INTERFACING WITH CYTHON

KONRAD HINSEN

CENTRE DE BIOPHYSIQUE MOLÉCULAIRE (ORLÉANS)

AND

SYNCHROTRON SOLEIL (ST AUBIN)

EXTENSION MODULES

- Python permits modules to be written in C.
 Such modules are called **extension modules**.
- Extension modules can define **extension types**, which are very similar to classes, but more efficient.
- Extension modules are usually compiled to produce shared libraries (Unix) or dynamic-link libraries (DLL, Windows). This causes certain restrictions on the C code in the module.
- De To client code, extension modules look just like Python modules.
- Many modules in the standard library are in fact extension modules.
- Many scientific packages (including NumPy) consist of a mix of Python modules and extension modules.
- Writing extension modules in plain C is both difficult and a lot of work. Nowadays most programmers use interface generators (SWIG, f2py, ...) or a special extension-module language: Cython.

CYTHON

- Described Compiler that compiles a Python module to a C extension module
 - → 5% acceleration at best!
- Language extensions for writing C in Python syntax
 - → hybrid Python/C programming

Applications:

- optimizing a Python function by translating it to C incrementally
- writing extension modules more conveniently
- writing interfaces to C libraries

EXAMPLE: PYTHON

```
def exp(x, terms = 50):
    sum = 0.
    power = 1.
    fact = 1.
    for i in range(terms):
        sum += power/fact
        power *= x
        fact *= i+1
    return sum
```

Note: This is not the best algorithm for calculating an exponential function!

EXAMPLE: CYTHON

Automatic conversion Python->C

Declaration of C variables

def exp(double x, int terms = 50):

cdef double sum

cdef double power

cdef double fact

cdef int i

sum = 0.

power = 1.

fact = 1.

Conversion to integer loop

for i in range(terms):

sum += power/fact

power *= x

fact *= i+1

Loop in C

return sum

Automatic conversion C->Python

COMPILING CYTHON MODULES

Use distutils as for C extension modules, with some modifications:

```
from distutils.core import setup, Extension
from Cython.Distutils import build_ext
                                  name of the package
setup (name = "Exponential",
                                  package version number
      version = "0.1",
                                                   name of the module
      ext_modules = [Extension('exp_cython',
                               ['exp_cython.pyx'])], source code files
      cmdclass = {'build_ext': build_ext}
```

Compile using: python setup.py build_ext --inplace

PYTHON FUNCTIONS VS C FUNCTIONS

Python function:

```
def exp(d)uble x, int terms = 50):
    cdef double sum
    cdef double power
    cdef double fact
    cdef int i
    sum = 0.
    power = 1.
    fact = 1.
    for i in range(terms):
        sum += power/fact
        power *= x
        fact *= i+1
    return sum
```

- Callable from Python code
- Python objects as arguments, automatic conversion to C values
- Return value converted to Python object

C function:

```
cdef double exp(double x, int terms = 50):
    cdef double sum
    cdef double power
    cdef double fact
    cdef int i
    sum = 0.
    power = 1.
    fact = 1.
    for i in range(terms):
        sum += power/fact
        power *= x
        fact *= i+1
    return sum
```

- Pure C function in Python syntax
- Callable only from a Cython module
- No data conversion whatsoever

IMPORTANT C DATA TYPES

Data type	Cname	Typical size
Integer	int	32 or 64 bits
Long integer	long	64 bits
Byte	char	8 bits
SP Real	float	32-bit IEEE
DP Real	double	64-bit IEEE

Note: all data type sizes are compiler-dependent!

NUMPY ARRAYS IN CYTHON

```
cimport numpy
import numpy
                                 Verification of Python data type
def array_sum(numpy.ndarray[double, ndim=1] a):
    cdef double sum
                                      Variable declarations in C
    cdef int i
    sum = 0.
    for i in range(a.shape[0]):
                                                   Loop in C
        sum += a[i]
    return sum ←
                               Automatic Conversion C->Python
```

COMPILING WITH NUMPY

```
from distutils.core import setup, Extension
from Cython.Distutils import build_ext
import numpy.distutils.misc_util
                                                                   locate the NumPy header files
include_dirs = numpy.distutils.misc_util.get_numpy_include_dirs()
setup (name = "ArraySum",
      version = "0.1",
       ext_modules = [Extension('array_sum',
                               ['array_sum.pyx'],
                               include_dirs=include_dirs)],
       cmdclass = {'build_ext': build_ext}
```

INTERFACING TO C CODE

GSL definitions:

```
cdef extern from "gsl/gsl_sf_bessel.h":
    ctypedef struct gsl_sf_result:
        double val
        double err
   int gsl_sf_bessel_I0_e(double x,
                          gsl_sf_result *result)
cdef extern from "gsl/gsl_errno.h":
    ctypedef void gsl_error_handler_t
   int GSL_SUCCESS
   int GSL_EUNDRFLW
    char *gsl_strerror(int gsl_errno)
   gsl_error_handler_t* gsl_set_error_handler_off()
gsl_set_error_handler_off()
```

Bessel function I0:

```
def I0(double x):
    cdef gsl_sf_result result
    cdef int status
    status = gsl_sf_bessel_I0_e(x, &result)
    if status == GSL_SUCCESS \
        or status == GSL_EUNDRFLW:
        return result.val
    raise ValueError(gsl_strerror(status))
```

EXERCICE: INTERFACING

The files ndtr.c, polevl.c, and mconf.h from the Cephes library (http://www.netlib.org/cephes/) contain the C functions erf() and erfc() plus routines used in them.

Provide a Python interface to erf and erfc. Write a Python script that verifies that erf(x)+erfc(x)=1 for several x.

Note: if you want to use the symbols erf and erfc for your Python functions, you will have to rename the C functions. This is done as follows:

```
cdef extern from "mconf.h":
    double c_erf "erf" (double x)
```