Study guide: Scientific software engineering; wave equation model

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Migrating loops to Cython

- Vectorization: 5-10 times slower than pure C or Fortran code
- Cython: extension of Python for translating functions to C
- Principle: declare variables with type

Declaring variables and annotating the code

Pure Python code:

```
def advance_scalar(u, u_1, u_2, f, x, y, t,
                   n, Cx2, Cy2, dt2, D1=2, D2=1):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    for i in Ix[1:-1]:
        for j in Iy[1:-1]:
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = D1*u_1[i,j] - D2*u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f(x[i], y[j], t[n])
```

- Copy this function and put it in a file with `.pyx` extension.
- Add type of variables:
    - `function(a, b)` → `cpdef function(int a, double b)`
    - `v = 1.2` → `cdef double v = 1.2`
    - Array declaration:
      `np.ndarray[np.float64_t, ndim=2, mode='c'] u`

Cython version of the functions

```
import numpy as np
cimport numpy as np
cimport cython
ctypedef np.float64_t DT     # data type

@cython.boundscheck(False)  # turn off array bounds check
@cython.wraparound(False)   # turn off negative indices (u[-1,-1])
cpdef advance(
    np.ndarray[DT, ndim=2, mode='c'] u,
    np.ndarray[DT, ndim=2, mode='c'] u_1,
    np.ndarray[DT, ndim=2, mode='c'] u_2,
    np.ndarray[DT, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):

    cdef int Nx, Ny, i, j
    cdef double u_xx, u_yy
    Nx = u.shape[0]-1
    Ny = u.shape[1]-1
    for i in xrange(1, Nx):
        for j in xrange(1, Ny):
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
```

Note: from now in we skip the code for setting boundary values

Visual inspection of the C translation

See how effective Cython can translate this code to C:

```
Terminal> cython -a wave2D_u0_loop_cy.pyx
```

Load `wave2D_u0_loop_cy.html` in a browser (white lines indicate code that was successfully translated to pure C, while yellow lines indicate code that is still in Python):

Raw output: wave2D_u0_loop_cy.c

```
import numpy as np
cimport numpy as np
cimport cython
ctypedef np.float64_t DT    # data type

@cython.boundscheck(False)  # turn off array bounds check
@cython.wraparound(False)   # turn off negative indices (u[-1,-1])
cpdef advance(
    np.ndarray[DT, ndim=2, mode='c'] u,
    np.ndarray[DT, ndim=2, mode='c'] u_1,
    np.ndarray[DT, ndim=2, mode='c'] u_2,
    np.ndarray[DT, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):

    cdef int Ix_start = 0
    cdef int Iy_start = 0
    cdef int Ix_end = u.shape[0]-1
    cdef int Iy_end = u.shape[1]-1
    cdef int i, j
    cdef double u_xx, u_yy

    for i in range(Ix_start+1, Ix_end):
        for j in range(Iy_start+1, Iy_end):
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
    # Boundary condition u=0
    j = Iy_start
    for i in range(Ix_start, Ix_end+1): u[i,j] = 0
    j = Iy_end
    for i in range(Ix_start, Ix_end+1): u[i,j] = 0
    i = Ix_start
    for j in range(Iy_start, Iy_end+1): u[i,j] = 0
    i = Iy_end
    for j in range(Iy_start, Iy_end+1): u[i,j] = 0
    return u
```

Can click on `wave2D_u0_loop_cy.c` to see the generated C code...

Building the extension module

- Cython code must be translated to C
- C code must be compiled
- Compiled C code must be linked to Python C libraries
- Result: *C extension module* (.so file) that can be loaded as a standard Python module
- Use a `setup.py` script to build the extension module

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

cymodule = 'wave2D_u0_loop_cy'
setup(
  name=cymodule
  ext_modules=[Extension(cymodule, [cymodule + '.pyx'],)],
  cmdclass={'build_ext': build_ext},
)
```

```
Terminal> python setup.py build_ext --inplace
```

Calling the Cython function from Python

```python
import wave2D_u0_loop_cy
advance = wave2D_u0_loop_cy.advance
...
for n in It[1:-1:                    # time loop
    f_a[:,:] = f(xv, yv, t[n])       # precompute, size as u
    u = advance(u, u_1, u_2, f_a, x, y, t, Cx2, Cy2, dt2)
```

Efficiency:

- 120×120 cells in space:
  - Pure Python: 1370 CPU time units
  - Vectorized numpy: 5.5
  - Cython: 1
- 60×60 cells in space:
  - Pure Python: 1000 CPU time units
  - Vectorized numpy: 6
  - Cython: 1

Migrating loops to Fortran

- Write the `advance` function in pure Fortran
- Use `f2py` to generate C code for calling Fortran from Python
- Full manual control of the translation to Fortran

The Fortran subroutine

```fortran
      subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
      integer Nx, Ny
      real*8 u(0:Nx,0:Ny), u_1(0:Nx,0:Ny), u_2(0:Nx,0:Ny)
      real*8 f(0:Nx, 0:Ny), Cx2, Cy2, dt2
      integer i, j
Cf2py intent(in, out) u

C     Scheme at interior points
      do j = 1, Ny-1
         do i = 1, Nx-1
            u(i,j) = 2*u_1(i,j) - u_2(i,j) +
     &      Cx2*(u_1(i-1,j) - 2*u_1(i,j) + u_1(i+1,j)) +
     &      Cy2*(u_1(i,j-1) - 2*u_1(i,j) + u_1(i,j+1)) +
     &      dt2*f(i,j)
         end do
      end do
```

Note: `Cf2py` comment declares `u` as input argument and return value back to Python

Building the Fortran module with f2py

```
Terminal> f2py -m wave2D_u0_loop_f77 -h wave2D_u0_loop_f77.pyf \
          --overwrite-signature wave2D_u0_loop_f77.f
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \
          -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

f2py changes the argument list (!)

```
>>> import wave2D_u0_loop_f77
>>> print wave2D_u0_loop_f77.__doc__
This module 'wave2D_u0_loop_f77' is auto-generated with f2py....
Functions:
  u = advance(u,u_1,u_2,f,cx2,cy2,dt2,
      nx=(shape(u,0)-1),ny=(shape(u,1)-1))
```

- Array limits have default values
- Examine doc strings from f2py!

How to avoid array copying

- Two-dimensional arrays are stored row by row in Python and C
- Two-dimensional arrays are stored column by column in Fortran
- `f2py` takes a copy of a `numpy` (C) array and transposes it when calling Fortran
- Such copies are time and memory consuming
- Remedy: declare `numpy` arrays with Fortran storage

```
order = 'Fortran' if version == 'f77' else 'C'
u   = zeros((Nx+1,Ny+1), order=order)
u_1 = zeros((Nx+1,Ny+1), order=order)
u_2 = zeros((Nx+1,Ny+1), order=order)
```

Option `-DF2PY_REPORT_ON_ARRAY_COPY=1` makes `f2py` write out array copying:

```
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \
          -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

Efficiency of translating to Fortran

- Same efficiency (in this example) as Cython and C
- About 5 times faster than vectorized `numpy` code
- $>$ 1000 faster than pure Python code

Migrating loops to C via Cython

- Write the `advance` function in pure C
- Use Cython to generate C code for calling C from Python
- Full manual control of the translation to C

The C code

- numpy arrays transferred to C are one-dimensional in C
- Need to translate [i,j] indices to single indices

```
/* Translate (i,j) index to single array index */
#define idx(i,j) (i)*(Ny+1) + j

void advance(double* u, double* u_1, double* u_2, double* f,
     double Cx2, double Cy2, double dt2,
     int Nx, int Ny)
{
  int i, j;
  /* Scheme at interior points */
  for (i=1; i<=Nx-1; i++) {
    for (j=1; j<=Ny-1; j++) {
        u[idx(i,j)] = 2*u_1[idx(i,j)] - u_2[idx(i,j)] +
        Cx2*(u_1[idx(i-1,j)] - 2*u_1[idx(i,j)] + u_1[idx(i+1,j)]) +
        Cy2*(u_1[idx(i,j-1)] - 2*u_1[idx(i,j)] + u_1[idx(i,j+1)]) +
        dt2*f[idx(i,j)];
}
    }
  }
}
```

The Cython interface file

```
import numpy as np
cimport numpy as np
cimport cython

cdef extern from "wave2D_u0_loop_c.h":
    void advance(double* u, double* u_1, double* u_2, double* f,
                 double Cx2, double Cy2, double dt2,
                 int Nx, int Ny)

@cython.boundscheck(False)
@cython.wraparound(False)
def advance_cwrap(
    np.ndarray[double, ndim=2, mode='c'] u,
    np.ndarray[double, ndim=2, mode='c'] u_1,
    np.ndarray[double, ndim=2, mode='c'] u_2,
    np.ndarray[double, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):
    advance(&u[0,0], &u_1[0,0], &u_2[0,0], &f[0,0],
            Cx2, Cy2, dt2,
            u.shape[0]-1, u.shape[1]-1)
    return u
```

Building the extension module

Compile and link the extension module with a setup.py file:

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

sources = ['wave2D_u0_loop_c.c', 'wave2D_u0_loop_c_cy.pyx']
module = 'wave2D_u0_loop_c_cy'
setup(
  name=module,
  ext_modules=[Extension(module, sources,
                         libraries=[], # C libs to link with
                         )],
  cmdclass={'build_ext': build_ext},
)
```

```
Terminal> python setup.py build_ext --inplace
```

In Python:

```
import wave2D_u0_loop_c_cy
advance = wave2D_u0_loop_c_cy.advance_cwrap
...
f_a[:,:] = f(xv, yv, t[n])
u = advance(u, u_1, u_2, f_a, Cx2, Cy2, dt2)
```

Migrating loops to C via f2py

- Write the `advance` function in pure C
- Use `f2py` to generate C code for calling C from Python
- Full manual control of the translation to C

The C code and the Fortran interface file

- Write the C function `advance` as before
- Write a Fortran 90 module defining the signature of the `advance` function
- Or: write a Fortran 77 function defining the signature and let `f2py` generate the Fortran 90 module

Fortran 77 signature (note `intent(c)`):

```
      subroutine advance(u, u_n, u_nm1, f, Cx2, Cy2, dt2, Nx, Ny)
Cf2py intent(c) advance
      integer Nx, Ny, N
      real*8 u(0:Nx,0:Ny), u_n(0:Nx,0:Ny), u_nm1(0:Nx,0:Ny)
      real*8 f(0:Nx, 0:Ny), Cx2, Cy2, dt2
Cf2py intent(in, out) u
Cf2py intent(c) u, u_n, u_nm1, f, Cx2, Cy2, dt2, Nx, Ny
      return
      end
```

Building the extension module

Generate Fortran 90 module (`wave2D_u0_loop_c_f2py.pyf`):

```
Terminal> f2py -m wave2D_u0_loop_c_f2py \
          -h wave2D_u0_loop_c_f2py.pyf --overwrite-signature \
          wave2D_u0_loop_c_f2py_signature.f
```

The compile and build step must list the C files:

```
Terminal> f2py -c wave2D_u0_loop_c_f2py.pyf \
          --build-dir tmp_build_c \
          -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_c.c
```

Migrating loops to C++ via f2py

- C++ can be used as an alternative to C
- C++ code often applies sophisticated arrays
- Challenge: translate from `numpy` C arrays to C++ array classes
- Can use SWIG to make C++ classes available as Python classes
- Easier (and more efficient):
  - Make C API to the C++ code
  - Wrap C API with `f2py`
  - Send `numpy` arrays to C API and let C translate `numpy` arrays into C++ array classes