Scientific software engineering; wave equation model

Hans Petter Langtangen[1,2]

[1]Center for Biomedical Computing, Simula Research Laboratory
[2]Department of Informatics, University of Oslo

Oct 20, 2015

> **Warning.**
>
> This document is in a very incomplete state!

Contents

List of Exercises

1 A 1D wave equation simulator

1.1 Mathematical model

Let u_t, u_{tt}, u_x, u_{xx} denote derivatives of u with respect to the subscript, i.e., u_{tt} is a second-order time derivative and u_x is a first-order space derivative. The initial-boundary value problem implemented in the `wave1D_dn_vc.py` code is

$$u_{tt} = (q(x)u_x)_x + f(x,t), \qquad\qquad x \in (0,L),\ t \in (0,T] \qquad (1)$$
$$u(x,0) = I(x), \qquad\qquad x \in [0,L] \qquad (2)$$
$$u_t(x,0) = V(t), \qquad\qquad x \in [0,L] \qquad (3)$$
$$u(0,t) = U_0(t) \text{ or } u_x(0,t) = 0, \qquad\qquad t \in (0,T] \qquad (4)$$
$$u(L,t) = U_L(t) \text{ or } u_x(L,t) = 0, \qquad\qquad t \in (0,T] \qquad (5)$$

We allow variable wave velocity $c^2(x) = q(x)$, and Dirichlet or homogeneous Neumann conditions at the boundaries.

1.2 Numerical discretization

The PDE is discretized by second-order finite differences in time and space, with arithmetic mean for the variable coefficient

$$[D_t D_t u = \varrho^{-1} D_x \overline{q}^x D_x u + f]_i^n . \qquad (6)$$

The Neumann boundary conditions are discretized by

$$[D_{2x} u]_i^n = 0,$$

at a boundary point i. The details of how the numerical scheme is worked out are described in Sections **??** and **??** in [1].

1.3 A solver function

The general initial-boundary value problem (1)-(5) solved by finite difference methods can be implemented in the following `solver` function (taken from the file `wave1D_dn_vc.py`). This function builds on simpler versions described in Sections **??**, **??** **??**, and **??** in [1]. There are several quite advanced constructs that will be commented upon later.

```
def solver(I, V, f, c, U_0, U_L, L, dt, C, T,
           user_action=None, version='scalar',
           stability_safety_factor=1.0):
    """Solve u_tt=(c^2*u_x)_x + f on (0,L)x(0,T]."""
    Nt = int(round(T/dt))
    t = np.linspace(0, Nt*dt, Nt+1)       # Mesh points in time

    # Find max(c) using a fake mesh and adapt dx to C and dt
    if isinstance(c, (float,int)):
```

```
        c_max = c
    elif callable(c):
        c_max = max([c(x_) for x_ in linspace(0, L, 101)])
    dx = dt*c_max/(stability_safety_factor*C)
    Nx = int(round(L/dx))
    x = np.linspace(0, L, Nx+1)          # Mesh points in space

    # Treat c(x) as array
    if isinstance(c, (float,int)):
        c = np.zeros(x.shape) + c
    elif callable(c):
        # Call c(x) and fill array c
        c_ = np.zeros(x.shape)
        for i in range(Nx+1):
            c_[i] = c(x[i])
        c = c_

    q = c**2
    C2 = (dt/dx)**2; dt2 = dt*dt    # Help variables in the scheme

    # Wrap user-given f, I, V, U_0, U_L if None or 0
    if f is None or f == 0:
        f = (lambda x, t: 0) if version == 'scalar' else \
            lambda x, t: np.zeros(x.shape)
    if I is None or I == 0:
        I = (lambda x: 0) if version == 'scalar' else \
            lambda x: np.zeros(x.shape)
    if V is None or V == 0:
        V = (lambda x: 0) if version == 'scalar' else \
            lambda x: np.zeros(x.shape)
    if U_0 is not None:
        if isinstance(U_0, (float,int)) and U_0 == 0:
            U_0 = lambda t: 0
    if U_L is not None:
        if isinstance(U_L, (float,int)) and U_L == 0:
            U_L = lambda t: 0

    # Make hash of all input data
    import hashlib, inspect
    data = inspect.getsource(I) + '_' + inspect.getsource(V) + \
           '_' + inspect.getsource(f) + '_' + str(c) + '_' + \
           ('None' if U_0 is None else inspect.getsource(U_0)) + \
           ('None' if U_L is None else inspect.getsource(U_L)) + \
           '_' + str(L) + str(dt) + '_' + str(C) + '_' + str(T) + \
           '_' + str(stability_safety_factor)
    hashed_input = hashlib.sha1(data).hexdigest()
    if os.path.isfile('.' + hashed_input + '_archive.npz'):
        # Simulation is already run
        return -1, hashed_input

    u   = np.zeros(Nx+1)   # Solution array at new time level
    u_1 = np.zeros(Nx+1)   # Solution at 1 time level back
    u_2 = np.zeros(Nx+1)   # Solution at 2 time levels back

    import time;  t0 = time.clock()  # CPU time measurement

    Ix = range(0, Nx+1)
    It = range(0, Nt+1)

    # Load initial condition into u_1
    for i in range(0,Nx+1):
        u_1[i] = I(x[i])

    if user_action is not None:
```

```
        user_action(u_1, x, t, 0)

    # Special formula for the first step
    for i in Ix[1:-1]:
        u[i] = u_1[i] + dt*V(x[i]) + \
        0.5*C2*(0.5*(q[i] + q[i+1])*(u_1[i+1] - u_1[i]) - \
                0.5*(q[i] + q[i-1])*(u_1[i] - u_1[i-1])) + \
        0.5*dt2*f(x[i], t[0])

    i = Ix[0]
    if U_0 is None:
        # Set boundary values (x=0: i-1 -> i+1 since u[i-1]=u[i+1]
        # when du/dn = 0, on x=L: i+1 -> i-1 since u[i+1]=u[i-1])
        ip1 = i+1
        im1 = ip1   # i-1 -> i+1
        u[i] = u_1[i] + dt*V(x[i]) + \
                0.5*C2*(0.5*(q[i] + q[ip1])*(u_1[ip1] - u_1[i])  - \
                        0.5*(q[i] + q[im1])*(u_1[i] - u_1[im1])) + \
        0.5*dt2*f(x[i], t[0])
    else:
        u[i] = U_0(dt)

    i = Ix[-1]
    if U_L is None:
        im1 = i-1
        ip1 = im1   # i+1 -> i-1
        u[i] = u_1[i] + dt*V(x[i]) + \
                0.5*C2*(0.5*(q[i] + q[ip1])*(u_1[ip1] - u_1[i])  - \
                        0.5*(q[i] + q[im1])*(u_1[i] - u_1[im1])) + \
        0.5*dt2*f(x[i], t[0])
    else:
        u[i] = U_L(dt)

    if user_action is not None:
        user_action(u, x, t, 1)

    # Update data structures for next step
    #u_2[:] = u_1;  u_1[:] = u  # safe, but slower
    u_2, u_1, u = u_1, u, u_2

    for n in It[1:-1]:
        # Update all inner points
        if version == 'scalar':
            for i in Ix[1:-1]:
                u[i] = - u_2[i] + 2*u_1[i] + \
                    C2*(0.5*(q[i] + q[i+1])*(u_1[i+1] - u_1[i])  - \
                        0.5*(q[i] + q[i-1])*(u_1[i] - u_1[i-1])) + \
                dt2*f(x[i], t[n])

        elif version == 'vectorized':
            u[1:-1] = - u_2[1:-1] + 2*u_1[1:-1] + \
            C2*(0.5*(q[1:-1] + q[2:])*(u_1[2:] - u_1[1:-1]) -
                0.5*(q[1:-1] + q[:-2])*(u_1[1:-1] - u_1[:-2])) + \
            dt2*f(x[1:-1], t[n])
        else:
            raise ValueError('version=%s' % version)

        # Insert boundary conditions
        i = Ix[0]
        if U_0 is None:
            # Set boundary values
            # x=0: i-1 -> i+1 since u[i-1]=u[i+1] when du/dn=0
            # x=L: i+1 -> i-1 since u[i+1]=u[i-1] when du/dn=0
            ip1 = i+1
```

6

```
            im1 = ip1
            u[i] = - u_2[i] + 2*u_1[i] + \
                   C2*(0.5*(q[i] + q[ip1])*(u_1[ip1] - u_1[i])  - \
                       0.5*(q[i] + q[im1])*(u_1[i] - u_1[im1])) + \
            dt2*f(x[i], t[n])
        else:
            u[i] = U_0(t[n+1])

        i = Ix[-1]
        if U_L is None:
            im1 = i-1
            ip1 = im1
            u[i] = - u_2[i] + 2*u_1[i] + \
                   C2*(0.5*(q[i] + q[ip1])*(u_1[ip1] - u_1[i])  - \
                       0.5*(q[i] + q[im1])*(u_1[i] - u_1[im1])) + \
            dt2*f(x[i], t[n])
        else:
            u[i] = U_L(t[n+1])

        if user_action is not None:
            if user_action(u, x, t, n+1):
                break

        # Update data structures for next step
        #u_2[:] = u_1;  u_1[:] = u  # safe, but slower
        u_2, u_1, u = u_1, u, u_2

    # Important to correct the mathematically wrong u=u_2 above
    # before returning u
    u = u_1
    cpu_time = t0 - time.clock()
    return cpu_time, hashed_input
```

Or maybe copy section by section...?

2 Saving large arrays in files

Numerical simulations produce large arrays as results and the software needs to store these arrays on disk. Several methods are available in Python. We recommend to use tailored solutions for large arrays and not standard file storage tools such as `pickle` (`cPickle` for speed in Python version 2) and `shelve`.

2.1 Using `savez` to store arrays in files

Storing individual arrays. The `numpy.storez` function can store a set of arrays to a named file in a zip archive. An associated function `numpy.load` can be used to read the file later. Basically, we call `numpy.storez(filename, **kwargs)`, where `kwargs` is a dictionary containing array names as keys and the corresponding array objects as values. Very often, the solution at a time point is given a natural name where the name of the variable and the time level counter are combined, e.g., `u11` or `v39`. Suppose `n` is the time level counter and we have two solution arrays, `u` and `v`, that we want to save to a zip archive. The appropriate code is

```
import numpy as np
u_name = 'u%04d' % n    # array name
v_name = 'v%04d' % n    # array name
kwargs = {u_name: u, v_name: v}    # keyword args for savez
fname = '.mydata%04d.dat' % n
np.savez(fname, **kwargs)
if n == 0:              # store x once
    np.savez('.mydata_x.dat', x=x)
```

Since the name of the array must be given as a keyword argument to `savez`, and the name must be constructed as shown, it becomes a little tricky to do the call, but with a dictionary `kwargs` and `**kwargs`, which sends each key-value pair as individual keyword arguments, the task gets accomplished.

Merging zip archives. Each separate call to `np.savez` creates a new file (zip archive) with extension `.npz`. It is very convenient if collect all results in one archive instead. This can be done by merging all the individual `.npz` files into a single zip archive:

```
def merge_zip_archives(individual_archives, archive_name):
    """
    Merge individual zip archives made with numpy.savez into
    one archive with name archive_name.
    The individual archives can be given as a list of names
    or as a Unix wild chard filename expression for glob.glob.
    The result of this function is that all the individual
    archives are deleted and the new single archive made.
    """
    import zipfile
    archive = zipfile.ZipFile(
        archive_name, 'w', zipfile.ZIP_DEFLATED,
        allowZip64=True)
    if isinstance(individual_archives, (list,tuple)):
        filenames = individual_archives
    elif isinstance(individual_archives, str):
        filenames = glob.glob(individual_archives)

    # Open each archive and write to the common archive
    for filename in filenames:
        f = zipfile.ZipFile(filename,  'r',
                            zipfile.ZIP_DEFLATED)
        for name in f.namelist():
            data = f.open(name, 'r')
            # Save under name without .npy
            archive.writestr(name[:-4], data.read())
        f.close()
        os.remove(filename)
    archive.close()
```

Here we remark that `savez` automatically adds the `.npz` extension to the names of the arrays we store. We do not want this extension in the final archive.

Reading arrays from zip archives. Archives created by `savez` or the merged archive we describe above with name of the form `myarchive.npz` can be conveniently read by the `numpy.load` function:

8

```
import numpy as np
array_names = np.load('myarchive.npz')
for array_name in array_names:
    # array_names[array_name] is the array itself
    # e.g. plot(array_names['t'], array_names[array_name])
```

2.2 Using `joblib` to store arrays in files

The Python package `joblib` has nice functionality for efficient storage of arrays
on disk. The following class applies this functionality so that one can save an
array, or in fact any Python data structure (e.g., a dictionary of arrays), to disk
under a certain name. Later, we can retrieve the object from its name. The
name of the directory under which the arrays are stored by `joblib` can be given
by the user.

```
class Storage(object):
    """
    Store large data structures (e.g. numpy arrays) efficiently
    using joblib.

    Use:

    >>> from Storage import Storage
    >>> storage = Storage(cachedir='tmp_u01', verbose=1)
    >>> import numpy as np
    >>> a = np.linspace(0, 1, 100000) # large array
    >>> b = np.linspace(0, 1, 100000) # large array
    >>> storage.save('a', a)
    >>> storage.save('b', b)
    >>> # later
    >>> a = storage.retrieve('a')
    >>> b = storage.retrieve('b')
    """
    def __init__(self, cachedir='tmp', verbose=1):
        """
        Parameters
        ----------
        cachedir: str
            Name of directory where objects are stored in files.
        verbose: bool, int
            Let joblib and this class speak when storing files
            to disk.
        """
        import joblib
        self.memory = joblib.Memory(cachedir=cachedir,
                                    verbose=verbose)
        self.verbose = verbose
        self.retrieve = self.memory.cache(
            self.retrieve, ignore=['data'])
        self.save = self.retrieve

    def retrieve(self, name, data=None):
        if self.verbose > 0:
            print 'joblib save of', name
        return data
```

The `retrive` and `save` functions, which do the work, seem quite magic. The
idea is that `joblib` looks at the `name` parameter and saves the return value `data`

9

to disk if the `name` parameter has not been used in a previous call. Otherwise, if `name` is already registered, `joblib` fetches the `data` object from file and returns it (this is example of a memoize function, see Section **??**in [2]).

2.3   Using a hash to create a file or directory name

The user of array storage techniques like those outlined in Sections 2.2 and 2.1 demand the user to assign a name for the file(s) or directory where the solution is to be stored. Ideally, this name should reflect parameters in the problem such that one can recognize an already run simulation. One technique is to make a hash string out of the input data. A hash string is a 40-character long hexadecimal string that uniquely reflects another potentially much longer string. (You may be used to hash strings from the Git version control system: every committed version of the files in Git is recognized by a hash string.)

Suppose you have some input data in the form of functions, `numpy` arrays, and other objects. To turn these input data into a string we may grab the source code of the functions, use a very efficient hash method for potentially large arrays, and simply convert all other objects via `str` to a string representation. The final string, merging all input data, is then converted to an SHA1 hash string such that we represent the input with a 40-character long string.

```
def myfunction(func1, func2, array1, array2, obj1, obj2):
    # Convert arguments to hash
    import inspect, joblib, hashlib
    data = (inspect.getsource(func1),
            inspect.getsource(func2),
            joblib.hash(array1),
            joblib.hash(array2),
            str(obj1),
            str(obj2))
    hash_input = hashlib.sha1(data).hexdigest()
```

It is wise to use `joblib.hash` and not try to do a `str(array1)`, since that string can be *very* long, and `joblib.hash` is more efficient than `hashlib` to turn these data into a hash.

> **Remark: turning function objects into their source code is unreliable!**
>
> The idea of turning a function object into a string via its source code may look smart, but is not a completely reliable solution. Suppose we have some function
>
> ```
> x0 = 0.1
> f = lambda x: 0 of x <= x0 else 1
> ```
>
> The source code will be `f = lambda x:  0 of x <= x0 else 1`, so if the calling code changes the value of `x0` (which `f` remembers - it is a closure), the source remains unchanged, the hash is the same, and the change in input

data is unnoticed. Consequently, the technique above must be used with care. The user can always just remove the stored files in disk and thereby force a recomputation (provided the software applies to hash to test if a zip archive or `joblib` subdirectory exists and if so avoids recomputation).

3   Software for the 1D wave equation

We use `numpy.storez` to store the solution at each time level on disk. Such actions must be taken care of outside the `solver` function, more precisely in the `user_action` function that is called at every time level.

We have in the `wave1D_dn_vc.py` code implemented the `user_action` callback function as a class `PlotAndStoreSolution` with a `__call__(self, x, t, t, n)` method for the `user_action` function. Basically, `__call__` stores and plots the solution. The storage makes use of the `numpy.savez` function for saving a set of arrays to a zip archive. Here, in this callback function, we want to save one array, `u`. Since there will be many such arrays, we introduce the array names `'u%04d' % n` and closely related filenames. The usage of `numpy.savez` in `__call__` goes like this:

```
from numpy import savez
name = 'u%04d' % n    # array name
kwargs = {name: u}    # keyword args for savez
fname = '.' + self.filename + '_' + name + '.dat'
self.t.append(t[n])   # store corresponding time value
savez(fname, **kwargs)
if n == 0:            # store x once
    savez('.' + self.filename + '_x.dat', x=x)
```

For example, if `n` is 10 and `self.filename` is `tmp`, the above call to `savez` becomes `savez('.tmp_u0010.dat', u0010=u)`. The actual filename becomes `.tmp_u0010.dat.npz`. The actual array name becomes `u0010.npy`.

Each `savez` call results in a file, so after the simulation we have one file per time level. Each file produced by `savez` is a zip archive. It makes sense to merge all the files into one. This is done in the `close_file` method in the `PlotAndStoreSolution` class. The code goes as follows.

```
class PlotAndStoreSolution:
    ...
    def close_file(self, hashed_input):
        """
        Merge all files from savez calls into one archive.
        hashed_input is a string reflecting input data
        for this simulation (made by solver).
        """
        if self.filename is not None:
            # Save all the time points where solutions are saved
            savez('.' + self.filename + '_t.dat',
                  t=array(self.t, dtype=float))
            # Merge all savez files to one zip archive
            archive_name = '.' + hashed_input + '_archive.npz'
```

11

```
            filenames = glob.glob('.' + self.filename + '*.dat.npz')
            merge_zip_archives(filenames, archive_name)
```

We use various `ZipFile` functionality to extract the content of the individual
files (each with name `filename`) and write it to the merged archive (`archive`).
There is only one array in each individual file (`filename`) so strictly speaking,
there is no need for the loop `for name in f.namelist()` (as `f.namelist()`
returns a list of length 1). However, in other applications where we compute
more arrays at each time level, `savez` will store all these and then there is need
for iterating over `f.namelist()`.

Instead of merging the archives written by `savez` we could make an alternative
implementation that writes all our arrays into one archive. This is the subject
of Exercise 1.

3.1 Making hash strings from input data

The `hashed_input` argument, used to name the resulting archive file with all
solutions, is supposed to be a hash reflecting all import parameters in the problem
such that this simulation has a unique name. The `hashed_input` string is made
in the `solver` function, using the `hashlib` and `inspect` modules, based on the
arguments to `solver`:

```
# Make hash of all input data
import hashlib, inspect
data = inspect.getsource(I) + '_' + inspect.getsource(V) + \
       '_' + inspect.getsource(f) + '_' + str(c) + '_' + \
       ('None' if U_0 is None else inspect.getsource(U_0)) + \
       ('None' if U_L is None else inspect.getsource(U_L)) + \
       '_' + str(L) + str(dt) + '_' + str(C) + '_' + str(T) + \
       '_' + str(stability_safety_factor)
hashed_input = hashlib.sha1(data).hexdigest()
```

NOTE: All this is now explained!

To get the source code of a function `f` as a string, we use `inspect.getsource(f)`.
All input, functions as well as variables, is then merged to a string `data`, and then
`hashlib.sha1` makes a unique, much shorter (40 characters long), fixed-length
string out of `data` that we can use in the archive filename.

> **Remark.**
>
> Note that the construction of the `data` string is not fool proof: if, e.g., `I`
> is a formula with parameters and the parameters change, the source code
> is still the same and `data` and hence the hash remains unaltered. The
> implementation must therefore be used with care!

3.2 Avoiding rerunning previously run cases

If the archive file whose name is based on `hashed_input` already exists, the simulation with the current set of parameters has been done before and one can avoid redoing the work. The `solver` function returns the CPU time and `hashed_input`, and a negative CPU time means that no simulation was run. In that case we should not call the `close_file` method above (otherwise we overwrite the archive with just the `self.t` array). The typical usage goes like

```
action = PlotAndStoreSolution(...)
dt = (L/Nx)/C  # choose the stability limit with given Nx
cpu, hashed_input = solver(
    I=lambda x: ...,
    V=0, f=0, c=1, U_0=lambda t: 0, U_L=None, L=1,
    dt=dt, C=C, T=T,
    user_action=action, version='vectorized',
    stability_safety_factor=1)
action.make_movie_file()
if cpu > 0:   # did we generate new data?
    action.close_file(hashed_input)
```

3.3 Verification

Exact solutions of the numerical equations are always attractive for verification purposes since the software should reproduce such solutions to machine precision. With Dirichlet boundary conditions we can construct a function that is linear in t and quadratic in x that is an exact solution of the scheme, while with Neumann conditions are left with testing just a constant solution (see comments in Section **??** in [1]).

A more general method for verification is to check the convergence rates.

Do convergence rates here! It is general...

4 Programming the solver with classes

Many who knows about class programming prefer to organize their software in terms of classes. We can easily port our function-based code in ... to a class version.

We will create a class `Problem` to hold the physical parameters of the problem and a class `Solver` to hold the numerical parameters and the solver function. In addition, it is convenient to collect the arrays that describe the mesh in a special `Mesh` class and make a class `Function` for a mesh function (mesh point values and its mesh).

4.1 Class Problem

4.2 Class Mesh

The `Mesh` class can be made valid for a space-time mesh in any number of space dimensions. To make versatile, the constructor accepts either a tuple/list of

number of cells in each spatial dimension or a tuple/list of cell spacings. In addition, we need the size of the hypercube mesh as a tuple/list of 2-tuples with lower and upper limits of the mesh coordinates in each direction. For 1D meshes it is more natural to just write the number of cells or the cell size and not wrap it in a list. We also need the time interval from `t0` to `T`. Giving no spatial discretization information implies a time mesh only, and vice versa. The `Mesh` class with documentation and a doc test should now be self-explanatory:

```
import numpy as np

class Mesh(object):
    """
    Holds data structures for a uniform mesh on a hypercube in
    space, plus a uniform mesh in time.

    ======== =================================================
    Argument             Explanation
    ======== =================================================
    L        List of 2-lists of min and max coordinates
             in each spatial direction.
    T        Final time in time mesh.
    Nt       Number of cells in time mesh.
    dt       Time step. Either Nt or dt must be given.
    N        List of number of cells in the spatial directions.
    d        List of cell sizes in the spatial directions.
             Either N or d must be given.
    ======== =================================================

    Users can access all the parameters mentioned above, plus
    ``x[i]`` and ``t`` for the coordinates in direction ``i``
    and the time coordinates, respectively.

    Examples:

    >>> from UniformFDMesh import Mesh
    >>>
    >>> # Simple space mesh
    >>> m = Mesh(L=[0,1], N=4)
    >>> print m.dump()
    space: [0,1] N=4 d=0.25
    >>>
    >>> # Simple time mesh
    >>> m = Mesh(T=4, dt=0.5)
    >>> print m.dump()
    time: [0,4] Nt=8 dt=0.5
    >>>
    >>> # 2D space mesh
    >>> m = Mesh(L=[[0,1], [-1,1]], d=[0.5, 1])
    >>> print m.dump()
    space: [0,1]x[-1,1] N=2x2 d=0.5,1
    >>>
    >>> # 2D space mesh and time mesh
    >>> m = Mesh(L=[[0,1], [-1,1]], d=[0.5, 1], Nt=10, T=3)
    >>> print m.dump()
    space: [0,1]x[-1,1] N=2x2 d=0.5,1 time: [0,3] Nt=10 dt=0.3

    """
    def __init__(self,
                 L=None, T=None, t0=0,
                 N=None, d=None,
                 Nt=None, dt=None):
```

14

```python
        if N is None and d is None:
            # No spatial mesh
            if Nt is None and dt is None:
                raise ValueError(
                    'Mesh constructor: either Nt or dt must be given')
            if T is None:
                raise ValueError(
                    'Mesh constructor: T must be given')
        if Nt is None and dt is None:
            if N is None and d is None:
                raise ValueError(
                    'Mesh constructor: either N or d must be given')
            if L is None:
                raise ValueError(
                    'Mesh constructor: L must be given')

        # Allow 1D interface without nested lists with one element
        if L is not None and isinstance(L[0], (float,int)):
            # Only an interval was given
            L = [L]
        if N is not None and isinstance(N, (float,int)):
            N = [N]
        if d is not None and isinstance(d, (float,int)):
            d = [d]

        # Set all attributes to None
        self.x = None
        self.t = None
        self.Nt = None
        self.dt = None
        self.N = None
        self.d = None
        self.t0 = t0

        if N is None and d is not None and L is not None:
            self.L = L
            if len(d) != len(L):
                raise ValueError(
                    'd has different size (no of space dim.) from '
                    'L: %d vs %d', len(d), len(L))
            self.d = d
            self.N = [int(round(float(self.L[i][1] -
                                      self.L[i][0])/d[i]))
                      for i in range(len(d))]
        if d is None and N is not None and L is not None:
            self.L = L
            if len(N) != len(L):
                raise ValueError(
                    'N has different size (no of space dim.) from '
                    'L: %d vs %d', len(N), len(L))
            self.N = N
            self.d = [float(self.L[i][1] - self.L[i][0])/N[i]
                      for i in range(len(N))]

        if Nt is None and dt is not None and T is not None:
            self.T = T
            self.dt = dt
            self.Nt = int(round(T/dt))
        if dt is None and Nt is not None and T is not None:
            self.T = T
            self.Nt = Nt
            self.dt = T/float(Nt)

        if self.N is not None:
```

```python
            self.x = [np.linspace(
                        self.L[i][0], self.L[i][1], self.N[i]+1)
                        for i in range(len(self.L))]
        if Nt is not None:
            self.t = np.linspace(self.t0, self.T, self.Nt+1)

    def get_num_space_dim(self):
        return len(self.d) if self.d is not None else 0

    def has_space(self):
        return self.d is not None

    def has_time(self):
        return self.dt is not None

    def dump(self):
        s = ''
        if self.has_space():
            s += 'space: ' + \
                'x'.join(['[%g,%g]' % (self.L[i][0], self.L[i][1])
                        for i in range(len(self.L))]) + ' N='
            s += 'x'.join([str(Ni) for Ni in self.N]) + ' d='
            s += ','.join([str(di) for di in self.d])
        if self.has_space() and self.has_time():
            s += ' '
        if self.has_time():
            s += 'time: ' + '[%g,%g]' % (self.t0, self.T) + \
                ' Nt=%g' % self.Nt + ' dt=%g' % self.dt
        return s
```

We rely on attribute access - not get/set functions!

Java programmers in particular are used to get/set functions in classes to access internal data. In Python, we usually apply direct access of the attribute, such as `m.N[i]` if `m` is a `Mesh` object. A widely used convention is to do this as long as access to an attribute does not require additional code. In that case, one applies a property construction. The original interface remains the same after a property is introduced (in contrast to Java), so user will not notice a change to properties.

The only argument against direct attribute access in class `Mesh` is that the attributes are read-only so we could avoid offering a set function. Instead, we rely on the user that she does not assign new values to the attributes.

4.3   Class Function

A class `Function` is handy to hold a mesh and corresponding values for a scalar or vector function over the mesh. Since we may have a time or space mesh, or a combined time and space mesh, with one or more components in the function, some if tests are needed for allocating the right array sizes. To help the user, an `indices` attribute with the name of the indices in the final array `u` for the

function values is made. The examples in the doc string should explain the functionality.

```
class Function(object):
    """
    A scalar or vector function over a mesh (of class Mesh).

    ========== ========================================================
    Argument                          Explanation
    ========== ========================================================
    mesh       Class Mesh object: spatial and/or temporal mesh.
    num_comp   Number of components in function (1 for scalar).
    space_only True if the function is defined on the space mesh
               only (to save space). False if function has values
               in space and time.
    ========== ========================================================

    The indexing of ``u``, which holds the mesh point values of the
    function, depends on whether we have a space and/or time mesh.

    Examples:

    >>> from UniformFDMesh import Mesh, Function
    >>>
    >>> # Simple space mesh
    >>> m = Mesh(L=[0,1], N=4)
    >>> print m.dump()
    space: [0,1] N=4 d=0.25
    >>> f = Function(m)
    >>> f.indices
    ['x0']
    >>> f.u.shape
    (5,)
    >>> f.u[4]  # space point 4
    0.0
    >>>
    >>> # Simple time mesh for two components
    >>> m = Mesh(T=4, dt=0.5)
    >>> print m.dump()
    time: [0,4] Nt=8 dt=0.5
    >>> f = Function(m, num_comp=2)
    >>> f.indices
    ['time', 'component']
    >>> f.u.shape
    (9, 2)
    >>> f.u[3,1]  # time point 3, comp=1 (2nd comp.)
    0.0
    >>>
    >>> # 2D space mesh
    >>> m = Mesh(L=[[0,1], [-1,1]], d=[0.5, 1])
    >>> print m.dump()
    space: [0,1]x[-1,1] N=2x2 d=0.5,1
    >>> f = Function(m)
    >>> f.indices
    ['x0', 'x1']
    >>> f.u.shape
    (3, 3)
    >>> f.u[1,2]  # space point (1,2)
    0.0
    >>>
    >>> # 2D space mesh and time mesh
    >>> m = Mesh(L=[[0,1],[-1,1]], d=[0.5,1], Nt=10, T=3)
    >>> print m.dump()
```

```
space: [0,1]x[-1,1] N=2x2 d=0.5,1 time: [0,3] Nt=10 dt=0.3
>>> f = Function(m, num_comp=2, space_only=False)
>>> f.indices
['time', 'x0', 'x1', 'component']
>>> f.u.shape
(11, 3, 3, 2)
>>> f.u[2,1,2,0]  # time step 2, space point (1,2), comp=0
0.0
>>> # Function with space data only
>>> f = Function(m, num_comp=1, space_only=True)
>>> f.indices
['x0', 'x1']
>>> f.u.shape
(3, 3)
>>> f.u[1,2]  # space point (1,2)
0.0
"""
def __init__(self, mesh, num_comp=1, space_only=True):
    self.mesh = mesh
    self.num_comp = num_comp
    self.indices = []

    # Create array(s) to store mesh point values
    if (self.mesh.has_space() and not self.mesh.has_time()) or \
       (self.mesh.has_space() and self.mesh.has_time() and \
        space_only):
        # Space mesh only
        if num_comp == 1:
            self.u = np.zeros(
                [self.mesh.N[i] + 1
                 for i in range(len(self.mesh.N))])
            self.indices = [
                'x'+str(i) for i in range(len(self.mesh.N))]
        else:
            self.u = np.zeros(
                [self.mesh.N[i] + 1
                 for i in range(len(self.mesh.N))] +
                [num_comp])
            self.indices = [
                'x'+str(i)
                for i in range(len(self.mesh.N))] +\
                ['component']
    if not self.mesh.has_space() and self.mesh.has_time():
        # Time mesh only
        if num_comp == 1:
            self.u = np.zeros(self.mesh.Nt+1)
            self.indices = ['time']
        else:
            # Need num_comp entries per time step
            self.u = np.zeros((self.mesh.Nt+1, num_comp))
            self.indices = ['time', 'component']
    if self.mesh.has_space() and self.mesh.has_time() \
       and not space_only:
        # Space-time mesh
        size = [self.mesh.Nt+1] + \
               [self.mesh.N[i]+1
                for i in range(len(self.mesh.N))]
        if num_comp > 1:
            self.indices = ['time'] + \
                           ['x'+str(i)
                            for i in range(len(self.mesh.N))] +\
                           ['component']
            size += [num_comp]
        else:
```

```
                self.indices = ['time'] + ['x'+str(i)
                                  for i in range(len(self.mesh.N))]
            self.u = np.zeros(size)
```

4.4 Class Solver

With the `Mesh` and `Function` classes in place, we can rewrite the `solver` function, but we put it as a method in class `Solver`:

hpl 1: Rewrite solver!

5 Migrating loops to Cython

We now consider the `wave2D_u0.py` code for solving the 2D linear wave equation with constant wave velocity and homogeneous Dirichlet boundary conditions $u = 0$. This code contains a `solver` function, which calls and `advance_*` function to advance the numerical scheme one level forward in time. The function `advance_scalar` applies standard Python loops to implement the scheme, while `advance_vectorized` performs corresponding vectorized arithmetics with array slices. The statements of this solver are explained in Section **??**, in particular Sections **??** and **??** in [1].

Although vectorization can bring down the CPU time dramatically compared with scalar code, there is still some factor 5-10 to win in these types of applications by implementing the finite difference scheme in compiled code, typically in Fortran, C, or C++. This can quite easily be done by adding a little extra code to our program. Cython is an extension of Python that offers the easiest way to nail our Python loops in the scalar code down to machine code and achieve the efficiency of C.

Cython can be viewed as an extended Python language where variables are declared with types and where functions are marked to be implemented in C. Migrating Python code to Cython is done by copying the desired code segments to functions (or classes) and placing them in one or more separate files with extension `.pyx`.

5.1 Declaring variables and annotating the code

Our starting point is the plain `advance_scalar` function for a scalar implementation of the updating algorithm for new values $u_{i,j}^{n+1}$:

```
def advance_scalar(u, u_1, u_2, f, x, y, t, n, Cx2, Cy2, dt2,
                   V=None, step1=False):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    if step1:
        dt = sqrt(dt2)  # save
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2  # redefine
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 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])
            if step1:
                u[i,j] += dt*V(x[i], y[j])
    # Boundary condition u=0
    j = Iy[0]
    for i in Ix: u[i,j] = 0
    j = Iy[-1]
    for i in Ix: u[i,j] = 0
    i = Ix[0]
    for j in Iy: u[i,j] = 0
    i = Ix[-1]
    for j in Iy: u[i,j] = 0
    return u
```

We simply take a copy of this function and put it in a file `wave2D_u0_loop_cy.pyx`. The relevant Cython implementation arises from declaring variables with types and adding some important annotations to speed up array computing in Cython. Let us first list the complete code in the `.pyx` file:

```
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
        int Iy_start = 0
        int Ix_end = u.shape[0]-1
        int Iy_end = u.shape[1]-1
        int i, j
        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 = Ix_end
    for j in range(Iy_start, Iy_end+1): u[i,j] = 0
    return u
```

This example may act as a recipe on how to transform array-intensive code with loops into Cython.

1. Variables are declared with types: for example, `double v` in the argument list instead of just `v`, and `cdef double v` for a variable `v` in the body of the function. A Python `float` object is declared as `double` for translation to C by Cython, while an `int` object is declared by `int`.

2. Arrays need a comprehensive type declaration involving

   - the type `np.ndarray`,
   - the data type of the elements, here 64-bit floats, abbreviated as `DT` through `ctypedef np.float64_t DT` (instead of `DT` we could use the full name of the data type: `np.float64_t`, which is a Cython-defined type),
   - the dimensions of the array, here `ndim=2` and `ndim=1`,
   - specification of contiguous memory for the array (`mode='c'`).

3. Functions declared with `cpdef` are translated to C but are also accessible from Python.

4. In addition to the standard `numpy` import we also need a special Cython import of `numpy`: `cimport numpy as np`, to appear *after* the standard import.

5. By default, array indices are checked to be within their legal limits. To speed up the code one should turn off this feature for a specific function by placing `@cython.boundscheck(False)` above the function header.

6. Also by default, array indices can be negative (counting from the end), but this feature has a performance penalty and is therefore here turned off by writing `@cython.wraparound(False)` right above the function header.

7. The use of index sets `Ix` and `Iy` in the scalar code cannot be successfully translated to C. One reason is that constructions like `Ix[1:-1]` involve negative indices, and these are now turned off. Another reason is that Cython loops must take the form `for i in xrange` or `for i in range` for being translated into efficient C loops. We have therefore introduced `Ix_start` as `Ix[0]` and `Ix_end` as `Ix[-1]` to hold the start and end of the values of index i. Similar variables are introduced for the j index. A loop `for i in Ix` is with these new variables written as `for i in range(Ix_start, Ix_end+1)`.

Array declaration syntax in Cython.

We have used the syntax `np.ndarray[DT, ndim=2, mode='c']` to declare `numpy` arrays in Cython. There is a simpler, alternative syntax, employ-

---

21

ing typed memory views, where the declaration looks like `double [:,:]`. However, the full support for this functionality is not yet ready, and in this text we use the full array declaration syntax.

5.2   Visual inspection of the C translation

Cython can visually explain how successfully it translated a code from Python to C. The command

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

produces an HTML file `wave2D_u0_loop_cy.html`, which can be loaded into a web browser to illustrate which lines of the code that have been translated to C. Figure 1 shows the illustrated code. Yellow lines indicate the lines that Cython did not manage to translate to efficient C code and that remain in Python. For the present code we see that Cython is able to translate all the loops with array computing to C, which is our primary goal.

Figure 1:   Visual illustration of Cython's ability to translate Python to C.

You can also inspect the generated C code directly, as it appears in the file `wave2D_u0_loop_cy.c`. Nevertheless, understanding this C code requires some familiarity with writing Python extension modules in C by hand. Deep down in the file we can see in detail how the compute-intensive statements have been translated into some complex C code that is quite different from what a human would write (at least if a direct correspondence to the mathematical notation was intended).

5.3 Building the extension module

Cython code must be translated to C, compiled, and linked to form what is known in the Python world as a *C extension module*. This is usually done by making a `setup.py` script, which is the standard way of building and installing Python software. For an extension module arising from Cython code, the following `setup.py` script is all we need to build and install the 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},
)
```

We run the script by

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

The `-inplace` option makes the extension module available in the current directory as the file `wave2D_u0_loop_cy.so`. This file acts as a normal Python module that can be imported and inspected:

```
>>> import wave2D_u0_loop_cy
>>> dir(wave2D_u0_loop_cy)
['__builtins__', '__doc__', '__file__', '__name__',
 '__package__', '__test__', 'advance', 'np']
```

The important output from the `dir` function is our Cython function `advance` (the module also features the imported `numpy` module under the name `np` as well as many standard Python objects with double underscores in their names).

The `setup.py` file makes use of the `distutils` package in Python and Cython's extension of this package. These tools know how Python was built on the computer and will use compatible compiler(s) and options when building other code in Cython, C, or C++. Quite some experience with building large program systems is needed to do the build process manually, so using a `setup.py` script is strongly recommended.

Simplified build of a Cython module.

When there is no need to link the C code with special libraries, Cython offers a shortcut for generating and importing the extension module:

```
import pyximport; pyximport.install()
```

23

> This makes the `setup.py` script redundant. However, in the `wave2D_u0.py` code we do not use `pyximport` and require an explicit build process of this and many other modules.

5.4 Calling the Cython function from Python

The `wave2D_u0_loop_cy` module contains our `advance` function, which we now may call from the Python program for the wave equation:

```
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. For a mesh consisting of 120×120 cells, the scalar Python code require 1370 CPU time units, the vectorized version requires 5.5, while the Cython version requires only 1! For a smaller mesh with 60×60 cells Cython is about 1000 times faster than the scalar Python code, and the vectorized version is about 6 times slower than the Cython version.

6 Migrating loops to Fortran

Instead of relying on Cython's (excellent) ability to translate Python to C, we can invoke a compiled language directly and write the loops ourselves. Let us start with Fortran 77, because this is a language with more convenient array handling than C (or plain C++). Or more precisely, we can with ease program with the same multi-dimensional indices in the Fortran code as in the `numpy` arrays in the Python code, while in C these arrays are one-dimensional and requires us to reduce multi-dimensional indices to a single index.

6.1 The Fortran subroutine

We write a Fortran subroutine `advance` in a file `wave2D_u0_loop_f77.f` for implementing the updating formula (**??**) and setting the solution to zero at the boundaries:

```
      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
      real*8 u_xx, u_yy
Cf2py intent(in, out) u

C     Scheme at interior points
```

```fortran
      do j = 1, Ny-1
         do i = 1, Nx-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) = 2*u_1(i,j) - u_2(i,j) + Cx2*u_xx + Cy2*u_yy +
     &               dt2*f(i,j)
         end do
      end do

C     Boundary conditions
      j = 0
      do i = 0, Nx
         u(i,j) = 0
      end do
      j = Ny
      do i = 0, Nx
         u(i,j) = 0
      end do
      i = 0
      do j = 0, Ny
         u(i,j) = 0
      end do
      i = Nx
      do j = 0, Ny
         u(i,j) = 0
      end do
      return
      end
```

This code is plain Fortran 77, except for the special `Cf2py` comment line, which
here specifies that `u` is both an input argument *and* an object to be returned
from the `advance` routine. Or more precisely, Fortran is not able return an array
from a function, but we need a *wrapper code* in C for the Fortran subroutine to
enable calling it from Python, and from this wrapper code one can return `u` to
the calling Python code.

Remark.

It is not strictly necessary to return `u` to the calling Python code since
the `advance` function will modify the elements of `u`, but the convention in
Python is to get all output from a function as returned values. That is,
the right way of calling the above Fortran subroutine from Python is

```python
u = advance(u, u_1, u_2, f, Cx2, Cy2, dt2)
```

The less encouraged style, which works and resembles the way the Fortran
subroutine is called from Fortran, reads

```python
advance(u, u_1, u_2, f, Cx2, Cy2, dt2)
```

6.2 Building the Fortran module with f2py

The nice feature of writing loops in Fortran is that, without much effort, the tool `f2py` can produce a C extension module such that we can call the Fortran version of `advance` from Python. The necessary commands to run are

```Terminal
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
```

The first command asks `f2py` to interpret the Fortran code and make a Fortran 90 specification of the extension module in the file `wave2D_u0_loop_f77.pyf`. The second command makes `f2py` generate all necessary wrapper code, compile our Fortran file and the wrapper code, and finally build the module. The build process takes place in the specified subdirectory `build_f77` so that files can be inspected if something goes wrong. The option `-DF2PY_REPORT_ON_ARRAY_COPY=1` makes `f2py` write a message for every array that is copied in the communication between Fortran and Python, which is very useful for avoiding unnecessary array copying (see below). The name of the module file is `wave2D_u0_loop_f77.so`, and this file can be imported and inspected as any other Python module:

```
>>> import wave2D_u0_loop_f77
>>> dir(wave2D_u0_loop_f77)
['__doc__', '__file__', '__name__', '__package__',
 '__version__', 'advance']
>>> 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))
```

Examine the doc strings!

Printing the doc strings of the module and its functions is extremely important after having created a module with `f2py`. The reason is that `f2py` makes Python interfaces to the Fortran functions that are different from how the functions are declared in the Fortran code (!). The rationale for this behavior is that `f2py` creates *Pythonic* interfaces such that Fortran routines can be called in the same way as one calls Python functions. Output data from Python functions is always returned to the calling code, but this is technically impossible in Fortran. Also, arrays in Python are passed to Python functions without their dimensions because that information is packed with the array data in the array objects. This is not possible in Fortran, however. Therefore, `f2py` removes array dimensions

---

from the argument list, and `f2py` makes it possible to return objects back to Python.

Let us follow the advice of examining the doc strings and take a close look at the documentation `f2py` has generated for our Fortran `advance` subroutine:

```
>>> print wave2D_u0_loop_f77.advance.__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))
.
advance - Function signature:
  u = advance(u,u_1,u_2,f,cx2,cy2,dt2,[nx,ny])
Required arguments:
  u : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  u_1 : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  u_2 : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  f : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  cx2 : input float
  cy2 : input float
  dt2 : input float
Optional arguments:
  nx := (shape(u,0)-1) input int
  ny := (shape(u,1)-1) input int
Return objects:
  u : rank-2 array('d') with bounds (nx + 1,ny + 1)
```

Here we see that the `nx` and `ny` parameters declared in Fortran are optional arguments that can be omitted when calling `advance` from Python.

We strongly recommend to print out the documentation of *every* Fortran function to be called from Python and make sure the call syntax is exactly as listed in the documentation.

6.3   How to avoid array copying

Multi-dimensional arrays are stored as a stream of numbers in memory. For a two-dimensional array consisting of rows and columns there are two ways of creating such a stream: *row-major ordering*, which means that rows are stored consecutively in memory, or *column-major ordering*, which means that the columns are stored one after each other. All programming languages inherited from C, including Python, apply the row-major ordering, but Fortran uses column-major storage. Thinking of a two-dimensional array in Python or C as a matrix, it means that Fortran works with the transposed matrix.

Fortunately, `f2py` creates extra code so that accessing `u(i,j)` in the Fortran subroutine corresponds to the element `u[i,j]` in the underlying `numpy` array (without the extra code, `u(i,j)` in Fortran would access `u[j,i]` in the `numpy` array). Technically, `f2py` takes a copy of our `numpy` array and reorders the data before sending the array to Fortran. Such copying can be costly. For 2D wave simulations on a 60×60 grid the overhead of copying is a factor of 5, which means that almost the whole performance gain of Fortran over vectorized `numpy` code is lost!

27

To avoid having `f2py` to copy arrays with C storage to the corresponding Fortran storage, we declare the arrays with Fortran storage:

```
order = 'Fortran' if version == 'f77' else 'C'
u   = zeros((Nx+1,Ny+1), order=order)   # solution array
u_1 = zeros((Nx+1,Ny+1), order=order)   # solution at t-dt
u_2 = zeros((Nx+1,Ny+1), order=order)   # solution at t-2*dt
```

In the compile and build step of using `f2py`, it is recommended to add an extra option for making `f2py` report on array copying:

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

It can sometimes be a challenge to track down which array that causes a copying. There are two principal reasons for copying array data: either the array does not have Fortran storage or the element types do not match those declared in the Fortran code. The latter cause is usually effectively eliminated by using `real*8` data in the Fortran code and `float64` (the default `float` type in `numpy`) in the arrays on the Python side. The former reason is more common, and to check whether an array before a Fortran call has the right storage one can print the result of `isfortran(a)`, which is `True` if the array `a` has Fortran storage.

Let us look at an example where we face problems with array storage. A typical problem in the `wave2D_u0.py` code is to set

```
f_a = f(xv, yv, t[n])
```

before the call to the Fortran `advance` routine. This computation creates a new array with C storage. An undesired copy of `f_a` will be produced when sending `f_a` to a Fortran routine. There are two remedies, either direct insertion of data in an array with Fortran storage,

```
f_a = zeros((Nx+1, Ny+1), order='Fortran')
...
f_a[:,:] = f(xv, yv, t[n])
```

or remaking the `f(xv, yv, t[n])` array,

```
f_a = asarray(f(xv, yv, t[n]), order='Fortran')
```

The former remedy is most efficient if the `asarray` operation is to be performed a large number of times.

Efficiency. The efficiency of this Fortran code is very similar to the Cython code. There is usually nothing more to gain, from a computational efficiency point of view, by implementing the *complete* Python program in Fortran or C. That will just be a lot more code for all administering work that is needed in

scientific software, especially if we extend our sample program `wave2D_u0.py` to handle a real scientific problem. Then only a small portion will consist of loops with intensive array calculations. These can be migrated to Cython or Fortran as explained, while the rest of the programming can be more conveniently done in Python.

7 Migrating loops to C via Cython

The computationally intensive loops can alternatively be implemented in C code. Just as Fortran calls for care regarding the storage of two-dimensional arrays, working with two-dimensional arrays in C is a bit tricky. The reason is that `numpy` arrays are viewed as one-dimensional arrays when transferred to C, while C programmers will think of u, `u_1`, and `u_2` as two dimensional arrays and index them like `u[i][j]`. The C code must declare u as `double* u` and translate an index pair `[i][j]` to a corresponding single index when u is viewed as one-dimensional. This translation requires knowledge of how the numbers in u are stored in memory.

7.1 Translating index pairs to single indices

Two-dimensional `numpy` arrays with the default C storage are stored row by row. In general, multi-dimensional arrays with C storage are stored such that the last index has the fastest variation, then the next last index, and so on, ending up with the slowest variation in the first index. For a two-dimensional u declared as `zeros((Nx+1,Ny+1))` in Python, the individual elements are stored in the following order:

```
u[0,0], u[0,1], u[0,2], ..., u[0,Ny], u[1,0], u[1,1], ...,
u[1,Ny], u[2,0], ..., u[Nx,0], u[Nx,1], ..., u[Nx, Ny]
```

Viewing u as one-dimensional, the index pair (i,j) translates to $i(N_y+1)+j$. So, where a C programmer would naturally write an index `u[i][j]`, the indexing must read `u[i*(Ny+1) + j]`. This is tedious to write, so it can be handy to define a C macro,

```
#define idx(i,j) (i)*(Ny+1) + j
```

so that we can write `u[idx(i,j)]`, which reads much better and is easier to debug.

> **Be careful with macro definitions.**
>
> Macros just perform simple text substitutions: `idx(hello,world)` is expanded to `(hello)*(Ny+1) + world`. The parenthesis in `(i)` are essential - using the natural mathematical formula `i*(Ny+1) + j` in the macro definition, `idx(i-1,j)` would expand to `i-1*(Ny+1) + j`, which is the

wrong formula. Macros are handy, but requires careful use. In C++, inline functions are safer and replace the need for macros.

7.2 The complete C code

The C version of our function `advance` can be coded as follows.

```c
#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;
  double u_xx, u_yy;
  /* Scheme at interior points */
  for (i=1; i<=Nx-1; i++) {
    for (j=1; j<=Ny-1; j++) {
      u_xx = u_1[idx(i-1,j)] - 2*u_1[idx(i,j)] + u_1[idx(i+1,j)];
      u_yy = u_1[idx(i,j-1)] - 2*u_1[idx(i,j)] + u_1[idx(i,j+1)];
      u[idx(i,j)] = 2*u_1[idx(i,j)] - u_2[idx(i,j)] +
        Cx2*u_xx + Cy2*u_yy + dt2*f[idx(i,j)];
    }
  }
  /* Boundary conditions */
  j = 0;  for (i=0; i<=Nx; i++) u[idx(i,j)] = 0;
  j = Ny; for (i=0; i<=Nx; i++) u[idx(i,j)] = 0;
  i = 0;  for (j=0; j<=Ny; j++) u[idx(i,j)] = 0;
  i = Nx; for (j=0; j<=Ny; j++) u[idx(i,j)] = 0;
}
```

7.3 The Cython interface file

All the code above appears in a file `wave2D_u0_loop_c.c`. We need to compile this file together with C wrapper code such that `advance` can be called from Python. Cython can be used to generate appropriate wrapper code. The relevant Cython code for interfacing C is placed in a file with extension `.pyx`. Here this file, called `wave2D_u0_loop_c_cy.pyx`, looks like

```python
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
```

We first declare the C functions to be interfaced. These must also appear in a C header file, `wave2D_u0_loop_c.h`,

```
extern void advance(double* u, double* u_1, double* u_2, double* f,
                    double Cx2, double Cy2, double dt2,
                    int Nx, int Ny);
```

The next step is to write a Cython function with Python objects as arguments. The name `advance` is already used for the C function so the function to be called from Python is named `advance_cwrap`. The contents of this function is simply a call to the `advance` version in C. To this end, the right information from the Python objects must be passed on as arguments to `advance`. Arrays are sent with their C pointers to the first element, obtained in Cython as `&u[0,0]` (the `&` takes the address of a C variable). The `Nx` and `Ny` arguments in `advance` are easily obtained from the shape of the `numpy` array `u`. Finally, `u` must be returned such that we can set `u = advance(...)` in Python.

7.4   Building the extension module

It remains to build the extension module. An appropriate `setup.py` file is

```
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},
)
```

All we need to specify is the `.c` file(s) and the `.pyx` interface file. Cython is automatically run to generate the necessary wrapper code. Files are then compiled and linked to an extension module residing in the file `wave2D_u0_loop_c_cy.so`. Here is a session with running `setup.py` and examining the resulting module in Python

————————————————————————— Terminal —————————————————————————

```
Terminal> python setup.py build_ext --inplace
Terminal> python
>>> import wave2D_u0_loop_c_cy as m
>>> dir(m)
['__builtins__', '__doc__', '__file__', '__name__', '__package__',
 '__test__', 'advance_cwrap', 'np']
```

The call to the C version of `advance` can go like this 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)
```

Efficiency. In this example, the C and Fortran code runs at the same speed, and there are no significant differences in the efficiency of the wrapper code. The overhead implied by the wrapper code is negligible as long as we do not work with very small meshes and consequently little numerical work in the `advance` function.

8 Migrating loops to C via f2py

An alternative to using Cython for interfacing C code is to apply `f2py`. The C code is the same, just the details of specifying how it is to be called from Python differ. The `f2py` tool requires the call specification to be a Fortran 90 module defined in a `.pyf` file. This file was automatically generated when we interfaced a Fortran subroutine. With a C function we need to write this module ourselves, or we can use a trick and let `f2py` generate it for us. The trick consists in writing the signature of the C function with Fortran syntax and place it in a Fortran file, here `wave2D_u0_loop_c_f2py_signature.f`:

```
      subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
Cf2py intent(c) advance
      integer Nx, Ny, N
      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
Cf2py intent(in, out) u
Cf2py intent(c) u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny
      return
      end
```

Note that we need a special `f2py` instruction, through a `Cf2py` comment line, to specify that all the function arguments are C variables. We also need to tell that the function is actually in C: `intent(c) advance`.

Since `f2py` is just concerned with the function signature and not the complete contents of the function body, it can easily generate the Fortran 90 module specification based solely on the signature above:

```
                          ┌──────────┐
──────────────────────────┤ Terminal ├──────────────────────────
                          └──────────┘
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 is as for the Fortran code, except that we list C files instead of Fortran 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
```

As when interfacing Fortran code with `f2py`, we need to print out the doc string to see the exact call syntax from the Python side. This doc string is identical for the C and Fortran versions of `advance`.

8.1 Migrating loops to C++ via f2py

C++ is a much more versatile language than C or Fortran and has over the last two decades become very popular for numerical computing. Many will therefore prefer to migrate compute-intensive Python code to C++. This is, in principle, easy: just write the desired C++ code and use some tool for interfacing it from Python. A tool like SWIG can interpret the C++ code and generate interfaces for a wide range of languages, including Python, Perl, Ruby, and Java. However, SWIG is a comprehensive tool with a correspondingly steep learning curve. Alternative tools, such as Boost Python, SIP, and Shiboken are similarly comprehensive. Simpler tools include PyBindGen,

A technically much easier way of interfacing C++ code is to drop the possibility to use C++ classes directly from Python, but instead make a C interface to the C++ code. The C interface can be handled by `f2py` as shown in the example with pure C code. Such a solution means that classes in Python and C++ cannot be mixed and that only primitive data types like numbers, strings, and arrays can be transferred between Python and C++. Actually, this is often a very good solution because it forces the C++ code to work on array data, which usually gives faster code than if fancy data structures with classes are used. The arrays coming from Python, and looking like plain C/C++ arrays, can be efficiently wrapped in more user-friendly C++ array classes in the C++ code, if desired.

9 Exercises

Exercise 1: Make an improved `numpy.savez` function

The `numpy.savez` function can save multiple arrays to a zip archive. Unfortunately, if we want to use `savez` in time-dependent problems and call it multiple times (once per time level), each call leads to a separate zip archive. It is more convenient to have all arrays in one archive, which can be read by `numpy.load`. Section 2 provides a recipe for merging all the individual zip archives into one archive. An alternative is to write a new `savez` function that allows multiple calls and storage into the same archive prior to a final `close` method to close the archive and make it ready for reading. Implement such an improved `savez` function as a class `Savez`.

The class should pass the following unit test:

```
def test_Savez():
    import tempfile, os
    tmp = 'tmp_testarchive'
    database = Savez(tmp)
    for i in range(4):
        array = np.linspace(0, 5+i, 3)
        kwargs = {'myarray_%02d' % i: array}
        database.savez(**kwargs)
    database.close()

    database = np.load(tmp+'.npz')

    expected = {
        'myarray_00': np.array([ 0. ,  2.5,  5. ]),
        'myarray_01': np.array([ 0.,  3.,  6.]),
        'myarray_02': np.array([ 0. ,  3.5,  7. ]),
        'myarray_03': np.array([ 0.,  4.,  8.]),
        }
    for name in database:
        computed = database[name]
        diff = np.abs(expected[name] - computed).max()
        assert diff < 1E-13
    database.close
    os.remove(tmp+'.npz')
```

Hint. Study the source code for function `savez` (or more precisely, function `_savez`).

Filename: `Savez`.

References

[1] H. P. Langtangen. Finite difference methods for wave motion. http://tinyurl.com/k3sdbuv/pub/wave.

[2] H. P. Langtangen. *Scaling of Differential Equations*. 2015. http://tinyurl.com/qfjgxmf/web.

Index