Slides from INF3331 lectures – combining Python with Fortran/C/C++

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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
- Alternative tools; ctypes, Instant, Cython

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

(Maybe 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*

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.
- Cython is a rapidly developing tool for integrating C and Python.
- The module `ctypes` provides C compatible data types in Python, and enables calling functions in shared libraries.

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)

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)
- Instant, Weave: simple tools for inlining C and C++ code in Python scripts
- 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)
```

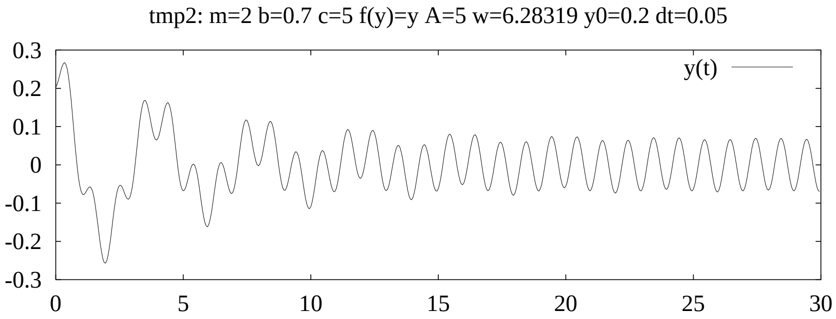
- The proxy class introduces overhead

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
- C++ class for wrapping NumPy arrays
- Alternative tools; instant, Weave
- 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) +
```

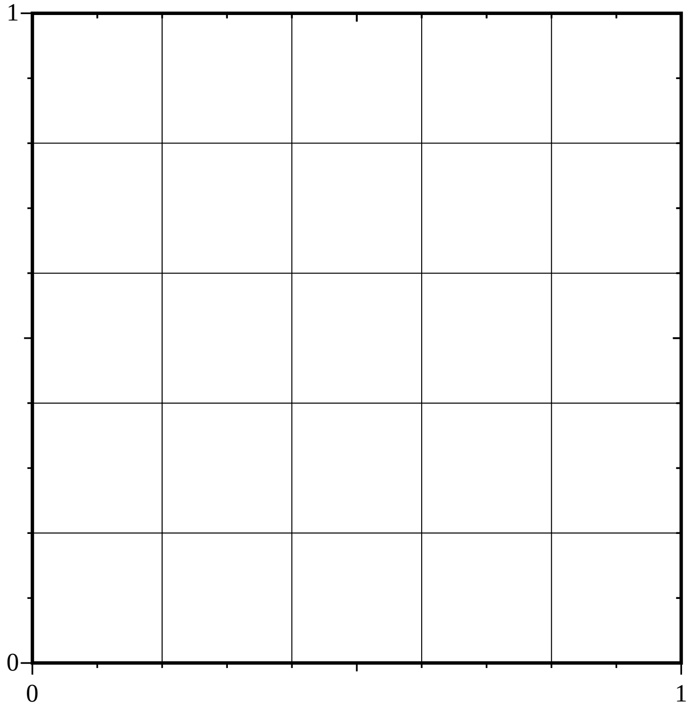
- Fortran/C/C++ version: (normalized) time 1.0
- NumPy vectorized evaluation of `f`: time 3.0
- Python loop version (version): time 140 (`math.sin`)
- Python loop version (version): time 350 (`numpy.sin`)

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)
- Inlining C/C++ code with Instant or Weave: 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), fu
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)
```

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());
```

The Instant tool (1)

- Instant allows inlining of C and C++ functions in Python codes
- A quick demo shows its potential

```
class Grid2Deff:
    ...
    def ext_gridloop1_instant(self, fstr):
        if not isinstance(fstr,str):
             raise TypeError, \
             ’fstr must be string expression, not %s’, type(fs

        #generate C source (fstr string must be valid C code)
        source = """
void gridloop1(double *a, int nx, int ny,
                        double *xcoor, double *ycoor)
{
# define index(a,i,j) a{i*ny+j}
   int i, j; double x, y;
   for (i = 0; i <nx; i++) {
      for (j = 0; j <= ny; j++){
         x = xcoor[i]; y = ycoor[i];
         index(a,i,j) = %s
      }
   }
}""" %fstr
```

The Instant tool (2)

```
 try:
    from instant import inline_with_numpy
    a = zeros((self.nx,self.ny))
    arrays = [['nx','ny','a'],
            ['nx','xcoor'],
            ['ny','ycoor']]
    self.gridloop1_instant = \
           inline_with_numpy(source, arrays=arrays)
except:
   self.gridloop1_instant = None
```

The Instant tool (3)

- `g` is a `Grid2Deff` instance
- We call `g.ext_gridloop_instant(fstr)` to make a C function from `fstr`
- Then we call

  ```
  a = zeros((g.nx,g.ny))
  g.gridloop1_instant(a,g.nx,g.ny,g.xcoor,g.ycoor)
  ```
- Instant detects any changes to the C code (e.g. `fstr`), and automatically recompiles

The Weave tool (1)

- Weave is an easy-to-use tool for inlining C++ snippets in Python codes
- Similar to instant, but with the added flexibility that the C++ code does not need to be a function
- Quick demo example

```
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 only recompiles the code if it has changed since last compilation

Summary

We have implemented several versions of `gridloop1` and `gridloop2`:

- Fortran subroutines, working on Fortran arrays, automatically wrapped by F2PY
- Hand-written C++ wrapper, working on a C++ class wrapper for NumPy arrays
- Instant and Weave for inlining C and C++ code

Comparison

- What is the most convenient approach in this case?
  Instant or Weave for inlining. Fortran if we want to interface external code.
- C++ is far more attracting for wrapping NumPy arrays than C, with classes allowing higher-level programming