self._prms)
```

Efficiency tests

- Test function: `sin(x) + x**3 + 2*x`

```
f1                : 1
StringFunction_v1: 13      (because of uncompiled eval)
StringFunction_v2:  2.3
StringFunction_v3: 22      (because of exec in __call__)
StringFunction_v4:  2.3
StringFunction_v5:  3.1    (because of loop in __call__)
```

Removing all overhead

- Instead of `eval` in `__call__` we may build a (lambda) function

```
class StringFunction:
    def _build_lambda(self):
        s = 'lambda ' + ', '.join(self._var)
        # add parameters as keyword arguments:
        if self._prms:
            s += ', ' + ', '.join(['%s=%s' % (k, self._prms[k]) \
                                   for k in self._prms])
        s += ': ' + self._f
        self.__call__ = eval(s, self._globals)
```

- For a call

```
f = StringFunction('A*sin(x)*exp(-b*t)', A=0.1, b=1,
                   independent_variables=('x','t'))
```

the `s` looks like

```
lambda x, t, A=0.1, b=1: return A*sin(x)*exp(-b*t)
```

Final efficiency test

- `StringFunction` objects are as efficient as similar hardcoded objects, i.e.,

```
class F:
    def __call__(self, x, y):
        return sin(x)*cos(y)
```

but there is some overhead associated with the `__call__` op.

- Trick: extract the underlying method and call it directly

```
f1 = F()
f2 = f1.__call__
# f2(x,y) is faster than f1(x,y)
```

Can typically reduce CPU time from 1.3 to 1.0

- Conclusion: now we can grab formulas from command-line, GUI, Web, anywhere, and turn them into callable Python functions *without any overhead*

Adding pretty print and reconstruction

- “Pretty print”:

```
class StringFunction:
    ...
    def __str__(self):
        return self._f  # just the string formula
```

- Reconstruction: `a = eval(repr(a))`

```
    # StringFunction('1+x+a*y',
                     independent_variables=('x','y'),
                     a=1)

    def __repr__(self):
        kwargs = ', '.join(['%s=%s' % (key, repr(value)) \
                     for key, value in self._prms.items()])
        return "StringFunction1(%s, independent_variable=%s"
          ", %s)" % (repr(self._f), repr(self._var), kwargs)
```

Examples on StringFunction functionality (1)

```
>>> from scitools.StringFunction import StringFunction
>>> f = StringFunction('1+sin(2*x)')
>>> f(1.2)
1.6754631805511511

>>> f = StringFunction('1+sin(2*t)', independent_variables='t')
>>> f(1.2)
1.6754631805511511

>>> f = StringFunction('1+A*sin(w*t)', independent_variables='t', \
                       A=0.1, w=3.14159)
>>> f(1.2)
0.94122173238695939
>>> f.set_parameters(A=1, w=1)
>>> f(1.2)
1.9320390859672263

>>> f(1.2, A=2, w=1)   # can also set parameters in the call
2.8640781719344526
```

Examples on StringFunction functionality (2)

```
>>> # function of two variables:
>>> f = StringFunction('1+sin(2*x)*cos(y)', \
                       independent_variables=('x','y'))
>>> f(1.2,-1.1)
1.3063874788637866

>>> f = StringFunction('1+V*sin(w*x)*exp(-b*t)', \
                       independent_variables=('x','t'))
>>> f.set_parameters(V=0.1, w=1, b=0.1)
>>> f(1.0,0.1)
1.0833098208613807
>>> str(f)  # print formula with parameters substituted by values
'1+0.1*sin(1*x)*exp(-0.1*t)'
>>> repr(f)
"StringFunction('1+V*sin(w*x)*exp(-b*t)',
independent_variables=('x', 't'), b=0.10000000000000001,
w=1, V=0.10000000000000001)"

>>> # vector field of x and y:
>>> f = StringFunction('[a+b*x,y]', \
                           independent_variables=('x','y'))
>>> f.set_parameters(a=1, b=2)
>>> f(2,1)  # [1+2*2, 1]
[5, 1]
```

Exercise

- Implement a class for vectors in 3D
- Application example:

```
>>> from Vec3D import Vec3D
>>> u = Vec3D(1, 0, 0)  # (1,0,0) vector
>>> v = Vec3D(0, 1, 0)
>>> print u**v # cross product
(0, 0, 1)
>>> len(u)     # Eucledian norm
1.0
>>> u[1]       # subscripting
0
>>> v[2]=2.5   # subscripting w/assignment
>>> u+v        # vector addition
(1, 1, 2.5)
>>> u-v        # vector subtraction
(1, -1, -2.5)
>>> u*v        # inner (scalar, dot) product
0
>>> str(u)     # pretty print
'(1, 0, 0)'
>>> repr(u)    # u = eval(repr(u))
'Vec3D(1, 0, 0)'
```

Exercise, 2nd part

- Make the arithmetic operators `+`, `-` and `*` more intelligent:

```
u = Vec3D(1, 0, 0)
v = Vec3D(0, -0.2, 8)
a = 1.2
u+v  # vector addition
a+v  # scalar plus vector, yields (1.2, 1, 9.2)
v+a  # vector plus scalar, yields (1.2, 1, 9.2)
a-v  # scalar minus vector
v-a  # scalar minus vector
a*v  # scalar times vector
v*a  # vector times scalar
```

Common tasks in Python

Overview

- file globbing, testing file types
- copying and renaming files, creating and moving to directories, creating directory paths, removing files and directories
- directory tree traversal
- parsing command-line arguments
- running an application
- file reading and writing
- list and dictionary operations
- splitting and joining text
- basics of Python classes
- writing functions

Python programming information

Man-page oriented information:

- `pydoc somemodule.somefunc`, `pydoc somemodule`
- `doc.html`! Links to lots of electronic information
- The Python Library Reference (go to the index)
- Python in a Nutshell
- Beazley's Python reference book
- Your favorite Python language book
- Google

These slides (and exercises) are closely linked to the "Python scripting for computational science" book, ch. 3 and 8

Preprocessor

- C and C++ programmers heavily utilize the "C preprocessor" for including files, excluding code blocks, defining constants, etc.
- `preprocess` is a (Python!) program that provides (most) "C preprocessor" functionality for Python, Perl, Ruby, shell scripts, makefiles, HTML, Java, JavaScript, PHP, Fortran, C, C++, ... (!)
- `preprocess` directives are typeset within comments
- Most important directives: `include`, `if/ifdef/ifndef/else/endif`, `define`
- See `pydoc preprocess` for documentation

```
# #if defined('DEBUG') and DEBUG >= 2
# write out debug info at level 2:
...
# #elif DEBUG == 0
# write out minimal debug info:
...
# #else
# no debug output
# #endif
```

How to use the preprocessor

- Include documentation or common code snippets in several files

```
#  #include "myfile.py"
```

- Exclude/include code snippets according to an variable (its value or just if the variable is defined)

```
# #ifdef MyDEBUG
....debug code....
# #endif
```

- Define variables with optional value

```
# #define MyDEBUG
```

```
# #define MyDEBUG 2
```

Such preprocessor variables can also be defined on the command line

```
preprocess -DMyDEBUG=2 myscript.p.py > myscript.py
```

- Naming convention: `.p.py` files are input, `.py` output

File globbing

- List all .ps and .gif files (Unix):

```
ls *.ps *.gif
```

- Cross-platform way to do it in Python:

```
import glob
filelist = glob.glob('*.ps') + glob.glob('*.gif')
```

This is referred to as file globbing

Testing file types

```
import os.path
print myfile,

if os.path.isfile(myfile):
     print 'is a plain file'
if os.path.isdir(myfile):
     print 'is a directory'
if os.path.islink(myfile):
     print 'is a link'

# the size and age:
size = os.path.getsize(myfile)
time_of_last_access       = os.path.getatime(myfile)
time_of_last_modification = os.path.getmtime(myfile)

# times are measured in seconds since 1970.01.01
days_since_last_access = \
(time.time() - os.path.getatime(myfile))/(3600*24)
```

More detailed file info

```
import stat

myfile_stat = os.stat(myfile)
filesize = myfile_stat[stat.ST_SIZE]
mode = myfile_stat[stat.ST_MODE]
if stat.S_ISREG(mode):
    print ’%(myfile)s is a regular file ’\
          ’with %(filesize)d bytes’ % vars()
```

Check out the `stat` module in Python Library Reference

Copy, rename and remove files

- Copy a file:

  ```
  import shutil
  shutil.copy(myfile, tmpfile)
  ```

- Rename a file:

  ```
  os.rename(myfile, ’tmp.1’)
  ```

- Remove a file:

  ```
  os.remove(’mydata’)
  # or os.unlink(’mydata’)
  ```

Path construction

- Cross-platform construction of file paths:

  ```
  filename = os.path.join(os.pardir, ’src’, ’lib’)

  # Unix:    ../src/lib
  # Windows: ..\src\lib

  shutil.copy(filename, os.curdir)

  # Unix:  cp ../src/lib .

  # os.pardir : ..
  # os.curdir : .
  ```

Directory management

- Creating and moving to directories:

  ```
  dirname = ’mynewdir’
  if not os.path.isdir(dirname):
      os.mkdir(dirname) # or os.mkdir(dirname,’0755’)
  os.chdir(dirname)
  ```

- Make complete directory path with intermediate directories:

  ```
  path = os.path.join(os.environ[’HOME’],’py’,’src’)
  os.makedirs(path)

  # Unix: mkdirhier $HOME/py/src
  ```

- Remove a non-empty directory tree:

  ```
  shutil.rmtree(’myroot’)
  ```

Basename/directory of a path

- Given a path, e.g.,

  ```
  fname = ’/home/hpl/scripting/python/intro/hw.py’
  ```

- Extract directory and basename:

  ```
  # basename: hw.py
  basename = os.path.basename(fname)

  # dirname: /home/hpl/scripting/python/intro
  dirname  = os.path.dirname(fname)

  # or
  dirname, basename = os.path.split(fname)
  ```

- Extract suffix:

  ```
  root, suffix = os.path.splitext(fname)
  # suffix: .py
  ```

Platform-dependent operations

- The operating system interface in Python is the same on Unix, Windows and Mac
- Sometimes you need to perform platform-specific operations, but how can you make a portable script?

  ```
  # os.name       : operating system name
  # sys.platform  : platform identifier

  # cmd:  string holding command to be run
  if os.name == ’posix’:            # Unix?
      failure, output = commands.getstatusoutput(cmd + ’&’)
  elif sys.platform[:3] == ’win’:   # Windows?
      failure, output = commands.getstatusoutput(’start ’ + cmd)
  else:
      # foreground execution:
      failure, output = commands.getstatusoutput(cmd)
  ```

Traversing directory trees (1)

- Run through all files in your home directory and list files that are larger than 1 Mb
- A Unix find command solves the problem:

  ```
  find $HOME -name ’*’ -type f -size +2000 \
       -exec ls -s {} \;
  ```

- This (and all features of Unix find) can be given a cross-platform implementation in Python

---

Traversing directory trees (2)

- Similar cross-platform Python tool:

  ```
  root = os.environ[’HOME’]  # my home directory
  os.path.walk(root, myfunc, arg)
  ```

  walks through a directory tree (`root`) and calls, for each directory `dirname`,

  ```
  myfunc(arg, dirname, files)  # files is list of (local) filenames
  ```

- `arg` is any user-defined argument, e.g. a nested list of variables

Example on finding large files

```
def checksize1(arg, dirname, files):
    for file in files:
        # construct the file’s complete path:
        filename = os.path.join(dirname, file)
        if os.path.isfile(filename):
            size = os.path.getsize(filename)
            if size > 1000000:
                print ’%.2fMb %s’ % (size/1000000.0,filename)

root = os.environ[’HOME’]
os.path.walk(root, checksize1, None)

# arg is a user-specified (optional) argument,
# here we specify None since arg has no use
# in the present example
```

Make a list of all large files

- Slight extension of the previous example
- Now we use the `arg` variable to build a list during the walk

```
def checksize1(arg, dirname, files):
    for file in files:
        filepath = os.path.join(dirname, file)
        if os.path.isfile(filepath):
            size = os.path.getsize(filepath)
            if size > 1000000:
                size_in_Mb = size/1000000.0
                arg.append((size_in_Mb, filename))

bigfiles = []
root = os.environ[’HOME’]
os.path.walk(root, checksize1, bigfiles)
for size, name in bigfiles:
    print name, ’is’, size, ’Mb’
```

arg must be a list or dictionary

- Let’s build a tuple of all files instead of a list:

```
def checksize1(arg, dirname, files):
    for file in files:
        filepath = os.path.join(dirname, file)
        if os.path.isfile(filepath):
            size = os.path.getsize(filepath)
            if size > 1000000:
                msg = ’%.2fMb %s’ % (size/1000000.0, filepath)
                arg = arg + (msg,)

bigfiles = []
os.path.walk(os.environ[’HOME’], checksize1, bigfiles)
for size, name in bigfiles:
    print name, ’is’, size, ’Mb’
```

- Now `bigfiles` is an empty list! Why? Explain in detail... (Hint: `arg` must be mutable)

Creating Tar archives

- Tar is a widepsread tool for packing file collections efficiently
- Very useful for software distribution or sending (large) collections of files in email
- Demo:

```
>>> import tarfile
>>> files = ’NumPy_basics.py’, ’hw.py’, ’leastsquares.py’
>>> tar = tarfile.open(’tmp.tar.gz’, ’w:gz’)  # gzip compression
>>> for file in files:
...     tar.add(file)
...
>>> # check what’s in this archive:
>>> members = tar.getmembers()  # list of TarInfo objects
>>> for info in members:
...     print ’%s: size=%d, mode=%s, mtime=%s’ % \
...           (info.name, info.size, info.mode,
...            time.strftime(’%Y.%m.%d’, time.gmtime(info.mtime)))
...
NumPy_basics.py: size=11898, mode=33261, mtime=2004.11.23
hw.py: size=206, mode=33261, mtime=2005.08.12
leastsquares.py: size=1560, mode=33261, mtime=2004.09.14
>>> tar.close()
```

- Compressions: uncompressed (`w:`), gzip (`w:gz`), bzip2 (`w:bz2`)

Reading Tar archives

```
>>> tar = tarfile.open(’tmp.tar.gz’, ’r’)
>>>
>>> for file in tar.getmembers():
...     tar.extract(file)       # extract file to current work.dir
...
>>> # do we have all the files?
>>> allfiles = os.listdir(os.curdir)
>>> for file in allfiles:
...     if not file in files:  print ’missing’, file
...
>>> hw = tar.extractfile(’hw.py’)  # extract as file object
>>> hw.readlines()
```

Measuring CPU time (1)

- The time module:

```
import time
e0 = time.time()     # elapsed time since the epoch
c0 = time.clock()    # total CPU time spent so far
# do tasks...
elapsed_time = time.time() - e0
cpu_time = time.clock() - c0
```

- The `os.times` function returns a list:

```
os.times()[0]  : user   time, current process
os.times()[1]  : system time, current process
os.times()[2]  : user   time, child processes
os.times()[3]  : system time, child processes
os.times()[4]  : elapsed time
```

- CPU time = user time + system time

Measuring CPU time (2)

- Application:

```
t0 = os.times()
# do tasks...
os.system(time_consuming_command) # child process
t1 = os.times()

elapsed_time = t1[4] - t0[4]
user_time    = t1[0] - t0[0]
system_time  = t1[1] - t0[1]
cpu_time     = user_time + system_time
cpu_time_system_call = t1[2]-t0[2] + t1[3]-t0[3]
```

- There is a special Python profiler for finding bottlenecks in scripts (ranks functions according to their CPU-time consumption)

A timer function

Let us make a function `timer` for measuring the efficiency of an arbitrary function. `timer` takes 4 arguments:

- a function to call
- a list of arguments to the function
- number of calls to make (repetitions)
- name of function (for printout)

```
def timer(func, args, repetitions, func_name):
    t0 = time.time();  c0 = time.clock()

    for i in range(repetitions):
        func(*args)  # old style: apply(func, args)

    print ’%s: elapsed=%g, CPU=%g’ % \
    (func_name, time.time()-t0, time.clock()-c0)
```

Parsing command-line arguments

- Running through `sys.argv[1:]` and extracting command-line info ’manually’ is easy
- Using standardized modules and interface specifications is better!
- Python’s `getopt` and `optparse` modules parse the command line
- `getopt` is the simplest to use
- `optparse` is the most sophisticated

Short and long options

- It is a ’standard’ to use either short or long options

```
-d dirname           # short options -d and -h
--directory dirname  # long options --directory and --help
```

- Short options have single hyphen,
  long options have double hyphen
- Options can take a value or not:

```
--directory dirname --help --confirm
-d dirname -h -i
```

- Short options can be combined

```
-iddirname   is the same as  -i -d dirname
```

Using the getopt module (1)

- Specify short options by the option letters, followed by colon if the option requires a value
- Example: `’id:h’`
- Specify long options by a list of option names, where names must end with = if the require a value
- Example: `[’help’,’directory=’,’confirm’]`

Using the getopt module (2)

- `getopt` returns a list of (option,value) pairs and a list of the remaining arguments
- Example:

```
--directory mydir -i file1 file2
```

makes `getopt` return

```
[(’--directory’,’mydir’), (’-i’,’’)]
[’file1’,’file2]’
```

Using the getopt module (3)

- Processing:

```
import getopt
try:
    options, args = getopt.getopt(sys.argv[1:], ’d:hi’,
                    [’directory=’, ’help’, ’confirm’])
except:
    # wrong syntax on the command line, illegal options,
    # missing values etc.

directory = None; confirm = 0  # default values
for option, value in options:
    if option in (’-h’, ’--help’):
        # print usage message
    elif option in (’-d’, ’--directory’):
        directory = value
    elif option in (’-i’, ’--confirm’):
        confirm = 1
```

Using the interface

- Equivalent command-line arguments:

```
-d mydir --confirm src1.c src2.c
--directory mydir -i src1.c src2.c
--directory=mydir --confirm src1.c src2.c
```

- Abbreviations of long options are possible, e.g.,

```
--d mydir --co
```

- This one also works: `-idmydir`

Writing Python data structures

- Write nested lists:

```
somelist = [’text1’, ’text2’]
a = [[1.3,somelist], ’some text’]
f = open(’tmp.dat’, ’w’)

# convert data structure to its string repr.:
f.write(str(a))
f.close()
```

- Equivalent statements writing to standard output:

```
print a
sys.stdout.write(str(a) + ’\n’)

# sys.stdin        standard input as file object
# sys.stdout       standard input as file object
```

Reading Python data structures

- `eval(s)`: treat string s as Python code
- `a = eval(str(a))` is a valid ’equation’ for basic Python data structures
- Example: read nested lists

```
f = open(’tmp.dat’, ’r’)  # file written in last slide
# evaluate first line in file as Python code:
newa = eval(f.readline())
```

results in

```
[[1.3, [’text1’, ’text2’]], ’some text’]

# i.e.
newa = eval(f.readline())
# is the same as
newa = [[1.3, [’text1’, ’text2’]], ’some text’]
```

Remark about str and eval

- `str(a)` is implemented as an object function `__str__`
- `repr(a)` is implemented as an object function `__repr__`
- `str(a)`: pretty print of an object
- `repr(a)`: print of all info for use with `eval`
- `a = eval(repr(a))`
- `str` and `repr` are identical for standard Python objects (lists, dictionaries, numbers)

Persistence

- Many programs need to have persistent data structures, i.e., data live after the program is terminated and can be retrieved the next time the program is executed
- `str`, `repr` and `eval` are convenient for making data structures persistent
- pickle, cPickle and shelve are other (more sophisticated) Python modules for storing/loading objects

Pickling

- Write *any* set of data structures to file using the cPickle module:

```
f = open(filename, ’w’)
import cPickle
cPickle.dump(a1, f)
cPickle.dump(a2, f)
cPickle.dump(a3, f)
f.close()
```

- Read data structures in again later:

```
f = open(filename, ’r’)
a1 = cPickle.load(f)
a2 = cPickle.load(f)
a3 = cPickle.load(f)
```

Shelving

- Think of shelves as dictionaries with file storage

```
import shelve
database = shelve.open(filename)
database[’a1’] = a1  # store a1 under the key ’a1’
database[’a2’] = a2
database[’a3’] = a3
# or
database[’a123’] = (a1, a2, a3)

# retrieve data:
if ’a1’ in database:
    a1 = database[’a1’]
# and so on

# delete an entry:
del database[’a2’]

database.close()
```

What assignment really means

```
>>> a = 3           # a refers to int object with value 3
>>> b = a           # b refers to a (int object with value 3)
>>> id(a), id(b )   # print integer identifications of a and b
(135531064, 135531064)
>>> id(a) == id(b)  # same identification?
True                # a and b refer to the same object
>>> a is b          # alternative test
True
>>> a = 4           # a refers to a (new) int object
>>> id(a), id(b)    # let’s check the IDs
(135532056, 135531064)
>>> a is b
False
>>> b     # b still refers to the int object with value 3
3
```

Assignment vs in-place changes

```
>>> a = [2, 6]     # a refers to a list [2, 6]
>>> b = a          # b refers to the same list as a
>>> a is b
True
>>> a = [1, 6, 3]  # a refers to a new list
>>> a is b
False
>>> b              # b still refers to the old list
[2, 6]

>>> a = [2, 6]
>>> b = a
>>> a[0] = 1       # make in-place changes in a
>>> a.append(3)    # another in-place change
>>> a
[1, 6, 3]
>>> b
[1, 6, 3]
>>> a is b         # a and b refer to the same list object
True
```

Assignment with copy

- What if we want b to be a copy of a?
- Lists: `a[:]` extracts a slice, which is a *copy* of all elements:

```
>>> b = a[:]   # b refers to a copy of elements in a
>>> b is a
False
```

  In-place changes in a will not affect b

- Dictionaries: use the `copy` method:

```
>>> a = {’refine’: False}
>>> b = a.copy()
>>> b is a
False
```

  In-place changes in a will not affect b

Running an application

- Run a stand-alone program:

```
cmd = ’myprog -c file.1 -p -f -q > res’
failure = os.system(cmd)
if failure:
  print ’%s: running myprog failed’ % sys.argv[0]
  sys.exit(1)
```

- Redirect output from the application to a list of lines:

```
pipe = os.popen(cmd)
output = pipe.readlines()
pipe.close()

for line in output:
  # process line
```

- Better tool: the `commands` module (next slide)

Running applications and grabbing the output

- A nice way to execute another program:

```
import commands
failure, output = commands.getstatusoutput(cmd)

if failure:
    print ’Could not run’, cmd; sys.exit(1)

for line in output.splitlines()  # or output.split(’\n’):
    # process line
```

  (`output` holds the output as a string)
- `output` holds both standard error and standard output (`os.popen` grabs only standard output so you do not see error messages)

Running applications in the background

- `os.system`, pipes, or `commands.getstatusoutput` terminates after the command has terminated
- There are two methods for running the script in parallel with the command:
  - run the command in the background

```
Unix:     add an ampersand (&) at the end of the command
Windows:  run the command with the ’start’ program
```

  - run the operating system command in a separate thread
- More info: see “Platform-dependent operations” slide and the `threading` module

---

The new standard: subprocess

- A module subprocess is the new standard for running stand-alone applications:

```
from subprocess import call
try:
    returncode = call(cmd, shell=True)
    if returncode:
        print ’Failure with returncode’, returncode; sys,exit(1)
except OSError, message:
    print ’Execution failed!\n’, message; sys.exit(1)
```

- More advanced use of subprocess applies its `Popen` object

```
from subprocess import Popen, PIPE
p = Popen(cmd, shell=True, stdout=PIPE)
output, errors = p.communicate()
```

Output pipe

- Open (in a script) a dialog with an interactive program:

```
pipe = Popen(’gnuplot -persist’, shell=True, stdin=PIPE).stdin
pipe.write(’set xrange [0:10]; set yrange [-2:2]\n’)
pipe.write(’plot sin(x)\n’)
pipe.write(’quit’)  # quit Gnuplot
```

- Same as "here documents" in Unix shells:

```
gnuplot <<EOF
set xrange [0:10]; set yrange [-2:2]
plot sin(x)
quit
EOF
```

Writing to and reading from applications

- In theory, `Popen` allows us to have two-way comminucation with an application (read/write), but this technique is not suitable for reliable two-way dialog (easy to get hang-ups)
- The `pexpect` module is the right tool for a two-way dialog with a stand-alone application

```
# copy files to remote host via scp and password dialog
cmd = ’scp %s %s@%s:%s’ % (filename, user, host, directory)
import pexpect
child = pexpect.spawn(cmd)
child.expect(’password:’)
child.sendline(’&%$hQxz?+MbH’)
child.expect(pexpect.EOF)  # important; wait for end of scp sessi
child.close()
```

- Complete example: `simviz1.py` version that runs `oscillator` on a remote machine (“supercomputer”) via `pexpect`:

```
src/py/examples/simviz/simviz1_ssh_pexpect.py
```

File reading

- Load a file into list of lines:

```
infilename = ’.myprog.cpp’
infile = open(infilename, ’r’)  # open file for reading

# load file into a list of lines:
lines = infile.readlines()

# load file into a string:
filestr = infile.read()
```

- Line-by-line reading (for large files):

```
while 1:
    line = infile.readline()
    if not line: break
    # process line
```

File writing

- Open a new output file:

```
outfilename = ’.myprog2.cpp’
outfile = open(outfilename, ’w’)
outfile.write(’some string\n’)
```

- Append to existing file:

```
outfile = open(outfilename, ’a’)
outfile.write(’....’)
```

Python types

- Numbers: `float`, `complex`, `int` (+ `bool`)
- Sequences: `list`, `tuple`, `str`, NumPy arrays
- Mappings: `dict` (dictionary/hash)
- Instances: user-defined class
- Callables: functions, callable instances

Numerical expressions

- Python distinguishes between strings and numbers:

```
b =  1.2       # b is a number
b = ’1.2’      # b is a string
a = 0.5 * b    # illegal: b is NOT converted to float
a = 0.5 * float(b)   # this works
```

- All Python objects are compard with

```
==   !=  <  >  <=  >=
```

Potential confusion

- Consider:

```
b = ’1.2’

if b < 100:    print b, ’< 100’
else:          print b, ’>= 100’
```

What do we test? string less than number!

- What we want is

```
if float(b) < 100:   # floating-point number comparison
# or
if b < str(100):     # string comparison
```

Boolean expressions

- A `bool` type is `True` or `False`
- Can mix `bool` with `int` 0 (false) or 1 (true)
- `if a:` evaluates a in a boolean context, same as `if bool(a):`
- Boolean tests:

```
>>> a = ’’
>>> bool(a)
False
>>> bool(’some string’)
True
>>> bool([])
False
>>> bool([1,2])
True
```

- Empty strings, lists, tuples, etc. evaluates to `False` in a boolean context

---

Setting list elements

- Initializing a list:

```
arglist = [myarg1, ’displacement’, "tmp.ps"]
```

- Or with indices (if there are already two list elements):

```
arglist[0] = myarg1
arglist[1] = ’displacement’
```

- Create list of specified length:

```
n = 100
mylist = [0.0]*n
```

- Adding list elements:

```
arglist = []  # start with empty list
arglist.append(myarg1)
arglist.append(’displacement’)
```

Getting list elements

- Extract elements form a list:

```
 filename, plottitle, psfile  = arglist
(filename, plottitle, psfile) = arglist
[filename, plottitle, psfile] = arglist
```

- Or with indices:

```
filename = arglist[0]
plottitle = arglist[1]
```

Traversing lists

- For each item in a list:

```
for entry in arglist:
    print ’entry is’, entry
```

- For-loop-like traversal:

```
start = 0;  stop = len(arglist);  step = 1
for index in range(start, stop, step):
    print ’arglist[%d]=%s’ % (index,arglist[index])
```

- Visiting items in reverse order:

```
mylist.reverse()  # reverse order
for item in mylist:
    # do something...
```

List comprehensions

- Compact syntax for manipulating all elements of a list:

```
y = [ float(yi) for yi in line.split() ]  # call function float
x = [ a+i*h for i in range(n+1) ]         # execute expression
```

(called list comprehension)

- Written out:

```
y = []
for yi in line.split():
    y.append(float(yi))
```

etc.

Map function

- `map` is an alternative to list comprehension:

```
y = map(float, line.split())
y = map(lambda i: a+i*h, range(n+1))
```

- `map` is faster than list comprehension but not as easy to read

Typical list operations

```
d = []               # declare empty list
d.append(1.2)        # add a number 1.2
d.append(’a’)        # add a text
d[0] = 1.3           # change an item
del d[1]             # delete an item
len(d)               # length of list
```

Nested lists

- Lists can be nested and heterogeneous
- List of string, number, list and dictionary:

```
>>> mylist = [’t2.ps’, 1.45, [’t2.gif’, ’t2.png’],\
          { ’factor’ : 1.0, ’c’ : 0.9} ]
>>> mylist[3]
{’c’: 0.90000000000000002, ’factor’: 1.0}
>>> mylist[3][’factor’]
1.0
>>> print mylist
[’t2.ps’, 1.45, [’t2.gif’, ’t2.png’],
 {’c’: 0.90000000000000002, ’factor’: 1.0}]
```

- Note: `print` prints all basic Python data structures in a nice format

---

Sorting a list

- In-place sort:

  `mylist.sort()`

  modifies `mylist`!

```
>>> print mylist
[1.4, 8.2, 77, 10]
>>> mylist.sort()
>>> print mylist
[1.4, 8.2, 10, 77]
```

- Strings and numbers are sorted as expected

Defining the comparison criterion

```
# ignore case when sorting:

def ignorecase_sort(s1, s2):
    s1 = s1.lower()
    s2 = s2.lower()
    if   s1 <  s2: return -1
    elif s1 == s2: return  0
    else:          return  1

# or a quicker variant, using Python’s built-in
# cmp function:
def ignorecase_sort(s1, s2):
    s1 = s1.lower();  s2 = s2.lower()
    return cmp(s1,s2)

# usage:
mywords.sort(ignorecase_sort)
```

Tuples (’constant lists’)

- Tuple = constant list; items cannot be modified

```
>>> s1=[1.2, 1.3, 1.4]   # list
>>> s2=(1.2, 1.3, 1.4)   # tuple
>>> s2=1.2, 1.3, 1.4     # may skip parenthesis
>>> s1[1]=0              # ok
>>> s2[1]=0              # illegal
Traceback (innermost last):
  File "<pyshell#17>", line 1, in ?
    s2[1]=0
TypeError: object doesn’t support item assignment

>>> s2.sort()
AttributeError: ’tuple’ object has no attribute ’sort’
```

- You cannot append to tuples, but you can add two tuples to form a new tuple

---

Dictionary operations

- Dictionary = array with text indices (keys)
  (even user-defined objects can be indices!)
- Also called hash or associative array
- Common operations:

```
d[’mass’]           # extract item corresp. to key ’mass’
d.keys()            # return copy of list of keys
d.get(’mass’,1.0)   # return 1.0 if ’mass’ is not a key
d.has_key(’mass’)   # does d have a key ’mass’?
d.items()           # return list of (key,value) tuples
del d[’mass’]       # delete an item
len(d)              # the number of items
```

Initializing dictionaries

- Multiple items:

```
d = { ’key1’ : value1, ’key2’ : value2 }
# or
d = dict(key1=value1, key2=value2)
```

- Item by item (indexing):

```
d[’key1’] = anothervalue1
d[’key2’] = anothervalue2
d[’key3’] = value2
```

Dictionary examples

- Problem: store MPEG filenames corresponding to a parameter with values 1, 0.1, 0.001, 0.00001

```
movies[1]       = ’heatsim1.mpeg’
movies[0.1]     = ’heatsim2.mpeg’
movies[0.001]   = ’heatsim5.mpeg’
movies[0.00001] = ’heatsim8.mpeg’
```

- Store compiler data:

```
g77 = {
  ’name’          : ’g77’,
  ’description’   : ’GNU f77 compiler, v2.95.4’,
  ’compile_flags’ : ’ -pg’,
  ’link_flags’    : ’ -pg’,
  ’libs’          : ’-lf2c’,
  ’opt’           : ’-O3 -ffast-math -funroll-loops’
}
```

Another dictionary example (1)

- Idea: hold command-line arguments in a dictionary `cmlargs[option]`, e.g., `cmlargs['infile']`, instead of separate variables
- Initialization: loop through `sys.argv`, assume options in pairs: –option value

```
arg_counter = 1
while arg_counter < len(sys.argv):
    option = sys.argv[arg_counter]
    option = option[2:]  # remove double hyphen
    if option in cmlargs:
        # next command-line argument is the value:
        arg_counter += 1
        value = sys.argv[arg_counter]
        cmlargs[cmlarg] = value
    else:
        # illegal option
    arg_counter += 1
```

Another dictionary example (2)

- Working with `cmlargs` in simviz1.py:

```
f = open(cmlargs[’case’] + ’.’, ’w’)
f.write(cmlargs[’m’]     + ’\n’)
f.write(cmlargs[’b’]     + ’\n’)
f.write(cmlargs[’c’]     + ’\n’)
f.write(cmlargs[’func’]  + ’\n’)
...
# make gnuplot script:
f = open(cmlargs[’case’] + ’.gnuplot’, ’w’)
f.write("""
set title ’%s: m=%s b=%s c=%s f(y)=%s A=%s w=%s y0=%s dt=%s’;
""" % (cmlargs[’case’],cmlargs[’m’],cmlargs[’b’],
       cmlargs[’c’],cmlargs[’func’],cmlargs[’A’],
       cmlargs[’w’],cmlargs[’y0’],cmlargs[’dt’]))
if not cmlargs[’noscreenplot’]:
    f.write("plot ’sim.dat’ title ’y(t)’ with lines;\n")
```

- Note: all `cmlargs[opt]` are (here) strings!

Environment variables

- The dictionary-like `os.environ` holds the environment variables:

```
os.environ[’PATH’]
os.environ[’HOME’]
os.environ[’scripting’]
```

- Write all the environment variables in alphabethic order:

```
sorted_env = os.environ.keys()
sorted_env.sort()

for key in sorted_env:
    print ’%s = %s’ % (key, os.environ[key])
```

Find a program

- Check if a given program is on the system:

```
program = ’vtk’
path = os.environ[’PATH’]
# PATH can be /usr/bin:/usr/local/bin:/usr/X11/bin
# os.pathsep is the separator in PATH
# (: on Unix, ; on Windows)
paths = path.split(os.pathsep)
for d in paths:
    if os.path.isdir(d):
        if os.path.isfile(os.path.join(d, program)):
             program_path = d; break

try:  # program was found if program_path is defined
    print ’%s found in %s’ % (program, program_path)
except:
    print ’%s not found’ % program
```

Cross-platform fix of previous script

- On Windows, programs usually end with `.exe` (binaries) or `.bat` (DOS scripts), while on Unix most programs have no extension
- We test if we are on Windows:

```
if sys.platform[:3] == ’win’:
    # Windows-specific actions
```

- Cross-platform snippet for finding a program:

```
for d in paths:
    if os.path.isdir(d):
        fullpath = os.path.join(dir, program)
        if sys.platform[:3] == ’win’:   # windows machine?
            for ext in ’.exe’, ’.bat’:  # add extensions
                if os.path.isfile(fullpath + ext):
                    program_path = d; break
        else:
            if os.path.isfile(fullpath):
                program_path = d; break
```

Splitting text

- Split string into words:

```
>>> files = ’case1.ps case2.ps    case3.ps’
>>> files.split()
[’case1.ps’, ’case2.ps’, ’case3.ps’]
```

- Can split wrt other characters:

```
>>> files = ’case1.ps, case2.ps, case3.ps’
>>> files.split(’, ’)
[’case1.ps’, ’case2.ps’, ’case3.ps’]
>>> files.split(’,  ’)  # extra erroneous space after comma...
[’case1.ps, case2.ps, case3.ps’]  # unsuccessful split
```

- Very useful when interpreting files

Example on using split (1)

- Suppose you have file containing numbers only
- The file can be formatted ’arbitrarily’, e.g,

```
1.432 5E-09
1.0

3.2 5 69 -111
4 7 8
```

- Get a list of all these numbers:

```
f = open(filename, ’r’)
numbers = f.read().split()
```

- String objects’s `split` function splits wrt sequences of whitespace (whitespace = blank char, tab or newline)

Example on using split (2)

- Convert the list of strings to a list of floating-point numbers, using `map`:

```
numbers = [ float(x) for x in f.read().split() ]
```

- Think about reading this file in Fortran or C!
  (quite some low-level code...)
- This is a good example of how scripting languages, like Python, yields flexible and compact code

Joining a list of strings

- Join is the opposite of split:

```
>>> line1 = ’iteration 12:    eps= 1.245E-05’
>>> line1.split()
[’iteration’, ’12:’, ’eps=’, ’1.245E-05’]
>>> w = line1.split()
>>> ’ ’.join(w)  # join w elements with delimiter ’ ’
’iteration 12: eps= 1.245E-05’
```

- Any delimiter text can be used:

```
>>> ’@@@’.join(w)
’iteration@@@12:@@@eps=@@@1.245E-05’
```

Common use of join/split

```
f = open(’myfile’, ’r’)
lines = f.readlines()            # list of lines
filestr = ’’.join(lines)         # a single string
# can instead just do
# filestr = file.read()

# do something with filestr, e.g., substitutions...

# convert back to list of lines:
lines = filestr.splitlines()
for line in lines:
    # process line
```

Text processing (1)

- Exact word match:

```
if line == ’double’:
   # line equals ’double’

if line.find(’double’) != -1:
   # line contains ’double’
```

- Matching with Unix shell-style wildcard notation:

```
import fnmatch
if fnmatch.fnmatch(line, ’double’):
   # line contains ’double’
```

  Here, double can be any valid wildcard expression, e.g.,

```
double*   [Dd]ouble
```

Text processing (2)

- Matching with full regular expressions:

```
import re
if re.search(r’double’, line):
    # line contains ’double’
```

  Here, double can be any valid regular expression, e.g.,

```
double[A-Za-z0-9_]*  [Dd]ouble  (DOUBLE|double)
```

Substitution

- Simple substitution:

```
newstring = oldstring.replace(substring, newsubstring)
```

- Substitute regular expression `pattern` by `replacement` in `str`:

```
import re
str = re.sub(pattern, replacement, str)
```

Various string types

- There are many ways of constructing strings in Python:

```
s1 = ’with forward quotes’
s2 = "with double quotes"
s3 = ’with single quotes and a variable: %(r1)g’ \
     % vars()
s4 = """as a triple double (or single) quoted string"""
s5 = """triple double (or single) quoted strings
allow multi-line text (i.e., newline is preserved)
with other quotes like ’ and  "
"""
```

- Raw strings are widely used for regular expressions

```
s6 = r’raw strings start with r and \ remains backslash’
s7 = r"""another raw string with a double backslash: \\ """
```

String operations

- String concatenation:

```
myfile = filename + ’_tmp’ + ’.dat’
```

- Substring extraction:

```
>>> teststr = ’0123456789’
>>> teststr[0:5]; teststr[:5]
’01234’
’01234’
>>> teststr[3:8]
’34567’
>>> teststr[3:]
’3456789’
```

Mutable and immutable objects

- The items/contents of mutable objects can be changed in-place
- Lists and dictionaries are mutable
- The items/contents of immutable objects cannot be changed in-place
- Strings and tuples are immutable

```
>>> s2=(1.2, 1.3, 1.4)   # tuple
>>> s2[1]=0              # illegal
```

Classes in Python

- Similar class concept as in Java and C++
- All functions are virtual
- No private/protected variables
  (the effect can be "simulated")
- Single and multiple inheritance
- Everything in Python is a class and works with classes
- Class programming is easier and faster than in C++ and Java (?)

The basics of Python classes

- Declare a base class `MyBase`:

```
class MyBase:

    def __init__(self,i,j):  # constructor
        self.i = i; self.j = j

    def write(self):         # member function
        print 'MyBase: i=',self.i,'j=',self.j
```

- `self` is a reference to this object
- Data members are prefixed by self:
  `self.i`, `self.j`
- All functions take `self` as first argument in the declaration, but not in the call

```
obj1 = MyBase(6,9); obj1.write()
```

Implementing a subclass

- Class `MySub` is a subclass of `MyBase`:

```
class MySub(MyBase):

    def __init__(self,i,j,k):  # constructor
        MyBase.__init__(self,i,j)
        self.k = k;

   def write(self):
        print 'MySub: i=',self.i,'j=',self.j,'k=',self.k
```

- Example:

```
# this function works with any object that has a write func:
def write(v): v.write()

# make a MySub instance
i = MySub(7,8,9)

write(i)   # will call MySub's write
```

Functions

- Python functions have the form

```
def function_name(arg1, arg2, arg3):
    # statements
    return something
```

- Example:

```
def debug(comment, variable):
    if os.environ.get('PYDEBUG', '0') == '1':
        print comment, variable
...
v1 = file.readlines()[3:]
debug('file %s (exclusive header):' % file.name, v1)

v2 = somefunc()
debug('result of calling somefunc:', v2)
```

This function prints any printable object!

Keyword arguments

- Can name arguments, i.e., keyword=default-value

```
def mkdir(dirname, mode=0777, remove=1, chdir=1):
    if os.path.isdir(dirname):
        if remove:  shutil.rmtree(dirname)
        elif :      return 0  # did not make a new directory
    os.mkdir(dir, mode)
    if chdir: os.chdir(dirname)
    return 1      # made a new directory
```

Calls look like

```
mkdir('tmp1')
mkdir('tmp1', remove=0, mode=0755)
mkdir('tmp1', 0755, 0, 1)             # less readable
```

- Keyword arguments make the usage simpler and improve documentation

Variable-size argument list

- Variable number of ordinary arguments:

```
def somefunc(a, b, *rest):
    for arg in rest:
        # treat the rest...

# call:
somefunc(1.2, 9, 'one text', 'another text')
#                ...........rest...........
```

- Variable number of keyword arguments:

```
def somefunc(a, b, *rest, **kw):
    #...
    for arg in rest:
        # work with arg...
    for key in kw.keys():
        # work kw[key]
```

Example

- A function computing the average and the max and min value of a series of numbers:

```
def statistics(*args):
    avg = 0;  n = 0;   # local variables
    for number in args:  # sum up all the numbers
        n = n + 1; avg = avg + number
    avg = avg / float(n) # float() to ensure non-integer division

    min = args[0]; max = args[0]
    for term in args:
        if term < min: min = term
        if term > max: max = term
    return avg, min, max  # return tuple
```

- Usage:

```
average, vmin, vmax = statistics(v1, v2, v3, b)
```

The Python expert's version...

- The `statistics` function can be written more compactly using (advanced) Python functionality:

```
def statistics(*args):
    return (reduce(operator.add, args)/float(len(args)),
            min(args), max(args))
```

- `reduce(op,a)`: apply operation `op` successively on all elements in list a (here all elements are added)
- `min(a)`, `max(a)`: find min/max of a list a

Call by reference

- Python scripts normally avoid call by reference and return all output variables instead
- Try to swap two numbers:

```
>>> def swap(a, b):
        tmp = b; b = a; a = tmp;

>>> a=1.2; b=1.3; swap(a, b)
>>> print a, b    # has a and b been swapped?
(1.2, 1.3)  # no...
```

- The way to do this particular task

```
>>> def swap(a, b):
    return (b,a)   # return tuple

# or smarter, just say  (b,a) = (a,b)  or simply  b,a = a,b
```

In-place list assignment

- Lists can be changed in-place in functions:

```
>>> def somefunc(mutable, item, item_value):
        mutable[item] = item_value

>>> a = [’a’,’b’,’c’]  # a list
>>> somefunc(a, 1, ’surprise’)
>>> print a
[’a’, ’surprise’, ’c’]
```

- This works for dictionaries as well
(but not tuples) and instances of user-defined classes

Input and output data in functions

- The Python programming style is to have input data as arguments and output data as return values

```
def myfunc(i1, i2, i3, i4=False, io1=0):
    # io1: input and output variable
    ...
    # pack all output variables in a tuple:
    return io1, o1, o2, o3

# usage:
a, b, c, d = myfunc(e, f, g, h, a)
```

- Only (a kind of) references to objects are transferred so returning a large data structure implies just returning a reference

---

Scope of variables

- Variables defined inside the function are local
- To change global variables, these must be declared as global inside the function

```
s = 1

def myfunc(x, y):
    z = 0  # local variable, dies when we leave the func.
    global s
    s = 2  # assignment requires decl. as global
    return y-1,z+1
```

- Variables can be global, local (in func.), and class attributes
- The scope of variables in nested functions may confuse newcomers (see ch. 8.7 in the course book)

Third-party Python modules

- Parnassus is a large collection of Python modules, see link from www.python.org
- Do not reinvent the wheel, search Parnassus!

Python modules

Contents

- Making a module
- Making Python aware of modules
- Packages
- Distributing and installing modules

More info

- Appendix B.1 in the course book
- Python electronic documentation:
Distributing Python Modules, Installing Python Modules

Make your own Python modules!

- Reuse scripts by wrapping them in classes or functions
- Collect classes and functions in library modules
- How? just put classes and functions in a file MyMod.py
- Put MyMod.py in one of the directories where Python can find it (see next slide)
- Say

  ```
  import MyMod
  # or
  import MyMod as M   # M is a short form
  # or
  from MyMod import *
  # or
  from MyMod import myspecialfunction, myotherspecialfunction
  ```

  in any script

How Python can find your modules

- Python has some ’official’ module directories, typically

  ```
  /usr/lib/python2.3
  /usr/lib/python2.3/site-packages
  ```

  + current working directory
- The environment variable `PYTHONPATH` may contain additional directories with modules

  ```
  unix> echo $PYTHONPATH
  /home/me/python/mymodules:/usr/lib/python2.2:/home/you/yourlibs
  ```

- Python’s `sys.path` list contains the directories where Python searches for modules
- `sys.path` contains ’official’ directories, plus those in `PYTHONPATH`)

Setting PYTHONPATH

- In a Unix Bash environment environment variables are normally set in `.bashrc`:

  ```
  export PYTHONTPATH=$HOME/pylib:$scripting/src/tools
  ```

- Check the contents:

  ```
  unix> echo $PYTHONPATH
  ```

- In a Windows environment one can do the same in `autoexec.bat`:

  ```
  set PYTHONPATH=C:\pylib;%scripting%\src\tools
  ```

- Check the contents:

  ```
  dos> echo %PYTHONPATH%
  ```

- Note: it is easy to make mistakes; `PYTHONPATH` may be different from what you think, so check `sys.path`

Summary of finding modules

- Copy your module file(s) to a directory already contained in `sys.path`

  ```
  unix or dos> python -c ’import sys; print sys.path’
  ```

- Can extend `PYTHONPATH`

  ```
  # Bash syntax:
  export PYTHONPATH=$PYTHONPATH:/home/me/python/mymodules
  ```

- Can extend `sys.path` in the script:

  ```
  sys.path.insert(0, ’/home/me/python/mynewmodules’)
  ```

  (insert first in the list)

Packages (1)

- A class of modules can be collected in a *package*
- Normally, a package is organized as module files in a directory tree
- Each subdirectory has a file `__init__.py`
  (can be empty)
- Packages allow “dotted modules names” like

  ```
  MyMod.numerics.pde.grids
  ```

  reflecting a file `MyMod/numerics/pde/grids.py`

Packages (2)

- Can import modules in the tree like this:

  ```
  from MyMod.numerics.pde.grids import fdm_grids
  ```

  ```
  grid = fdm_grids()
  grid.domain(xmin=0, xmax=1, ymin=0, ymax=1)
  ...
  ```

  Here, class `fdm_grids` is in module `grids` (file `grids.py`) in the directory `MyMod/numerics/pde`
- Or

  ```
  import MyMod.numerics.pde.grids
  grid = MyMod.numerics.pde.grids.fdm_grids()
  grid.domain(xmin=0, xmax=1, ymin=0, ymax=1)
  #or
  import MyMod.numerics.pde.grids as Grid
  grid = Grid.fdm_grids()
  grid.domain(xmin=0, xmax=1, ymin=0, ymax=1)
  ```

- See ch. 6 of the Python Tutorial (part of the electronic doc)

Test/doc part of a module

- Module files can have a test/demo script at the end:

  ```
  if __name__ == ’__main__’:
      infile = sys.argv[1]; outfile = sys.argv[2]
      for i in sys.argv[3:]:
          create(infile, outfile, i)
  ```

- The block is executed if the module file is run as a script
- The tests at the end of a module often serve as good examples on the usage of the module

Public/non-public module variables

- Python convention: add a leading underscore to non-public functions and (module) variables

  ```
  _counter = 0
  ```

  ```
  def _filename():
      """Generate a random filename."""
      ...
  ```

- After a standard import `import MyMod`, we may access

  ```
  MyMod._counter
  n = MyMod._filename()
  ```

  but after a `from MyMod import *` the names with leading underscore are *not* available
- Use the underscore to tell users what is public and what is not
- Note: non-public parts can be changed in future releases

Installation of modules/packages

- Python has its own build/installation system: Distutils
- Build: compile (Fortran, C, C++) into module
  (only needed when modules employ compiled code)
- Installation: copy module files to “install” directories
- Publish: make module available for others through PyPi
- Default installation directory:

```
os.path.join(sys.prefix, ’lib’, ’python’ + sys.version[0:3],
             ’site-packages’)
# e.g. /usr/lib/python2.3/site-packages
```

- Distutils relies on a `setup.py` script

A simple setup.py script

- Say we want to distribute two modules in two files

```
MyMod.py  mymodcore.py
```

- Typical `setup.py` script for this case:

```
#!/usr/bin/env python
from distutils.core import setup

setup(name=’MyMod’,
      version=’1.0’,
      description=’Python module example’,
      author=’Hans Petter Langtangen’,
      author_email=’hpl@ifi.uio.no’,
      url=’http://www.simula.no/pymod/MyMod’,
      py_modules=[’MyMod’, ’mymodcore’],
     )
```

---

setup.py with compiled code

- Modules can also make use of Fortran, C, C++ code
- `setup.py` can also list C and C++ files; these will be compiled with the same options/compiler as used for Python itself
- SciPy has an extension of Distutils for “intelligent” compilation of Fortran files
- Note: `setup.py` eliminates the need for makefiles
- Examples of such `setup.py` files are provided in the section on mixing Python with Fortran, C and C++

Installing modules

- Standard command:

```
python setup.py install
```

- If the module contains files to be compiled, a two-step procedure can be invoked

```
python setup.py build
# compiled files and modules are made in subdir. build/
python setup.py install
```

Controlling the installation destination

- `setup.py` has many options
- Control the destination directory for installation:

```
python setup.py install --home=$HOME/install
# copies modules to /home/hpl/install/lib/python
```

- Make sure that `/home/hpl/install/lib/python` is registered in your `PYTHONPATH`

How to learn more about Distutils

- Go to the official electronic Python documentation
- Look up “Distributing Python Modules”
  (for packing modules in `setup.py` scripts)
- Look up “Installing Python Modules”
  (for running `setup.py` with various options)

Doc strings

Contents

- How to document *usage* of Python functions, classes, modules
- Automatic testing of code (through doc strings)

More info

- App. B.1/B.2 in the course book
- HappyDoc, Pydoc, Epydoc manuals
- Style guide for doc strings (see `doc.html`)

Doc strings (1)

- Doc strings = first string in functions, classes, files
- Put user information in doc strings:

```
def ignorecase_sort(a, b):
    """Compare strings a and b, ignoring case."""
    ...
```

- The doc string is available at run time and explains the purpose and usage of the function:

```
>>> print ignorecase_sort.__doc__
’Compare strings a and b, ignoring case.’
```

Doc strings (2)

- Doc string in a class:

```
class MyClass:
    """Fake class just for exemplifying doc strings."""

    def __init__(self):
        ...
```

- Doc strings in modules are a (often multi-line) string starting in the top of the file

```
"""
This module is a fake module
for exemplifying multi-line
doc strings.
"""
```

Doc strings (3)

- The doc string serves two purposes:
  - documentation in the source code
  - on-line documentation through the attribute `__doc__`
  - documentation generated by, e.g., HappyDoc
- HappyDoc: Tool that can extract doc strings and automatically produce overview of Python classes, functions etc.
- Doc strings can, e.g., be used as balloon help in sophisticated GUIs (cf. IDLE)
- Providing doc strings is a good habit!

Doc strings (4)

There is an official style guide for doc strings:

- PEP 257 "Docstring Conventions" from http://www.python.org/dev/peps/
- Use triple double quoted strings as doc strings
- Use complete sentences, ending in a period

```
def somefunc(a, b):
    """Compare a and b."""
```

Automatic doc string testing (1)

- The `doctest` module enables automatic testing of interactive Python sessions embedded in doc strings

```
class StringFunction:
    """
    Make a string expression behave as a Python function
    of one variable.
    Examples on usage:
    >>> from StringFunction import StringFunction
    >>> f = StringFunction(’sin(3*x) + log(1+x)’)
    >>> p = 2.0; v = f(p)  # evaluate function
    >>> p, v
    (2.0, 0.81919679046918392)
    >>> f = StringFunction(’1+t’, independent_variables=’t’)
    >>> v = f(1.2)  # evaluate function of t=1.2
    >>> print "%.2f" % v
    2.20
    >>> f = StringFunction(’sin(t)’)
    >>> v = f(1.2)  # evaluate function of t=1.2
    Traceback (most recent call last):
        v = f(1.2)
    NameError: name ’t’ is not defined
    """
```

Automatic doc string testing (2)

- Class `StringFunction` is contained in the module `StringFunction`
- Let `StringFunction.py` execute two statements when run as a script:

```
def _test():
    import doctest, StringFunction
    return doctest.testmod(StringFunction)

if __name__ == ’__main__’:
    _test()
```

- Run the test:

```
python StringFunction.py       # no output: all tests passed
python StringFunction.py  -v   # verbose output
```

Quick Python review

Python info

- `doc.html` is the resource portal for the course; load it into a web browser from

  `http://www.ifi.uio.no/~inf3330/scripting/doc.html`

  and make a bookmark
- `doc.html` has links to the electronic Python documentation, F2PY, SWIG, Numeric/numarray, and lots of things used in the course
- The course book “Python scripting for computational science” (the PDF version is fine for searching)
- Python in a Nutshell (by Martelli)
- Programming Python 2nd ed. (by Lutz)
- Python Essential Reference (Beazley)
- Quick Python Book

Electronic Python documentation

- Python Tutorial
- Python Library Reference (start with the index!)
- Python Reference Manual (less used)
- Extending and Embedding the Python Interpreter
- Quick references from `doc.html`
- `pydoc anymodule`, `pydoc anymodule.anyfunc`

Python variables

- Variables are not declared
- Variables hold references to objects of any type

```
a = 3      # reference to an int object containing 3
a = 3.0    # reference to a float object containing 3.0
a = ’3.’   # reference to a string object containing ’3.’
a = [’1’, 2]  # reference to a list object containing
              # a string ’1’ and an integer 2
```

- Test for a variable’s type:

```
if isinstance(a, int):            # int?
if isinstance(a, (list, tuple)):  # list or tuple?
```

Common types

- Numbers: `int`, `float`, `complex`
- Sequences: `str` (string), `list`, `tuple`, NumPy array
- Mappings: `dict` (dictionary/hash)
- User-defined type in terms of a class

Numbers

- Integer, floating-point number, complex number

```
a = 3         # int
a = 3.0       # float
a = 3 + 0.1j  # complex (3, 0.1)
```

List and tuple

- List:

```
a = [1, 3, 5, [9.0, 0]]   # list of 3 ints and a list
a[2] = ’some string’
a[3][0] = 0               # a is now [1,3,5,[0,0]]
b = a[0]                  # b refers first element in a
```

- Tuple (“constant list”):

```
a = (1, 3, 5, [9.0, 0])   # tuple of 3 ints and a list
a[3] = 5                  # illegal! (tuples are const/final)
```

- Traversing list/tuple:

```
for item in a:            # traverse list/tuple a
    # item becomes, 1, 3, 5, and [9.0,0]
```

Dictionary

- Making a dictionary:

```
a = {’key1’: ’some value’, ’key2’: 4.1}
a[’key1’] = ’another string value’
a[’key2’] = [0, 1]  # change value from float to string
a[’another key’] = 1.1E+7   # add a new (key,value) pair
```

- Important: no natural sequence of (key,value) pairs!
- Traversing dictionaries:

```
for key in some_dict:
    # process key and corresponding value in some_dict[key]
```

Strings

- Strings apply different types of quotes

```
s = ’single quotes’
s = "double quotes"
s = """triple quotes are
used for multi-line
strings
"""
s = r’raw strings start with r and backslash \ is preserved’
s = ’\t\n’  # tab + newline
s = r’\t\n’  # a string with four characters: \t\n
```

- Some useful operations:

```
if sys.platform.startswith(’win’):  # Windows machine?
    ...
file = infile[:-3] + ’.gif’  # string slice of infile
answer = answer.lower()      # lower case
answer = answer.replace(’ ’, ’_’)
words = line.split()
```

NumPy arrays

- Efficient arrays for numerical computing

```
from Numeric import *     # classical, widely used module
from numarray import *    # alternative version
```

-
```
a = array([[1, 4], [2, 1]], Float)  # 2x2 array from list
a = zeros((n,n), Float)             # nxn array with 0
```

- Indexing and slicing:

```
for i in xrange(a.shape[0]):
    for j in xrange(a.shape[1]):
        a[i,j] = ...
b = a[0,:]  # reference to 1st row
b = a[:,1]  # reference to 2nd column
```

- Avoid loops and indexing, use operations that compute with whole arrays at once (in efficient C code)

Mutable and immutable types

- Mutable types allow in-place modifications

```
>>> a = [1, 9, 3.2, 0]
>>> a[2] = 0
>>> a
[1, 9, 0, 0]
```

Types: list, dictionary, NumPy arrays, class instances

- Immutable types do not allow in-place modifications

```
>>> s = ’some string containing x’
>>> s[-1] = ’y’  # try to change last character - illegal!
TypeError: object doesn’t support item assignment
>>> a = 5
>>> b = a    # b is a reference to a (integer 5)
>>> a = 9    # a becomes a new reference
>>> b        # b still refers to the integer 5
5
```

Types: numbers, strings

Operating system interface

- Run arbitrary operating system command:

```
cmd = ’myprog -f -g 1.0 < input’
failure, output = commands.getstatusoutput(cmd)
```

- Use `commands.getstatsoutput` for running applications
- Use Python (cross platform) functions for listing files, creating directories, traversing file trees, etc.

```
psfiles = glob.glob(’*.ps’) + glob.glob(’*.eps’)
allfiles = os.listdir(os.curdir)
os.mkdir(’tmp1’); os.chdir(’tmp1’)
print os.getcwd()  # current working dir.

def size(arg, dir, files):
    for file in files:
        fullpath = os.path.join(dir,file)
        s = os.path.getsize(fullpath)
        arg.append((fullpath, s))  # save name and size
name_and_size = []
os.path.walk(os.curdir, size, name_and_size)
```

Files

- Open and read:

```
f = open(filename, ’r’)
filestr = f.read()    # reads the whole file into a string
lines = f.readlines() # reads the whole file into a list of lines

for line in f:        # read line by line
    <process line>

while True:           # old style, more flexible reading
    line = f.readline()
    if not line: break
    <process line>

f.close()
```

- Open and write:

```
f = open(filename, ’w’)
f.write(somestring)
f.writelines(list_of_lines)
print >> f, somestring
```

Functions

- Two types of arguments: positional and keyword

```
def myfync(pos1, pos2, pos3, kw1=v1, kw2=v2):
    ...
```

3 positional arguments, 2 keyword arguments (keyword=default-value)

- Input data are arguments, output variables are returned as a tuple

```
def somefunc(i1, i2, i3, io1):
    """i1,i2,i3: input, io1: input and output"""
    ...
    o1 = ...; o2 = ...; o3 = ...; io1 = ...
    ...
    return o1, o2, o3, io1
```

Example: a grep script (1)

- Find a string in a series of files:

```
grep.py ’Python’ *.txt *.tmp
```

- Python code:

```
def grep_file(string, filename):
    res = {}  # result: dict with key=line no. and value=line
    f = open(filename, ’r’)
    line_no = 1
    for line in f:
        #if line.find(string) != -1:
        if re.search(string, line):
            res[line_no] = line
        line_no += 1
```

Example: a grep script (2)

- Let us put the previous function in a file `grep.py`
- This file defines a module `grep` that we can import
- Main program:

```
import sys, re, glob, grep

grep_res = {}
string = sys.argv[1]
for filespec in sys.argv[2:]:
    for filename in glob.glob(filespec):
        grep_res[filename] = grep.grep(string, filename)

# report:
for filename in grep_res:
    for line_no in grep_res[filename]:
        print ’%-20s.%5d: %s’ % (filename, line_no,
                                grep_res[filename][line_no])
```

Interactive Python

- Just write `python` in a terminal window to get an *interactive Python shell*:

```
>>> 1269*1.24
1573.5599999999999
>>> import os; os.getcwd()
’/home/hpl/work/scripting/trunk/lectures’
>>> len(os.listdir(’modules’))
60
```

- We recommend to use IPython as interactive shell

```
Unix/DOS> ipython
In [1]: 1+1
Out[1]: 2
```

IPython and the Python debugger

- Scripts can be run from IPython:

  ```
  In [1]:run scriptfile arg1 arg2 ...
  ```

  e.g.,

  ```
  In [1]:run datatrans2.py .datatrans_infile tmp1
  ```

- IPython is integrated with Python's `pdb` debugger
- `pdb` can be automatically invoked when an exception occurs:

  ```
  In [29]:%pdb on  # invoke pdb automatically
  In [30]:run datatrans2.py infile tmp2
  ```

More on debugging

- This happens when the infile name is wrong:

  ```
  /home/work/scripting/src/py/intro/datatrans2.py
        7     print "Usage:",sys.argv[0], "infile outfile"; sys.exi
        8
  ----> 9 ifile = open(infilename, 'r')  # open file for reading
       10 lines = ifile.readlines()      # read file into list of l
       11 ifile.close()
  ```

  ```
  IOError: [Errno 2] No such file or directory: 'infile'
  > /home/work/scripting/src/py/intro/datatrans2.py(9)?()
  -> ifile = open(infilename, 'r')  # open file for reading
  (Pdb) print infilename
  infile
  ```