Slides from INF3331 lectures

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About this course

Teachers

- Joakim Sundnes
- Glenn Lines
- Guest lecturers TBD
- We use Python to create efficient working (or problem solving) environments
- We also use Python to develop large-scale simulation software (which solves partial differential equations)
- We believe high-level languages such as Python constitute a promising way of making flexible and user-friendly software!
- Some of our research migrates into this course
- There are lots of opportunities for master projects related to this course

Contents

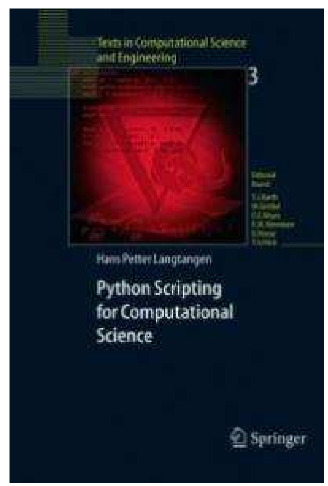
- Scripting in general
- Quick Python introduction (first two weeks)
- Python problem solving
- More advanced Python (class programming++)
- Regular expressions
- Combining Python with C, C++ and Fortran
- The Python C API and the NumPy C API
- Distributing Python modules (incl. extension modules)
- Verifying/testing (Python) software
- Documenting Python software
- Optimizing Python code
- Python coding standards and 'Pythonic' programming
- Basic Bash programming

What you will learn

- Scripting in general, but with most examples taken from scientific computing
- Jump into useful scripts and dissect the code
- Learning by doing
- Find examples, look up man pages, Web docs and textbooks on demand
- Get the overview
- Customize existing code
- Have fun and work with useful things

Teaching material (1)

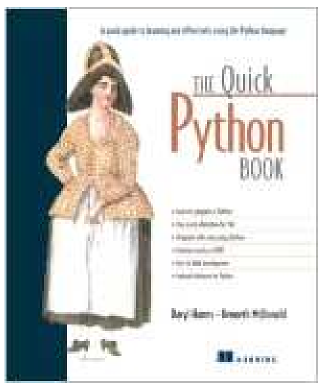
- Slides from lectures
  (by Skavhaug, Sundnes, Langtangen et al), download from
  `http://www.uio.no/studier/emner/matnat/ifi/INF3331/h11/inf3331.pdf`
- Associated book (for the Python material):
  H. P. Langtangen: *Python Scripting for Computational Science*, 3rd edition, Springer 2008

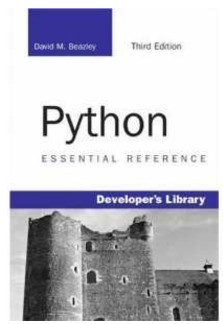


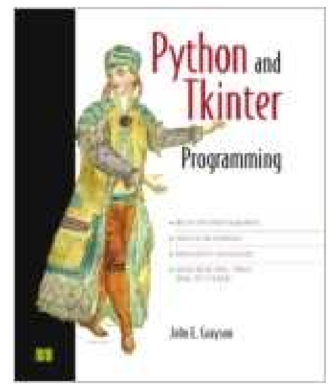
- You must find the rest: manuals, textbooks, google

Teaching material (2)

- Good Python litterature:
  Harms and McDonald: The Quick Python Book (tutorial+advanced)
  Beazley: Python Essential Reference
  Grayson: Python and Tkinter Programming







Lectures and groups (1)

- Lectures Tuesdays 10.15-12.00
- Groups Thursday 14.15, Monday 10.15, (Friday 10.15)
- Slides will be updated as we go. Printing the entire pdf file in August is not recommended.
- Topics for the lecture, updated slides and page numbers will be made available one week before each lecture.
- Groups and exercises are the core of the course; problem solving is in focus.

Lectures and groups (2)

- Tuesday 23rd:
  - “User survey”
  - Intro/motivation; scripting vs regular programming
- Tuesday 30th:
  - First encounter with Python

What is a script?

- Very high-level, often short, program
  written in a high-level scripting language
- Scripting languages: Unix shells, Tcl, Perl, Python, Ruby, Scheme, Rexx, JavaScript, VisualBasic, ...
- This course: Python
  \+ a taste of Bash (Unix shell)

Characteristics of a script

- Glue other programs together
- Extensive text processing
- File and directory manipulation
- Often special-purpose code
- Many small interacting scripts may yield a big system
- Perhaps a special-purpose GUI on top
- Portable across Unix, Windows, Mac
- Interpreted program (no compilation+linking)

Why not stick to Java or C/C++?

Features of scripting languages compared with Java, C/C++ and Fortran:

- shorter, more high-level programs
- much faster software development
- more convenient programming
- you feel more productive

Two main reasons:

- no variable declarations,
  but lots of consistency checks at run time
- lots of standardized libraries and tools

Scripts yield short code

- Consider reading real numbers from a file, where each line can contain an arbitrary number of real numbers:

```
1.1  9   5.2
1.762543E-02
0 0.01 0.001

9 3 7
```

- Python solution:

```
F = open(filename, 'r')
n = F.read().split()
```

Using regular expressions (1)

- Suppose we want to read complex numbers written as text

```
(-3, 1.4)  or  (-1.437625E-9, 7.11)  or  (  4, 2 )
```

- Python solution:

```
m = re.search(r'\(\s*([^,]+)\s*,\s*([^,]+)\s*\)',
              '(-3,1.4)')
re, im = [float(x) for x in m.groups()]
```

Using regular expressions (2)

- Regular expressions like

  ```
  \(\s*([^,]+)\s*,\s*([^,]+)\s*\)
  ```

  constitute a powerful language for specifying text patterns
- Doing the same thing, without regular expressions, in Fortran and C requires quite some low-level code at the character array level
- Remark: we could read pairs (-3, 1.4) without using regular expressions,

  ```
  s = '(-3,  1.4 )'
  re, im = s[1:-1].split(',')
  ```

Script variables are not declared

- Example of a Python function:

```
def debug(leading_text, variable):
    if os.environ.get('MYDEBUG', '0') == '1':
        print leading_text, variable
```

- Dumps any printable variable
(number, list, hash, heterogeneous structure)
- Printing can be turned on/off by setting the environment variable `MYDEBUG`

The same function in C++

- Templates can be used to mimic dynamically typed languages
- Not as quick and convenient programming:

```
template <class T>
void debug(std::ostream& o,
           const std::string& leading_text,
           const T& variable)
{
  char* c = getenv("MYDEBUG");
  bool defined = false;
  if (c != NULL) {  // if MYDEBUG is defined ...
    if (std::string(c) == "1") {  // if MYDEBUG is true ...
      defined = true;
    }
  }
  if (defined) {
    o <<  leading_text << " " << variable << std::endl;
  }
}
```

The relation to OOP

- Object-oriented programming can also be used to parameterize types
- Introduce base class A and a range of subclasses, all with a (virtual) print function
- Let `debug` work with `var` as an A reference
- Now `debug` works for all subclasses of A
- Advantage: complete control of the legal variable types that `debug` are allowed to print (may be important in big systems to ensure that a function can allow make transactions with certain objects)
- Disadvantage: much more work, much more code, less reuse of `debug` in new occasions

Flexible function interfaces

- User-friendly environments (Matlab, Maple, Mathematica, S-Plus, ...) allow flexible function interfaces
- Novice user:

```
# f is some data
plot(f)
```

- More control of the plot:

```
plot(f, label='f', xrange=[0,10])
```

- More fine-tuning:

```
plot(f, label='f', xrange=[0,10], title='f demo',
     linetype='dashed', linecolor='red')
```

Keyword arguments

- Keyword arguments = function arguments with keywords and default values, e.g.,

```
def plot(data, label='', xrange=None, title='',
         linetype='solid', linecolor='black', ...)
```

- The sequence and number of arguments in the call can be chosen by the user

Classification of languages (1)

- Many criteria can be used to classify computer languages
- Dynamically vs statically typed languages
  Python (dynamic):

```
c = 1                 # c is an integer
c = [1,2,3]           # c is a list
```

C (static):

```
double c; c = 5.2;    # c can only hold doubles
c = "a string..."     # compiler error
```

Classification of languages (2)

- Weakly vs strongly typed languages
  Perl (weak):

```
$b = '1.2'
$c = 5*$b;    # implicit type conversion: '1.2' -> 1.2
```

  Python (strong):

```
b = '1.2'
c = 5*b       # illegal; no implicit type conversion
```

Classification of languages (3)

- Interpreted vs compiled languages
- Dynamically vs statically typed (or type-safe) languages
- High-level vs low-level languages (Python-C)
- Very high-level vs high-level languages (Python-C)
- Scripting vs system languages

Turning files into code (1)

- Code can be constructed and executed at run-time
- Consider an input file with the syntax

```
a = 1.2
no of iterations = 100
solution strategy = 'implicit'
c1 = 0
c2 = 0.1
A = 4
c3 = StringFunction('A*sin(x)')
```

- How can we read this file and define variables `a`, `no_of_iterations`, `solution_strategi`, `c1`, `c2`, `A` with the specified values?
- And can we make `c3` a function `c3(x)` as specified?

Yes!

Turning files into code (2)

- The answer lies in this short and generic code:

```
file = open('inputfile.dat', 'r')
for line in file:
    # first replace blanks on the left-hand side of = by _
    variable, value = line.split('=').strip()
    variable = re.sub(' ', '_', variable)
    exec(variable + '=' + value)   # magic...
```

- This cannot be done in Fortran, C, C++ or Java!

Scripts can be slow

- Perl and Python scripts are first compiled to byte-code
- The byte-code is then *interpreted*
- Text processing is usually as fast as in C
- Loops over large data structures might be very slow

```
for i in range(len(A)):
    A[i] = ...
```

- Fortran, C and C++ compilers are good at optimizing such loops at compile time and produce very efficient assembly code (e.g. 100 times faster)
- Fortunately, long loops in scripts can easily be migrated to Fortran or C

Scripts may be fast enough (1)

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 (!)
- Remark: in practice, 100 000 data points are written and read in binary format, resulting in much smaller differences

Scripts may be fast enough (2)

Read a text in a human language and generate random nonsense text in that language (from "The Practice of Programming" by B. W. Kernighan and R. Pike, 1999):

Language	CPU-time	lines of code
C	0.30	150
Java	9.2	105
C++ (STL-deque)	11.2	70
C++ (STL-list)	1.5	70
Awk	2.1	20
Perl	1.0	18

Machine: Pentium II running Windows NT

When scripting is convenient (1)

- The application's main task is to connect together existing components
- The application includes a graphical user interface
- The application performs extensive string/text manipulation
- The design of the application code is expected to change significantly
- CPU-time intensive parts can be migrated to C/C++ or Fortran

When scripting is convenient (2)

- The application can be made short if it operates heavily on list or hash structures
- The application is supposed to communicate with Web servers
- The application should run without modifications on Unix, Windows, and Macintosh computers, also when a GUI is included

When to use C, C++, Java, Fortran

- Does the application implement complicated algorithms and data structures?
- Does the application manipulate large datasets so that execution speed is critical?
- Are the application's functions well-defined and changing slowly?
- Will type-safe languages be an advantage, e.g., in large development teams?

Some personal applications of scripting

- Get the power of Unix also in non-Unix environments
- Automate manual interaction with the computer
- Customize your own working environment and become more efficient
- Increase the reliability of your work
  (what you did is documented in the script)
- Have more fun!

Some business applications of scripting

- Python and Perl are very popular in the open source movement and Linux environments
- Python, Perl and PHP are widely used for creating Web services (Django, SOAP, Plone)
- Python and Perl (and Tcl) replace 'home-made' (application-specific) scripting interfaces
- Many companies want candidates with Python experience

What about mission-critical operations?

- Scripting languages are free
- What about companies that do mission-critical operations?
- Can we use Python when sending a man to Mars?
- Who is responsible for the quality of products?

The reliability of scripting tools

- Scripting languages are developed as a world-wide collaboration of volunteers (open source model)
- The open source community as a whole is responsible for the quality
- There is a single repository for the source codes (plus mirror sites)
- This source is read, tested and controlled by a very large number of people (and experts)
- The reliability of *large* open source projects like Linux, Python, and Perl appears to be very good - at least as good as commercial software

Practical problem solving

- Problem: you are not an expert (yet)
- Where to find detailed info, and how to understand it?
- The efficient programmer navigates quickly in the jungle of textbooks, man pages, README files, source code examples, Web sites, news groups, ... and has a gut feeling for what to look for
- The aim of the course is to improve your practical problem-solving abilities
- *You think you know when you learn, are more sure when you can write, even more when you can teach, but certain when you can program* (Alan Perlis)

Basic Python Constructs

First encounter with Python

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

from math import sin
import sys

x = float(sys.argv[1])
print "Hello world, sin(%g) = %g." % (x, sin(x))
```

Running the Script

Code in file hw.py.
Run with command:

```
> python hw.py 0.5
Hello world, sin(0.5) = 0.479426.
```

Linux alternative if file is executable (chmod a+x hw.py):

```
> ./hw.py 0.5
Hello world, sin(0.5) = 0.479426.
```

Quick Run Through

On *nix; find out what kind of script language (interpreter) to use:

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

Access library functions:

```
from math import sin
import sys
```

Read command line argument and convert it to a floating point:

```
x = float(sys.argv[1])
```

Print out the result using a format string:

```
print "Hello world, sin(%g) = %g." % (x, sin(x))
```

Simple Assignments

```
a = 10 # a is a variable referencing an
       # integer object of value 10

b = True # b is a boolean variable

a = b # a is now a boolean as well
      # (referencing the same object as b)

b = increment(4) # b is the value returned by a function

is_equal = a == b # is_equal is True if a == b
```

Simple control structures

- Loops:

```
while condition:
    <block of statements>
```

Here, `condition` must be a boolean expression (or have a boolean interpretation), for example: `i < 10` or `!found`

```
for element in somelist:
    <block of statements>
```

Note that `element` is a copy of the list items, not a reference into the list!

- Conditionals:

```
if condition:
    <block of statements>
elif condition:
    <block of statements>
else:
    <block of statements>
```

Ranges and Loops

- `range(start, stop, increment)` constructs a list. Typically, it is used in for loops:

```
for i in range(10):
    print i
```

- `xrange(start, stop, increment)` is better for fat loops since it constructs an iterator:

```
for i in xrange(10000000):
    sum += sin(i*pi*x)
```

- Looping over lists can be done in several ways:

```
names = ["Ola", "Per", "Kari"]
surnames = ["Olsen", "Pettersen", "Bremnes"]
for name, surname in zip(names, surnames):
    print name, surname # join element by element

for i, name in enumerate(names):
    print i, name # join list index and item
```

Lists and Tuples

```
mylist  = ['a string', 2.5, 6, 'another string']
mytuple = ('a string', 2.5, 6, 'another string')
mylist[1]  = -10
mylist.append('a third string')
mytuple[1] = -10  # illegal: cannot change a tuple
```

A tuple is a constant list (immutable)

List functionality

`a = []`	initialize an empty list
`a = [1, 4.4, 'run.py']`	initialize a list
`a.append(elem)`	add `elem` object to the end
`a + [1,3]`	add two lists
`a[3]`	index a list element
`a[-1]`	get last list element
`a[1:3]`	slice: copy data to sublist (here: index 1, 2)
`del a[3]`	delete an element (index `3`)
`a.remove(4.4)`	remove an element (with value `4.4`)
`a.index('run.py')`	find index corresponding to an element's value
`'run.py' in a`	test if a value is contained in the list

More list functionality

`a.count(v)`	count how many elements that have the value `v`
`len(a)`	number of elements in list `a`
`min(a)`	the smallest element in `a`
`max(a)`	the largest element in `a`
`min(["001", 100])`	tricky!
`sum(a)`	add all elements in `a`
`a.sort()`	sort list `a` (changes `a`)
`as = sorted(a)`	sort list `a` (return new list)
`a.reverse()`	reverse list `a` (changes `a`)
`b[3][0][2]`	nested list indexing
`isinstance(a, list)`	is `True` if `a` is a list

Functions and arguments

- User-defined functions:

```
def split(string, char):
    position = string.find(char)
    if  position > 0:
        return string[:position+1], string[position+1:]
    else:
        return string, ""

# function call:
message = "Heisann"
print split(message, "i")
```

  prints out `('Hei', 'sann')`.

- Positional arguments must appear before keyword arguments:

```
def split(message, char="i"):
    [...]
```

How to find more Python information

- The book contains only fragments of the Python language (intended for real beginners!)
- These slides are even briefer
- Therefore you will need to look up more Python information
- Primary reference: The official Python documentation at `docs.python.org`
- Very useful: The Python Library Reference, especially the index
- Example: what can I find in the `math` module? Go to the Python Library Reference index, find "math", click on the link and you get to a description of the module
- Alternative: `pydoc math` in the terminal window (briefer)
- Note: for a newbie it is difficult to read manuals (intended for experts) – you will need a lot of training; just browse, don't read everything, try to dig out the key info

eval and exec

- Evaluating string expressions with `eval`:

```
>>> x = 20
>>> r = eval('x + 1.1')
>>> r
21.1
>>> type(r)
<type 'float'>
```

- Executing strings with Python code, using `exec`:

```
exec("""
def f(x):
    return %s
""" % sys.argv[1])
```

Exceptions

- Handling exceptions:

```
try:
    <statements>
except ExceptionType1:
    <provide a remedy for ExceptionType1 errors>
except ExceptionType2, ExceptionType3, ExceptionType4:
    <provide a remedy for three other types of errors>
except:
    <provide a remedy for any other errors>
...
```

- Raising exceptions:

```
if z < 0:
    raise ValueError\
          ('z=%s is negative - cannot do log(z)' % z)
a = math.log(z)
```

File reading and writing

- Reading a file:

```
infile = open(filename, 'r')
for line in infile:
    # process line

lines = infile.readlines()
for line in lines:
    # process line

for i in xrange(len(lines)):
    # process lines[i] and perhaps next line lines[i+1]

fstr = infile.read()
# process the while file as a string fstr

infile.close()
```

- Writing a file:

```
outfile = open(filename, 'w')   # new file or overwrite
outfile = open(filename, 'a')   # append to existing file
outfile.write("""Some string
....
""")
```

Dictionary functionality

`a = {}`	initialize an empty dictionary
`a = {'point':[2,7], 'value':3}`	initialize a dictionary
`a = dict(point=[2,7], value=3)`	initialize a dictionary
`a['hide'] = True`	add new key-value pair to a dictionary
`a['point']`	get value corresponding to key `point`
`'value' in a`	`True` if `value` is a key in the dictionary
`del a['point']`	delete a key-value pair from the dictionary
`a.keys()`	list of keys
`a.values()`	list of values
`len(a)`	number of key-value pairs in dictionary `a`
`for key in a:`	loop over keys in unknown order
`for key in sorted(a.keys()):`	loop over keys in alphabetic order
`isinstance(a, dict)`	is `True` if `a` is a dictionary

String operations

```
s = 'Berlin: 18.4 C at 4 pm'
s[8:17]           # extract substring
s.find(':')       # index where first ':' is found
s.split(':')      # split into substrings
s.split()         # split wrt whitespace
'Berlin' in s     # test if substring is in s
s.replace('18.4', '20')
s.lower()         # lower case letters only
s.upper()         # upper case letters only
s.split()[4].isdigit()
s.strip()         # remove leading/trailing blanks
', '.join(list_of_words)
```

Modules

Import module as namespace:

```
import sys
x = float(sys.argv[1])
```

Import module member `argv` into current namespace:

```
from sys import argv
x = float(argv[1])
```

Import everything from sys into current namespace (evil)

```
from sys import *
x = float(argv[1])
```

Import `argv` into current namespace under an alias

```
from sys import argv as a
x = float(a[1])
```

Frequently encountered 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

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 = os.system(cmd + '&')
elif sys.platform[:3] == 'win':   # Windows?
  failure = os.system('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) filena
  ```

- `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 files:
...     if not file in allfiles:  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
- a dictionary of keyword arguments to the function
- number of calls to make (repetitions)
- name of function (for printout)

```
def timer(func, args, kwargs, repetitions, func_name):
    t0 = time.time();  c0 = time.clock()

    for i in xrange(repetitions):
        func(*args, **kwargs)

    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 they 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)  # wait for end of scp session
child.close()
```

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 (probably) 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

# 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)

#Best variant:
mywords.sort(key=lambda s: s.lower())
```

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
```

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 divis

    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
```

Arguments are like variables

- Consider a function

```
def swap(a, b):
    b = 2*b
    return b, a
```

- Calling `swap(A, B)` is inside `swap` equivalent to

```
a = A
b = B
b = 2*b
return b, a
```

- Arguments are transferred in the same way as we assign objects to variables (using the assignment operator =)
- This may help to explain how arguments in functions get their values

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']
```

- Note: `mutable` is a name for the same object as `a`, and we use this name to change the object in-place
- 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)

Regular expressions

Contents

- Motivation for regular expression
- Regular expression syntax
- Lots of examples on problem solving with regular expressions
- Many examples related to scientific computations

More info

- Ch. 8.2 in the course book
- Regular Expression HOWTO for Python (see `doc.html`)
- perldoc perlrequick (intro), perldoc perlretut (tutorial), perldoc perlre (full reference)
- “Text Processing in Python” by Mertz (Python syntax)
- “Mastering Regular Expressions” by Friedl (Perl syntax)
- Note: the core syntax is the same in Perl, Python, Ruby, Tcl, Egrep, Vi/Vim, Emacs, ..., so books about these tools also provide info on regular expressions

Motivation

- Consider a simulation code with this type of output:

```
t=2.5  a: 1.0 6.2 -2.2   12 iterations and eps=1.38756E-05
t=4.25  a: 1.0 1.4   6 iterations and eps=2.22433E-05
>> switching from method AQ4 to AQP1
t=5  a: 0.9   2 iterations and eps=3.78796E-05
t=6.386  a: 1.0 1.1525   6 iterations and eps=2.22433E-06
>> switching from method AQP1 to AQ2
t=8.05  a: 1.0   3 iterations and eps=9.11111E-04
...
```

- You want to make two graphs:
  - iterations vs t
  - eps vs t
- How can you extract the relevant numbers from the text?

Regular expressions

- Some structure in the text, but `line.split()` is too simple (different no of columns/words in each line)
- Regular expressions constitute a powerful language for formulating structure and extract parts of a text
- Regular expressions look cryptic for the novice
- regex/regexp: abbreviations for regular expression

Specifying structure in a text

```
t=6.386  a: 1.0 1.1525   6 iterations and eps=2.22433E-06
```

- Structure: t=, number, 2 blanks, a:, some numbers, 3 blanks, integer, ’ iterations and eps=’, number
- Regular expressions constitute a language for specifying such structures
- Formulation in terms of a regular expression:

  ```
  t=(.*)\s{2}a:.*\s+(\d+) iterations and eps=(.*)
  ```

Dissection of the regex

- A regex usually contains special characters introducing freedom in the text:

```
t=(.*)\s{2}a:.*\s+(\d+) iterations and eps=(.*)
```

```
t=6.386  a: 1.0 1.1525   6 iterations and eps=2.22433E-06
```

```
.          any character
.*         zero or more . (i.e. any sequence of characters)
(.*)       can extract the match for .* afterwards
\s         whitespace (spacebar, newline, tab)
\s{2}      two whitespace characters
a:         exact text
.*         arbitrary text
\s+        one or more whitespace characters
\d+        one or more digits (i.e. an integer)
(\d+)      can extract the integer later
iterations and eps=     exact text
```

Using the regex in Python code

```
pattern = \
r"t=(.*)\s{2}a:.*\s+(\d+) iterations and eps=(.*)"

t = []; iterations = []; eps = []

# the output to be processed is stored in the list of lines

for line in lines:

    match = re.search(pattern, line)

    if match:
        t.append          (float(match.group(1)))
        iterations.append(int  (match.group(2)))
        eps.append        (float(match.group(3)))
```

Result

- Output text to be interpreted:

```
t=2.5  a: 1 6 -2   12 iterations and eps=1.38756E-05
t=4.25  a: 1.0 1.4   6 iterations and eps=2.22433E-05
>> switching from method AQ4 to AQP1
t=5  a: 0.9   2 iterations and eps=3.78796E-05
t=6.386  a: 1 1.15   6 iterations and eps=2.22433E-06
>> switching from method AQP1 to AQ2
t=8.05  a: 1.0   3 iterations and eps=9.11111E-04
```

- Extracted Python lists:

```
t = [2.5, 4.25, 5.0, 6.386, 8.05]
iterations = [12, 6, 2, 6, 3]
eps = [1.38756e-05, 2.22433e-05, 3.78796e-05,
       2.22433e-06, 9.11111E-04]
```

Another regex that works

- Consider the regex

  `t=(.*)\s+a:.*\s+(\d+)\s+.*=(.*)`

  compared with the previous regex

  `t=(.*)\s{2}a:.*\s+(\d+) iterations and eps=(.*)`

- Less structure
- How 'exact' does a regex need to be?
- The degree of preciseness depends on the probability of making a wrong match

Failure of a regex

- Suppose we change the regular expression to

  ```
  t=(.*)\s+a:.*(\d+).*=(.*)
  ```

- It works on most lines in our test text but not on

  ```
  t=2.5  a: 1 6 -2   12 iterations and eps=1.38756E-05
  ```

- 2 instead of 12 (iterations) is extracted
  (why? see later)
- Regular expressions constitute a powerful tool, but you need to develop understanding and experience

List of special regex characters

```
.       # any single character except a newline
^       # the beginning of the line or string
$       # the end of the line or string
*       # zero or more of the last character
+       # one or more of the last character
?       # zero or one of the last character

[A-Z]   # matches all upper case letters
[abc]   # matches either a or b or c
[^b]    # does not match b
[^a-z]  # does not match lower case letters
```

Context is important

```
.*     # any sequence of characters (except newline)
[.*]   # the characters . and *

^no    # the string ’no’ at the beginning of a line
[^no]  # neither n nor o

A-Z    # the 3-character string ’A-Z’ (A, minus, Z)
[A-Z]  # one of the chars A, B, C, ..., X, Y, or Z
```

More weird syntax...

- The OR operator:

```
(eg|le)gs  # matches eggs or legs
```

- Short forms of common expressions:

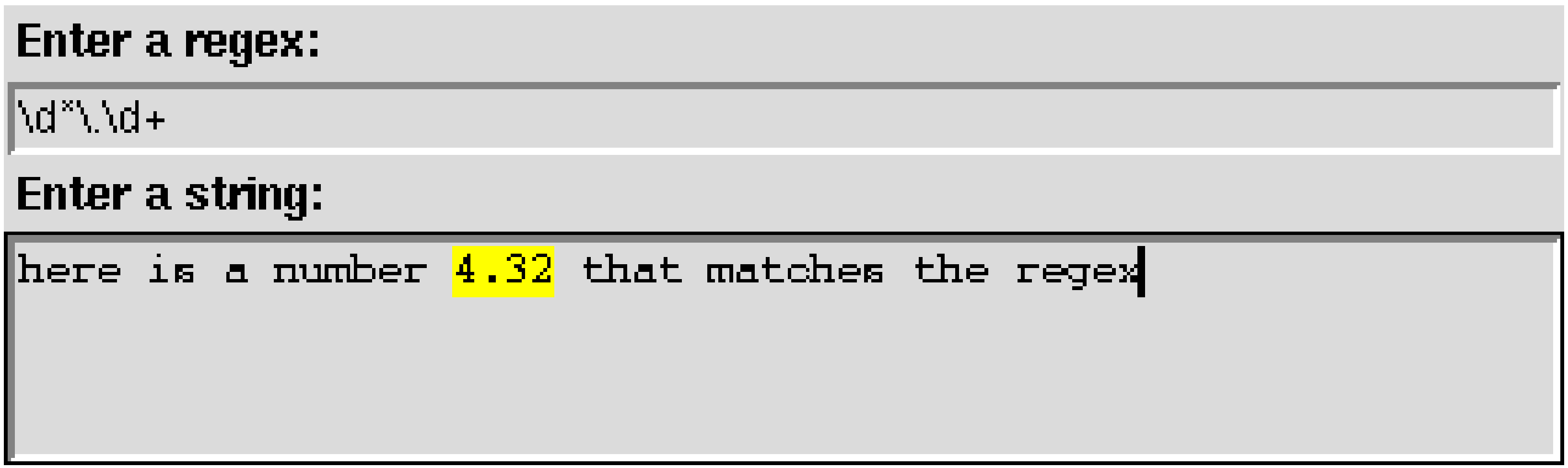
```
\n     # a newline
\t     # a tab
\w     # any alphanumeric (word) character
       # the same as [a-zA-Z0-9_]
\W     # any non-word character
       # the same as [^a-zA-Z0-9_]
\d     # any digit, same as [0-9]
\D     # any non-digit, same as [^0-9]
\s     # any whitespace character: space,
       # tab, newline, etc
\S     # any non-whitespace character
\b     # a word boundary, outside [] only
\B     # no word boundary
```

Quoting special characters

```
\.       # a dot
\|       # vertical bar
\[       # an open square bracket
\)       # a closing parenthesis
\*       # an asterisk
\^       # a hat
\/       # a slash
\\       # a backslash
\{       # a curly brace
\?       # a question mark
```

GUI for regex testing

src/tools/regexdemo.py:



The part of the string that matches the regex is high-lighted

Regex for a real number

- Different ways of writing real numbers:
  -3, 42.9873, 1.23E+1, 1.2300E+01, 1.23e+01
- Three basic forms:
  - integer: -3
  - decimal notation: 42.9873, .376, 3.
  - scientific notation: 1.23E+1, 1.2300E+01, 1.23e+01, 1e1

A simple regex

- Could just collect the legal characters in the three notations:

```
[0-9.Ee\-+]+
```

- Downside: this matches text like

```
12-24
24.-
--E1--
+++++
```

- How can we define precise regular expressions for the three notations?

Decimal notation regex

- Regex for decimal notation:

```
-?\d*\.\d+

# or equivalently (\d is [0-9])
-?[0-9]*\.[0-9]+
```

- Problem: this regex does not match '3.'
- The fix

```
-?\d*\.\d*
```

  is ok but matches text like '-.' and (much worse!) '.'
- Trying it on

```
'some text. 4. is a number.'
```

  gives a match for the first period!

Fix of decimal notation regex

- We need a digit before OR after the dot
- The fix:

  ```
  -?(\d*\.\d+|\d+\.\d*)
  ```

- A more compact version (just "OR-ing" numbers without digits after the dot):

  ```
  -?(\d*\.\d+|\d+\.)
  ```

Combining regular expressions

- Make a regex for integer or decimal notation:

  `(integer OR decimal notation)`

  using the OR operator and parenthesis:

  ```
  -?(\d+|(\d+\.\d*|\d*\.\d+))
  ```

- Problem: `22.432` gives a match for `22`
  (i.e., just digits? yes - `22` - match!)

Check the order in combinations!

- Remedy: test for the most complicated pattern first

  ```
  (decimal notation OR integer)
  ```

  ```
  -?((\d+\.\d*|\d*\.\d+)|\d+)
  ```

- Modularize the regex:

  ```
  real_in = r'\d+'
  real_dn = r'(\d+\.\d*|\d*\.\d+)'
  real = '-?(' + real_dn + '|' + real_in + ')'
  ```

Scientific notation regex (1)

- Write a regex for numbers in scientific notation
- Typical text: `1.27635E+01`, `-1.27635e+1`
- Regular expression:

```
-?\d\.\d+[Ee][+\-]\d\d?
```

- = optional minus, one digit, dot, at least one digit, E or e, plus or minus, one digit, optional digit

Scientific notation regex (2)

- Problem: `1e+00` and `1e1` are not handled
- Remedy: zero or more digits behind the dot, optional e/E, optional sign in exponent, more digits in the exponent (`1e001`):

```
-?\d\.?\d*[Ee][+\-]?\d+
```

Making the regex more compact

- A pattern for integer or decimal notation:

```
-?((\d+\.\d*|\d*\.\d+)|\d+)
```

- Can get rid of an OR by allowing the dot and digits behind the dot be optional:

```
-?(\d+(\.\d*)?|\d*\.\d+)
```

- Such a number, followed by an optional exponent (a la `e+02`), makes up a general real number (!)

```
-?(\d+(\.\d*)?|\d*\.\d+)([eE][+\-]?\d+)?
```

A more readable regex

- Scientific OR decimal OR integer notation:

```
-?(\d\.?\d*[Ee][+\-]?\d+|(\d+\.\d*|\d*\.\d+)|\d+)
```

  or better (modularized):

```
real_in = r'\d+'
real_dn = r'(\d+\.\d*|\d*\.\d+)'
real_sn = r'(\d\.?\d*[Ee][+\-]?\d+'
real = '-?(' + real_sn + '|' + real_dn + '|' + real_in + ')'
```

- Note: first test on the most complicated regex in OR expressions

Groups (in introductory example)

- Enclose parts of a regex in () to extract the parts:

```
pattern = r"t=(.*)\s+a:.*\s+(\d+)\s+.*=(.*)"
# groups:     ( )          (   )      ( )
```

  This defines three groups (t, iterations, eps)

- In Python code:

```
match = re.search(pattern, line)
if match:
    time = float(match.group(1))
    iter = int  (match.group(2))
    eps  = float(match.group(3))
```

- The complete match is group 0 (here: the whole line)

Regex for an interval

- Aim: extract lower and upper limits of an interval:

  ```
  [ -3.14E+00, 29.6524]
  ```

- Structure: bracket, real number, comma, real number, bracket, with embedded whitespace

Easy start: integer limits

- Regex for real numbers is a bit complicated
- Simpler: integer limits

```
pattern = r'\[\d+,\d+\]'
```

but this does must be fixed for embedded white space or negative numbers a la

```
[ -3   , 29  ]
```

- Remedy:

```
pattern = r'\[\s*-?\d+\s*,\s*-?\d+\s*\]'
```

- Introduce groups to extract lower and upper limit:

```
pattern = r'\[\s*(-?\d+)\s*,\s*(-?\d+)\s*\]'
```

Testing groups

In an interactive Python shell we write

```
>>> pattern = r'\[\s*(-?\d+)\s*,\s*(-?\d+)\s*\]'
>>> s = "here is an interval: [ -3, 100] ..."
>>> m = re.search(pattern, s)
>>> m.group(0)
[ -3, 100]
>>> m.group(1)
-3
>>> m.group(2)
100
>>> m.groups()   # tuple of all groups
('-3', '100')
```

Named groups

- Many groups? inserting a group in the middle changes other group numbers...
- Groups can be given *logical names* instead
- Standard group notation for interval:

```
# apply integer limits for simplicity: [int,int]
\[\s*(-?\d+)\s*,\s*(-?\d+)\s*\]
```

- Using named groups:

```
\[\s*(?P<lower>-?\d+)\s*,\s*(?P<upper>-?\d+)\s*\]
```

- Extract groups by their names:

```
match.group('lower')
match.group('upper')
```

Regex for an interval; real limits

- Interval with general real numbers:

```
real_short = r’\s*(-?(\d+(\.\d*)?|\d*\.\d+)([eE][+\-]?\d+)?)\s
interval = r"\[" + real_short + "," + real_short + r"\]"
```

- Example:

```
>>> m = re.search(interval, ’[-100,2.0e-1]’)
>>> m.groups()
(’-100’, ’100’, None, None, ’2.0e-1’, ’2.0’, ’.0’, ’e-1’)
```

  i.e., lots of (nested) groups; only group 1 and 5 are of interest

Handle nested groups with named groups

- Real limits, previous regex resulted in the groups

  ```
  ('-100', '100', None, None, '2.0e-1', '2.0', '.0', 'e-1')
  ```

- Downside: many groups, difficult to count right
- Remedy 1: use named groups for the outer left and outer right groups:

  ```
  real1 = \
   r"\s*(?P<lower>-?(\d+(\.\d*)?|\d*\.\d+)([eE][+\-]?\d+)?)\s*"
  real2 = \
   r"\s*(?P<upper>-?(\d+(\.\d*)?|\d*\.\d+)([eE][+\-]?\d+)?)\s*"
  interval = r"\[" + real1 + "," + real2 + r"\]"
  ...
  match = re.search(interval, some_text)
  if match:
      lower_limit = float(match.group('lower'))
      upper_limit = float(match.group('upper'))
  ```

Simplify regex to avoid nested groups

- Remedy 2: reduce the use of groups
- Avoid nested OR expressions (recall our first tries):

```
real_sn = r"-?\d\.?\d*[Ee][+\-]\d+"
real_dn = r"-?\d*\.\d*"
real = r"\s*(" + real_sn + "|" + real_dn + "|" + real_in + r")
interval = r"\[" + real + "," + real + r"\]"
```

- Cost: (slightly) less general and safe regex

Extracting multiple matches (1)

- `re.findall` finds all matches (`re.search` finds the first)

```
>>> r = r"\d+\.\d*"
>>> s = "3.29 is a number, 4.2 and 0.5 too"
>>> re.findall(r,s)
['3.29', '4.2', '0.5']
```

- Application to the interval example:

```
lower, upper = re.findall(real, '[-3, 9.87E+02]')
# real: regex for real number with only one group!
```

Extracting multiple matches (1)

- If the regex contains groups, `re.findall` returns the matches of all groups - this might be confusing!

```
>>> r = r"(\d+)\.\d*"
>>> s = "3.29 is a number, 4.2 and 0.5 too"
>>> re.findall(r,s)
['3', '4', '0']
```

- Application to the interval example:

```
>>> real_short = r"([+\-]?(\d+(\.\d*)?|\d*\.\d+)([eE][+\-]?\d+
>>> # recall: real_short contains many nested groups!
>>> g = re.findall(real_short, '[-3, 9.87E+02]')
>>> g
[('-3', '3', '', ''), ('9.87E+02', '9.87', '.87', 'E+02')]
>>> limits = [ float(g1) for g1, g2, g3, g4 in g ]
>>> limits
[-3.0, 987.0]
```

Making a regex simpler

- Regex is often a question of structure *and context*
- Simpler regex for extracting interval limits:

```
\[(.*),(.*)\]
```

- It works!

```
>>> l = re.search(r'\[(.*),(.*)\]',
                  ' [-3.2E+01,0.11  ]').groups()
>>> l
('-3.2E+01', '0.11  ')

# transform to real numbers:
>>> r = [float(x) for x in l]
>>> r
[-32.0, 0.11]
```

Failure of a simple regex (1)

- Let us test the simple regex on a more complicated text:

  ```
  >>> l = re.search(r'\[(.*),(.*)\]', \
      ' [-3.2E+01,0.11  ] and [-4,8]').groups()
  >>> l
  ('-3.2E+01,0.11  ] and [-4', '8')
  ```

  Regular expressions can surprise you...!

- Regular expressions are greedy, they attempt to find the longest possible match, here from `[` to the last (!) comma
- We want a shortest possible match, up to the first comma, i.e., a non-greedy match
- Add a `?` to get a non-greedy match:

  ```
  \[(.*?),(.*?)\]
  ```

- Now `l` becomes

  ```
  ('-3.2E+01', '0.11  ')
  ```

Failure of a simple regex (2)

- Instead of using a non-greedy match, we can use

  `\[([^,]*),([^\]]*)\]`

- Note: only the first group (here first interval) is found by `re.search`, use `re.findall` to find all

Failure of a simple regex (3)

- The simple regexes

```
\[([^,]*),([^\]]*)\]
\[(.*?),(.*?)\]
```

  are not fool-proof:

```
>>> l = re.search(r'\[([^,]*),([^\]]*)\]',
                  ' [e.g., exception]').groups()
>>> l
('e.g.', ' exception')
```

- 100 percent reliable fix: use the detailed real number regex inside the parenthesis
- The simple regex is ok for personal code

Application example

- Suppose we, in an input file to a simulator, can specify a grid using this syntax:

```
domain=[0,1]x[0,2] indices=[1:21]x[0:100]
domain=[0,15] indices=[1:61]
domain=[0,1]x[0,1]x[0,1] indices=[0:10]x[0:10]x[0:20]
```

- Can we easily extract domain and indices limits and store them in variables?

Extracting the limits

- Specify a regex for an interval with real number limits
- Use re.findall to extract multiple intervals
- Problems: many nested groups due to complicated real number specifications
- Various remedies: as in the interval examples, see fdmgrid.py
- The bottom line: a very simple regex, utilizing the surrounding structure, works well

Utilizing the surrounding structure

- We can get away with a simple regex, because of the surrounding structure of the text:

```
indices = r"\[([^:,]*):([^\]]*)\]"  # works
domain  = r"\[([^,]*),([^\]]*)\]"   # works
```

- Note: these ones do not work:

```
indices = r"\[([^:]*):([^\]]*)\]"
indices = r"\[(.*?):(.*?)\]"
```

They match too much:

```
domain=[0,1]x[0,2] indices=[1:21]x[1:101]
       [.....................:
```

we need to exclude commas (i.e. left bracket, anything but comma or colon, colon, anythin but right bracket)

Splitting text

- Split a string into words:

```
line.split(splitstring)
# or
string.split(line, splitstring)
```

- Split wrt a regular expression:

```
>>> files = "case1.ps, case2.ps,    case3.ps"
>>> import re
>>> re.split(r",\s*", files)
['case1.ps', 'case2.ps', 'case3.ps']
```

```
>>> files.split(", ")  # a straight string split is undesired
['case1.ps', 'case2.ps', '   case3.ps']
>>> re.split(r"\s+", "some    words   in a text")
['some', 'words', 'in', 'a', 'text']
```

- Notice the effect of this:

```
>>> re.split(r" ", "some    words   in a text")
['some', '', '', '', 'words', '', '',  'in', 'a', 'text']
```

Pattern-matching modifiers (1)

- ...also called flags in Python regex documentation
- Check if a user has written "yes" as answer:

```
if re.search('yes', answer):
```

- Problem: "YES" is not recognized; try a fix

```
if re.search(r'(yes|YES)', answer):
```

- Should allow "Yes" and "YEs" too...

```
if re.search(r'[yY][eE][sS]', answer):
```

- This is hard to read and case-insensitive matches occur frequently - there must be a better way!

Pattern-matching modifiers (2)

```
if re.search('yes', answer,  re.IGNORECASE):
# pattern-matching modifier: re.IGNORECASE
# now we get a match for 'yes', 'YES', 'Yes' ...

# ignore case:
re.I  or  re.IGNORECASE

# let ^ and $ match at the beginning and
# end of every line:
re.M  or  re.MULTILINE

# allow comments and white space:
re.X  or  re.VERBOSE

# let . (dot) match newline too:
re.S  or  re.DOTALL

# let e.g. \w match special chars (?, ?, ...):
re.L  or  re.LOCALE
```

Comments in a regex

- The `re.X` or `re.VERBOSE` modifier is very useful for inserting comments explaning various parts of a regular expression
- Example:

```
# real number in scientific notation:
real_sn = r"""
-?                # optional minus
\d\.\d+            # a number like 1.4098
[Ee][+\-]\d\d?  # exponent, E-03, e-3, E+12
"""

match = re.search(real_sn, 'text with a=1.92E-04 ',
                  re.VERBOSE)

# or when using compile:
c = re.compile(real_sn, re.VERBOSE)
match = c.search('text with a=1.9672E-04 ')
```

Substitution

- Substitute `float` by `double`:

```
# filestr contains a file as a string
filestr = re.sub('float', 'double', filestr)
```

- In general:

```
re.sub(pattern, replacement, str)
```

- If there are groups in pattern, these are accessed by

```
\1      \2      \3      ...
\g<1>   \g<2>   \g<3>   ...
```

```
\g<lower>  \g<upper> ...
```

  in `replacement`

Example: strip away C-style comments

- C-style comments could be nice to have in scripts for commenting out large portions of the code:

```
/*
while 1:
    line = file.readline()
    ...
...
*/
```

- Write a script that strips C-style comments away
- Idea: match comment, substitute by an empty string

Trying to do something simple

- Suggested regex for C-style comments:

```
comment = r'/\*.*\*/'

# read file into string filestr
filestr = re.sub(comment, '', filestr)
```

  i.e., match everything between `/*` and `*/`
- Bad: . does not match newline
- Fix: `re.S` or `re.DOTALL` modifier makes . match newline:

```
comment = r'/\*.*\*/'
c_comment = re.compile(comment, re.DOTALL)
filestr = c_comment.sub(comment, '', filestr)
```

- OK? No!

Testing the C-comment regex (1)

Test file:

```
/********************************************/
/* File myheader.h                          */
/********************************************/

#include <stuff.h>  // useful stuff

class MyClass
{
  /* int r; */  float q;
  // here goes the rest class declaration
}

/* LOG HISTORY of this file:
 * $ Log: somefile,v $
 * Revision 1.2  2000/07/25 09:01:40  hpl
 * update
 *
 * Revision 1.1.1.1  2000/03/29 07:46:07  hpl
 * register new files
 *
*/
```

Testing the C-comment regex (2)

- The regex

  ```
  /\*.*\*/  with re.DOTALL (re.S)
  ```

  matches the whole file (i.e., the whole file is stripped away!)
- Why? a regex is by default greedy, it tries the longest possible match, here the whole file
- A question mark makes the regex non-greedy:

  ```
  /\*.*?\*/
  ```

Testing the C-comment regex (3)

- The non-greedy version works
- OK? Yes - the job is done, almost...

```
const char* str ="/* this is a comment */"
```

gets stripped away to an empty string...

Substitution example

- Suppose you have written a C library which has many users
- One day you decide that the function

  ```
  void superLibFunc(char* method, float x)
  ```

  would be more natural to use if its arguments were swapped:

  ```
  void superLibFunc(float x, char* method)
  ```

- All users of your library must then update their application codes - can you automate?

Substitution with backreferences

- You want locate all strings on the form

  ```
  superLibFunc(arg1, arg2)
  ```

  and transform them to

  ```
  superLibFunc(arg2, arg1)
  ```

- Let `arg1` and `arg2` be groups in the regex for the superLibFunc calls
- Write out

  ```
  superLibFunc(\2, \1)

  # recall: \1 is group 1, \2 is group 2 in a re.sub command
  ```

Regex for the function calls (1)

- Basic structure of the regex of calls:

  ```
  superLibFunc\s*\(\s*arg1\s*,\s*arg2\s*\)
  ```

  but what should the `arg1` and `arg2` patterns look like?

- Natural start: `arg1` and `arg2` are valid C variable names

  ```
  arg = r"[A-Za-z_0-9]+"
  ```

- Fix; digits are not allowed as the first character:

  ```
  arg = "[A-Za-z_][A-Za-z_0-9]*"
  ```

Regex for the function calls (2)

- The regex

  ```
  arg = "[A-Za-z_][A-Za-z_0-9]*"
  ```

  works well for calls with variables, but we can call `superLibFunc` with numbers too:

  ```
  superLibFunc ("relaxation", 1.432E-02);
  ```

- Possible fix:

  ```
  arg = r"[A-Za-z0-9_.\-+\"]+"
  ```

  but the disadvantage is that `arg` now also matches

  ```
  .+-32skj  3.ejks
  ```

Constructing a precise regex (1)

- Since `arg2` is a float we can make a precise regex: legal C variable name OR legal real variable format

```
arg2 = r"([A-Za-z_][A-Za-z_0-9]*|" + real + \
        "|float\s+[A-Za-z_][A-Za-z_0-9]*" + ")"
```

where `real` is our regex for formatted real numbers:

```
real_in = r"-?\d+"
real_sn = r"-?\d\.\d+[Ee][+\-]\d\d?"
real_dn = r"-?\d*\.\d+"
real = r"\s*("+ real_sn +"|"+ real_dn +"|"+ real_in +r")\s*"
```

Constructing a precise regex (2)

- We can now treat variables and numbers in calls
- Another problem: should swap arguments in a user's definition of the function:

  ```
  void superLibFunc(char* method, float x)
  ```

  to

  ```
  void superLibFunc(float x, char* method)
  ```

  Note: the argument names (`x` and `method`) can also be omitted!
- Calls and declarations of superLibFunc can be written on more than one line and with embedded C comments!
- Giving up?

A simple regex may be sufficient

- Instead of trying to make a precise regex, let us make a very simple one:

  ```
  arg = '.+'    # any text
  ```

- "Any text" may be precise enough since we have the surrounding structure,

  ```
  superLibFunc\s*(\s*arg\s*,\s*arg\s*)
  ```

  and assume that a C compiler has checked that `arg` is a valid C code text in this context

Refining the simple regex

- A problem with `.+` appears in lines with more than one calls:

  ```
  superLibFunc(a,x);  superLibFunc(ppp,qqq);
  ```

- We get a match for the first argument equal to

  ```
  a,x);  superLibFunc(ppp
  ```

- Remedy: non-greedy regex (see later) or

  ```
  arg = r"[^,]+"
  ```

  This one matches multi-line calls/declarations, also with embedded comments (`.+` does not match newline unless the `re.S` modifier is used)

Swapping of the arguments

- Central code statements:

```
arg = r"[^,]+"
call = r"superLibFunc\s*\(\s*(%s),\s*(%s)\)" % (arg,arg)

# load file into filestr

# substutite:
filestr = re.sub(call, r"superLibFunc(\2, \1)", filestr)

# write out file again
fileobject.write(filestr)
```

Files: src/py/intro/swap1.py

Testing the code

- Test text:

```
superLibFunc(a,x);  superLibFunc(qqq,ppp);
superLibFunc ( method1, method2 );
superLibFunc(3method /* illegal name! */, method2 ) ;
superLibFunc(  _method1,method_2) ;
superLibFunc (
              method1 /* the first method we have */ ,
          super_method4 /* a special method that
                               deserves a two-line comment...
             ) ;
```

- The simple regex successfully transforms this into

```
superLibFunc(x, a);  superLibFunc(ppp, qqq);
superLibFunc(method2 , method1);
superLibFunc(method2 , 3method /* illegal name! */) ;
superLibFunc(method_2, _method1) ;
superLibFunc(super_method4 /* a special method that
                               deserves a two-line comment...
             , method1 /* the first method we have */ ) ;
```

- Notice how powerful a small regex can be!!
- Downside: cannot handle a function call as argument

Shortcomings

- The simple regex

  ```
  [^,]+
  ```

  breaks down for comments with comma(s) and function calls as arguments, e.g.,

  ```
  superLibFunc(m1, a /* large, random number */);
  superLibFunc(m1, generate(c, q2));
  ```

  The regex will match the longest possible string ending with a comma, in the first line

  ```
  m1, a /* large,
  ```

  but then there are no more commas ...

- A complete solution should *parse* the C code

More easy-to-read regex

- The `superLibFunc` call with comments and named groups:

```
call = re.compile(r"""
     superLibFunc  # name of function to match
     \s*           # possible whitespace
     \(            # parenthesis before argument list
     \s*           # possible whitespace
     (?P<arg1>%s)  # first argument plus optional whitespace
     ,             # comma between the arguments
     \s*           # possible whitespace
     (?P<arg2>%s)  # second argument plus optional whitespace
     \)            # closing parenthesis
     """ % (arg,arg), re.VERBOSE)

# the substitution command:
filestr = call.sub(r"superLibFunc(\g<arg2>,
                   \g<arg1>)",filestr)
```

Files: src/py/intro/swap2.py

Example

- Goal: remove C++/Java comments from source codes
- Load a source code file into a string:

```
filestr = open(somefile, 'r').read()
# note: newlines are a part of filestr
```

- Substitute comments *// some text...* by an empty string:

```
filestr = re.sub(r'//.*', '', filestr)
```

- Note: . (dot) does not match newline; if it did, we would need to say

```
filestr = re.sub(r'//[^\n]*', '', filestr)
```

Failure of a simple regex

- How will the substitution

```
filestr = re.sub(r'//[^\n]*', '', filestr)
```

  treat a line like

```
const char* heading = "------------//------------";
```

  ???

Regex debugging (1)

- The following useful function demonstrate how to extract matches, groups etc. for examination:

```
def debugregex(pattern, str):
    s = "does ’" + pattern + "’ match ’" + str + "’?\n"
    match = re.search(pattern, str)
    if match:
        s += str[:match.start()] + "[" + \
             str[match.start():match.end()] + \
             "]" + str[match.end():]
        if len(match.groups()) > 0:
            for i in range(len(match.groups())):
                s += "\ngroup %d: [%s]" % \
                     (i+1,match.groups()[i])
    else:
        s += "No match"
    return s
```

Regex debugging (2)

- Example on usage:

```
>>> print debugregex(r"(\d+\.\d*)",
                     "a= 51.243 and b =1.45")

does '(\d+\.\d*)' match 'a= 51.243 and b =1.45'?
a= [51.243] and b =1.45
group 1: [51.243]
```

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/yourlib
  ```
- 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 --prefix=$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
    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
```

Numerical Python

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

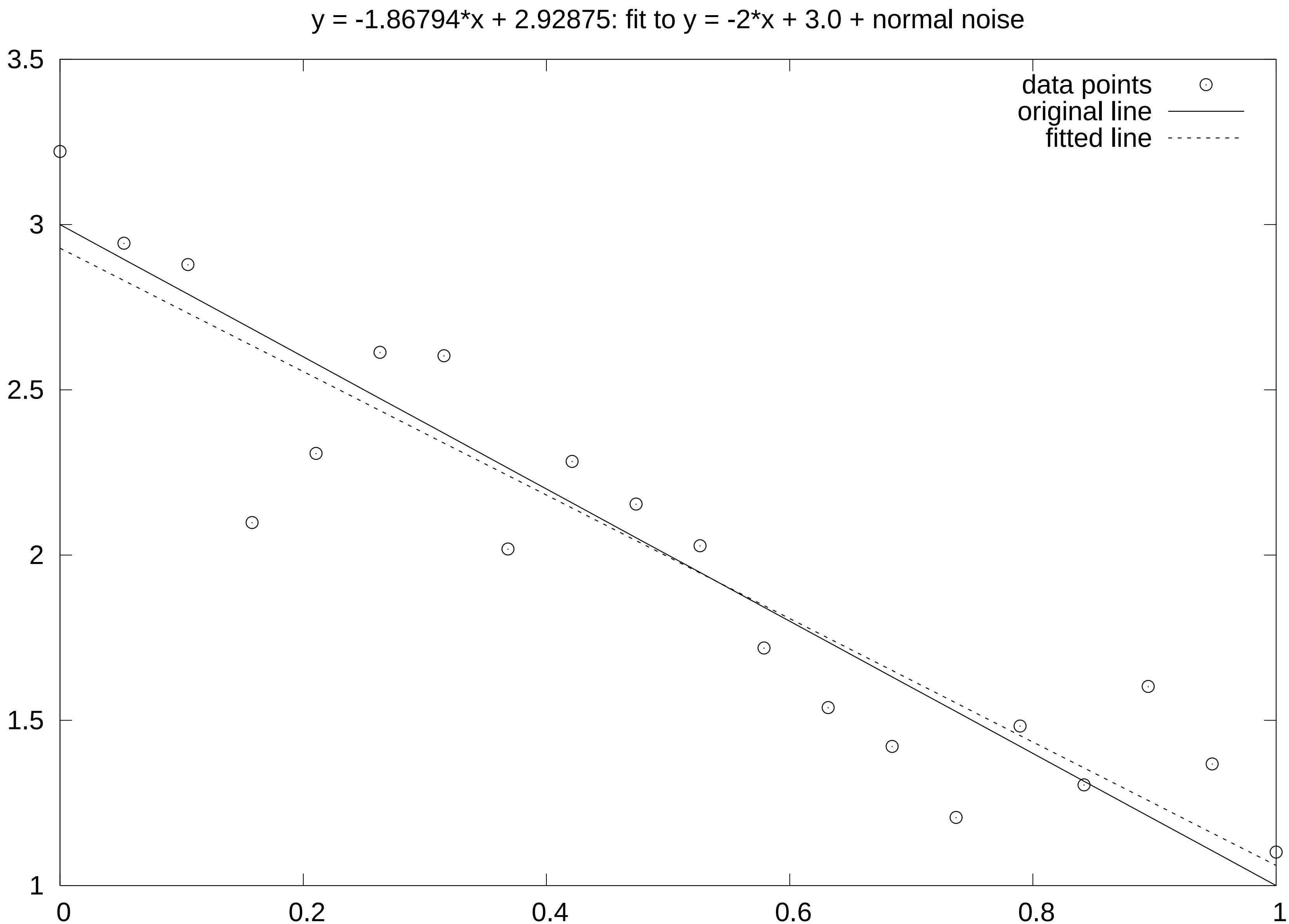
# goal: fit a line to the data points x, y

# 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



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)
```

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(-5, 5, 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: `seq(start, stop, increment)`

```
>>> 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.]
```

- The package `scitools` is available at `http://code.google.com/p/scitools/`

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 agair
>>> 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

Note: all integer indices in Python start at 0!

```
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,::2]   # a[i,j] for i=1,2 and j=0,2,4
array([[  6.,   8.,  10.],
       [ 12.,  14.,  16.]])

>>> a[::3,2::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, None, 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[2,:]          # extract 2nd row of a
>>> print a[2,0]
12.0
>>> b[0] = 2
>>> print a[2,0]
2.0                     # change in b is reflected in a!
```

- Take a copy to avoid referencing via slices:

```
>>> b = a[2,:].copy()
>>> print a[2,0]
12.0
>>> b[0] = 2         # b and a are two different arrays now
>>> print a[2,0]
12.0                 # a is not affected by change in b
```

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.ravel():
    print e
```

  Use `ravel()` only when reading elements, for assigning it is better to use `shape` or `reshape` first!

- 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
```

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
```

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])
```

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

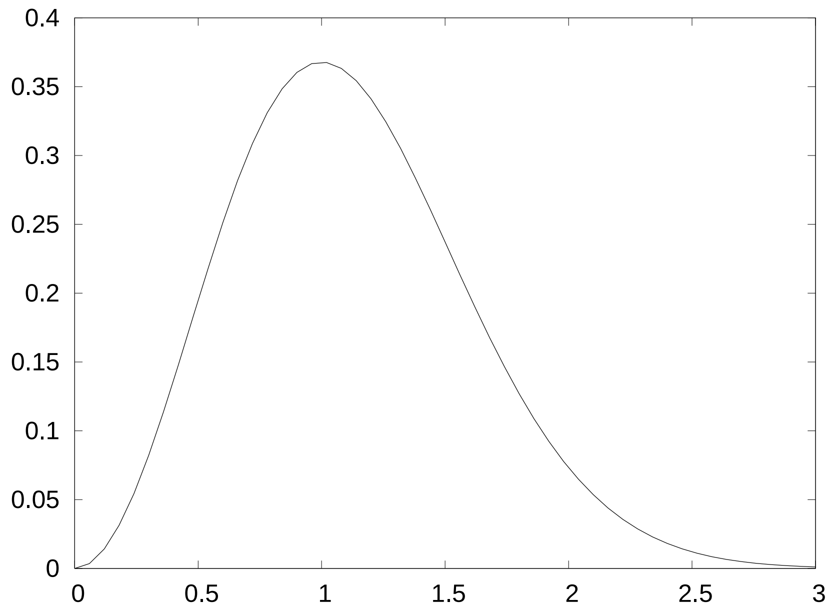
- Easyviz is a light-weight interface to many plotting packages, using a Matlab-like syntax
- Goal: write your program using Easyviz (“Matlab”) syntax and postpone your choice of plotting package
- Note: some powerful plotting packages (Vtk, R, matplotlib, ...) may be troublesome to install, while Gnuplot 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
```



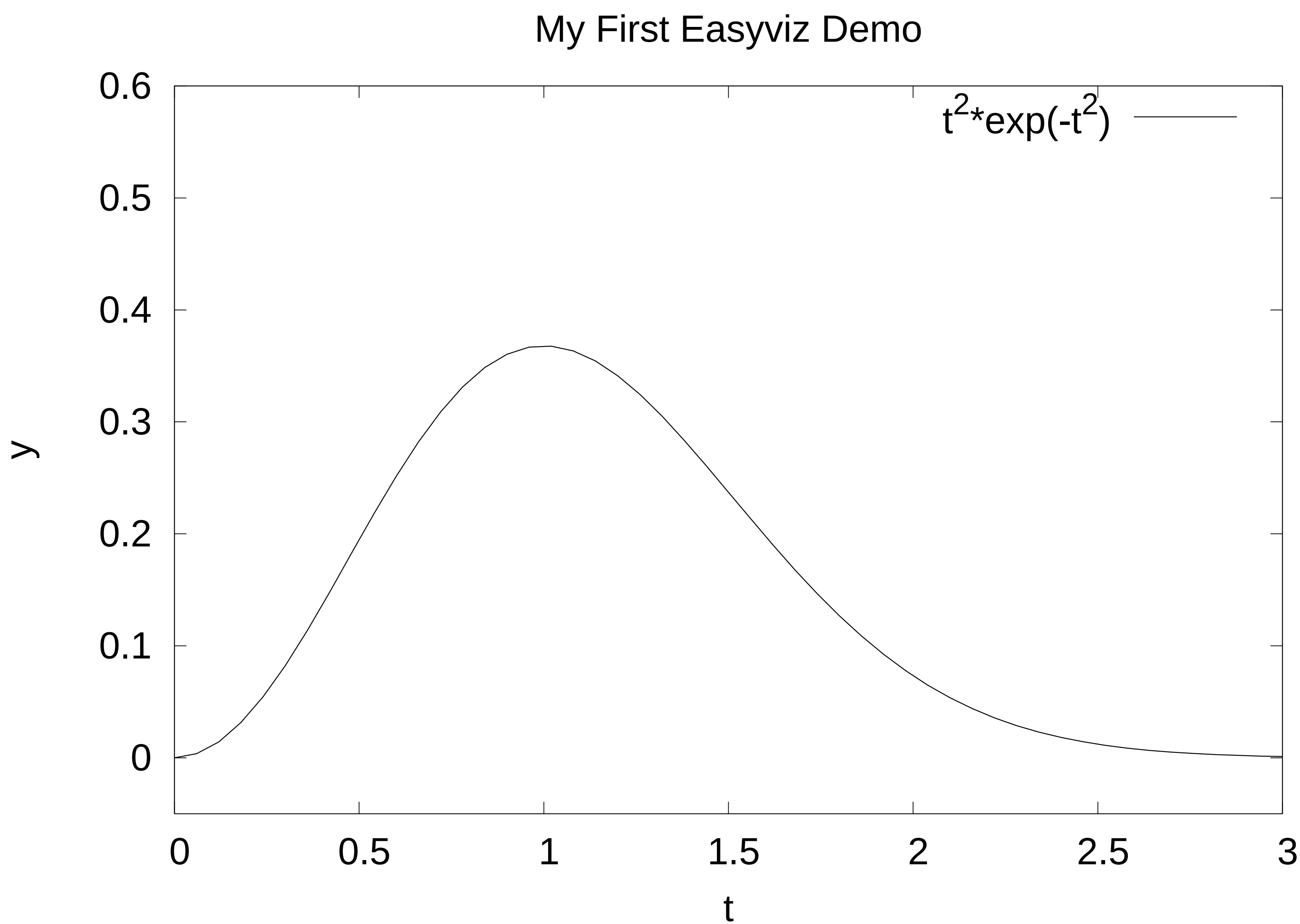
Decorating the plot

```
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)

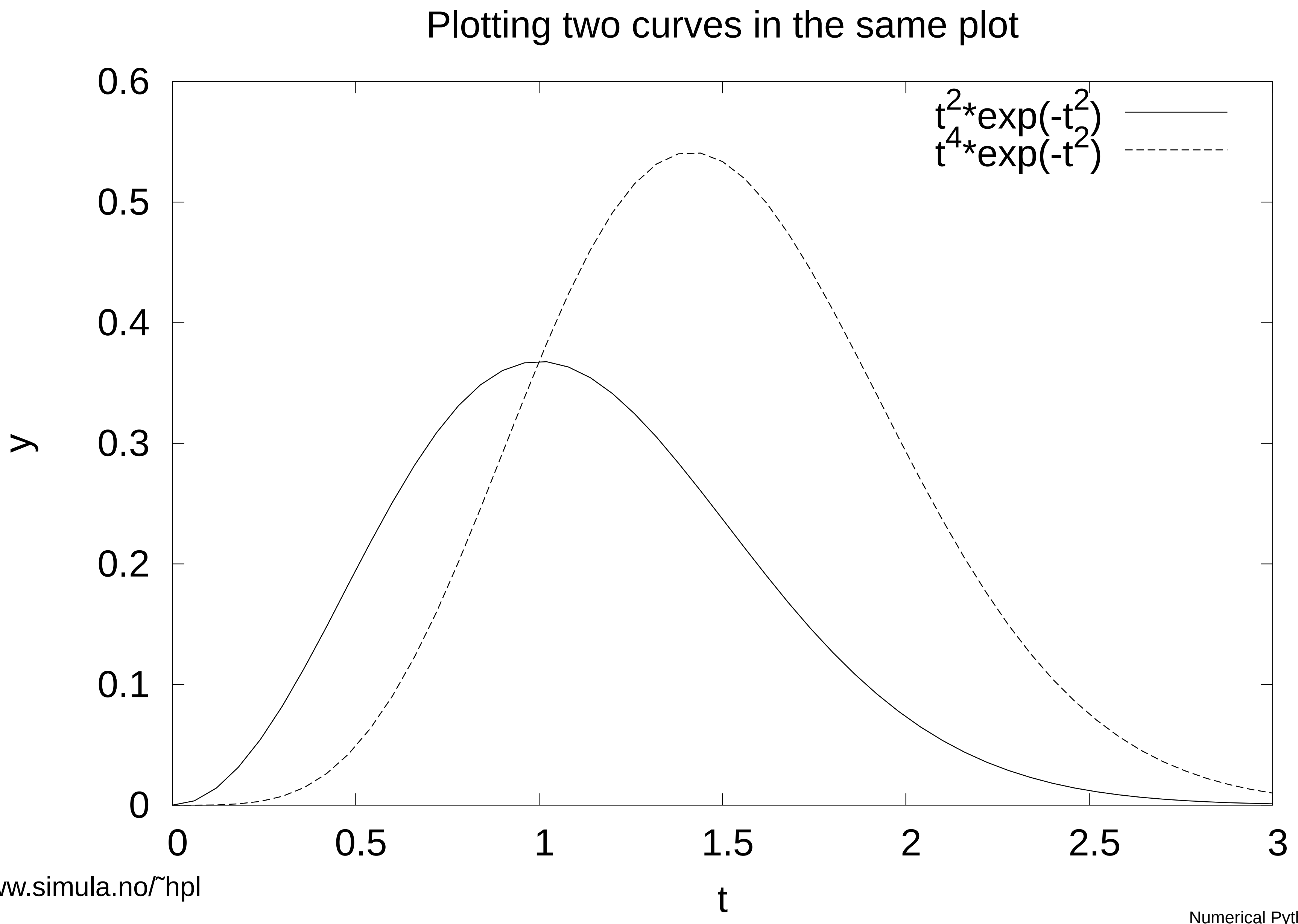
def f2(t):
    return t**2*f1(t)

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])

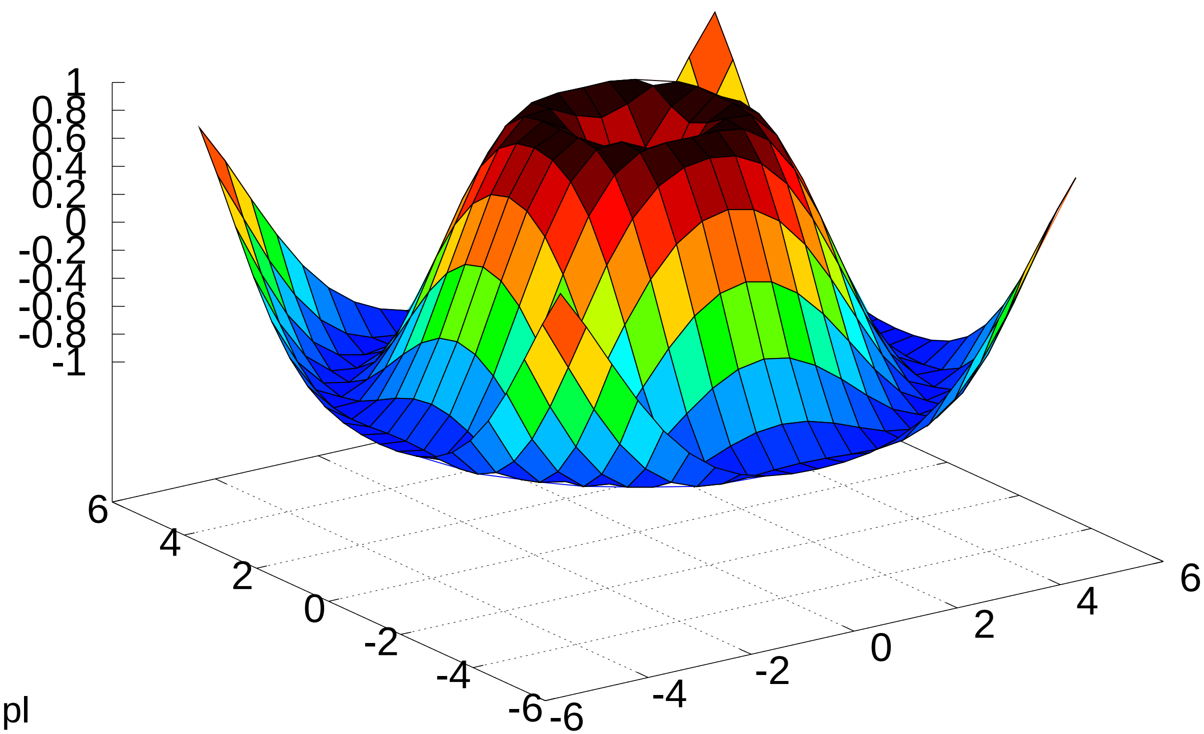
x = linspace(xmin, xmax, 101)
y = eval(formula)
plot(x, y, title=formula)
```

- 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)
```

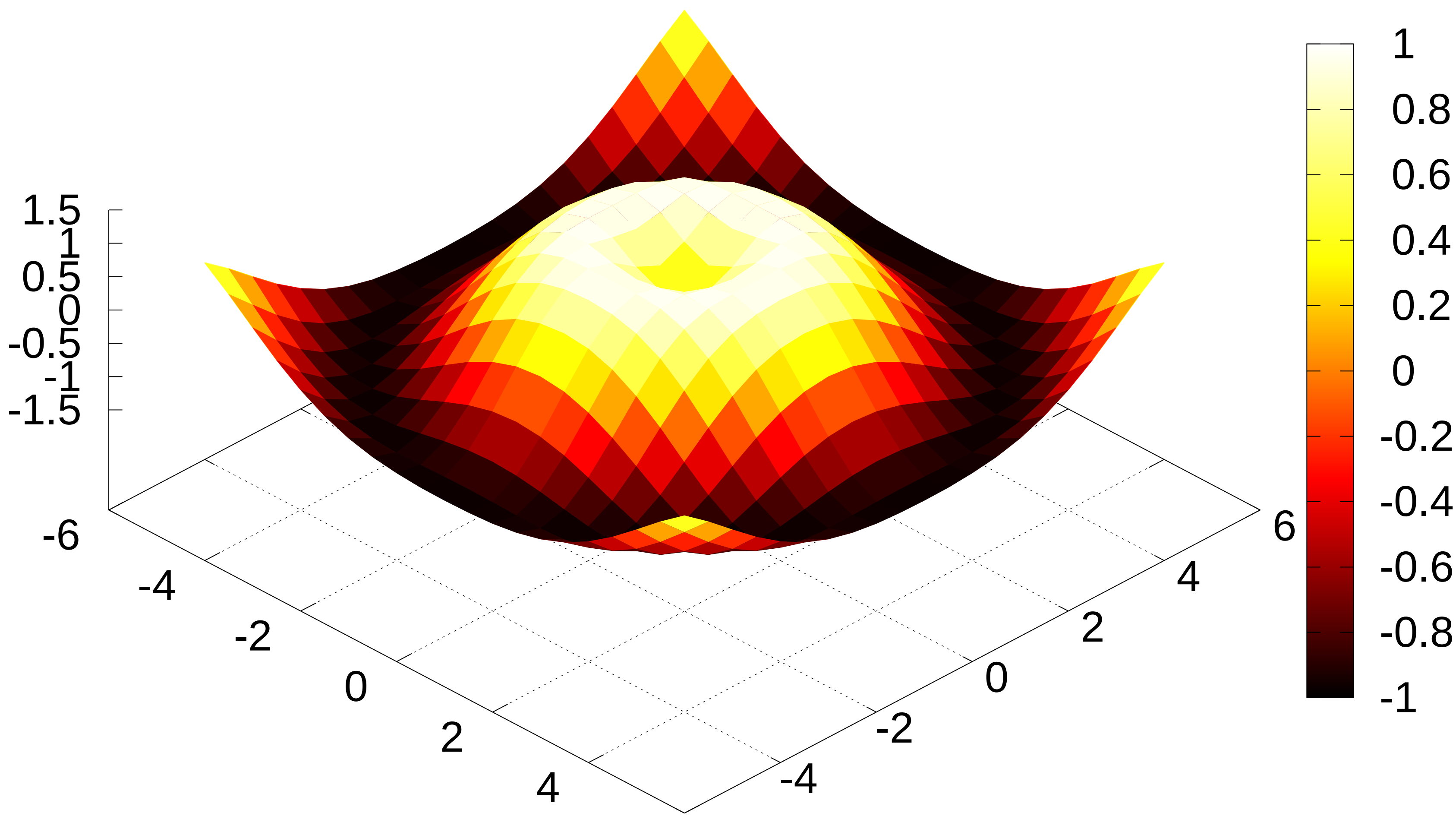


Adding plot features

```
# 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://code.google.com/p/scitools/wiki/EasyvizDocumentation`

- Download SciTools (incl. Easyviz):

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

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 an object, even the source code
- 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 `_classname__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

- Bad 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

- Bad 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)
```

Alternative solution: Closure

- Make a function that locks the namespace and constructs and returns a tailor made function

```
def F(a=1,b=1,c=1):

    def f(x, y):
        return a + b*x + c*y*y

    return f

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 $\Rightarrow$ 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,
                    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, 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)
>>> 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
```

Python optimalization

Optimization of C, C++, and Fortran

- Compilers do a good job for C, C++, and Fortran.
- The type system makes agressive optimization possible.
- Examples: code inlining, loop unrolling, and memory prefetching.

Python optimization

- No compiler.
- No type declaration of variables.
- No inlining and no loop unrolling.
- Probably inefficient in Python:

```
def f(a, b):
    return a + b
```

Manual timing

- Use `time.time()`.
- Simple statements should be placed in a loop.
- Make sure constant machine load.
- Run the tests several times, choose the fastest.

The `timeit` module (1)

- Usage:

```
import timeit
timer =
timeit.Timer(stmt="a+=1",setup="a=0")
time = timer.timeit(number=10000) #or
times = timer.repeat(repeat=5,
number=10000)
```

The `timeit` module (2)

- Isolates the global namespace.
- Automatically wraps the code in a for–loop.
- Users can provide their own timer (callback).
- Time a user defined function:
  ```
  from __main__ import my_func
  ```

Profiling modules

- Prior to code optimization, hotspots and bottlenecks must be located.
  "First make it work. Then make it right. Then make it fast."
  - Kent Beck
- Two modules: `profile` and `hotshot`.
- `profile` works for all Python versions.
- `hotshot` introduced in Python version 2.2.

The `profile` module (1)

- As a script: `profile.py script.py`
- As a module:

```
import profile
pr = profile.Profile()
res = pr.run("function()", "filename")
res.print\_stats()
```

- Profile data saved to "filename" can be viewed with the `pstats` module.

The `profile` module (2)

- `profile.calibrate(number)` finds the profiling overhead.
- Remove profiling overhead:
  `pr = profile.Profile(bias=overhead)`
- Profile a single function call:

```
pr = profile.Profile()
pr.runcall(func, *args, **kwargs)
```

The `hotshot` module

- Similar to `profile`, but mostly implemented in C.
- Smaller performance impact than `profile`.
- Useage:

```
import hotshot
pr = hotshot.Profile("filename")
pr.run(cmd)
pr.close() # Close log-file and end profiler
```

- Read profile data:

```
import hotshot.stats
data = hotshot.stats.load("filename")# profile.Stats instance
data.print_stats()
```

The `pstats` module

- There are many ways to view profiling data.
- The module `pstats` provides the class `Stats` for creating profiling reports:

```
import pstats
data = pstats.Stats("filename")
data.print_stats()
```

- The method `sort_stats(key, *keys)` is used to sort future output.
- Common used keys: `'calls', 'cumulative', 'time'`.

Pure Python performance tips

- Place references to functions in the local namespace.

```
from math import *
def f(x):
    for i in xrange(len(x)):
        x[i] = sin(x[i]) # Slow
    return x

def g(x):
    loc_sin = sin # Local reference
    for i in xrange(len(x)):
        x[i] = loc_sin(x[i]) # Faster
    return x
```

- Reason: Local namespace is searched first.

More local references

- Local references to instance methods of global objects are even more important, as we need only one dictionary look–up to find the method instead of three (local, global, instance–dictionary).

```
class Dummy(object):
    def f(self): pass

d = Dummy()

def f():
    loc_f=d.f
    for i in xrange(10000): loc_f()
```

- Calling `loc_f()` instead of `d.f()` is 40% faster in this example.

Exceptions should never happen

- Use `if/else` instead of `try/except`
- Example:

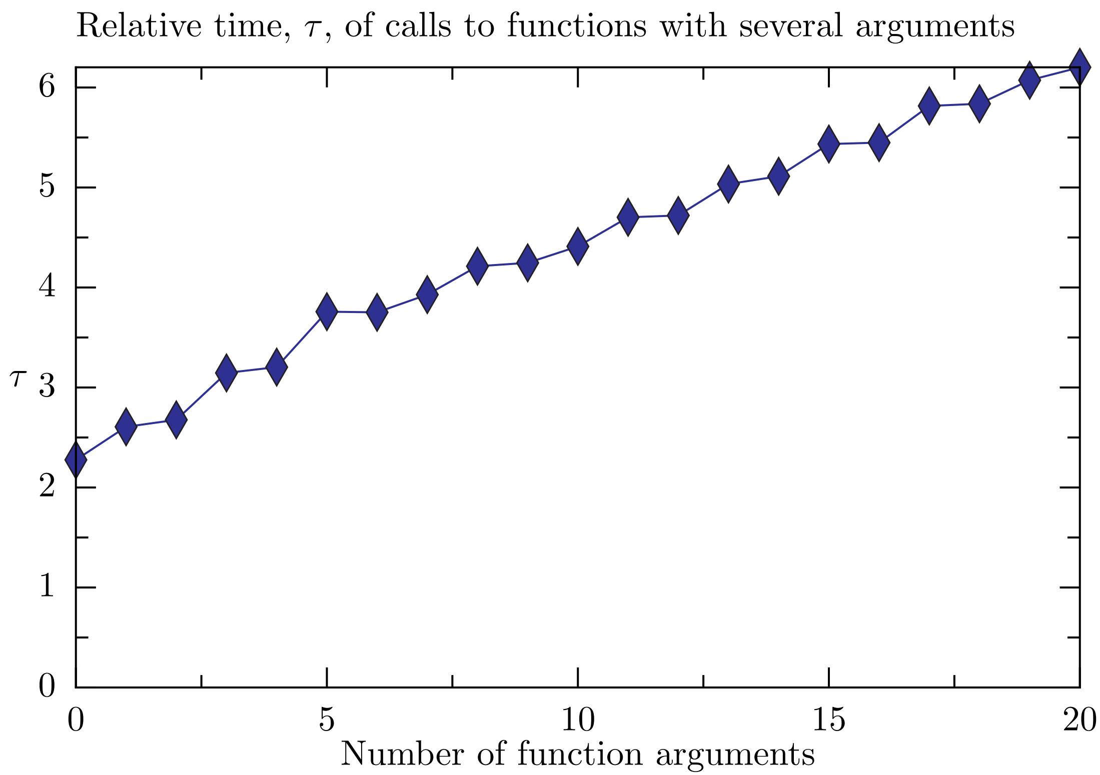
```
x = 0
try: 1.0/x
except: 0
```

```
if not (x==0): 1.0/x
else: 0
```

- `if/else` is more than 20 times faster.

Function calls

- The time of calling a function grows linearly with the number of arguments:



Numerical Python

- Vectorized computations are fast:

```
import numarray # Array functions
x = numarray.arange(-1,1,0.01)
y = numarray.sin(x)

import math # Scalar functions
y = numarray.zeros(len(x), type=numarray.Float)
for i in xrange(len(x)):
    y[i] = math.sin(x[i])
```

- The speedup is a factor of 20.

Resizing arrays

- The `resize` method of arrays is very slow.
- Increasing the array size by one in a loop is about 300-350 times slower than appending elements to a Python list.
- Best approach; allocate the memory once, and assign values later.

`Numeric` vs. `numarray`

- `Numeric` is the old array module in Python
- Still very popular, and will probably live for many years
- The difference between pointwise and array evaluation of a vector is about 13 for `Numeric` (20 for `numarray`)
- Vectorized functions work on scalars as well, but at a high price
- Using `numarray.sin` instead of `math.sin` on a scalar value is slower by a factor of 12. `Numeric.sin` only slower by a factor of 4

Conclusions

- Python scripts can often be heavily optimized.
- The results given here may vary on different architectures and Python versions
- Be extremely careful about the `from numarray import *`.

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

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)
- F77 code in a file `hw.f`:

```
      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
- Comments 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`
- Run F2PY (-m module name, -c for compile+link):

```
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)
```

- In Python, `hw` appears as a module with Python code...
- 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
- Output arguments must be explicitly specified!

General adjustment of interfaces to Fortran

- 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, as generated by F2PY:

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

Check F2PY-generated doc strings

- What happened to our hw3 subroutine?
- F2PY generates doc strings that document the interface:

```
>>> import hw
>>> print hw.__doc__       # brief module doc string
Functions:
  hw1 = hw1(r1,r2)
  hw2(r1,r2)
  hw3(r1,r2,s)

>>> print hw.hw3.__doc__  # more detailed function doc string
hw3 - Function signature:
  hw3(r1,r2,s)
Required arguments:
  r1 : input float
  r2 : input float
  s : input float
```

- We see that hw3 assumes s is *input* argument!
- Remedy: adjust the interface

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 always 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 (as generated by F2PY):

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

Specification of input/output arguments; .pyf file

- 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; .f file

- 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
```

Specification of input/output arguments; .f90 file

- With Fortran 90:

```
subroutine somef(i1, i2, o1, o2, o3, o4, io1)
real*8 i1, i2, o1, o2, o3, o4, io1
!f2py  intent(in) i1
!f2py  intent(in) i2
!f2py  intent(out) o1
!f2py  intent(out) o2
!f2py  intent(out) o3
!f2py  intent(out) o4
!f2py  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.. -fPIC -I/some/path/include/python2.5 \
    -c ../hw.c hw_wrap.c
gcc -shared -fPIC -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 -fPIC -I.. -I$root/include/python$ver -c ../hw.c hw_wrap.c
gcc -shared -fPIC -o _hw.so hw.o hw_wrap.o

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

this script make_module_1.sh is found here:

http://www.ifi.uio.no/~inf3331/scripting/src/py/mixed/hw/C/swig-hw/

- 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

- 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++ -fPIC -I.. -I$root/include/python$ver \
    -c ../hw.cpp hw_wrap.cxx
g++ -shared -fPIC -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 = _hw.new_HelloWorld()
_hw.HelloWorld_set(hw, 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)
```

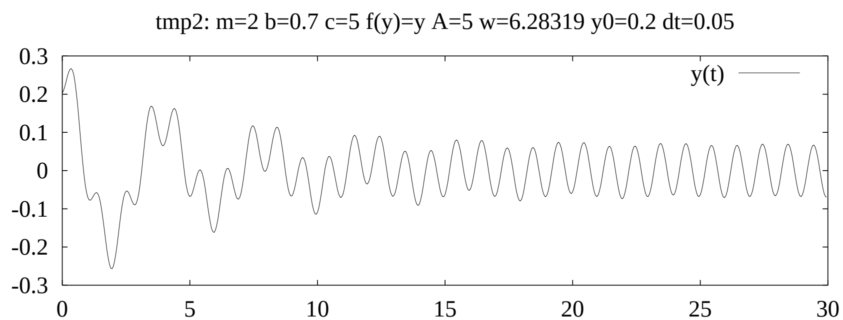
- The proxy class introduces overhead

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

Example on what we can do

- 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)
```

Principles

- 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), order='Fortran')
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

Mixed language numerical Python

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) +
```

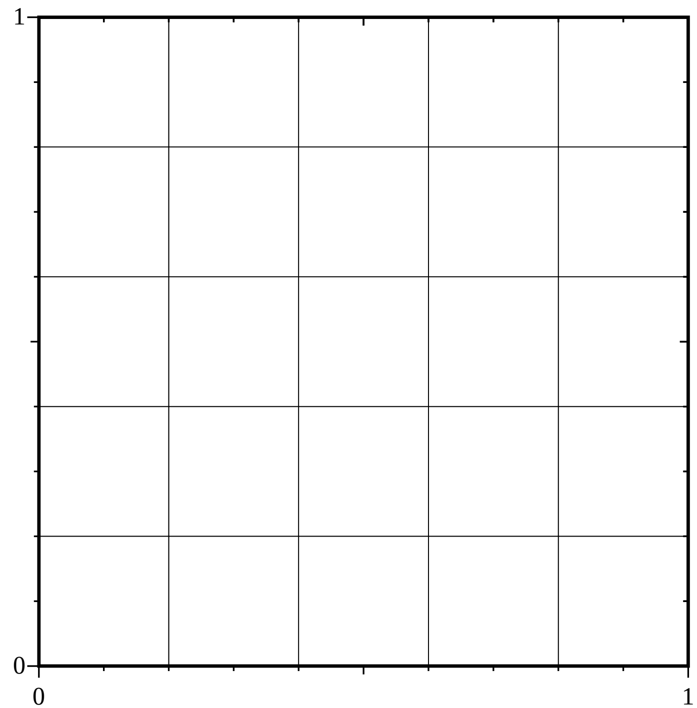
- Fortran/C/C++ version: (normalized) time 1.0
- NumPy vectorized evaluation of `f`: time 3.0
- Python loop version (version): time 140 (`math.sin`)
- Python loop version (version): time 350 (`numarray.sin`)

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

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 xrange(lx):
            x = self.xcoor[i]
            for j in xrange(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), fun
      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), fun
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 vectorize(func):

    def vec77(a, xcoor, ycoor, nx, ny):
        """Vectorized function to be called from extension module."""
        x = xcoor[:,NewAxis];  y = ycoor[NewAxis,:]
        a[:,:] = func(x, y)  # in-place modification of a

    return vec77

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

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 vectorize(func):

    def vec77(a, xcoor, ycoor, nx, ny):
        """Vectorized function to be called from extension module."""
        x = xcoor[:,NewAxis];  y = ycoor[NewAxis,:]
        a = func(x, y)

    return vec77
```

- 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 `fcb` 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)

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`
- Warning: manual writing of extension modules is very much more complicated than using F2PY on Fortran code! You need to know C quite well...

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);

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

First debugging example

- 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 (2)

```
(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 (ini
```

- 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

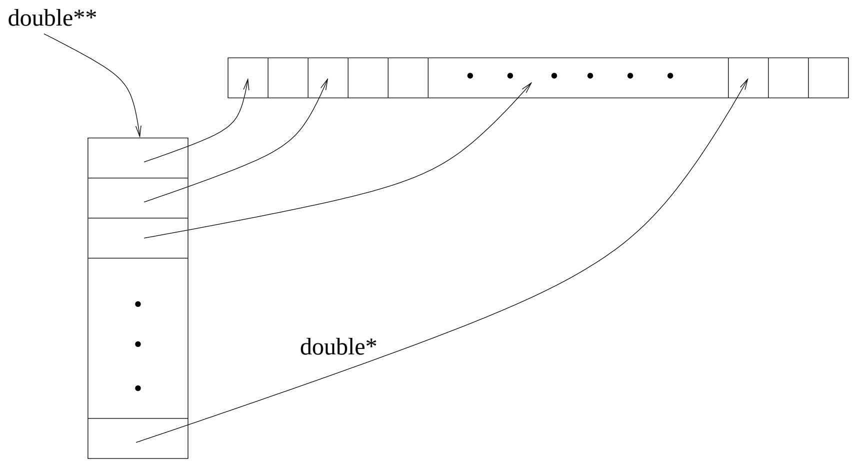
Problems

- 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, ...)

Basic Bash programming

Overview of Unix shells

- The original scripting languages were (extensions of) command interpreters in operating systems
- Primary example: Unix shells
- Bourne shell (`sh`) was the first major shell
- C and TC shell (`csh` and `tcsh`) had improved command interpreters, but were less popular than Bourne shell for programming
- Bourne Again shell (Bash/`bash`): GNU/FSF improvement of Bourne shell
- Other Bash-like shells: Korn shell (`ksh`), Z shell (`zsh`)
- Bash is the dominating Unix shell today

Why learn Bash?

- Learning Bash means learning Unix
- Learning Bash means learning the roots of scripting (Bourne shell is a subset of Bash)
- Shell scripts, especially in Bourne shell and Bash, are frequently encountered on Unix systems
- Bash is widely available (open source) and the dominating command interpreter and scripting language on today's Unix systems
- Shell scripts are often used to glue more advanced scripts in Perl and Python

More information

- Greg Wilson's excellent online course:
  `http://www.swc.scipy.org`
- `man bash`
- "Introduction to and overview of Unix" link in `doc.html`

Scientific Hello World script

- Let's start with a script writing "Hello, World!"
- Scientific computing extension: compute the sine of a number as well
- The script (hw.sh) should be run like this:

  ```
  ./hw.sh 3.4
  ```

  or (less common):

  ```
  bash 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

Remark

- We use plain Bourne shell (`/bin/sh`) when special features of Bash (`/bin/bash`) are not needed
- Most of our examples can in fact be run under Bourne shell (and of course also Bash)
- Note that Bourne shell (`/bin/sh`) is usually just a link to Bash (`/bin/bash`) on Linux systems
  (Bourne shell is proprietary code, whereas Bash is open source)

The code

File hw.sh:

```
#!/bin/sh
r=$1  # store first command-line argument in r
s=‘echo "s($r)" | bc -l‘

# print to the screen:
echo "Hello, World! sin($r)=$s"
```

Comments

- The first line specifies the interpreter of the script (here `/bin/sh`, could also have used `/bin/bash`)
- The command-line variables are available as the script variables

```
$1  $2  $3  $4 and so on
```

- Variables are initialized as

```
r=$1
```

while the *value* of `r` requires a dollar prefix:

```
my_new_variable=$r  # copy r to my_new_variable
```

Bash and math

- Bourne shell and Bash have very little built-in math, we therefore need to use bc, Perl or Awk to do the math

```
s=‘echo "s($r)" | bc -l‘
s=‘perl -e ’$s=sin($ARGV[0]); print $s;’ $r‘
s=‘awk "BEGIN { s=sin($r); print s;}"‘
# or shorter:
s=‘awk "BEGIN {print sin($r)}"‘
```

- Back quotes means executing the command inside the quotes and assigning the output to the variable on the left-hand-side

```
some_variable=‘some Unix command‘

# alternative notation:
some_variable=$(some Unix command)
```

The bc program

- bc = interactive calculator
- Documentation: man bc
- bc -l means bc with math library
- Note: sin is s, cos is c, exp is e
- echo sends a text to be interpreted by bc and bc responds with output (which we assign to s)

```
variable=‘echo "math expression" | bc -l‘
```

Printing

- The `echo` command is used for writing:

  ```
  echo "Hello, World! sin($r)=$s"
  ```

  and variables can be inserted in the text string (variable interpolation)

- Bash also has a printf function for format control:

  ```
  printf "Hello, World! sin(%g)=%12.5e\n" $r $s
  ```

- `cat` is usually used for printing multi-line text (see next slide)

Convenient debugging tool: -x

- Each source code line is printed prior to its execution of you -x as option to `/bin/sh` or `/bin/bash`
- Either in the header

  ```
  #!/bin/sh -x
  ```

  or on the command line:

  ```
  unix> /bin/sh -x hw.sh
  unix> sh -x hw.sh
  unix> bash -x hw.sh
  ```

- Very convenient during debugging

File reading and writing

- Bourne shell and Bash are not much used for file reading and manipulation; usually one calls up Sed, Awk, Perl or Python to do file manipulation
- File writing is efficiently done by ’here documents’:

```
cat > myfile <<EOF
multi-line text
can now be inserted here,
and variable interpolation
a la $myvariable is
supported. The final EOF must
start in column 1 of the
script file.
EOF
```

Simulation and visualization script

- Typical application in numerical simulation:
  - run a simulation program
  - run a visualization program and produce graphs
- Programs are supposed to run in batch
- Putting the two commands in a file, with some glue, makes a classical Unix script

Setting default parameters

```
#!/bin/sh

pi=3.14159
m=1.0; b=0.7; c=5.0; func="y"; A=5.0;
w=‘echo 2*$pi | bc‘
y0=0.2; tstop=30.0; dt=0.05; case="tmp1"
screenplot=1
```

Parsing command-line options

```
# read variables from the command line, one by one:
while [ $# -gt 0 ]  # $# = no of command-line args.
do
    option = $1; # load command-line arg into option
    shift;       # eat currently first command-line arg
    case "$option" in
        -m)
            m=$1; shift; ;;  # load next command-line arg
        -b)
            b=$1; shift; ;;
        ...
        *)
            echo "$0: invalid option \"$option\""; exit ;;
    esac
done
```

Alternative to case: if

`case` is standard when parsing command-line arguments in Bash, but if-tests can also be used. Consider

```
case "$option" in
    -m)
        m=$1; shift; ;;  # load next command-line arg
    -b)
        b=$1; shift; ;;
    *)
        echo "$0: invalid option \"$option\""; exit ;;
esac
```

versus

```
if [ "$option" == "-m" ]; then
    m=$1; shift;  # load next command-line arg
elif [ "$option" == "-b" ]; then
    b=$1; shift;
else
    echo "$0: invalid option \"$option\""; exit
fi
```

Creating a subdirectory

```
dir=$case
# check if $dir is a directory:
if [ -d $dir ]
  # yes, it is; remove this directory tree
  then
    rm -r $dir
fi
mkdir $dir   # create new directory $dir
cd $dir      # move to $dir

# the 'then' statement can also appear on the 1st line:
if [ -d $dir ]; then
  rm -r $dir
fi

# another form of if-tests:
if test -d $dir; then
  rm -r $dir
fi

# and a shortcut:
[ -d $dir ] && rm -r $dir
test -d $dir && rm -r $dir
```

Writing an input file

'Here document' for multi-line output:

```
# write to $case.i the lines that appear between
# the EOF symbols:

cat > $case.i <<EOF
        $m
        $b
        $c
        $func
        $A
        $w
        $y0
        $tstop
        $dt
EOF
```

Running the simulation

- Stand-alone programs can be run by just typing the name of the program
- If the program reads data from standard input, we can put the input in a file and *redirect input*:

```
oscillator < $case.i
```

- Can check for successful execution:

```
# the shell variable $? is 0 if last command
# was successful, otherwise $? != 0

if [ "$?" != "0" ]; then
  echo "running oscillator failed"; exit 1
fi

# exit n sets $? to n
```

Remark (1)

- Variables can in Bash be integers, strings or arrays
- For safety, declare the type of a variable if it is not a string:

```
declare -i i   # i is an integer
declare -a A   # A is an array
```

Remark (2)

- Comparison of two integers use a syntax different comparison of two strings:

```
if [ $i -lt 10 ]; then          # integer comparison
if [ "$name" == "10" ]; then    # string  comparison
```

- Unless you have declared a variable to be an integer, assume that all variables are strings and use double quotes (strings) when comparing variables in an if test

```
if [ "$?" != "0" ]; then  # this is safe
if [  $?  !=  0  ]; then  # might be unsafe
```

Making plots

- Make Gnuplot script:

```
echo "set title '$case: m=$m ...'" > $case.gnuplot
...
# contiune writing with a here document:
cat >> $case.gnuplot <<EOF
set size ratio 0.3 1.5, 1.0;
...
plot 'sim.dat' title 'y(t)' with lines;
...
EOF
```

- Run Gnuplot:

```
gnuplot -geometry 800x200 -persist $case.gnuplot
if [ "$?" != "0" ]; then
  echo "running gnuplot failed"; exit 1
fi
```

Some common tasks in Bash

- file writing
- for-loops
- running an application
- pipes
- writing functions
- file globbing, testing file types
- copying and renaming files, creating and moving to directories, creating directory paths, removing files and directories
- directory tree traversal
- packing directory trees

File writing

```
outfilename="myprog2.cpp"

# append multi-line text (here document):
cat >> $filename <<EOF
/*
  This file, "$outfilename", is a version
  of "$infilename" where each line is numbered.
*/
EOF

# other applications of cat:
cat myfile                # write myfile to the screen
cat myfile >  yourfile # write myfile to yourfile
cat myfile >> yourfile # append myfile to yourfile
cat myfile | wc           # send myfile as input to wc
```

For-loops

- The for element in list construction:

```
files=`/bin/ls *.tmp`
# we use /bin/ls in case ls is aliased

for file in $files
do
  echo removing $file
  rm -f $file
done
```

- Traverse command-line arguments:

```
for arg; do
  # do something with $arg
done

# or full syntax; command-line args are stored in $@
for arg in $@; do
  # do something with $arg
done
```

Counters

- Declare an integer counter:

```
declare -i counter
counter=0
# arithmetic expressions must appear inside (( ))
((counter++))
echo $counter  # yields 1
```

- For-loop with counter:

```
declare -i n; n=1
for arg in $@; do
  echo "command-line argument no. $n is <$arg>"
  ((n++))
done
```

C-style for-loops

```
declare -i i
for ((i=0; i<$n; i++)); do
  echo $c
done
```

Example: bundle files

- Pack a series of files into one file
- Executing this single file as a Bash script packs out all the individual files again (!)
- Usage:

```
bundle file1 file2 file3 > onefile  # pack
bash onefile # unpack
```

- Writing `bundle` is easy:

```
#/bin/sh
for i in $@; do
    echo "echo unpacking file $i"
    echo "cat > $i <<EOF"
    cat $i
    echo "EOF"
done
```

The bundle output file

- Consider 2 fake files; file1

```
Hello, World!
No sine computations today
```

  and file2

```
1.0 2.0 4.0
0.1 0.2 0.4
```

- Running `bundle file1 file2` yields the output

```
echo unpacking file file1
cat > file1 <<EOF
Hello, World!
No sine computations today
EOF
echo unpacking file file2
cat > file2 <<EOF
1.0 2.0 4.0
0.1 0.2 0.4
EOF
```

Running an application

- Running in the foreground:

```
cmd="myprog -c file.1 -p -f -q";
$cmd < my_input_file

# output is directed to the file res
$cmd < my_input_file > res

# process res file by Sed, Awk, Perl or Python
```

- Running in the background:

```
myprog -c file.1 -p -f -q < my_input_file &
```

or stop a foreground job with Ctrl-Z and then type `bg`

Pipes

- Output from one command can be sent as input to another command via a pipe

```
# send files with size to sort -rn
# (reverse numerical sort) to get a list
# of files sorted after their sizes:

/bin/ls -s | sort -r


cat $case.i | oscillator
# is the same as
oscillator < $case.i
```

- Make a new application: sort all files in a directory tree `root`, with the largest files appearing first, and equip the output with paging functionality:

```
du -a root | sort -rn | less
```

Numerical expressions

Numerical expressions can be evaluated using bc:

```
echo "s(1.2)" | bc -l  # the sine of 1.2
# -l loads the math library for bc

echo "e(1.2) + c(0)" | bc -l  # exp(1.2)+cos(0)

# assignment:
s=‘echo "s($r)" | bc -l‘

# or using Perl:
s=‘perl -e "print sin($r)"‘
```

Functions

```
# compute x^5*exp(-x) if x>0, else 0 :

function calc() {
   echo "
   if ( $1 >= 0.0 ) {
      ($1)^5*e(-($1))
   } else {
      0.0
   } " | bc -l
}

# function arguments: $1 $2 $3 and so on
# return value: last statement

# call:
r=4.2
s=‘calc $r‘
```

Another function example

```
#!/bin/bash

function statistics {
  avg=0; n=0
  for i in $@; do
    avg=‘echo $avg + $i | bc -l‘
    n=‘echo $n + 1 | bc -l‘
  done
  avg=‘echo $avg/$n | bc -l‘

  max=$1; min=$1; shift;
  for i in $@; do
    if [ ‘echo "$i < $min" | bc -l‘ != 0 ]; then
      min=$i; fi
    if [ ‘echo "$i > $max" | bc -l‘ != 0 ]; then
      max=$i; fi
  done
  printf "%.3f %g %g\n" $avg $min $max
}
```

Calling the function

```
statistics 1.2 6 -998.1 1 0.1

# statistics returns a list of numbers
res=‘statistics 1.2 6 -998.1 1 0.1‘

for r in $res; do echo "result=$r"; done

echo "average, min and max = $res"
```

File globbing

- List all .ps and .gif files using wildcard notation:

```
files=`ls *.ps *.gif`

# or safer, if you have aliased ls:
files=`/bin/ls *.ps *.gif`

# compress and move the files:
gzip $files
for file in $files; do
  mv ${file}.gz $HOME/images
```

Testing file types

```
if [ -f $myfile ]; then
    echo "$myfile is a plain file"
fi

# or equivalently:
if test -f $myfile; then
    echo "$myfile is a plain file"
fi

if [ ! -d $myfile ]; then
    echo "$myfile is NOT a directory"
fi

if [ -x $myfile ]; then
    echo "$myfile is executable"
fi

[ -z $myfile ] && echo "empty file $myfile"
```

Rename, copy and remove files

```
# rename $myfile to tmp.1:
mv $myfile tmp.1

# force renaming:
mv -f $myfile tmp.1

# move a directory tree my tree to $root:
mv mytree $root

# copy myfile to $tmpfile:
cp myfile $tmpfile

# copy a directory tree mytree recursively to $root:
cp -r mytree $root

# remove myfile and all files with suffix .ps:
rm myfile *.ps

# remove a non-empty directory tmp/mydir:
rm -r tmp/mydir
```

Directory management

```
# make directory:
$dir = "mynewdir";
mkdir $mynewdir
mkdir -m 0755 $dir  # readable for all
mkdir -m 0700 $dir  # readable for owner only
mkdir -m 0777 $dir  # all rights for all

# move to $dir
cd $dir
# move to $HOME
cd

# create intermediate directories (the whole path):
mkdirhier $HOME/bash/prosjects/test1
# or with GNU mkdir:
mkdir -p  $HOME/bash/prosjects/test1
```

The find command

Very useful command!

- `find` visits all files in a directory tree and can execute one or more commands for every file
- Basic example: find the `oscillator` codes

```
find $scripting/src -name 'oscillator*' -print
```

- Or find all PostScript files

```
find $HOME \( -name '*.ps' -o -name '*.eps' \) -print
```

- We can also run a command for each file:

```
find rootdir -name filenamespec -exec command {} \; -print
# {} is the current filename
```

Applications of find (1)

- Find all files larger than 2000 blocks a 512 bytes (=1Mb):

```
find $HOME -name '*' -type f -size +2000 -exec ls -s {} \;
```

- Remove all these files:

```
find $HOME -name '*' -type f -size +2000 \
     -exec ls -s {} \; -exec rm -f {} \;
```

or ask the user for permission to remove:

```
find $HOME -name '*' -type f -size +2000 \
     -exec ls -s {} \; -ok rm -f {} \;
```

Applications of find (2)

- Find all files not being accessed for the last 90 days:

  ```
  find $HOME -name '*' -atime +90 -print
  ```

  and move these to /tmp/trash:

  ```
  find $HOME -name '*' -atime +90 -print \
       -exec mv -f {} /tmp/trash \;
  ```

- Note: this one does seemingly nothing...

  ```
  find ~hpl/projects -name '*.tex'
  ```

  because it lacks the `-print` option for printing the name of all *.tex files (common mistake)

Tar and gzip

- The `tar` command can pack single files or all files in a directory tree into one file, which can be unpacked later

  ```
  tar -cvf myfiles.tar mytree file1 file2

  # options:
  # c: pack, v: list name of files, f: pack into file

  # unpack the mytree tree and the files file1 and file2:
  tar -xvf myfiles.tar

  # options:
  # x: extract (unpack)
  ```

- The tarfile can be compressed:

  ```
  gzip mytar.tar

  # result: mytar.tar.gz
  ```

Two find/tar/gzip examples

- Pack all PostScript figures:

```
tar -cvf ps.tar `find $HOME -name '*.ps' -print`
gzip ps.tar
```

- Pack a directory but remove CVS directories and redundant files

```
# take a copy of the original directory:
cp -r myhacks /tmp/oblig1-hpl
# remove CVS directories
find /tmp/oblig1-hpl -name CVS -print -exec rm -rf {} \;
# remove redundant files:
find /tmp/oblig1-hpl \( -name '*~' -o -name '*.bak' \
 -o -name '*.log' \) -print -exec rm -f {} \;
# pack files:
tar -cf oblig1-hpl.tar /tmp/tar/oblig1-hpl.tar
gzip oblig1-hpl.tar
# send oblig1-hpl.tar.gz as mail attachment
```

Advanced Python

Contents

- Subclassing built-in types
  (Ex: dictionary with default values, list with elements of only one type)
- Assignment vs. copy; deep vs. shallow copy
  (in-place modifications, mutable vs. immutable types)
- Iterators and generators
- Building dynamic class interfaces (at run time)
- Inspecting classes and modules (`dir`)

More info

- Ch. 8.5 in the course book
- copy module (Python Library Reference)
- Python in a Nutshell

Determining a variable's type (1)

- Different ways of testing if an object a is a list:

```
if isinstance(a, list):
    ...
if type(a) == type([]):
    ...
import types
if type(a) == types.ListType:
    ...
```

- `isinstance` is the recommended standard
- `isinstance` works for subclasses:

```
isinstance(a, MyClass)
```

  is true if a is an instance of a class that is a subclass of `MyClass`

Determining a variable's type (2)

- Can test for more than one type:

```
if isinstance(a, (list, tuple)):
    ...
```

or test if `a` belongs to a class of types:

```
import operator
if operator.isSequenceType(a):
    ...
```

A sequence type allows indexing and for-loop iteration (e.g.: tuple, list, string, NumPy array)

Subclassing built-in types

- One can easily modify the behaviour of a built-in type, like list, tuple, dictionary, NumPy array, by subclassing the type
- Old Python: `UserList`, `UserDict`, `UserArray` (in Numeric) are special base-classes
- Now: the types `list`, `tuple`, `dict`, `NumArray` (in numarray) can be used as base classes
- Examples:
  1. dictionary with default values
  2. list with items of one type

Dictionaries with default values

- Goal: if a key does not exist, return a default value

```
>>> d = defaultdict(0)
>>> d[4] = 2.2   # assign
>>> d[4]
2.2000000000000002
>>> d[6]         # non-existing key, return default
0
```

- Implementation:

```
class defaultdict(dict):
    def __init__(self, default_value):
        self.default = default_value
        dict.__init__(self)

    def __getitem__(self, key):
        return self.get(key, self.default)

    def __delitem__(self, key):
        if self.has_key(key):  dict.__delitem__(self, key)
```

List with items of one type

- Goal: raise exception if a list element is not of the same type as the first element
- Implementation:

```
class typedlist(list):
    def __init__(self, somelist=[]):
        list.__init__(self, somelist)
        for item in self:
            self._check(item)

    def _check(self, item):
        if len(self) > 0:
            item0class = self.__getitem__(0).__class__
            if not isinstance(item, item0class):
                raise TypeError, 'items must be %s, not %s' \
                % (item0class.__name__, item.__class__.__name_
```

Class typedlist cont.

- Need to call `_check` in all methods that modify the list
- What are these methods?

```
>>> dir([])  # get a list of all list object functions
['__add__', ..., '__iadd__', ..., '__setitem__',
 '__setslice__', ..., 'append', 'extend', 'insert', ...]
```

- Idea: call `_check`, then call similar function in base class `list`

Class typedlist; modification methods

```
def __setitem__(self, i, item):
    self._check(item); list.__setitem__(self, i, item)

def append(self, item):
    self._check(item); list.append(self, item)

def insert(self, index, item):
    self._check(item); list.insert(self, index, item)

def __add__(self, other):
    return typedlist(list.__add__(self, other))

def __iadd__(self, other):
    return typedlist(list.__iadd__(self, other))

def __setslice__(self, slice, somelist):
    for item in somelist:  self._check(item)
    list.__setslice__(self, slice, somelist)

def extend(self, somelist):
    for item in somelist:  self._check(item)
    list.extend(self, somelist)
```

Using typedlist objects

```
>>> from typedlist import typedlist
>>> q = typedlist((1,4,3,2))  # integer items
>>> q = q + [9,2,3]           # add more integer items
>>> q
[1, 4, 3, 2, 9, 2, 3]
>>> q += [9.9,2,3]            # oops, a float...
Traceback (most recent call last):
...
TypeError: items must be int, not float

>>> class A:
        pass
>>> class B:
        pass
>>> q = typedlist()
>>> q.append(A())
>>> q.append(B())
Traceback (most recent call last):
...
TypeError: items must be A, not B
```

Copy and assignment

- What actually happens in an assignment b=a?
- Python objects act as references, so b=a makes a reference b pointing to the same object as a refers to
- *In-place* changes in a will be reflected in b
- What if we want b to become a copy of a?

Examples of assignment; numbers

```
>>> 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
```

Examples of assignment; lists

```
>>> 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
```

Examples of assignment; dicts

```
>>> a = {'q': 6, 'error': None}
>>> b = a
>>> a['r'] = 2.5
>>> a
{'q': 6, 'r': 2.5, 'error': None}
>>> a is b
True
>>> a = 'a string'   # make a refer to a new (string) object
>>> b                # new contents in a do not affect b
{'q': 6, 'r': 2.5, 'error': None}
```

Copying objects

- 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

The copy module

- The copy module allows a deep or shallow copy of an object
- Deep copy: copy everything to the new object
- Shallow copy: let the new (copy) object have references to attributes in the copied object
- Usage:

```
b_assign  = a                     # assignment (make reference)
b_shallow = copy.copy(a)          # shallow copy
b_deep    = copy.deepcopy(a)      # deep copy
```

Examples on copy (1)

- Test class:

```
class A:
    def __init__(self, value=None):
        self.x = x
    def __repr__(self):
        return 'x=%s' % self.x
```

- Session:

```
>>> a = A(-99)                          # make instance a
>>> b_assign  = a                       # assignment
>>> b_shallow = copy.copy(a)            # shallow copy
>>> b_deep    = copy.deepcopy(a)        # deep copy
>>> a.x = 9                             # let's change a!
>>> print 'a.x=%s, b_assign.x=%s, b_shallow.x=%s, b_deep.x=%s' %\
          (a.x, b_assign.x, b_shallow.x, b_deep.x)
a.x=9, b_assign.x=9, b_shallow.x=-99, b_deep.x=-99
```

shallow refers the original `a.x`, deep holds a copy of `a.x`

Examples on copy (2)

- Let a have a mutable object (list here), allowing in-place modifications

```
>>> a = A([-2,3])
>>> b_assign  = a
>>> b_shallow = copy.copy(a)
>>> b_deep    = copy.deepcopy(a)
>>> a.x[0] = 8  # in-place modification
>>> print 'a.x=%s, b_assign.x=%s, b_shallow.x=%s, b_deep.x=%s'
    % (a.x, b_assign.x, b_shallow.x, b_deep.x)
a.x=[8,3], b_assign.x=[8,3], b_shallow.x=[8,3], b_deep.x=[-2,3
```

shallow refers the original object and reflects in-place changes, deep holds a copy

Examples on copy (3)

- Increase complexity: a holds a heterogeneous list

```
>>> a = [4,3,5,['some string',2], A(-9)]
>>> b_assign  = a
>>> b_shallow = copy.copy(a)
>>> b_deep    = copy.deepcopy(a)
>>> b_slice   = a[0:5]
>>> a[3] = 999; a[4].x = -6
>>> print 'b_assign=%s\nb_shallow=%s\nb_deep=%s\nb_slice=%s' %
          (b_assign, b_shallow, b_deep, b_slice)
b_assign=[4, 3, 5, 999, x=-6]
b_shallow=[4, 3, 5, ['some string', 2], x=-6]
b_deep=[4, 3, 5, ['some string', 2], x=-9]
b_slice=[4, 3, 5, ['some string', 2], x=-6]
```

Generating code at run time

- With `exec` and `eval` we can generate code at run time
- `eval` evaluates expressions given as text:

```
x = 3.2
e = 'x**2 + sin(x)'
v = eval(e)                          # evaluate an expression
v = x**2 + sin(x)                    # equivalent to the previous line
```

- `exec` executes arbitrary text as Python code:

```
s = 'v = x**2 + sin(x)'  # complete statement stored in a stri
exec s                   # run code in s
```

- `eval` and `exec` are recommended to be run in user-controlled namespaces

Fancy application

- Consider an input file with this format:

```
set heat conduction = 5.0
set dt = 0.1
set rootfinder = bisection
set source = V*exp(-q*t) is function of (t) with V=0.1, q=1
set bc = sin(x)*sin(y)*exp(-0.1*t) is function of (x,y,t)
```

  (last two lines specifies a `StringFunction` object)

- Goal: convert this text to Python data for further processing

```
heat_conduction, dt : float variables
rootfinder          : string
source, bc          : StringFunction instances
```

- Means: regular expressions, string operations, `StringFunction`, `exec`, `eval`

Implementation (1)

```
# target line:
# set some name of variable = some value
from scitools import misc

def parse_file(somefile):
    namespace = {}    # holds all new created variables
    line_re = re.compile(r'set (.*?)=(.*)$')
    for line in somefile:
        m = line_re.search(line)
        if m:
            variable = m.group(1).strip()
            value = m.group(2).strip()
            # test if value is a StringFunction specification:
            if value.find('is function of') >= 0:
                # interpret function specification:
                value = eval(string_function_parser(value))
            else:
                value = misc.str2obj(value)  # string -> object
            # space in variables names is illegal
            variable = variable.replace(' ', '_')
            code = 'namespace["%s"] = value' % variable
            exec code
    return namespace
```

Implementation (2)

```
# target line (with parameters A and q):
# expression is a function of (x,y) with A=1, q=2
# or (no parameters)
# expression is a function of (t)

def string_function_parser(text):
    m = re.search(r'(.*) is function of \((.*)\)( with .+)?', text
    if m:
        expr = m.group(1).strip();  args = m.group(2).strip()
        # the 3rd group is optional:
        prms = m.group(3)
        if prms is None:  # the 3rd group is optional
            prms = ''     # works fine below
        else:
            prms = ''.join(prms.split()[1:])  # strip off 'with'

        # quote arguments:
        args = ', '.join(["'%s'" % v for v in args.split(',')])
        if args.find(',') < 0:  # single argument?
            args = args + ','   # add comma in tuple
        args = '(' + args + ')' # tuple needs parenthesis

        s = "StringFunction('%s', independent_variables=%s, %s)" %
            (expr, args, prms)
        return s
```

Testing the general solution

```
>>> import somemod
>>> newvars = somemod.parse_file(testfile)
>>> globals().update(newvars)  # let new variables become global
>>> heat_conduction, type(heat_conduction)
(5.0, <type 'float'>)
>>> dt, type(dt)
(0.10000000000000001, <type 'float'>)
>>> rootfinder, type(rootfinder)
('bisection', <type 'str'>)
>>> source, type(source)
(StringFunction('V*exp(-q*t)', independent_variables=('t',),
 q=1, V=0.10000000000000001), <type 'instance'>)
>>> bc, type(bc)
(StringFunction('sin(x)*sin(y)*exp(-0.1*t)',
 independent_variables=('x', 'y', 't'), ), <type 'instance'>)
>>> source(1.22)
0.029523016692401424
>>> bc(3.14159, 0.1, 0.001)
2.6489044508054893e-07
```

Iterators

- Typical Python `for` loop,

  ```
  for item in some_sequence:
      # process item
  ```

  allows *iterating* over any object `some_sequence` that supports such iterations
- Most built-in types offer iterators
- User-defined classes can also implement iterators

Iterating with built-in types

```
for element in some_list:

for element in some_tuple:

for s in some_NumPy_array:  # iterates over first index

for key in some_dictionary:

for line in file_object:

for character in some_string:
```

Iterating with user-defined types

- Implement `__iter__`, returning an iterator object (can be `self`) containing a `next` function
- Implement `next` for returning the next element in the iteration sequence, or raise `StopIteration` if beyond the last element

Example using iterator object

```
class MySeq:
    def __init__(self, *data):
        self.data = data

    def __iter__(self):
        return MySeqIterator(self.data)

# iterator object:
class MySeqIterator:
    def __init__(self, data):
        self.index = 0
        self.data = data

    def next(self):
        if self.index < len(self.data):
            item = self.data[self.index]
            self.index += 1  # ready for next call
            return item
        else:  # out of bounds
            raise StopIteration
```

Example without separate iterator object

```
class MySeq2:
    def __init__(self, *data):
        self.data = data

    def __iter__(self):
        self.index = 0
        return self

    def next(self):
        if self.index < len(self.data):
            item = self.data[self.index]
            self.index += 1  # ready for next call
            return item
        else:  # out of bounds
            raise StopIteration
```

Example on application

- Use iterator:

```
>>> obj = MySeq(1, 9, 3, 4)
>>> for item in obj:
        print item,
1 9 3 4
```

- Write out as complete code:

```
obj = MySeq(1, 9, 3, 4)
iterator = iter(obj)   # iter(obj) means obj.__iter__()
while True:
    try:
        item = iterator.next()
    except StopIteration:
        break
    # process item:
    print item
```

Remark

- Could omit the iterator in this sample class and just write

  ```
  for item in obj.data:
      print item
  ```

  since the `self.data` list already has an iterator...

A more comprehensive example

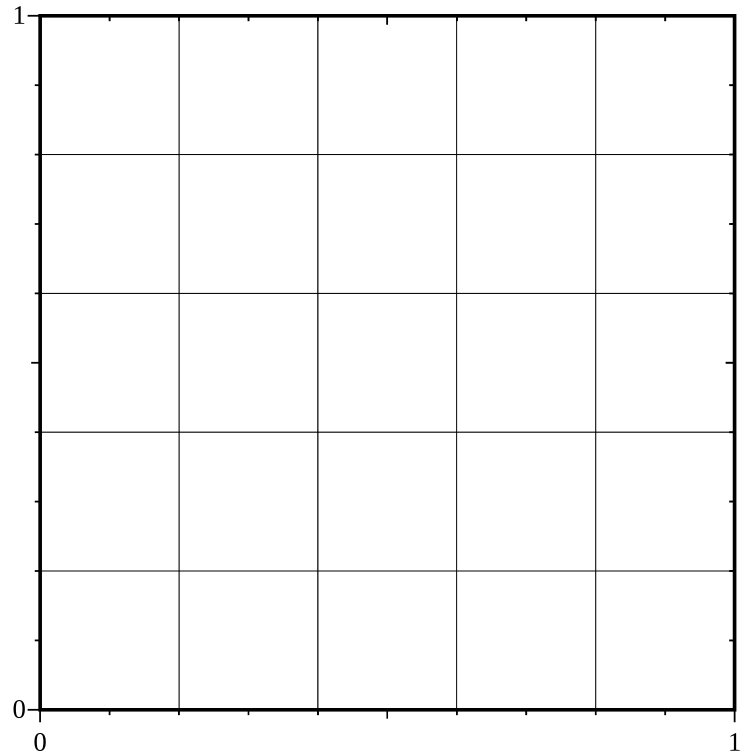
- Consider class `Grid2D` for uniform, rectangular 2D grids:

```
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, Float)
        self.ycoor = sequence(ymin, ymax, dy, Float)

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

- Make iterators for internal points, boundary points, and corner points (useful for finite difference methods on such grids)

A uniform rectangular 2D grid



Potential sample code

```
# this is what we would like to do:

for i, j in grid.interior():
    <process interior point with index (i,j)>

for i, j in grid.boundary():
    <process boundary point with index (i,j)>

for i, j in grid.corners():
    <process corner point with index (i,j)>

for i, j in grid.all():  # visit all points
    <process grid point with index (i,j)>
```

Implementation overview

- Derive a subclass `Grid2Dit` equipped with iterators
- Let `Grid2Dit` be its own iterator (for convenience)
- `interior`, `boundary`, `corners` must set an indicator for the type of desired iteration
- `__iter__` initializes the two iteration indices (i,j) and returns `self`
- `next` must check the iteration type (interior, boundary, corners) and call an appropriate method
- `_next_interior`, `_next_boundary`, `_next_corners`, find next (i,j) index pairs or raise `StopIteration`
- We also add a possibility to iterate over all points (easy)

Implementation; interior points

```
# iterator domains:
INTERIOR=0; BOUNDARY=1; CORNERS=2; ALL=3

class Grid2Dit(Grid2D):
    def interior(self):
        self._iterator_domain = INTERIOR
        return self

    def __iter__(self):
        if self._iterator_domain == INTERIOR:
            self._i = 1; self._j = 1
        return self

    def _next_interior(self):
        if self._i >= len(self.xcoor)-1:
            self._i = 1;  self._j += 1  # start on a new row
        if self._j >= len(self.ycoor)-1:
            raise StopIteration # end of last row
        item = (self._i, self._j)
        self._i += 1  #  walk along rows...
        return item

    def next(self):
        if self._iterator_domain == INTERIOR:
            return self._next_interior()
```

Application; interior points

```
>>> # make a grid with 3x3 points:
>>> g = Grid2Dit(dx=1.0, dy=1.0, xmin=0, xmax=2.0, ymin=0, ymax=2.
>>> for i, j in g.interior():
        print g.xcoor[i], g.ycoor[j]
1.0 1.0
```

Correct (only one interior point!)

Implementation; boundary points (1)

```
# boundary parts:
RIGHT=0; UPPER=1; LEFT=2; LOWER=3

class Grid2Dit(Grid2D):
    ...
    def boundary(self):
        self._iterator_domain = BOUNDARY
        return self

    def __iter__(self):
        ...
        elif self._iterator_domain == BOUNDARY:
            self._i = len(self.xcoor)-1; self._j = 1
            self._boundary_part = RIGHT
        ...
        return self

    def next(self):
        ...
        elif self._iterator_domain == BOUNDARY:
            return self._next_boundary()
        ...
```

Implementation; boundary points (1)

```
def _next_boundary(self):
    """Return the next boundary point."""
    if self._boundary_part == RIGHT:
        if self._j < len(self.ycoor)-1:
            item = (self._i, self._j)
            self._j += 1  # move upwards
        else: # switch to next boundary part:
            self._boundary_part = UPPER
            self._i = 1;  self._j = len(self.ycoor)-1
    if self._boundary_part == UPPER:
        ...
    if self._boundary_part == LEFT:
        ...
    if self._boundary_part == LOWER:
        if self._i < len(self.xcoor)-1:
            item = (self._i, self._j)
            self._i += 1  # move to the right
        else: # end of (interior) boundary points:
            raise StopIteration
    if self._boundary_part == LOWER:
        ...
    return item
```

Application; boundary points

```
>>> g = Grid2Dit(dx=1.0, dy=1.0, xmax=2.0, ymax=2.0)
>>> for i, j in g.boundary():
        print g.xcoor[i], g.ycoor[j]
2.0 1.0
1.0 2.0
0.0 1.0
1.0 0.0
```

(i.e., one boundary point at the middle of each side)

A vectorized grid iterator

- The one-point-at-a-time iterator shown is slow for large grids
- A faster alternative is to generate index slices (ready for use in arrays)

```
grid = Grid2Ditv(dx=1.0, dy=1.0, xmax=2.0, ymax=2.0)
```

```
grid = Grid2Ditv(dx=1.0, dy=1.0, xmax=2.0, ymax=2.0)

for imin,imax, jmin,jmax in grid.interior():
    # yields slice (1:2,1:2)

for imin,imax, jmin,jmax in grid.boundary():
    # yields slices (2:3,1:2) (1:2,2:3) (0:1,1:2) (1:2,0:1)

for imin,imax, jmin,jmax in grid.corners():
    # yields slices (0:1,0:1) (2:3,0:1) (2:3,2:3) (0:1,2:3)
```

Typical application

2D diffusion equation (finite difference method):

```
for imin,imax, jmin,jmax in grid.interior():
    u[imin:imax, jmin:jmax] = \
      u[imin:imax, jmin:jmax] + h*(
      u[imin:imax, jmin-1:jmax-1] - 2*u[imin:imax, jmin:jmax] + \
      u[imin:imax, jmin+1:jmax+1] + \
      u[imin-1:imax-1, jmin:jmax] - 2*u[imin:imax, jmin:jmax] + \
      u[imin+1:imax+1, jmin:jmax])

for imin,imax, jmin,jmax in grid.boundary():
    u[imin:imax, jmin:jmax] = \
      u[imin:imax, jmin:jmax] + h*(
      u[imin:imax, jmin-1:jmax-1] - 2*u[imin:imax, jmin:jmax] + \
      u[imin:imax, jmin+1:jmax+1] + \
      u[imin-1:imax-1, jmin:jmax] - 2*u[imin:imax, jmin:jmax] + \
      u[imin+1:imax+1, jmin:jmax])
```

Implementation (1)

```
class Grid2Ditv(Grid2Dit):
    """Vectorized version of Grid2Dit."""
    def __iter__(self):
        nx = len(self.xcoor)-1;  ny = len(self.ycoor)-1
        if self._iterator_domain == INTERIOR:
            self._indices = [(1,nx, 1,ny)]
        elif self._iterator_domain == BOUNDARY:
            self._indices = [(nx,nx+1, 1,ny),
                             (1,nx, ny,ny+1),
                             (0,1, 1,ny),
                             (1,nx, 0,1)]
        elif self._iterator_domain == CORNERS:
            self._indices = [(0,1, 0,1),
                             (nx, nx+1, 0,1),
                             (nx,nx+1, ny,ny+1),
                             (0,1, ny,ny+1)]
        elif self._iterator_domain == ALL:
            self._indices = [(0,nx+1, 0,ny+1)]
        self._indices_index = 0
        return self
```

Implementation (2)

```
class Grid2Ditv(Grid2Dit):
    ...
    def next(self):
        if self._indices_index <= len(self._indices)-1:
            item = self._indices[self._indices_index]
            self._indices_index += 1
            return item
        else:
            raise StopIteration
```

Generators

- Generators enable writing iterators in terms of a single function (no `__iter__` and `next` methods)

```
for item in some_func(some_arg1, some_arg2):
    # process item
```

- The generator implements a loop and jumps for each element back to the calling code with a return-like `yield` statement

```
class MySeq3:
    def __init__(self, *data):
        self.data = data

def items(obj):                                    # generator
    for item in obj.data:
        yield item

for item in items(obj):                            # use generator
    print item
```

Generator-list relation

- A generator can also be implemented as a standard function returning a list
- Generator:

```
def mygenerator(...):
    ...
    for i in some_object:
        yield i
```

- Implemented as standard function returning a list:

```
def mygenerator(...):
    ...
    return [i for i in some_object]
```

- The usage is the same:

```
for i in mygenerator(...):
    # process i
```

Generators as short cut for iterators

- Consider our `MySeq` and `MySeq2` classes with iterators
- With a generator we can implement exactly the same functionality very compactly:

```
class MySeq4:
    def __init__(self, *data):
        self.data = data

    def __iter__(self):
        for item in obj.data:
            yield item

obj = MySeq4(1,2,3,4,6,1)
for item in obj:
    print item
```

Exercise

- Implement a sparse vector (most elements are zeros and not stored; use a dictionary for storage with integer keys (element no.))
- Functionality:

```
>>> a = SparseVec(4)
>>> a[2] = 9.2
>>> a[0] = -1
>>> print a
[0]=-1 [1]=0 [2]=9.2 [3]=0
>>> print a.nonzeros()
{0: -1, 2: 9.2}
```

Exercise cont.

```
>>> b = SparseVec(5)
>>> b[1] = 1
>>> print b
[0]=0 [1]=1 [2]=0 [3]=0 [4]=0
>>> print b.nonzeros()
{1: 1}
>>> c = a + b
>>> print c
[0]=-1 [1]=1 [2]=9.2 [3]=0 [4]=0
>>> print c.nonzeros()
{0: -1, 1: 1, 2: 9.2}
>>> for ai, i in a:  # SparseVec iterator
        print 'a[%d]=%g ' % (i, ai),
a[0]=-1  a[1]=0  a[2]=9.2  a[3]=0
```

Inspecting class interfaces

- What type of attributes and methods are available in this object `s`?
- Use `dir(s)`!

```
>>> dir(()) # what's in a tuple?
['__add__', '__class__', '__contains__', ...
 '__repr__', '__rmul__', '__setattr__', '__str__']
>>> # try some user-defined object:
>>> class A:
        def __init__(self):
                self.a = 1
                self.b = 'some string'
        def method1(self, c):
                self.c = c

>>> a = A()
>>> dir(a)
['__doc__', '__init__', '__module__', 'a', 'b', 'method1']
```

Dynamic class interfaces

- Dynamic languages (like Python) allows adding attributes to instances at run time
- Advantage: can tailor iterfaces according to input data
- Simplest use: mimic C structs by classes

```
>>> class G: pass  # completely empty class

>>> g = G()        # instance with no data (almost)
>>> dir(g)
['__doc__', '__module__']  # no user-defined attributes

>>> # add instance attributes:
>>> g.xmin=0; g.xmax=4; g.ymin=0; g.ymax=1
>>> g.xmax
4
```

Generating properties

- Adding a property to some class A:

```
A.x = property(fget=lambda self: self._x) # grab A's _x attrib
```

(“`self`” is supplied as first parameter)

- Example: a 1D/2D/3D point class, implemented as a NumPy array (with all built-in stuff), but with attributes (properties) `x`, `y`, `z` for convenient extraction of coordinates

```
>>> p1 = Point((0,1)); p2 = Point((1,2))
>>> p3 = p1 + p2
>>> p3
[ 1.  3.]
>>> p3.x, p3.y
(1.0, 3.0)
>>> p3.z # should raise an exception
Traceback (most recent call last):
...
AttributeError: 'NumArray' object has no attribute 'z'
```

Implementation

Must use numarray or numpy version of NumPy (where the array is an instance of a class such that we can add new class attributes):

```
class Point(object):
    """Extend NumPy array objects with properties."""
    def __new__(self, point):
        # __new__ is a constructor in new-style classes,
        # but can return an object of any type (!)

        a = array(point, Float)

        # define read-only attributes x, y, and z:
        if len(point) >= 1:
            NumArray.x = property(fget=lambda o: o[0])
            # or a.__class__.x = property(fget=lambda o: o[0])
        if len(point) >= 2:
            NumArray.y = property(fget=lambda o: o[1])
        if len(point) == 3:
            NumArray.z = property(fget=lambda o: o[2])
        return a
```

Note

- Making a `Point` instance actually makes a NumArray instance with extra data
- In addition it has read-only attributes `x`, `y` and `z`, depending on the no of dimensions in the initialization

```
>>> p = Point((1.1,))  # 1D point
>>> p.x
1.1
>>> p.y
Traceback (most recent call last):
...
AttributeError: 'NumArray' object has no attribute 'y'
```

- Can be done in C++ with advanced template meta programming

Automatic generation of properties

- Suppose we have a set of non-public attributes for which we would like to generate read-only properties
- Three lines of code are enough:

```
for v in variables:
    exec('%s.%s = property(fget=lambda self: self._%s' % \
         (self.__class__.__name__, v, v))
```

- Application: list the variable names as strings and collect in list/tuple:

```
variables = ('counter', 'nx, 'x', 'help', 'coor')
```

- This gives read-only property `self.counter` returning the value of non-public attribute `self._counter` (initialized elsewhere), etc.

Adding a new method on the fly: setattr

- That A class should have a method hw!
- Add it on the fly, if you need it:

```
>>> class A:
        pass

>>> def hw(self, r, file=sys.stdout):
        file.write('Hi! sin(%g)=%g')

>>> def func_to_method(func, class_, method_name=None):
        setattr(class_, method_name or func.__name__, func)

>>> func_to_method(hw, A)  # add hw as method in class A
>>> a = A()
>>> dir(a)
['__doc__', '__module__', 'hw']
>>> a.hw(1.2)
'Hi! sin(1.2)=0.932039'
```

Adding a new method: subclassing

- We can also subclass to add a new method:

```
class B(A):
    def hw(self, r, file=sys.stdout):
        file.write('Hi! sin(%g)=%g' % (r,math.sin(r)))
```

- Sometimes you want to extend a class with methods *without changing the class name*:

```
from A import A as A_old   # import class A from module fi
class A(A_old):
    def hw(self, r, file=sys.stdout):
        file.write('Hi! sin(%g)=%g' % (r,math.sin(r)))
```

- The new A class is now a subclass of the old A class, but for users it looks like the original class was extended
- With this technique you can extend libraries without touching the original source code and without introducing new subclass names

Adding another class' method as new method (1)

- Suppose we have a module file `A.py` with

```
class A:
    def __init__(self):
        self.v = 'a'
    def func1(self, x):
        print '%s.%s, self.v=%s' % (self.__class__.__name__, \
                                    self.func1.__name__, self.
```

- Can we "steel" `A.func1` and attach it as method in another class? Yes, but this new method will not accept instances of the new class as `self` (see next example)

Adding another class' method as new method (2)

```
>>> class B:
...     def __init__(self):
...         self.v = 'b'
...     def func2(self, x):
...         print '%s.%s, self.v=%s' % (self.__class__.__name__, \
...                                     self.func2.__name__, self.
>>> import A
>>> a = A.A()
>>> b = B()
>>> print dir(b)
['__doc__', '__init__', '__module__', 'func2', 'v']
>>> b.func2(3)                 # works of course fine
B.func2, self.v=b
>>> setattr(B, 'func1', a.func1)
>>> print dir(b)               # does the created b get a new func1?
['__doc__', '__init__', '__module__', 'func1', 'func2', 'v']
>>> b.func1(3)
A.func1, self.v=a              # note: self is a!
```

Adding another class' method as new method (3)

```
>>> def func3(self, x):         # stand-alone function
...     print '%s.%s, self.v=%s' % (self.__class__.__name__, \
...                             self.func3.__name__, self.v)
...
>>> setattr(B, 'func3', func3)
>>> b.func3(3)                  # function -> method
B.func3, self.v=b
>>>
>>> setattr(B, 'func1', A.A.func1)  # unbound method
>>> print dir(B)
['__doc__', '__init__', '__module__', 'func1', 'func2', 'func3']
>>> b.func1(3)
Traceback (most recent call last):
  File "<input>", line 1, in ?
TypeError: unbound method func1() must be called with A
instance as first argument (got int instance instead)
>>> B.func1(a,3)
A.func1, self.v=a
>>> B.func1(b,3)
Traceback (most recent call last):
  File "<input>", line 1, in ?
TypeError: unbound method func1() must be called with A
instance as first argument (got B instance instead)
```

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 li

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.
      8
----> 9 ifile = open(infilename, 'r')  # open file for reading
     10 lines = ifile.readlines()      # read file into list o
     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
```

Software engineering

Version control systems

Why?

- Can retrieve old versions of files
- Can print history of incremental changes
- Very useful for programming or writing teams
- Contains an official repository
- Programmers work on *copies* of repository files
- Conflicting modifications by different team members are detected
- Can serve as a backup tool as well
- So simple to use that there are no arguments against using version control systems!

Some svn commands

- svn: a modern version control system, with commands much like the older widespread CVS tool
- See `http://www.third-bit.com/swc/www/swc.html`
- Or the course book for a quick introduction
- `svn import/checkout`: start with CVS
- `svn add`: register a new file
- `svn commit`: check files into the repository
- `svn remove`: remove a file
- `svn move`: move/rename a file
- `svn update`: update file tree from repository
- See also `svn help`

Contents

- How to verify that scripts work as expected
- Regression tests
- Regression tests with numerical data
- `doctest` module for doc strings with tests/examples
- Unit tests

More info

- Appendix B.4 in the course book
- `doctest`, `unittest` module documentation

Verifying scripts

How can you know that a script works?

- Create some tests, save (what you think are) the correct results
- Run the tests frequently, compare new results with the old ones
- Evaluate discrepancies
- If new and old results are equal, one believes that the script still works
- This approach is called *regression testing*

The limitation of tests

Program testing can be a very effective way to show the presence of bugs, but is hopelessly inadequate for showing their absence. -Dijkstra, 1972

Three different types of tests

- Regression testing:
  test a complete application ("problem solving")
- Tests embedded in source code (doc string tests):
  test user functionality of a function, class or module
  (Python grabs out interactive tests from doc strings)
- Unit testing:
  test a single method/function or small pieces of code
  (emphasized in Java and extreme programming (XP))

Info: App. B.4 in the course book
doctest and unittest module documentation (Py Lib.Ref.)

Regression testing

- Create a number of tests
- Each test is run as a script
- Each such script writes some key results to a file
- This file must be compared with a previously generated ’exact’ version of the file

A suggested set-up

- Say the name of a script is `myscript`
- Say the name of a test for `myscript` is `test1`
- `test1.verify`: script for testing
- `test1.verify` runs `myscript` and directs/copies important results to `test1.v`
- Reference ('exact') output is in `test1.r`
- Compare `test1.v` with `test1.r`
- The first time `test1.verify` is run, copy `test1.v` to `test1.r` (if the results seem to be correct)

Recursive run of all tests

- Regression test scripts `*.verify` are distributed around in a directory tree
- Go through all files in the directory tree
- If a file has suffix `.verify`, say `test.verify`, execute `test.verify`
- Compare `test.v` with `test.r` and report differences

File comparison

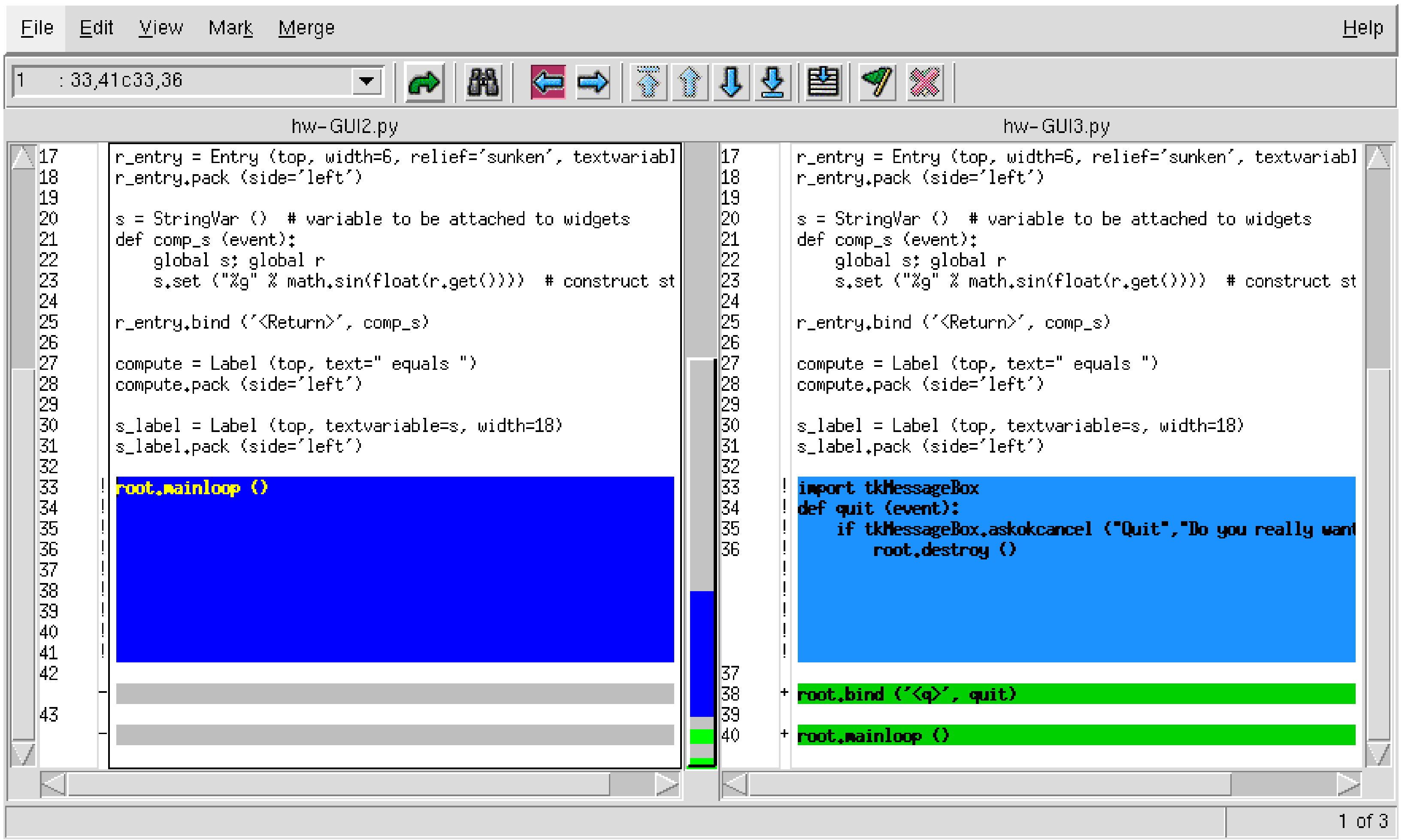
- How can we determine if two (text) files are equal?

  ```
  some_diff_program test1.v test1.r > test1.diff
  ```

- Unix `diff`:
  output is not very easy to read/interpret,
  tied to Unix
- Perl script `diff.pl`:
  easy readable output, but very slow for large files
- Tcl/Tk script `tkdiff.tcl`:
  very readable graphical output
- `gvimdiff` (part of the Vim editor):
  highlights differences in parts of long lines
- Other tools: emacs `ediff`, `diff.py`, `windiff` (Windows only)

tkdiff.tcl

tkdiff.tcl hw-GUI2.py hw-GUI3.py



Example

- We want to write a regression test for src/ex/circle.py (solves equations for circular movement of a body)

  ```
  python circle.py 5 0.1
  ```

  ```
  # 5: no of circular rotations
  # 0.1: time step used in numerical method
  ```

- Output from circle.py:

  ```
  xmin xmax ymin ymax
  x1 y1
  x2 y2
  ...
  end
  ```

  `xmin`, `xmax`, `ymin`, `ymax`: bounding box for all the `x1,y1`, `x2,y2` etc. coordinates

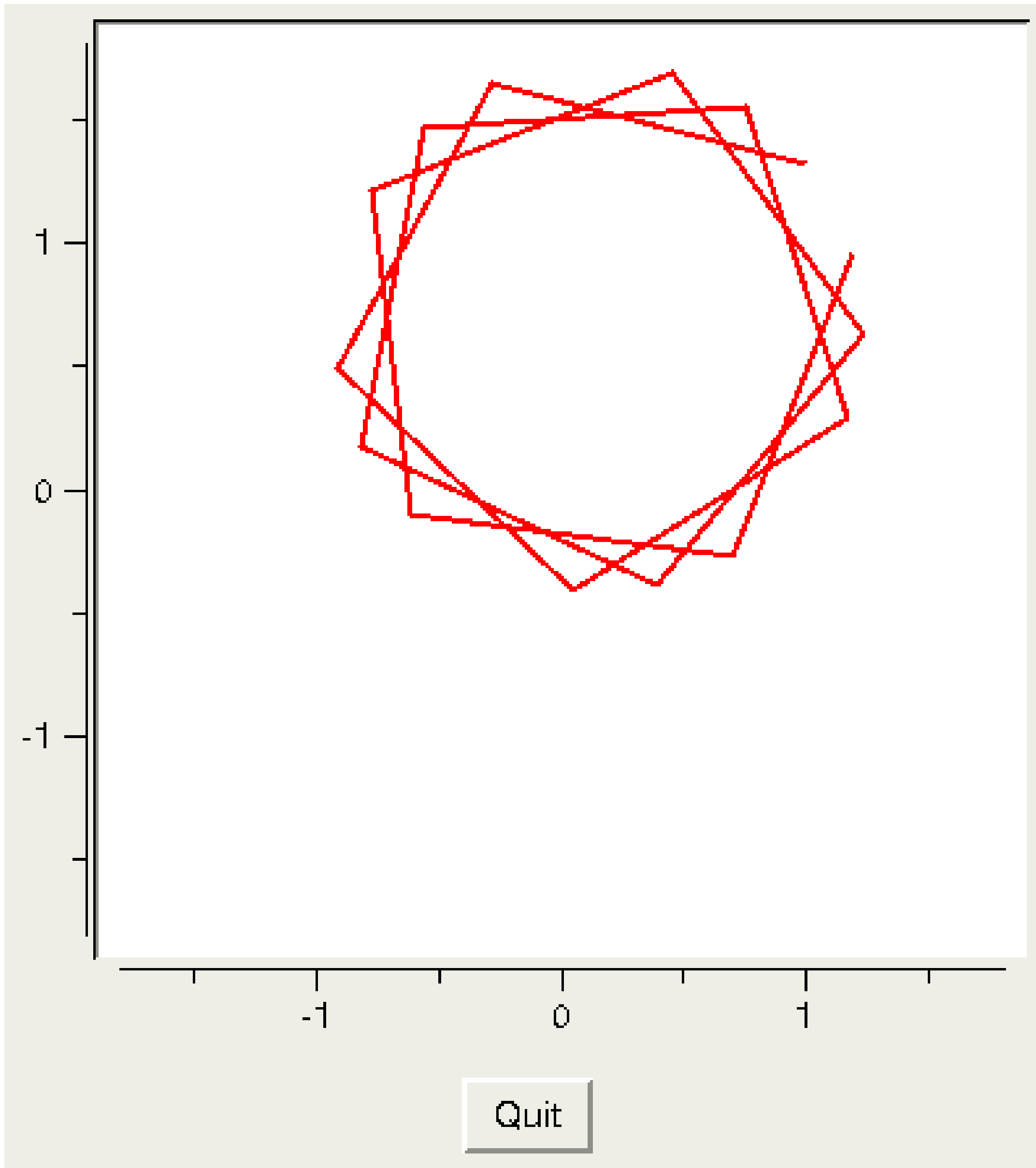
Establishing correct results

- When is the output correct? (for later use as reference)
- Exact result from `circle.py`, `x1,y1`, `x2,y2` etc., are points on a circle
- Numerical approximation errors imply that the points deviate from a circle
- One can get a visual impression of the accuracy of the results from

  ```
  python circle.py 3 0.21 | plotpairs.py
  ```

  Try different time step values!

Plot of approximate circle



Regression test set-up

- Test script: circle.verify
- Simplest version of circle.verify (Bourne shell):

```
#!/bin/sh
./circle.py 3 0.21 > circle.v
```

- Could of course write it in Python as well:

```
#!/usr/bin/env python
import os
os.system("./circle.py 3 0.21 > circle.v")
# or completely cross platform:
os.system(os.path.join(os.curdir,"circle.py") + \
          " 3 0.21 > circle.v")
```

The .v file with key results

- How does `circle.v` look like?

```
-1.8 1.8 -1.8 1.8
1.0 1.31946891451
-0.278015372225 1.64760748997
-0.913674369652 0.491348066081
0.048177073882 -0.411890560708
1.16224152523 0.295116238827
end
```

- If we believe circle.py is working correctly, `circle.v` is copied to `circle.r`
- `circle.r` now contains the reference ('exact') results

Executing the test

- Manual execution of the regression test:

```
./circle.verify
diff.py circle.v circle.r > circle.log
```

- View `circle.log`; if it is empty, the test is ok; if it is non-empty, one must judge the quality of the new results in `circle.v` versus the old ('exact') results in `circle.r`

Automating regression tests

- We have made a Python module Regression for automating regression testing
- `scitools regression` is a script, using the Regression module, for executing all `*.verify` test scripts in a directory tree, run a diff on `*.v` and `*.r` files and report differences in HTML files
- Example:

```
scitools regression verify .
```

  runs all regression tests in the current working directory and all subdirectories

Presentation of results of tests

- Output from the `scitools regression` command are two files:
  - `verify_log.htm`: overview of tests and no of differing lines between `.r` and `.v` files
  - `verify_log_details.htm`: detailed diff
- If all results (`verify_log.htm`) are ok, update latest results (`*.v`) to reference status (`*.r`) in a directory tree:

```
scitools regression update .
```

- The update is important if just changes in the output format have been performed (this may cause large, insignificant differences!)

Running a single test

- One can also run `scitools regression` on a single test (instead of traversing a directory tree):

```
scitools regression verify circle.verify
scitools regression update circle.verify
```

Tools for writing test files

- Our Regression module also has a class `TestRun` for simplifying the writing of robust *.verify scripts
- Example: `mytest.verify`

```
import Regression
test = Regression.TestRun("mytest.v")
# mytest.v is the output file

# run script to be tested (myscript.py):
test.run("myscript.py", options="-g -p 1.0")
# runs myscript.py -g -p 1.0

# append file data.res to mytest.v
test.append("data.res")
```

- Many different options are implemented, see the book

Numerical round-off errors

- Consider `circle.py`, what about numerical round-off errors when the regression test is run on different hardware?

  ```
  -0.16275412    # Linux PC
  -0.16275414    # Sun machine
  ```

  The difference is not significant wrt testing whether circle.py works correctly
- Can easily get a difference between each output line in `circle.v` and `circle.r`
- How can we judge if `circle.py` is really working?
- Answer: try to ignore round-off errors when comparing `circle.v` and `circle.r`

Tools for numeric data

- Class `TestRunNumerics` in the Regression module extends class `TestRun` with functionality for ignoring round-off errors
- Idea: write real numbers with (say) five significant digits only
- `TestRunNumerics` modifies all real numbers in `*.v`, after the file is generated
- Problem: small bugs can arise and remain undetected
- Remedy: create another file `*.vd` (and `*.rd`) with a *few* selected data (floating-point numbers) written with all significant digits

Example on a .vd file

- The `*.vd` file has a compact format:

```
## field 1
number of floats
float1
float2
float3
...
## field 2
number of floats
float1
float2
float3
...
## field 3
...
```

A test with numeric data

- Example file: src/ex/circle2.verify (and circle2.r, circle2.rd)
- We have a made a tool that can visually compare `*.vd` and `*.rd` in the form of two curves

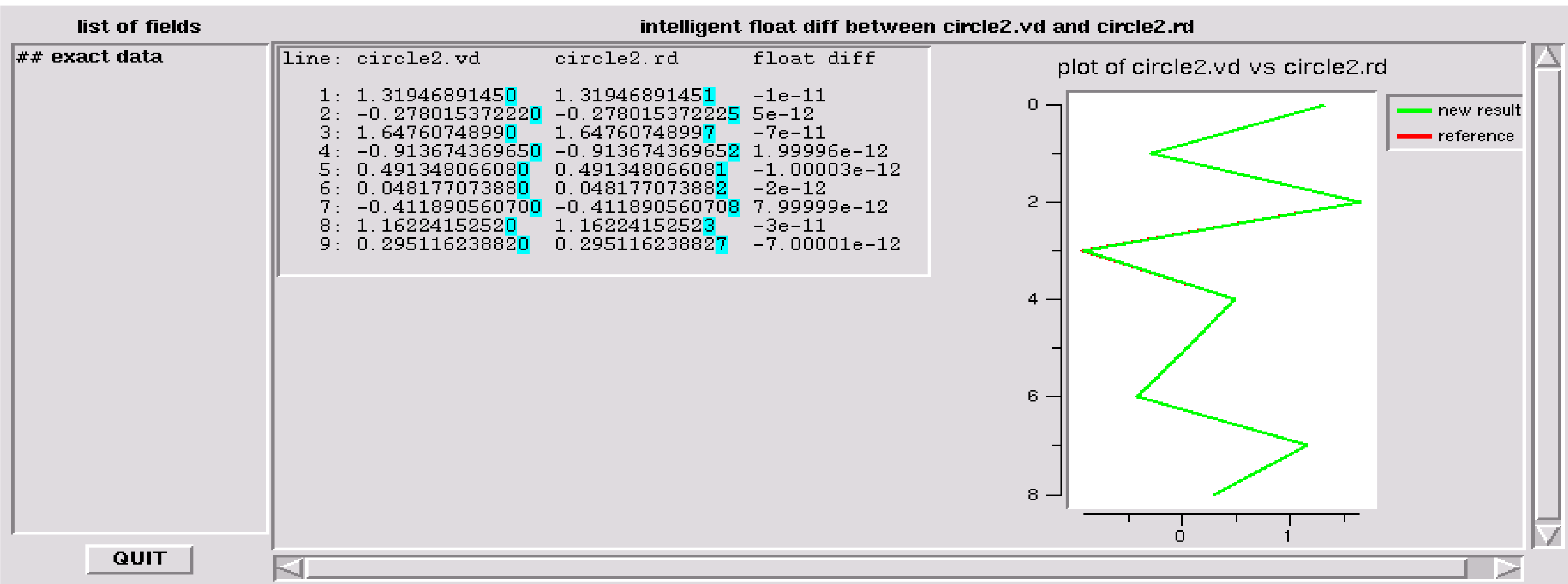
```
scitools regression verify circle2.verify
scitools floatdiff circle2.vd circle2.rd

# usually no diff in the above test, but we can fake
# a diff for illustrating scitools floatdiff:
perl -pi.old~~ -e 's/\d$/0/;' circle2.vd
scitools floatdiff circle2.vd circle2.rd
```

- Random curve deviation imply round-off errors only
- Trends in curve deviation may be caused by bugs

The floatdiff GUI

```
scitools floatdiff circle2.vd circle2.rd
```



Automatic doc string testing

- The doctest module can grab out interactive sessions from doc strings, run the sessions, and compare new output with the output from the session text
- Advantage: doc strings shows example on usage and these examples can be automatically verified at any time

Example

```
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
    """
```

The magic code enabling testing

```
def _test():
    import doctest, StringFunction
    return doctest.testmod(StringFunction)

if __name__ == '__main__':
    _test()
```

Example on output (1)

```
Running StringFunction.StringFunction.__doc__
Trying: from StringFunction import StringFunction
Expecting: nothing
ok
Trying: f = StringFunction('sin(3*x) + log(1+x)')
Expecting: nothing
ok
Trying: p = 2.0; v = f(p)  # evaluate function
Expecting: nothing
ok
Trying: p, v
Expecting: (2.0, 0.81919679046918392)
ok
Trying: f = StringFunction('1+t', independent_variables='t')
Expecting: nothing
ok
Trying: v = f(1.2)  # evaluate function of t=1.2
Expecting: nothing
ok
```

Example on output (1)

```
Trying: v = f(1.2)  # evaluate function of t=1.2
Expecting:
Traceback (most recent call last):
    v = f(1.2)
NameError: name 't' is not defined
ok
0 of 9 examples failed in StringFunction.StringFunction.__doc__
...
Test passed.
```

Unit testing

- Aim: test all (small) pieces of code
  (each class method, for instance)
- Cornerstone in extreme programming (XP)
- The Unit test framework was first developed for Smalltalk and then ported to Java (JUnit)
- The Python module unittest implements a version of JUnit
- While regression tests and doc string tests verify the overall functionality of the software, unit tests verify all the small pieces
- Unit tests are particularly useful when the code is restructured or newcomers perform modifications
- Write tests first, then code (!)

Using the unit test framework

- Unit tests are implemented in classes derived from class `TestCase` in the unittest module
- Each test is a method, whose name is prefixed by `test`
- Generated and correct results are compared using methods `assert*` or `failUnless*` inherited from class `TestCase`
- Example:

```
from scitools.StringFunction import StringFunction
import unittest

class TestStringFunction(unittest.TestCase):

    def test_plain1(self):
        f = StringFunction('1+2*x')
        v = f(2)
        self.failUnlessEqual(v, 5, 'wrong value')
```

Tests with round-off errors

- Compare v with correct answer to 6 decimal places:

```
def test_plain2(self):
    f = StringFunction('sin(3*x) + log(1+x)')
    v = f(2.0)
    self.failUnlessAlmostEqual(v, 0.81919679046918392, 6,
                               'wrong value')
```

More examples

```
def test_independent_variable_t(self):
    f = StringFunction('1+t', independent_variables='t')
    v = '%.2f' % f(1.2)

    self.failUnlessEqual(v, '2.20', 'wrong value')

# check that a particular exception is raised:
def test_independent_variable_z(self):
    f = StringFunction('1+z')

    self.failUnlessRaises(NameError, f, 1.2)

def test_set_parameters(self):
    f = StringFunction('a+b*x')
    f.set_parameters('a=1; b=4')
    v = f(2)

    self.failUnlessEqual(v, 9, 'wrong value')
```

Initialization of unit tests

- Sometimes a common initialization is needed before running unit tests
- This is done in a method `setUp`:

```
class SomeTestClass(unittest.TestCase):
    ...
    def setUp(self):
        <initializations for each test go here...>
```

Run the test

- Unit tests are normally placed in a separate file
- Enable the test:

```
if __name__ == '__main__':
    unittest.main()
```

- Example on output:

```
.....
----------------------------------------------------------------------
Ran 5 tests in 0.002s

OK
```

If some tests fail...

- This is how it looks like when unit tests fail:

```
==================================================================
FAIL: test_plain1 (__main__.TestStringFunction)
------------------------------------------------------------------
Traceback (most recent call last):
  File "./test_StringFunction.py", line 16, in test_plain1
    self.failUnlessEqual(v, 5, 'wrong value')
  File "/some/where/unittest.py", line 292, in failUnlessEqual
    raise self.failureException, \
AssertionError: wrong value
```

More about unittest

- The unittest module can do much more than shown here
- Multiple tests can be collected in test suites
- Look up the description of the unittest module in the Python Library Reference!
- There is an interesting scientific extension of unittest in the SciPy package

Contents

- How to make man pages out of the source code
- Doc strings
- Tools for automatic documentation
- Pydoc
- HappyDoc
- Epydoc

Write code and doc strings, autogenerate documentation!

More info

- App. B.2.2 in the course book
- Manuals for HappyDoc and Epydoc (see `doc.html`)
- `pydoc -h`

Man page documentation (1)

- Man pages = list of implemented functionality (preferably with examples)
- Advantage: man page as part of the source code
  - helps to document the code
  - increased reliability: doc details close to the code
  - easy to update doc when updating the code

Python tools for man page doc

- Pydoc: comes with Python
- HappyDoc: third-party tool
- HappyDoc support StructuredText, an “invisible”/natural markup of the text

Pydoc

- Suppose you have a module `doc` in `doc.py`
- View a structured documentation of classes, methods, functions, with arguments and doc strings:

  ```
  pydoc doc.py
  ```

  (try it out on `src/misc/doc.py`)
- Or generate HTML:

  ```
  pydoc -w doc.py
  firefox\emp\{doc.html\}  # view generated file
  ```

- You can view any module this way (including built-ins)

  ```
  pydoc math
  ```

Advantages of Pydoc

- Pydoc gives complete info on classes, methods, functions
- Note: the Python Library Reference does not have *complete* info on interfaces
- Search for modules whose doc string contains “keyword”:

  ```
  pydoc -k keyword
  ```

  e.g. find modules that do someting with dictionaries:

  ```
  pydoc -k dictionary
  ```

  (searches all reachable modules (`sys.path`))

HappyDoc

- HappyDoc gives more comprehensive and sophisticated output than Pydoc
- Try it:

```
cp $scripting/src/misc/doc.py .
happydoc doc.py
cd doc  # generated subdirectory
firefox index.html  # generated root of documentation
```

- HappyDoc supports StructuredText, which enables easy markup of plain ASCII text

Example on StructuredText

See `src/misc/doc.py` for more examples and references

```
Simple formatting rules

  Paragraphs are separated by blank lines. Words in running
  text can be *emphasized*.  Furthermore, text in single
  forward quotes, like 's = sin(r)', is typeset as code.
  Examples of lists are given in the 'func1' function
  in class 'MyClass' in the present module.
  Hyperlinks are also available, see the 'README.txt' file
  that comes with HappyDoc.

Headings

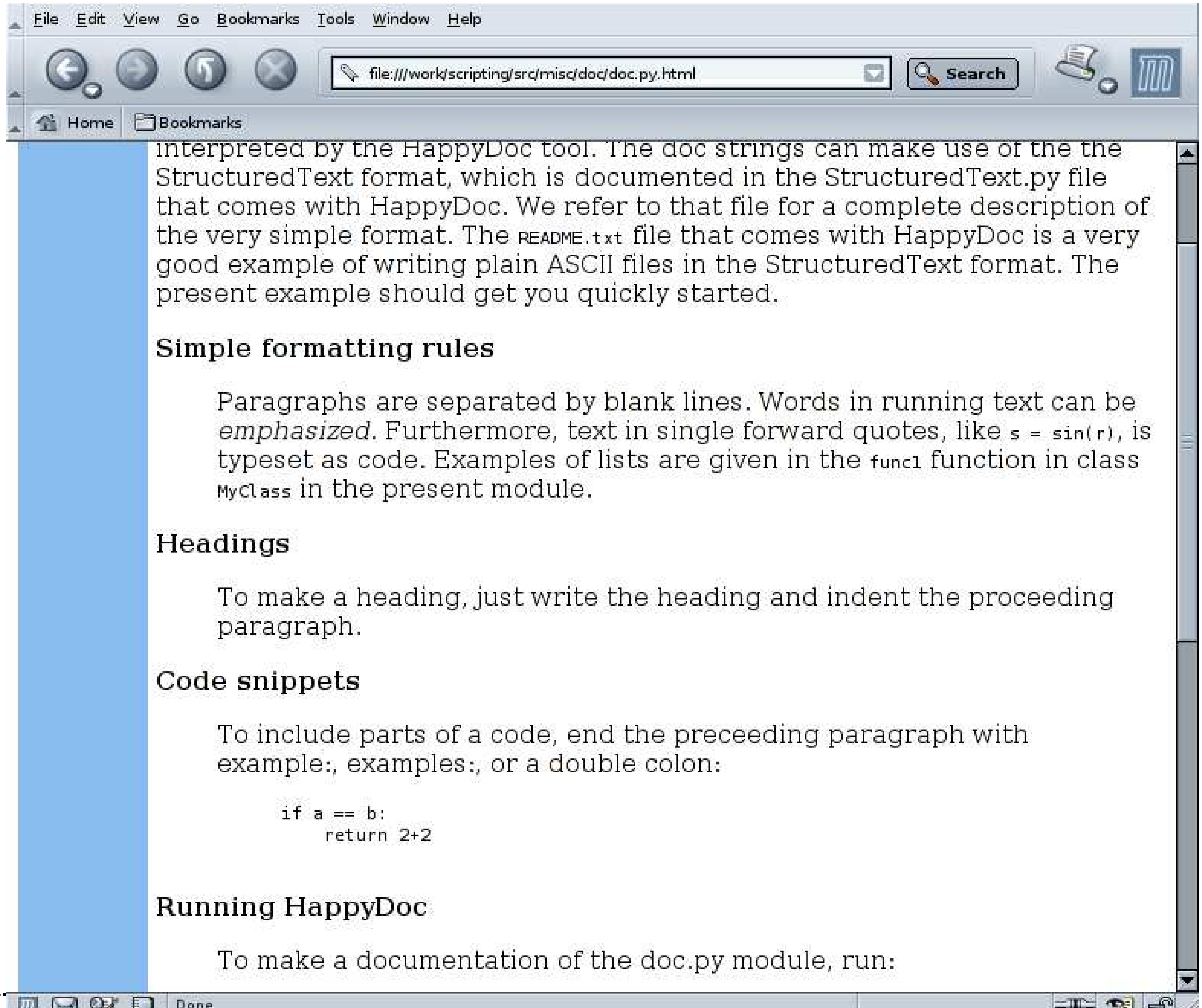
  To make a heading, just write the heading and
  indent the proceeding paragraph.

Code snippets

  To include parts of a code, end the preceeding paragraph
  with example:, examples:, or a double colon::

      if a == b:
          return 2+2
```

Browser result



Epydoc

- Epydoc is like Pydoc; it generates HTML, LaTeX and PDF
- Generate HTML document of a module:

```
epydoc --html -o tmp -n 'My First Epydoc Test' docex_epydoc.py
firefox tmp/index.html
```

- Can document large packages (nice toc/navigation)

Docutils

- Docutils is a coming tool for extracting documentation from source code
- Docutils supports an extended version of StructuredText
- See link in `doc.html` for more info

POD (1)

- POD = Plain Old Documentation
- Perl's documentation system
- POD applies tags and blank lines for indicating the formatting style

```
=head1 SYNOPSIS

 use File::Basename;

 ($name,$path,$suffix) = fileparse($fullname,@suff)
 fileparse_set_fstype($os_string);
 $basename = basename($fullname,@suffixlist);
 $dirname = dirname($fullname);

=head1 DESCRIPTION

=over 4

=item fileparse_set_fstype
...
=cut
```

POD (2)

- Perl ignores POD directives and text
- Filters transform the POD text to nroff, HTML, LaTeX, ASCII, ...
- Disadvantage: only Perl scripts can apply POD
- Example: src/sdf/simviz1-poddoc.pl

Build tools, by Kent-Andre Mardal

- Unix systems have an enormous amount of useful software
- Each package has its own huge set of command-line options
- The overwhelming software makes it hard to discover useful packages
- Here we will try to present some of the "most useful" commands
- These slides are therefore organized as a set of commands

gcc fundamentals

gcc - GNU project C and C++ compiler

Commonly used flags

- `-I`<directory-for-hearders>
- `-L`<directory-for-libraries>
- `-l`<libname> e.g. -lpython means libpython.so or libpython.a
- `-D`macro
- `-E` stop after the preprocessing stage
- `-o` file (place output in file)

gcc fundamentals

- `-O1` .. `-O3` optimize
- `-pg` generate extra code to write profile information (used py `gprof`)
- `-g` produce debugging information
- `-shared` produce a shared object
- `-fpic` generate position-independent code suitable for use in a shared library

gcc fundamentals

A compilation command:

`g++ -pg -Dgpp_Cplusplus -Wall -O` (*flags*)
`-DPOINTER_ARITHMETIC -DNUMT=double` (*preprocessor flags*)
`-I. -I/usr/X11/include -I/dp/include` (*include directories*)
`-o Poisson1.o -c Poisson1.cpp`

A linking command:

`g++ -pg -L. -L/dp/lib/linux/opt` (*flags and lib dirs*)
` -o app ./Poisson1.o -ldpU -larr3 -larr2` (*libs*++)

Notice that the order of `-I`, `-l` and `-L` matters

Use `-fpic` and `-shared` to compile shared libraries

-D and -E

Look at the file
`$scripting/src/py/mixed/Grid2D/C++/plain/NumPyArray.h`

```
class NumPyArray_Float
{

...

double  operator() (int i) const {
#ifdef INDEX_CHECK
    assert(a->nd == 1 && i >= 0 && i < a->dimensions[0]);
#endif
    return *((double*) (a->data + i*a->strides[0]));
  }

};
```

-D and -E

Typically index checking reduce performance significantly, but is very useful during debugging

Therefore index checking can be turned on/off at compile time with the `-DINDEX_CHECK` macro

```
~/src/py/mixed/Grid2D/C++/plain >gcc -E  NumPyArray.h  \
  2>/dev/null  | grep assert
```

i.e. no calls to assert

On the other hand, when using the `-DINDEX_CHECK` macro

```
~/src/py/mixed/Grid2D/C++/plain >gcc -E -DINDEX_CHECK   \
  NumPyArray.h  2>/dev/null  | grep assert \
    assert(a->nd == 1 && i >= 0 && i < a->dimensions[0]);
```

gdb

gdb - The GNU Debugger

Gdb is powerful!

However, you get far by knowing just one gdb command

```
where
```

The command `where` gives you the line number where the crash occurred

Remember to compile with the command line option `-g`

There are several graphical front-ends to gdb, but `ddd` is recommended

gdb example

```
gdb python
(gdb) run
>>> import Heat1D
>>> simulator = Heat1D.Heat1D()
>>> simulator.scan()
>>> simulator.n = 120
>>> simulator.solveProblem()

Program received signal SIGSEGV, Segmentation fault.
[Switching to Thread 16384 (LWP 17287)]
0x406b1431 in TimePrm::initTimeLoop() at gen/TimePrm.cpp:51
51        if (stationary_simulation)
Current language:  auto; currently c++
(gdb) where
#0  0x406b1431 in TimePrm::initTimeLoop() (this=0x0)
at gen/TimePrm.cpp:51
#1  0x4061571c in Heat1D::timeLoop() (this=0x81ed920)
at Heat1D.cpp:205
...
```

WAD

WAD - Wrapped Application Debugger

WAD is a Python module that turns segmentation faults etc. to Python exceptions

```
try:
  solveProblem()
except SegFault, s:
  print s
```

(It has been a while since the last release)

gprof

gprof - display call graph profile data

compile and link with `-pg`

```
gcc -pg -c test.c -o test.o
gcc -pg -shared -o app -o test.o -lm
app <command-line arguments>
gprof app | head -10
```

```
Each sample counts as 0.01 seconds.
  %   cumulative   self
 time  seconds   seconds   name
 87.72    6.43   6.43    MatBand::factLU()
  1.64    6.55   0.12    BasisFuncAtPt::calcJacobiEtc(Mat&)
  1.36    6.65   0.10    MatBand::forwBackLU(Vec&, Vec&)
  1.36    6.75   0.10    MatSimple::fill(double)
  0.82    6.81   0.06    sv_single2multiple(int, int, int)
```

make

make - utility to maintain groups of programs

A typical make command is

```
file :  dependency-file1 dependency-file2
  <tab>    rule to make file from dependency-file1
  <tab>    and dependency-file2
```

Notice that whitespace, tab and newline are important (This is the standard newbie problem)

`make` checks whether the time stamp on the dependencies are newer than the time stamp on `file`

If these are newer then `make` applies the rule to make a newer `file`

make

- All variables are on the form `$(VARIABLE)`
- General rules can be made, e.g. for compiling .c files to .o files

```
    .c.o:
            gcc $(INCLUDES) $(FLAGS)  -c $<
```

- $< holds the name of the dependency
- `.c.o` means that the `file.o` is made from `file.c`
- If the variable `$(VAR)` is not defined then the corresponding environment variable is used

Sample Makefile

```
INCLUDES = -I$(SOFTWARE)/include/python2.2/ -I.
SWIG_INCLUDES = -I$(SOFTWARE)/src/SWIG-1.3.19/Lib
Lib/python
FLAGS = -fpic -DHAVE_CONFIG_H -g
LIB_PATH = -L$(SOFTWARE)/lib

.c.o:
        gcc $(INCLUDES) $(FLAGS)  -c $<

default: _simple.so

simple_wrap.c: simple.h simple.c
        swig -python $(SWIG_INCLUDES) simple.i

_simple.so:  simple_wrap.o simple.o
        gcc -shared simple_wrap.o  simple.o -o _simple.so \
        -lswigpy -lnumpy  $(LIB_PATH)
```

make command line options

- `make -f file` forces `make` to use `file` as the makefile
- `make -n` tells make to print out the commands instead of executing them
- `make -j n` tells make to run `n` processes in parallel if possible
- `make -w` forces make to print out the working directory before and after execution

autoconf

autoconf - generate configuration scripts

`autoconf` is a tool for producing (stand-alone) shell scripts that adapt Makefiles to a Unix system

`autoconf` typically makes a Bourne shell script called `configure`

`configure` generates a `Makefile` based on `Makefile.in`

`configure` is based on `configure.in`

The goal when using `autoconf` is to make the following installation procedure possible

```
./configure
make
make install
```

Makefile.in

`configure` generates `Makefile` by replacing @ enclosed words such as `@prefix@` and `@CFLAGS@`

Example (lines) from the `Makefile.pre.in` in the Python distribution

```
CC=                @CC@
CXX=               @CXX@
AR=                @AR@
RANLIB=            @RANLIB@
srcdir=            @srcdir@
...

Modules/getbuildinfo.o: $(srcdir)/Modules/getbuildinfo.c
                $(CC) -c $(PY_CFLAGS) -DBUILD=‘cat buildno‘ \
                -o $@ $(srcdir)/Modules/getbuildinfo.c
```

configure.in

`autoscan` generates a preliminary `configure.in` file

`autoscan` examine a directory tree (either SRCDIR or the current directory) and creates `configure.scan`

`configure.scan` is modified and copied to `configure.in`

Libraries

Libraries can be

- static - code included in the executable during linking
  all symbols are defined in the executable
- dynamic - code is loaded during execution
- shared - the same library is shared by all its users

In practice we usually only distinguish between shared (.so) and static (.a) libraries

The standard format for both libraries (and executables) are now ELF.

Libraries

- .a : static library in containing raw object files stored in an archive made by `ar`
  ```
  > file /usr/lib/libz.a /usr/lib/libz.a:
  current ar archive
  ```
- .so : shared and dynamic library
  ```
  > file /usr/lib/libz.so.1.2.1
  /usr/lib/libz.so.1.2.1:  ELF 32-bit LSB shared
  object, Intel 80386, version 1 (SYSV), stripped
  ```

The command `file` is useful to determine the type of a file

Common Problem

A common problem when using shared libraries !

```
python
>>> import some_module
ImportError: _some_module.so:
>>>          undefined symbol: vertCases
```

Typically `vertCases` is defined in a library somewhere

We need to locate it.

In the following we will describe shortly various tools

See also: The inside story on shared libraries and dynamic loading `http://ieeexplore.ieee.org/xpl/abs_free.jsp?arNumber=947112`

nm

nm - list symbols from object files

```
~ >nm -o /home/kent-and/stable/lib/*.a \
   | grep daxpy | grep " T "
/home/kent-and/stable/lib/blas.a:daxpy.o:
  00000000 T daxpy_
/home/kent-and/stable/lib/libblas.a:daxpy.o:
  00000000 T daxpy_
```

```
nm gridloop.o  | grep NumPy
000003b0 T _Z4dumpRSoRK16NumPyArray_Float
000001e0 T _ZN16NumPyArray_Float6createEi
...
```

c++filt

c++filt - Demangle C++ and Java symbols

What is this ?

```
000003b0 T _Z4dumpRSoRK16NumPyArray_Float
```

```
>c++filt _Z4dumpRSoRK16NumPyArray_Float
dump(std::ostream&, NumPyArray_Float const&)
```

ranlib

ranlib - generate index to archive

- static libraries (suffix .a) are a collection of object files
- it usually have a index table that can be printed out with `nm`
- if not, this index table can be generate with `ranlib`
- `ranlib libpython.a`

objdump

objdump - display information from object files

```
~/stable/src/Python-2.2 >objdump -a libpython2.2.a \
  | egrep -2 readline

readline.o:   file format elf32-i386
rw-r--r-- 5889/15889 67224 Sep 8 10:38 2003 readline.o
```

ar

ar - create, modify, and extract from archives

remove readline.o from libpython2.2.a

```
ar d  libpython2.2.a readline.o
```

insert it again

```
ar cr  libpython2.2.a readline.o
```

readelf

readelf - Displays information about ELF files
Useful for finding symbols that are undefined

```
readelf -s _simple.so  | grep -v UND
```

ldd

ldd - print shared library dependencies

```
~ >ldd libvtkRenderingPython.so
    libvtkGraphics.so => libvtkGraphics.so (0x40175000)
    libvtkImaging.so => libvtkImaging.so (0x4034c000)
    libvtkFiltering.so => libvtkFiltering.so (0x40439000)
    libvtkCommonPython.so => not found
    libpthread.so.0 => not found
    libdl.so.2 => /lib/libdl.so.2 (0x4073d000)
    libGL.so.1 => /usr/X11R6/lib/libGL.so.1 (0x40741000)
    libvtkCommon.so => libvtkCommon.so (0x407b4000)
```

libraries that are not found must be found for proper execution

indent

indent - changes the appearance of a C program by inserting or deleting whitespace

- `indent` indent the C code according to a certain standard
- `indent -gnu file.c` indent according to the GNU standard
- `indent` is highly configurable
- Many similar programs

Further reading

- `info`, e.g. `info binutils`
- `man` pages
- tutorial shared and static libraries
  `http://users.actcom.co.il/˜choo/lupg/tutorials/libraries/unix-c-libraries.html`
- The inside story on shared libraries and dynamic loading
  `http://ieeexplore.ieee.org/xpl/abs_free.jsp?arNumber=947112`
- Lots of documentation: `www.gnu.org`