# Study guide: Finite difference methods for wave motion

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Mar 23, 2016

## Finite difference methods for waves on a string

Waves on a string can be modeled by the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

u(x,t) is the displacement of the string Demo of waves on a string.

#### The complete initial-boundary value problem

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \ t \in (0, T]$$
 (1)

$$u(x,0)=I(x), \hspace{1cm} x\in [0,L] \hspace{1cm} (2)$$

$$\frac{\partial}{\partial t}u(x,0) = 0,$$
  $x \in [0,L]$  (3)

$$u(0,t) = 0,$$
  $t \in (0,T]$  (4)

$$u(L,t) = 0, t \in (0,T] (5)$$

#### Input data in the problem

- Initial condition u(x,0) = I(x): initial string shape
- Initial condition  $u_t(x,0) = 0$ : string starts from rest
- $c = \sqrt{T/\varrho}$ : velocity of waves on the string
- (T is the tension in the string,  $\varrho$  is density of the string)

• Two boundary conditions on u: u = 0 means fixed ends (no displacement)

Rule for number of initial and boundary conditions:

- $u_{tt}$  in the PDE: two initial conditions, on u and  $u_t$
- $u_t$  (and no  $u_{tt}$ ) in the PDE: one initial conditions, on u
- $u_{xx}$  in the PDE: one boundary condition on u at each boundary point

#### Demo of a vibrating string (C = 0.8)

- Our numerical method is sometimes exact (!)
- Our numerical method is sometimes subject to serious non-physical effects

#### Demo of a vibrating string (C = 1.0012)

Ooops!

#### Step 1: Discretizing the domain

Mesh in time:

$$0 = t_0 < t_1 < t_2 < \dots < t_{N_t - 1} < t_{N_t} = T$$

$$\tag{6}$$

Mesh in space:

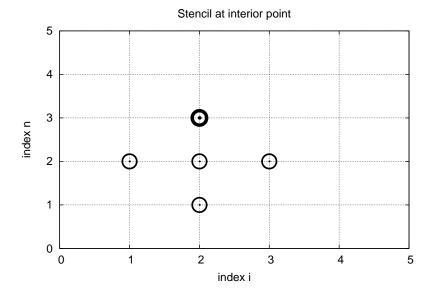
$$0 = x_0 < x_1 < x_2 < \dots < x_{N_x - 1} < x_{N_x} = L \tag{7}$$

Uniform mesh with constant mesh spacings  $\Delta t$  and  $\Delta x$ :

$$x_i = i\Delta x, \ i = 0, \dots, N_x, \quad t_i = n\Delta t, \ n = 0, \dots, N_t$$
 (8)

#### The discrete solution

- The numerical solution is a mesh function:  $u_i^n \approx u_e(x_i, t_n)$
- $\bullet$  Finite difference stencil (or scheme): equation for  $u_i^n$  involving neighboring space-time points



Step 2: Fulfilling the equation at the mesh points

Let the PDE be satisfied at all *interior* mesh points:

$$\frac{\partial^2}{\partial t^2} u(x_i, t_n) = c^2 \frac{\partial^2}{\partial x^2} u(x_i, t_n), \tag{9}$$

for  $i = 1, ..., N_x - 1$  and  $n = 1, ..., N_t - 1$ .

For n = 0 we have the initial conditions u = I(x) and  $u_t = 0$ , and at the boundaries  $i = 0, N_x$  we have the boundary condition u = 0.

#### Step 3: Replacing derivatives by finite differences

Widely used finite difference formula for the second-order derivative:

$$\frac{\partial^2}{\partial t^2} u(x_i, t_n) \approx \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = [D_t D_t u]_i^n$$

and

$$\frac{\partial^2}{\partial x^2} u(x_i, t_n) \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = [D_x D_x u]_i^n$$

#### Step 3: Algebraic version of the PDE

Replace derivatives by differences:

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2},\tag{10}$$

In operator notation:

$$[D_t D_t u = c^2 D_x D_x]_i^n \tag{11}$$

#### Step 3: Algebraic version of the initial conditions

- Need to replace the derivative in the initial condition  $u_t(x,0) = 0$  by a finite difference approximation
- The differences for  $u_{tt}$  and  $u_{xx}$  have second-order accuracy
- Use a centered difference for  $u_t(x,0)$

$$[D_{2t}u]_i^n = 0, \quad n = 0 \quad \Rightarrow \quad u_i^{n-1} = u_i^{n+1}, \quad i = 0, \dots, N_x$$

The other initial condition u(x,0) = I(x) can be computed by

$$u_i^0 = I(x_i), \quad i = 0, \dots, N_x$$

#### Step 4: Formulating a recursive algorithm

- Nature of the algorithm: compute u in space at  $t = \Delta t, 2\Delta t, 3\Delta t, ...$
- Three time levels are involved in the general discrete equation: n+1, n, n-1
- $u_i^n$  and  $u_i^{n-1}$  are then already computed for  $i = 0, \ldots, N_x$ , and  $u_i^{n+1}$  is the unknown quantity

Write out  $[D_t D_t u = c^2 D_x D_x]_i^n$  and solve for  $u_i^{n+1}$ .

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2 \left( u_{i+1}^n - 2u_i^n + u_{i-1}^n \right)$$
 (12)

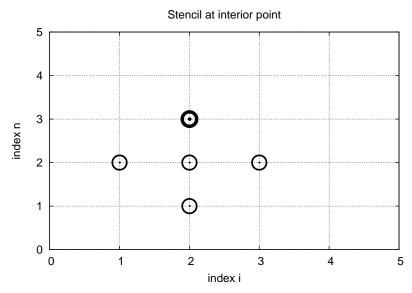
#### The Courant number

$$C = c \frac{\Delta t}{\Delta x},\tag{13}$$

is known as the (dimensionless) Courant number

**Observe.** There is only one parameter, C, in the discrete model: C lumps mesh parameters  $\Delta t$  and  $\Delta x$  with the only physical parameter, the wave velocity c. The value C and the smoothness of I(x) govern the quality of the numerical solution.

#### The finite difference stencil



#### The stencil for the first time level

- Problem: the stencil for n=1 involves  $u_i^{-1}$ , but time  $t=-\Delta t$  is outside the mesh
- $\bullet$  Remedy: use the initial condition  $u_t=0$  together with the stencil to eliminate  $u_i^{-1}$

Initial condition:

$$[D_{2t}u = 0]_i^0 \quad \Rightarrow \quad u_i^{-1} = u_i^1$$

Insert in stencil  $[D_t D_t u = c^2 D_x D_x]_i^0$  to get

$$u_i^1 = u_i^0 - \frac{1}{2}C^2 \left( u_{i+1}^n - 2u_i^n + u_{i-1}^n \right)$$
 (14)

#### The algorithm

- 1. Compute  $u_i^0 = I(x_i)$  for  $i = 0, \dots, N_x$
- 2. Compute  $u_i^1$  by (14) and set  $u_i^1=0$  for the boundary points i=0 and  $i=N_x$ , for  $n=1,2,\ldots,N-1$ ,
- 3. For each time level  $n = 1, 2, \ldots, N_t 1$ 
  - (a) apply (12) to find  $u_i^{n+1}$  for  $i = 1, \dots, N_x 1$
  - (b) set  $u_i^{n+1} = 0$  for the boundary points i = 0,  $i = N_x$ .

#### Moving finite difference stencil

web page or a movie file.

#### Sketch of an implementation (1)

• Arrays:

```
- \mathbf{u}[\mathbf{i}] stores u_i^{n+1}

- \mathbf{u}_1[\mathbf{i}] stores u_i^n

- \mathbf{u}_2[\mathbf{i}] stores u_i^{n-1}
```

Naming convention. u is the unknown to be computed (a spatial mesh function), u\_k is the computed spatial mesh function k time steps back in time.

#### PDE solvers should save memory

Important to minimize the memory usage. The algorithm only needs to access the three most recent time levels, so we need only three arrays for  $u_i^{n+1}$ ,  $u_i^n$ , and  $u_i^{n-1}$ ,  $i = 0, \ldots, N_x$ . Storing all the solutions in a two-dimensional array of size  $(N_x + 1) \times (N_t + 1)$  would be possible in this simple one-dimensional PDE problem, but not in large 2D problems and not even in small 3D problems.

#### Sketch of an implementation (2)

```
# Given mesh points as arrays x and t (x[i], t[n])
dx = x[1] - x[0]
dt = t[1] - t[0]
C = c*dt/dx
                       # Courant number
Nt = len(t)-1
C2 = C**2
                       # Help variable in the scheme
# Set initial condition u(x,0) = I(x)
for i in range(0, Nx+1):
    u_1[i] = I(x[i])
\# Apply special formula for first step, incorporating du/dt=0
for i in range(1, Nx):
   u[i] = u_1[i] - 0.5*C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])
u[0] = 0; u[Nx] = 0 # Enforce boundary conditions
# Switch variables before next step
u_2[:], u_1[:] = u_1, u
for n in range(1, Nt):
```

#### Verification

- Think about testing and verification before you start implementing the algorithm!
- Powerful testing tool: method of manufactured solutions and computation of convergence rates
- Will need a source term in the PDE and  $u_t(x,0) \neq 0$
- Even more powerful method: exact solution of the scheme

#### A slightly generalized model problem

Add source term f and nonzero initial condition  $u_t(x,0)$ :

$$u_{tt} = c^2 u_{xx} + f(x, t), (15)$$

$$u(x,0) = I(x), x \in [0,L] (16)$$

$$u_t(x,0) = V(x),$$
  $x \in [0,L]$  (17)

$$u(0,t) = 0, (18)$$

$$u(L,t) = 0, (19)$$

#### Discrete model for the generalized model problem

$$[D_t D_t u = c^2 D_x D_x + f]_i^n \tag{20}$$

Writing out and solving for the unknown  $u_i^{n+1}$ :

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \Delta t^2 f_i^n$$
 (21)

#### Modified equation for the first time level

Centered difference for  $u_t(x,0) = V(x)$ :

$$[D_{2t}u = V]_i^0 \quad \Rightarrow \quad u_i^{-1} = u_i^1 - 2\Delta t V_i,$$

Inserting this in the stencil (21) for n = 0 leads to

$$u_i^1 = u_i^0 - \Delta t V_i + \frac{1}{2} C^2 \left( u_{i+1}^n - 2u_i^n + u_{i-1}^n \right) + \frac{1}{2} \Delta t^2 f_i^n$$
 (22)

#### Using an analytical solution of physical significance

- Standing waves occur in real life on a string
- Can be analyzed mathematically (known exact solution)

$$u_{\rm e}(x,y,t)) = A \sin\left(\frac{\pi}{L}x\right) \cos\left(\frac{\pi}{L}ct\right)$$
 (23)

- PDE data: f=0, boundary conditions  $u_{\rm e}(0,t)=u_{\rm e}(L,0)=0$ , initial conditions  $I(x)=A\sin\left(\frac{\pi}{L}x\right)$  and V=0
- Note:  $u_i^{n+1} \neq u_e(x_i, t_{n+1})$ , and we do not know the error, so testing must aim at reproducing the expected convergence rates

#### Manufactured solution: principles

- Disadvantage with the previous physical solution: it does not test  $V \neq 0$  and  $f \neq 0$
- Method of manufactured solution:
  - Choose some  $u_{e}(x,t)$
  - Insert in PDE and fit f
  - Set boundary and initial conditions compatible with the chosen  $u_{\rm e}(x,t)$

#### Manufactured solution: example

$$u_{\rm e}(x,t) = x(L-x)\sin t$$

PDE  $u_{tt} = c^2 u_{xx} + f$ :

$$-x(L-x)\sin t = -2\sin t + f \quad \Rightarrow f = (2 - x(L-x))\sin t$$

Implied initial conditions:

$$u(x,0) = I(x) = 0$$
  
 $u_t(x,0) = V(x) = -x(L-x)$ 

Boundary conditions:

$$u(x,0) = u(x,L) = 0$$

#### Testing a manufactured solution

- Introduce common mesh parameter:  $h = \Delta t$ ,  $\Delta x = ch/C$
- This h keeps C and  $\Delta t/\Delta x$  constant
- Select coarse mesh h:  $h_0$
- Run experiments with  $h_i = 2^{-i}h_0$  (halving the cell size),  $i = 0, \dots, m$
- Record the error  $E_i$  and  $h_i$  in each experiment
- Compute pariwise convergence rates  $r_i = \ln E_{i+1}/E_i/\ln h_{i+1}/h_i$
- Verification:  $r_i \to 2$  as i increases

#### Constructing an exact solution of the discrete equations

- Manufactured solution with computation of convergence rates: much manual work
- Simpler and more powerful: use an exact solution for  $u_i^n$
- A linear or quadratic  $u_e$  in x and t is often a good candidate

#### Analytical work with the PDE problem

Here, choose  $u_e$  such that  $u_e(x,0) = u_e(L,0) = 0$ :

$$u_{e}(x,t) = x(L-x)(1+\frac{1}{2}t),$$

Insert in the PDE and find f:

$$f(x,t) = 2(1+t)c^2$$

Initial conditions:

$$I(x) = x(L - x), \quad V(x) = \frac{1}{2}x(L - x)$$

#### Analytical work with the discrete equations (1)

We want to show that  $u_e$  also solves the discrete equations! Useful preliminary result:

$$[D_t D_t t^2]^n = \frac{t_{n+1}^2 - 2t_n^2 + t_{n-1}^2}{\Delta t^2} = (n+1)^2 - n^2 + (n-1)^2 = 2$$
 (24)

$$[D_t D_t t]^n = \frac{t_{n+1} - 2t_n + t_{n-1}}{\Delta t^2} = \frac{((n+1) - n + (n-1))\Delta t}{\Delta t^2} = 0$$
 (25)

Hence,

$$[D_t D_t u_e]_i^n = x_i (L - x_i) [D_t D_t (1 + \frac{1}{2}t)]^n = x_i (L - x_i) \frac{1}{2} [D_t D_t t]^n = 0$$

#### Analytical work with the discrete equations (1)

$$[D_x D_x u_e]_i^n = (1 + \frac{1}{2}t_n)[D_x D_x (xL - x^2)]_i = (1 + \frac{1}{2}t_n)[LD_x D_x x - D_x D_x x^2]_i$$
$$= -2(1 + \frac{1}{2}t_n)$$

Now,  $f_i^n = 2(1 + \frac{1}{2}t_n)c^2$  and we get

$$[D_t D_t u_e - c^2 D_x D_x u_e - f]_i^n = 0 - c^2 (-1)2(1 + \frac{1}{2}t_n + 2(1 + \frac{1}{2}t_n)c^2 = 0$$

Moreover,  $u_{\rm e}(x_i,0)=I(x_i)$ ,  $\partial u_{\rm e}/\partial t=V(x_i)$  at t=0, and  $u_{\rm e}(x_0,t)=u_{\rm e}(x_{N_x},0)=0$ . Also the modified scheme for the first time step is fulfilled by  $u_{\rm e}(x_i,t_n)$ .

#### Testing with the exact discrete solution

- We have established that  $u_i^{n+1} = u_e(x_i, t_{n+1}) = x_i(L x_i)(1 + t_{n+1}/2)$
- Run one simulation with one choice of c,  $\Delta t$ , and  $\Delta x$
- Check that  $\max_i |u_i^{n+1} u_e(x_i, t_{n+1})| < \epsilon, \epsilon \sim 10^{-14}$  (machine precision + some round-off errors)
- This is the simplest and best verification test

Later we show that the exact solution of the discrete equations can be obtained by C=1 (!)

## **Implementation**

#### The algorithm

- 1. Compute  $u_i^0 = I(x_i)$  for  $i = 0, \dots, N_x$
- 2. Compute  $u_i^1$  by (14) and set  $u_i^1 = 0$  for the boundary points i = 0 and  $i = N_x$ , for n = 1, 2, ..., N 1,
- 3. For each time level  $n = 1, 2, \dots, N_t 1$ 
  - (a) apply (12) to find  $u_i^{n+1}$  for  $i = 1, ..., N_x 1$
  - (b) set  $u_i^{n+1} = 0$  for the boundary points i = 0,  $i = N_x$ .

#### What do to with the solution?

- Different problem settings demand different actions with the computed  $u_i^{n+1}$  at each time step
- Solution: let the solver function make a callback to a user function where the user can do whatever is desired with the solution
- Advantage: solver just solves and user uses the solution

```
def user_action(u, x, t, n):
    # u[i] at spatial mesh points x[i] at time t[n]
    # plot u
# or store u
```

#### Making a solver function (1)

We specify  $\Delta t$  and C, and let the solver function compute  $\Delta x = c\Delta t/C$ .

```
def solver(I, V, f, c, L, dt, C, T, user_action=None):
    """Solve u_tt=c^2*u_xx + f on (0,L)x(0,T]."""
    Nt = int(round(T/dt))
    t = linspace(0, Nt*dt, Nt+1)  # Mesh points in time
    dx = dt*c/float(C)
    Nx = int(round(L/dx))
    x = linspace(0, L, Nx+1)  # Mesh points in space
    dx = x[1] - x[0]
    C2 = C**2  # Help variable in the scheme
```

```
if f is None or f == 0:
    f = lambda x, t: 0
if V is None or V == 0:
    V = lambda x: 0

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

import time; t0 = time.clock()  # for measuring CPU time

# 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)
```

## Making a solver function (2)

#### Making a solver function (3)

```
def solver(I, V, f, c, L, Nx, C, T, user_action=None):
    ...
# Time loop
```

#### Verification: exact quadratic solution

Exact solution of the PDE problem and the discrete equations:  $u_{\rm e}(x,t)=x(L-x)(1+\frac{1}{2}t)$ 

```
def test_quadratic():
    """Check that u(x,t)=x(L-x)(1+t/2) is exactly reproduced."""
    def u_exact(x, t):
       return x*(L-x)*(1 + 0.5*t)
    def I(x):
       return u_exact(x, 0)
    def V(x):
       return 0.5*u_exact(x, 0)
    def f(x, t):
       return 2*(1 + 0.5*t)*c**2
   L = 2.5
    c = 1.5
    C = 0.75
   Nx = 6 # Very coarse mesh for this exact test
   dt = C*(L/Nx)/c
   T = 18
```

```
def assert_no_error(u, x, t, n):
    u_e = u_exact(x, t[n])
    diff = np.abs(u - u_e).max()
    tol = 1E-13
    assert diff < tol

solver(I, V, f, c, L, dt, C, T,
    user_action=assert_no_error)</pre>
```

#### Visualization: animating u(x,t)

Make a viz function for animating the curve, with plotting in a user\_action function plot\_u:

```
def viz(
   I, V, f, c, L, dt, C, T, # PDE parameters
                              # Interval for u in plots
    umin, umax,
    animate=True,
                             # Simulation with animation?
    tool='matplotlib',
                            # 'matplotlib' or 'scitools'
    solver_function=solver, # Function with numerical algorithm
    """Run solver and visualize u at each time level."""
    def plot_u_st(u, x, t, n):
        """user_action function for solver."""
       plt.plot(x, u, 'r-',
                 xlabel='x', ylabel='u',
                 axis=[0, L, umin, umax],
                 title='t=%f' % t[n], show=True)
        # Let the initial condition stay on the screen for 2
        # seconds, else insert a pause of 0.2 s between each plot
        time.sleep(2) if t[n] == 0 else time.sleep(0.2)
       plt.savefig('frame_%04d.png' % n) # for movie making
    class PlotMatplotlib:
        def __call__(self, u, x, t, n):
            """user_action function for solver."""
            if n == 0:
                plt.ion()
                self.lines = plt.plot(x, u, 'r-')
                plt.xlabel('x'); plt.ylabel('u')
                plt.axis([0, L, umin, umax])
                plt.legend(['t=%f' % t[n]], loc='lower left')
            else:
                self.lines[0].set_ydata(u)
                plt.legend(['t=%f' % t[n]], loc='lower left')
```

```
plt.draw()
        time.sleep(2) if t[n] == 0 else time.sleep(0.2)
        plt.savefig('tmp_%04d.png' % n) # for movie making
if tool == 'matplotlib':
    import matplotlib.pyplot as plt
   plot_u = PlotMatplotlib()
elif tool == 'scitools':
    import scitools.std as plt # scitools.easyviz interface
   plot_u = plot_u_st
import time, glob, os
# Clean up old movie frames
for filename in glob.glob('tmp_*.png'):
    os.remove(filename)
# Call solver and do the simulaton
user_action = plot_u if animate else None
u, x, t, cpu = solver_function(
    I, V, f, c, L, dt, C, T, user_action)
# Make video files
fps = 4 # frames per second
codec2ext = dict(flv='flv', libx264='mp4', libvpx='webm',
                 libtheora='ogg') # video formats
filespec = 'tmp_%04d.png'
movie_program = 'ffmpeg' # or 'avconv'
for codec in codec2ext:
    ext = codec2ext[codec]
    cmd = '%(movie_program)s -r %(fps)d -i %(filespec)s '\
          '-vcodec %(codec)s movie.%(ext)s' % vars()
    os.system(cmd)
if tool == 'scitools':
    # Make an HTML play for showing the animation in a browser
   plt.movie('tmp_*.png', encoder='html', fps=fps,
              output_file='movie.html')
return cpu
```

Note: plot\_u is function inside function and remembers the local variables in viz (known as a closure).

#### Making movie files

- Store spatial curve in a file, for each time level
- Name files like 'something\_%04d.png' % frame\_counter
- Combine files to a movie

```
Terminal> scitools movie encoder=html output_file=movie.html \
fps=4 frame_*.png # web page with a player

Terminal> avconv -r 4 -i frame_%04d.png -c:v flv movie.flv

Terminal> avconv -r 4 -i frame_%04d.png -c:v libtheora movie.ogg

Terminal> avconv -r 4 -i frame_%04d.png -c:v libx264 movie.mp4

Terminal> avconv -r 4 -i frame_%04d.png -c:v libpvx movie.webm
```

#### Important.

- Zero padding (%04d) is essential for correct sequence of frames in something\_\*.png (Unix alphanumeric sort)
- Remove old frame\_\*.png files before making a new movie

#### Running a case

- Vibrations of a guitar string
- Triangular initial shape (at rest)

$$I(x) = \begin{cases} ax/x_0, & x < x_0 \\ a(L-x)/(L-x_0), & \text{otherwise} \end{cases}$$
 (26)

Appropriate data:

• L=75 cm,  $x_0=0.8L,\,a=5$  mm, time frequency  $\nu=440$  Hz

#### Implementation of the case

```
def guitar(C):
    """Triangular wave (pulled guitar string)."""
    L = 0.75
    x0 = 0.8*L
    a = 0.005
    freq = 440
    wavelength = 2*L
    c = freq*wavelength
    omega = 2*pi*freq
    num_periods = 1
    T = 2*pi/omega*num_periods
# Choose dt the same as the stability limit for Nx=50
```

Program: wave1D\_u0.py.

## Resulting movie for C = 0.8

Movie of the vibrating string

#### The benefits of scaling

- It is difficult to figure out all the physical parameters of a case
- And it is not necessary because of a powerful: scaling

Introduce new x, t, and u without dimension:

$$\bar{x} = \frac{x}{L}, \quad \bar{t} = \frac{c}{L}t, \quad \bar{u} = \frac{u}{a}$$

Insert this in the PDE (with f = 0) and dropping bars

$$u_{tt} = u_{xx}$$

Initial condition: set a = 1, L = 1, and  $x_0 \in [0, 1]$  in (26).

In the code: set a=c=L=1, x0=0.8, and there is no need to calculate with wavelengths and frequencies to estimate c!

Just one challenge: determine the period of the waves and an appropriate end time (see the text for details).

#### Vectorization

- Problem: Python loops over long arrays are slow
- One remedy: use vectorized (numpy) code instead of explicit loops
- Other remedies: use Cython, port spatial loops to Fortran or C
- Speedup: 100-1000 (varies with  $N_x$ )

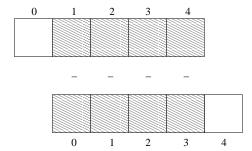
Next: vectorized loops

#### Operations on slices of arrays

• Introductory example: compute  $d_i = u_{i+1} - u_i$ 

```
n = u.size
for i in range(0, n-1):
    d[i] = u[i+1] - u[i]
```

- Note: all the differences here are independent of each other.
- Therefore  $d = (u_1, u_2, \dots, u_n) (u_0, u_1, \dots, u_{n-1})$
- In numpy code: u[1:n] u[0:n-1] or just u[1:] u[:-1]



#### Test the understanding

Newcomers to vectorization are encouraged to choose a small array u, say with five elements, and simulate with pen and paper both the loop version and the vectorized version.

#### Vectorization of finite difference schemes (1)

Finite difference schemes basically contains differences between array elements with shifted indices. Consider the updating formula

```
for i in range(1, n-1):
u2[i] = u[i-1] - 2*u[i] + u[i+1]
```

The vectorization consists of replacing the loop by arithmetics on slices of arrays of length  ${\tt n-2}$ :

```
u2 = u[:-2] - 2*u[1:-1] + u[2:]

u2 = u[0:n-2] - 2*u[1:n-1] + u[2:n] # alternative
```

Note: u2 gets length n-2.

If u2 is already an array of length n, do update on "inner" elements

```
u2[1:-1] = u[:-2] - 2*u[1:-1] + u[2:]

u2[1:n-1] = u[0:n-2] - 2*u[1:n-1] + u[2:n] # alternative
```

#### Vectorization of finite difference schemes (2)

Include a function evaluation too:

```
def f(x):
    return x**2 + 1

# Scalar version
for i in range(1, n-1):
    u2[i] = u[i-1] - 2*u[i] + u[i+1] + f(x[i])

# Vectorized version
u2[1:-1] = u[:-2] - 2*u[1:-1] + u[2:] + f(x[1:-1])
```

#### Vectorized implementation in the solver function

Scalar loop:

```
for i in range(1, Nx):
    u[i] = 2*u_1[i] - u_2[i] + \
        C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
```

Vectorized loop:

```
u[1:-1] = -u_2[1:-1] + 2*u_1[1:-1] + 

C2*(u_1[:-2] - 2*u_1[1:-1] + u_1[2:])
```

```
u[1:Nx] = 2*u_1[1:Nx] - u_2[1:Nx] + 
C2*(u_1[0:Nx-1] - 2*u_1[1:Nx] + u_1[2:Nx+1])
```

Program: wave1D\_u0v.py

#### Verification of the vectorized version

```
def test_quadratic():
    11 11 11
    Check the scalar and vectorized versions for
    a quadratic u(x,t)=x(L-x)(1+t/2) that is exactly reproduced.
    \# The following function must work for x as array or scalar
    u_{exact} = lambda x, t: x*(L - x)*(1 + 0.5*t)
    I = lambda x: u_exact(x, 0)
    V = lambda x: 0.5*u_exact(x, 0)
    # f is a scalar (zeros_like(x) works for scalar x too)
    f = lambda x, t: np.zeros_like(x) + 2*c**2*(1 + 0.5*t)
   L = 2.5
    c = 1.5
    C = 0.75
    Nx = 3 # Very coarse mesh for this exact test
    dt = C*(L/Nx)/c
    T = 18
    def assert_no_error(u, x, t, n):
        u_e = u_exact(x, t[n])
        tol = 1E-13
        diff = np.abs(u - u_e).max()
        assert diff < tol
    solver(I, V, f, c, L, dt, C, T,
           user_action=assert_no_error, version='scalar')
    solver(I, V, f, c, L, dt, C, T,
           user_action=assert_no_error, version='vectorized')
```

#### Note:

- Compact code with lambda functions
- ullet The scalar f value needs careful coding: return constant array if vectorized code, else number

#### Efficiency measurements

- Run wave1D\_u0v.py for  $N_x$  as 50,100,200,400,800 and measuring the CPU time
- Observe substantial speed-up: vectorized version is about  $N_x/5$  times faster

Much bigger improvements for 2D and 3D codes!

## Generalization: reflecting boundaries

- Boundary condition u = 0: u changes sign
- Boundary condition  $u_x = 0$ : wave is perfectly reflected
- How can we implement  $u_x$ ? (more complicated than u=0)

Demo of boundary conditions

#### Neumann boundary condition

$$\frac{\partial u}{\partial n} \equiv \boldsymbol{n} \cdot \nabla u = 0 \tag{27}$$

For a 1D domain [0, L]:

$$\left. \frac{\partial}{\partial n} \right|_{x=L} = \frac{\partial}{\partial x}, \quad \left. \frac{\partial}{\partial n} \right|_{x=0} = -\frac{\partial}{\partial x}$$

Boundary condition terminology:

- $u_x$  specified: Neumann condition
- u specified: Dirichlet condition

#### Discretization of derivatives at the boundary (1)

- How can we incorporate the condition  $u_x = 0$  in the finite difference scheme?
- We used centeral differences for  $u_{tt}$  and  $u_{xx}$ :  $\mathcal{O}(\Delta t^2, \Delta x^2)$  accuracy
- Also for  $u_t(x,0)$
- ullet Should use central difference for  $u_x$  to preserve second order accuracy

$$\frac{u_{-1}^n - u_1^n}{2\Delta x} = 0 (28)$$

#### Discretization of derivatives at the boundary (2)

$$\frac{u_{-1}^n-u_1^n}{2\Delta x}=0$$

- Problem:  $u_{-1}^n$  is outside the mesh (fictitious value)
- $\bullet$  Remedy: use the stencil at the boundary to eliminate  $u_{-1}^n;$  just replace  $u_{-1}^n$  by  $u_1^n$

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + 2C^2 \left( u_{i+1}^n - u_i^n \right), \quad i = 0$$
 (29)

#### Visualization of modified boundary stencil

Discrete equation for computing  $u_0^3$  in terms of  $u_0^2$ ,  $u_0^1$ , and  $u_1^2$ : Animation in a web page or a movie file.

#### Implementation of Neumann conditions

- Use the general stencil for interior points also on the boundary
- Replace  $u_{i-1}^n$  by  $u_{i+1}^n$  for i=0
- Replace  $u_{i+1}^n$  by  $u_{i-1}^n$  for  $i = N_x$

```
i = 0
ip1 = i+1
im1 = ip1  # i-1 -> i+1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])

i = Nx
im1 = i-1
ip1 = im1  # i+1 -> i-1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])

# Or just one loop over all points

for i in range(0, Nx+1):
    ip1 = i+1 if i < Nx else i-1
    im1 = i-1 if i > 0 else i+1
    u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

Program wave1D\_dn0.py

#### Moving finite difference stencil

web page or a movie file.

#### Index set notation

- Tedious to write index sets like  $i=0,\ldots,N_x$  and  $n=0,\ldots,N_t$
- $\bullet$  Notation not valid if i or n starts at 1 instead...
- Both in math and code it is advantageous to use index sets
- $i \in \mathcal{I}_x$  instead of  $i = 0, \dots, N_x$
- Definition:  $\mathcal{I}_x = \{0, \dots, N_x\}$
- The first index:  $i = \mathcal{I}_x^0$
- The last index:  $i = \mathcal{I}_x^{-1}$
- All interior points:  $i \in \mathcal{I}_x^i$ ,  $\mathcal{I}_x^i = \{1, \dots, N_x 1\}$
- $\mathcal{I}_x^-$  means  $\{0,\ldots,N_x-1\}$
- $\mathcal{I}_x^+$  means  $\{1,\ldots,N_x\}$

#### Index set notation in code

Notation	Python
$\mathcal{I}_x$	Ix
$\mathcal{I}_x^0$	Ix[0]
$\mathcal{I}_x^{-1}$	Ix[-1]
$\mathcal{I}_x^-$	Ix[1:]
$\mathcal{I}_x^+$	Ix[:-1]
$\mathcal{I}_x^i$	Ix[1:-1]

#### Index sets in action (1)

Index sets for a problem in the x, t plane:

$$\mathcal{I}_x = \{0, \dots, N_x\}, \quad \mathcal{I}_t = \{0, \dots, N_t\},$$
 (30)

Implemented in Python as

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

#### Index sets in action (2)

A finite difference scheme can with the index set notation be specified as

$$\begin{aligned} u_i^{n+1} &= -u_i^{n-1} + 2u_i^n + C^2 \left( u_{i+1}^n - 2u_i^n + u_{i-1}^n \right), \quad i \in \mathcal{I}_x^i, \ n \in \mathcal{I}_t^i \\ u_i &= 0, \quad i = \mathcal{I}_x^0, \ n \in \mathcal{I}_t^i \\ u_i &= 0, \quad i = \mathcal{I}_r^{-1}, \ n \in \mathcal{I}_t^i \end{aligned}$$

Corresponding implementation:

Program wave1D\_dn.py

#### Alternative implementation via ghost cells

- $\bullet$  Instead of modifying the stencil at the boundary, we extend the mesh to cover  $u^n_{-1}$  and  $u^n_{N_x+1}$
- The extra left and right cell are called *ghost cells*
- The extra points are called *ghost points*
- The  $u_{-1}^n$  and  $u_{N_x+1}^n$  values are called *ghost values*
- Update ghost values as  $u_{i-1}^n = u_{i+1}^n$  for i = 0 and  $i = N_x$
- Then the stencil becomes right at the boundary

#### Implementation of ghost cells (1)

Add ghost points:

```
u = zeros(Nx+3)
u_1 = zeros(Nx+3)
u_2 = zeros(Nx+3)

x = linspace(0, L, Nx+1) # Mesh points without ghost points
```

- A major indexing problem arises with ghost cells since Python indices *must* start at 0.
- u[-1] will always mean the last element in u
- Math indexing:  $-1, 0, 1, 2, \ldots, N_x + 1$
- Python indexing: 0,..,Nx+2
- Remedy: use index sets

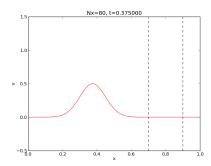
#### Implementation of ghost cells (2)

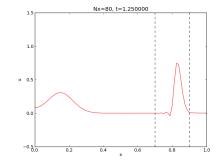
```
u = zeros(Nx+3)
Ix = range(1, u.shape[0]-1)
# Boundary values: u[Ix[0]], u[Ix[-1]]
# Set initial conditions
for i in Ix:
   u_1[i] = I(x[i-Ix[0]]) # Note i-Ix[0]
# Loop over all physical mesh points
for i in Ix:
   u[i] = -u_2[i] + 2*u_1[i] + 
          C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
# Update ghost values
i = Ix[0] # x=0 boundary
u[i-1] = u[i+1]
                # x=L boundary
i = Ix[-1]
u[i-1] = u[i+1]
```

Program: wave1D\_dn0\_ghost.py.

## Generalization: variable wave velocity

Heterogeneous media: varying c = c(x)





## The model PDE with a variable coefficient

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) + f(x, t) \tag{31}$$

This equation sampled at a mesh point  $(x_i, t_n)$ :

$$\frac{\partial^2}{\partial t^2}u(x_i,t_n) = \frac{\partial}{\partial x}\left(q(x_i)\frac{\partial}{\partial x}u(x_i,t_n)\right) + f(x_i,t_n),$$

#### Discretizing the variable coefficient (1)

The principal idea is to first discretize the outer derivative.

Define

$$\phi = q(x) \frac{\partial u}{\partial x}$$

Then use a centered derivative around  $x = x_i$  for the derivative of  $\phi$ :

$$\left[\frac{\partial \phi}{\partial x}\right]_{i}^{n} \approx \frac{\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}}{\Delta x} = [D_{x}\phi]_{i}^{n}$$

#### Discretizing the variable coefficient (2)

Then discretize the inner operators:

$$\phi_{i+\frac{1}{2}} = q_{i+\frac{1}{2}} \left[ \frac{\partial u}{\partial x} \right]_{i+\frac{1}{2}}^{n} \approx q_{i+\frac{1}{2}} \frac{u_{i+1}^{n} - u_{i}^{n}}{\Delta x} = [qD_{x}u]_{i+\frac{1}{2}}^{n}$$

Similarly,

$$\phi_{i-\frac{1}{2}} = q_{i-\frac{1}{2}} \left[ \frac{\partial u}{\partial x} \right]_{i-\frac{1}{2}}^{n} \approx q_{i-\frac{1}{2}} \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x} = [qD_{x}u]_{i-\frac{1}{2}}^{n}$$

#### Discretizing the variable coefficient (3)

These intermediate results are now combined to

$$\left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_{i}^{n} \approx \frac{1}{\Delta x^{2}}\left(q_{i+\frac{1}{2}}\left(u_{i+1}^{n}-u_{i}^{n}\right)-q_{i-\frac{1}{2}}\left(u_{i}^{n}-u_{i-1}^{n}\right)\right)$$
(32)

In operator notation:

$$\left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_{i}^{n} \approx \left[D_{x}qD_{x}u\right]_{i}^{n} \tag{33}$$

**Remark.** Many are tempted to use the chain rule on the term  $\frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right)$ , but this is not a good idea!

#### Computing the coefficient between mesh points

- Given q(x): compute  $q_{i+\frac{1}{2}}$  as  $q(x_{i+\frac{1}{2}})$
- Given q at the mesh points:  $q_i$ , use an average

$$q_{i+\frac{1}{2}} \approx \frac{1}{2} (q_i + q_{i+1}) = [\overline{q}^x]_i \qquad \text{(arithmetic mean)}$$
 (34)

$$q_{i+\frac{1}{2}} \approx 2\left(\frac{1}{q_i} + \frac{1}{q_{i+1}}\right)^{-1}$$
 (harmonic mean) (35)

$$q_{i+\frac{1}{2}} \approx (q_i q_{i+1})^{1/2}$$
 (geometric mean) (36)

The arithmetic mean in (34) is by far the most used averaging technique.

## Discretization of variable-coefficient wave equation in operator notation

$$[D_t D_t u = D_x \overline{q}^x D_x u + f]_i^n \tag{37}$$

We clearly see the type of finite differences and averaging! Write out and solve wrt  $u_i^{n+1}$ :

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta t}{\Delta x}\right)^2 \times \left(\frac{1}{2}(q_i + q_{i+1})(u_{i+1}^n - u_i^n) - \frac{1}{2}(q_i + q_{i-1})(u_i^n - u_{i-1}^n)\right) + \Delta t^2 f_i^n$$
(38)

#### Neumann condition and a variable coefficient

Consider  $\partial u/\partial x = 0$  at  $x = L = N_x \Delta x$ :

$$\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \quad u_{i+1}^n = u_{i-1}^n, \quad i = N_x$$

Insert  $u_{i+1}^n = u_{i-1}^n$  in the stencil (38) for  $i = N_x$  and obtain

$$u_i^{n+1} \approx -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta t}{\Delta x}\right)^2 2q_i(u_{i-1}^n - u_i^n) + \Delta t^2 f_i^n$$

(We have used  $q_{i+\frac{1}{2}} + q_{i-\frac{1}{2}} \approx 2q_i$ .)

Alternative: assume dq/dx = 0 (simpler).

#### Implementation of variable coefficients

Assume c[i] holds  $c_i$  the spatial mesh points

Here: C2=(dt/dx)\*\*2 Vectorized version:

```
 \begin{array}{l} 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]) \end{array}
```

Neumann condition  $u_x = 0$ : same ideas as in 1D (modified stencil or ghost cells).

#### A more general model PDE with variable coefficients

$$\varrho(x)\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) + f(x, t) \tag{39}$$

A natural scheme is

$$[\rho D_t D_t u = D_x \overline{q}^x D_x u + f]_i^n \tag{40}$$

Or

$$[D_t D_t u = \varrho^{-1} D_x \overline{q}^x D_x u + f]_i^n \tag{41}$$

No need to average  $\rho$ , just sample at i

#### Generalization: damping

Why do waves die out?

- Damping (non-elastic effects, air resistance)
- 2D/3D: conservation of energy makes an amplitude reduction by  $1/\sqrt{r}$  (2D) or 1/r (3D)

Simplest damping model (for physical behavior, see demo):

$$\frac{\partial^2 u}{\partial t^2} + b \frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} + f(x, t), \tag{42}$$

 $b \ge 0$ : prescribed damping coefficient.

Discretization via centered differences to ensure  $\mathcal{O}(\Delta t^2)$  error:

$$[D_t D_t u + b D_{2t} u = c^2 D_x D_x u + f]_i^n (43)$$

Need special formula for  $u_i^1$  + special stencil (or ghost cells) for Neumann conditions.

## Building a general 1D wave equation solver

The program wave1D\_dn\_vc.py solves a fairly general 1D wave equation:

$$u_t = (c^2(x)u_x)_x + f(x,t),$$
  $x \in (0,L), t \in (0,T]$  (44)

$$u(x,0) = I(x),$$
  $x \in [0,L]$  (45)

$$u_t(x,0) = V(t),$$
  $x \in [0,L]$  (46)

$$u(0,t) = U_0(t) \text{ or } u_x(0,t) = 0,$$
  $t \in (0,T]$  (47)

$$u(L,t) = U_L(t) \text{ or } u_x(L,t) = 0,$$
  $t \in (0,T]$  (48)

Can be adapted to many needs.

#### Collection of initial conditions

The function pulse in wave1D\_dn\_vc.py offers four initial conditions:

- 1. a rectangular pulse ("plug")
- 2. a Gaussian function (gaussian)

- 3. a "cosine hat": one period of  $1 + \cos(\pi x, x \in [-1, 1])$
- 4. half a "cosine hat": half a period of  $\cos \pi x,\,x\in[-\frac{1}{2},\frac{1}{2}]$

Can locate the initial pulse at x = 0 or in the middle

```
>>> import wave1D_dn_vc as w
>>> w.pulse(loc='left', pulse_tp='cosinehat', Nx=50, every_frame=10)
```

## Finite difference methods for 2D and 3D wave equations

Constant wave velocity c:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \text{ for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d, \ t \in (0, T]$$
(49)

Variable wave velocity:

$$\varrho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot (q \nabla u) + f \text{ for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d, \ t \in (0, T]$$
 (50)

#### Examples on wave equations written out in 2D/3D

3D, constant c:

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

2D, variable c:

$$\varrho(x,y)\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(q(x,y)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(q(x,y)\frac{\partial u}{\partial y}\right) + f(x,y,t) \tag{51}$$

Compact notation:

$$u_{tt} = c^2(u_{xx} + u_{yy} + u_{zz}) + f, (52)$$

$$\varrho u_{tt} = (qu_x)_x + (qu_z)_z + (qu_z)_z + f \tag{53}$$

## Boundary and initial conditions

We need one boundary condition at each point on  $\partial\Omega$ :

- 1. u is prescribed (u = 0 or known incoming wave)
- 2.  $\partial u/\partial n = \mathbf{n} \cdot \nabla u$  prescribed (= 0: reflecting boundary)
- 3. open boundary (radiation) condition:  $u_t + \mathbf{c} \cdot \nabla u = 0$  (let waves travel undisturbed out of the domain)

PDEs with second-order time derivative need two initial conditions:

- 1. u = I,
- 2.  $u_t = V$ .

#### Example: 2D propagation of Gaussian function

#### Mesh

- Mesh point:  $(x_i, y_i, z_k, t_n)$
- x direction:  $x_0 < x_1 < \cdots < x_{N_x}$
- y direction:  $y_0 < y_1 < \cdots < y_{N_y}$
- z direction:  $z_0 < z_1 < \cdots < z_{N_z}$
- $u_{i,j,k}^n \approx u_{\mathrm{e}}(x_i, y_j, z_k, t_n)$

#### Discretization

$$[D_t D_t u = c^2 (D_x D_x u + D_y D_y u) + f]_{i,i,k}^n,$$

Written out in detail:

$$\frac{u_{i,j}^{n+1} - 2u_{i,j}^n + u_{i,j}^{n-1}}{\Delta t^2} = c^2 \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + c^2 \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} + f_{i,j}^n,$$

 $u_{i,j}^{n-1}$  and  $u_{i,j}^n$  are known, solve for  $u_{i,j}^{n+1}$ :

$$u_{i,j}^{n+1} = 2u_{i,j}^n + u_{i,j}^{n-1} + c^2 \Delta t^2 [D_x D_x u + D_y D_y u]_{i,j}^n$$

#### Special stencil for the first time step

- The stencil for  $u_{i,j}^1$  (n=0) involves  $u_{i,j}^{-1}$  which is outside the time mesh
- Remedy: use discretized  $u_t(x,0) = V$  and the stencil for n = 0 to develop a special stencil (as in the 1D case)

$$[D_{2t}u = V]_{i,j}^{0} \Rightarrow u_{i,j}^{-1} = u_{i,j}^{1} - 2\Delta t V_{i,j}$$
$$u_{i,j}^{n+1} = u_{i,j}^{n} - 2\Delta V_{i,j} + \frac{1}{2}c^{2}\Delta t^{2}[D_{x}D_{x}u + D_{y}D_{y}u]_{i,j}^{n}$$

#### Variable coefficients (1)

3D wave equation:

$$\varrho u_{tt} = (qu_x)_x + (qu_y)_y + (qu_z)_z + f(x, y, z, t)$$

Just apply the 1D discretization for each term:

$$[\varrho D_t D_t u = (D_x \overline{q}^x D_x u + D_y \overline{q}^y D_y u + D_z \overline{q}^z D_z u) + f]_{i,j,k}^n$$
(54)

Need special formula for  $u_{i,j,k}^1$  (use  $[D_{2t}u=V]^0$  and stencil for n=0).

#### Variable coefficients (2)

Written out:

$$\begin{split} u_{i,j,k}^{n+1} &= -u_{i,j,k}^{n-1} + 2u_{i,j,k}^n + \\ &= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} (\frac{1}{2} (q_{i,j,k} + q_{i+1,j,k}) (u_{i+1,j,k}^n - u_{i,j,k}^n) - \\ &\qquad \frac{1}{2} (q_{i-1,j,k} + q_{i,j,k}) (u_{i,j,k}^n - u_{i-1,j,k}^n)) + \\ &= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} (\frac{1}{2} (q_{i,j,k} + q_{i,j+1,k}) (u_{i,j+1,k}^n - u_{i,j,k}^n) - \\ &\qquad \frac{1}{2} (q_{i,j-1,k} + q_{i,j,k}) (u_{i,j,k}^n - u_{i,j-1,k}^n)) + \\ &= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} (\frac{1}{2} (q_{i,j,k} + q_{i,j,k+1}) (u_{i,j,k+1}^n - u_{i,j,k}^n) - \\ &\qquad \frac{1}{2} (q_{i,j,k-1} + q_{i,j,k}) (u_{i,j,k}^n - u_{i,j,k-1}^n)) + \\ &+ \Delta t^2 f_{i,j,k}^n \end{split}$$

## Neumann boundary condition in 2D

Use ideas from 1D! Example:  $\frac{\partial u}{\partial n}$  at y=0,  $\frac{\partial u}{\partial n}=-\frac{\partial u}{\partial y}$  Boundary condition discretization:

$$[-D_{2y}u = 0]_{i,0}^n \quad \Rightarrow \quad \frac{u_{i,1}^n - u_{i,-1}^n}{2\Delta y} = 0, \ i \in \mathcal{I}_x$$

Insert  $u_{i,-1}^n = u_{i,1}^n$  in the stencil for  $u_{i,j=0}^{n+1}$  to obtain a modified stencil on the boundary.

Pattern: use interior stencil also on the bundary, but replace j-1 by j+1 Alternative: use ghost cells and ghost values

## Implementation of 2D/3D problems

$$u_t = c^2(u_{xx} + u_{yy}) + f(x, y, t),$$
  $(x, y) \in \Omega, \ t \in (0, T]$  (55)

$$u(x, y, 0) = I(x, y), \tag{56}$$

$$u_t(x, y, 0) = V(x, y), \qquad (x, y) \in \Omega \qquad (57)$$

$$u = 0, (x, y) \in \partial\Omega, \ t \in (0, T] (58)$$

$$\Omega = [0, L_x] \times [0, L_y]$$

Discretization:

$$[D_t D_t u = c^2 (D_x D_x u + D_y D_y u) + f]_{i,j}^n,$$

#### Algorithm

- 1. Set initial condition  $u_{i,j}^0 = I(x_i, y_j)$
- 2. Compute  $u_{i,j}^1 = \cdots$  for  $i \in \mathcal{I}_x^i$  and  $j \in \mathcal{I}_y^i$
- 3. Set  $u_{i,j}^1 = 0$  for the boundaries  $i = 0, N_x, j = 0, N_y$
- 4. For  $n = 1, 2, ..., N_t$ :
  - (a) Find  $u_{i,j}^{n+1} = \cdots$  for  $i \in \mathcal{I}_x^i$  and  $j \in \mathcal{I}_y^i$
  - (b) Set  $u_{i,j}^{n+1} = 0$  for the boundaries  $i = 0, N_x, j = 0, N_y$

#### Scalar computations: mesh

Program: wave2D\_u0.py

 Mesh:

#### Scalar computations: arrays

Store  $u_{i,j}^{n+1}$ ,  $u_{i,j}^{n}$ , and  $u_{i,j}^{n-1}$  in three two-dimensional arrays:

```
u = zeros((Nx+1,Ny+1))  # solution array
u_1 = zeros((Nx+1,Ny+1))  # solution at t-dt
u_2 = zeros((Nx+1,Ny+1))  # solution at t-2*dt
```

 $u_{i,j}^{n+1}$  corresponds to u[i,j], etc.

#### Scalar computations: initial condition

```
Ix = range(0, u.shape[0])
Iy = range(0, u.shape[1])
It = range(0, t.shape[0])

for i in Ix:
    for j in Iy:
        u_1[i,j] = I(x[i], y[j])

if user_action is not None:
    user_action(u_1, x, xv, y, yv, t, 0)
```

Arguments xv and yv: for vectorized computations

#### Scalar computations: primary stencil

```
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_x = 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
```

D1 and D2: allow advance\_scalar to be used also for  $u_{i,j}^1$ :

#### Vectorized computations: mesh coordinates

Mesh with  $30 \times 30$  cells: vectorization reduces the CPU time by a factor of 70 (!).

Need special coordinate arrays xv and yv such that I(x,y) and f(x,y,t) can be vectorized:

```
from numpy import newaxis
xv = x[:,newaxis]
yv = y[newaxis,:]
```

```
u_1[:,:] = I(xv, yv)
f_a[:,:] = f(xv, yv, t)
```

#### Vectorized computations: stencil

```
def advance_vectorized(u, u_1, u_2, f_a, Cx2, Cy2, dt2,
                       V=None, step1=False):
    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
    u_x = u_1[:-2,1:-1] - 2*u_1[1:-1,1:-1] + u_1[2:,1:-1]
    u_yy = u_1[1:-1,:-2] - 2*u_1[1:-1,1:-1] + u_1[1:-1,2:]
    u[1:-1,1:-1] = D1*u_1[1:-1,1:-1] - D2*u_2[1:-1,1:-1] + \
                  Cx2*u_xx + Cy2*u_yy + dt2*f_a[1:-1,1:-1]
    if step1:
       u[1:-1,1:-1] += dt*V[1:-1, 1:-1]
    # Boundary condition u=0
    j = 0
    u[:,j] = 0
    j = u.shape[1]-1
   u[:,j] = 0
    i = 0
    u[i,:] = 0
    i = u.shape[0]-1
   u[i,:] = 0
    return u
```

## Verification: quadratic solution (1)

Manufactured solution:

$$u_{e}(x, y, t) = x(L_{x} - x)y(L_{y} - y)(1 + \frac{1}{2}t)$$
(59)

Requires  $f = 2c^2(1 + \frac{1}{2}t)(y(L_y - y) + x(L_x - x)).$ 

This  $u_e$  is ideal because it also solves the discrete equations!

#### Verification: quadratic solution (2)

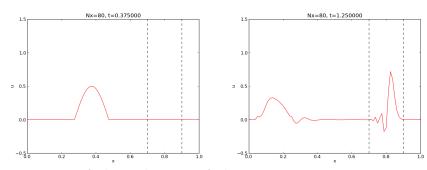
- $\bullet \ [D_t D_t 1]^n = 0$
- $\bullet \ [D_t D_t t]^n = 0$

- $\bullet \ [D_t D_t t^2] = 2$
- $D_t D_t$  is a linear operator:  $[D_t D_t (au + bv)]^n = a[D_t D_t u]^n + b[D_t D_t v]^n$

$$[D_x D_x u_e]_{i,j}^n = [y(L_y - y)(1 + \frac{1}{2}t)D_x D_x x(L_x - x)]_{i,j}^n$$
$$= y_j (L_y - y_j)(1 + \frac{1}{2}t_n)2$$

- $\bullet$  Similar calculations for  $[D_yD_yu_{\rm e}]_{i,j}^n$  and  $[D_tD_tu_{\rm e}]_{i,j}^n$  terms
- Must also check the equation for  $u_{i,j}^1$

## Analysis of the difference equations



#### Properties of the solution of the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Solutions:

$$u(x,t) = g_R(x - ct) + g_L(x + ct)$$

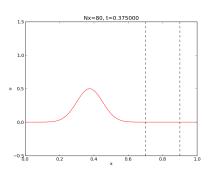
If u(x,0) = I(x) and  $u_t(x,0) = 0$ :

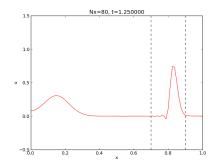
$$u(x,t) = \frac{1}{2}I(x-ct) + \frac{1}{2}I(x+ct)$$

Two waves: one traveling to the right and one to the left

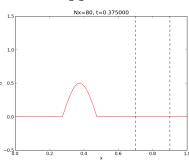
## Demo of the splitting of I(x) into two waves Simulation of a case with variable wave velocity

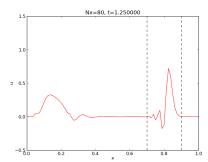
A wave propagates perfectly (C=1) and hits a medium with 1/4 of the wave velocity (C=0.25). A part of the wave is reflected and the rest is transmitted.





Let us change the shape of the initial condition slightly and see what happens





Representation of waves as sum of sine/cosine waves

Build I(x) of wave components  $e^{ikx} = \cos kx + i\sin kx$ :

$$I(x) \approx \sum_{k \in K} b_k e^{ikx}$$

- $\bullet\,$  Fit  $b_k$  by a least squares or projection method
- k is the frequency of a component ( $\lambda = 2\pi/k$  is the wave length in space)
- K is some set of all k needed to approximate I(x) well
- $b_k$  must be computed (Fourier coefficients)

Since  $u(x,t) = \frac{1}{2}I(x-ct) + \frac{1}{2}I(x+ct)$ , the exact solution is

$$u(x,t) = \frac{1}{2} \sum_{k \in K} b_k e^{ik(x-ct)} + \frac{1}{2} \sum_{k \in K} b_k e^{ik(x+ct)}$$

Our interest: one component  $e^{i(kx-\omega t)}$ ,  $\omega=kc$ 

## A similar wave component is also a solution of the finite difference scheme (!)

Idea: a similar discrete  $u_q^n = e^{i(kx_q - \tilde{\omega}t_n)}$  solution (corresponding to the exact  $e^{i(kx - \omega t)}$ ) solves

$$[D_t D_t u = c^2 D_x D_x u]_q^n$$

Note: we expect numerical frequency  $\tilde{\omega} \neq \omega$ 

- How accurate is  $\tilde{\omega}$  compared to  $\omega$ ?
- What about the wave amplitude (can  $\tilde{\omega}$  become complex)?

#### Preliminary results

$$[D_t D_t e^{i\omega t}]^n = -\frac{4}{\Delta t^2} \sin^2\left(\frac{\omega \Delta t}{2}\right) e^{i\omega n \Delta t}$$

By  $\omega \to k$ ,  $t \to x$ ,  $n \to q$ ) it follows that

$$[D_x D_x e^{ikx}]_q = -\frac{4}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) e^{ikq\Delta x}$$

#### Insertion of the numerical wave component

Inserting a basic wave component  $u=e^{i(kx_q-\tilde{\omega}t_n)}$  in the scheme requires computation of

$$\begin{split} [D_t D_t e^{ikx} e^{-i\tilde{\omega}t}]_q^n &= [D_t D_t e^{-i\tilde{\omega}t}]^n e^{ikq\Delta x} \\ &= -\frac{4}{\Delta t^2} \sin^2 \left(\frac{\tilde{\omega}\Delta t}{2}\right) e^{-i\tilde{\omega}n\Delta t} e^{ikq\Delta x} \\ [D_x D_x e^{ikx} e^{-i\tilde{\omega}t}]_q^n &= [D_x D_x e^{ikx}]_q e^{-i\tilde{\omega}n\Delta t} \\ &= -\frac{4}{\Delta x^2} \sin^2 \left(\frac{k\Delta x}{2}\right) e^{ikq\Delta x} e^{-i\tilde{\omega}n\Delta t} \end{split}$$

#### The equation for $\tilde{\omega}$

The complete scheme,

$$[D_t D_t e^{ikx} e^{-i\tilde{\omega}t} = c^2 D_x D_x e^{ikx} e^{-i\tilde{\omega}t}]_q^n$$

leads to an equation for  $\tilde{\omega}$  (which can readily be solved):

$$\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C^2\sin^2\left(\frac{k\Delta x}{2}\right), \quad C = \frac{c\Delta t}{\Delta x} \text{ (Courant number)}$$

Taking the square root:

$$\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C\sin\left(\frac{k\Delta x}{2}\right)$$

#### The numerical dispersion relation

Can easily solve for an explicit formula for  $\tilde{\omega}$ :

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left( C \sin \left( \frac{k \Delta x}{2} \right) \right)$$

Note:

• This  $\tilde{\omega} = \tilde{\omega}(k, c, \Delta x, \Delta t)$  is the numerical dispersion relation

• Inserting  $e^{kx-\omega t}$  in the PDE leads to  $\omega = kc$ , which is the analytical/exact dispersion relation

• Speed of waves might be easier to imagine:

- Exact speed:  $c = \omega/k$ ,

- Numerical speed:  $\tilde{c} = \tilde{\omega}/k$ 

 $\bullet$  We shall investigate  $\tilde{c}/c$  to see how wrong the speed of a numerical wave component is

## The special case C = 1 gives the exact solution

• For  $C=1, \, \tilde{\omega}=\omega$ 

• The numerical solution is exact (at the mesh points), regardless of  $\Delta x$  and  $\Delta t = c^{-1}\Delta x!$ 

• The only requirement is constant c

• The numerical scheme is then a simple-to-use analytical solution method for the wave equation

#### Computing the error in wave velocity

• Introduce  $p = k\Delta x/2$  (the important dimensionless spatial discretization parameter)

• p measures no of mesh points in space per wave length in space

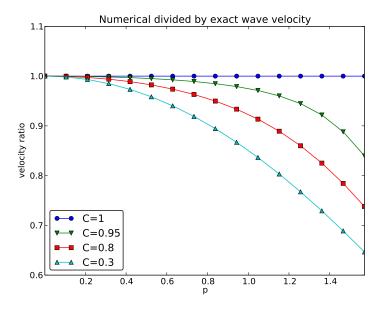
• Shortest possible wave length in mesh:  $\lambda = 2\Delta x$ ,  $k = 2\pi/\lambda = \pi/\Delta x$ , and  $p = k\Delta x/2 = \pi/2 \implies p \in (0, \pi/2]$ 

• Study error in wave velocity through  $\tilde{c}/c$  as function of p

$$r(C,p) = \frac{\tilde{c}}{c} = \frac{2}{kc\Delta t} \sin^{-1}(C\sin p) = \frac{2}{kC\Delta x} \sin^{-1}(C\sin p) = \frac{1}{Cp} \sin^{-1}(C\sin p)$$
  
Can plot  $r(C,p)$  for  $p \in (0,\pi/2], C \in (0,1]$ 

#### Visualizing the error in wave velocity

```
def r(C, p):
    return 1/(C*p)*asin(C*sin(p))
```



Note: the shortest waves have the largest error, and short waves move too slowly.

#### Taylor expanding the error in wave velocity

For small p, Taylor expand  $\tilde{\omega}$  as polynomial in p:

```
>>> C, p = symbols('C p')
>>> rs = r(C, p).series(p, 0, 7)
>>> print rs
1 - p**2/6 + p**4/120 - p**6/5040 + C**2*p**2/6 -
C**2*p**4/12 + 13*C**2*p**6/720 + 3*C**4*p**4/40 -
```

```
C**4*p**6/16 + 5*C**6*p**6/112 + O(p**7)

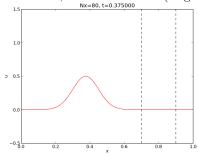
>>> # Drop the remainder O(...) term
>>> rs = rs.removeO()
>>> # Factorize each term
>>> rs = [factor(term) for term in rs.as_ordered_terms()]
>>> rs = sum(rs)
>>> print rs
p**6*(C - 1)*(C + 1)*(225*C**4 - 90*C**2 + 1)/5040 +
p**4*(C - 1)*(C + 1)*(3*C - 1)*(3*C + 1)/120 +
p**2*(C - 1)*(C + 1)/6 + 1
```

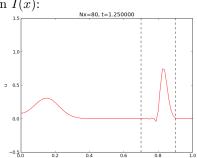
Leading error term is  $\frac{1}{6}(C^2-1)p^2$  or

$$\frac{1}{6} \left(\frac{k\Delta x}{2}\right)^2 (C^2 - 1) = \frac{k^2}{24} \left(c^2 \Delta t^2 - \Delta x^2\right) = \mathcal{O}(\Delta t^2, \Delta x^2)$$

## Example on effect of wrong wave velocity (1)

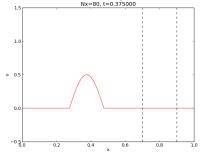
Smooth wave, few short waves (large k) in I(x):

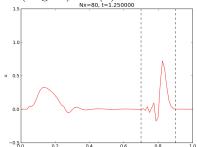




#### Example on effect of wrong wave velocity (1)

Not so smooth wave, significant short waves (large k) in I(x):





#### Stability

$$\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C\sin\left(\frac{k\Delta x}{2}\right)$$

- Exact  $\omega$  is real
- Complex  $\tilde{\omega}$  will lead to exponential growth of the amplitude
- Stability criterion: real  $\tilde{\omega}$
- Then  $\sin(\tilde{\omega}\Delta t/2) \in [-1,1]$
- $k\Delta x/2$  is always real, so right-hand side is in [-C, C]
- Then we must have  $C \leq 1$

Stability criterion:

$$C = \frac{c\Delta t}{\Delta x} \le 1$$

#### Why C > 1 leads to non-physical waves

Recall that right-hand side is in [-C, C]. Then C > 1 means

$$\underbrace{\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right)}_{\geq 1} = C\sin\left(\frac{k\Delta x}{2}\right)$$

- $|\sin x| > 1$  implies complex x
- Here: complex  $\tilde{\omega} = \tilde{\omega}_r \pm i\tilde{\omega}_i$
- One  $\tilde{\omega}_i < 0$  gives  $\exp(i \cdot i\tilde{\omega}_i) = \exp(-\tilde{\omega}_i)$  and exponential growth
- This wave component will after some time dominate the solution give an overall exponentially increasing amplitude (non-physical!)

## Extending the analysis to 2D (and 3D)

$$u(x, y, t) = g(k_x x + k_y y - \omega t)$$

is a typically solution of

$$u_{tt} = c^2(u_{xx} + u_{yy})$$

Can build solutions by adding complex Fourier components of the form

$$e^{i(k_x x + k_y y - \omega t)}$$

#### Discrete wave components in 2D

$$[D_t D_t u = c^2 (D_x D_x u + D_y D_y u)]_{q,r}^n$$

This equation admits a Fourier component

$$u_{q,r}^n = e^{i(k_x q \Delta x + k_y r \Delta y - \tilde{\omega} n \Delta t)}$$

Inserting the expression and using formulas from the 1D analysis:

$$\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C_x^2 \sin^2 p_x + C_y^2 \sin^2 p_y$$

where

$$C_x = \frac{c\Delta t}{\Delta x}, \quad C_y = \frac{c\Delta t}{\Delta y}, \quad p_x = \frac{k_x \Delta x}{2}, \quad p_y = \frac{k_y \Delta y}{2}$$

#### Stability criterion in 2D

R<br/>real-valued  $\tilde{\omega}$  requires

$$C_x^2 + C_y^2 \le 1$$

or

$$\Delta t \le \frac{1}{c} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1/2}$$

#### Stability criterion in 3D

$$\Delta t \le \frac{1}{c} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2}$$

For  $c^2=c^2(\boldsymbol{x})$  we must use the worst-case value  $\bar{c}=\sqrt{\max_{\boldsymbol{x}\in\Omega}c^2(\boldsymbol{x})}$  and a safety factor  $\beta\leq 1$ :

$$\Delta t \le \beta \frac{1}{\bar{c}} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2}$$

#### Numerical dispersion relation in 2D (1)

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left( \left( C_x^2 \sin^2 p_x + C_y^2 \sin_y^p \right)^{\frac{1}{2}} \right)$$

For visualization, introduce  $\theta$ :

$$k_x = k \sin \theta$$
,  $k_y = k \cos \theta$ ,  $p_x = \frac{1}{2}kh \cos \theta$ ,  $p_y = \frac{1}{2}kh \sin \theta$ 

Also:  $\Delta x = \Delta y = h$ . Then  $C_x = C_y = c\Delta t/h \equiv C$ .

Now  $\tilde{\omega}$  depends on

- ullet C reflecting the number cells a wave is displaced during a time step
- $\bullet$  kh reflecting the number of cells per wave length in space
- $\theta$  expressing the direction of the wave

## Numerical dispersion relation in 2D (2)

$$\frac{\tilde{c}}{c} = \frac{1}{Ckh} \sin^{-1} \left( C \left( \sin^2 \left( \frac{1}{2} kh \cos \theta \right) + \sin^2 \left( \frac{1}{2} kh \sin \theta \right) \right)^{\frac{1}{2}} \right)$$

Can make color contour plots of  $1 - \tilde{c}/c$  in *polar coordinates* with  $\theta$  as the angular coordinate and kh as the radial coordinate.

## Numerical dispersion relation in 2D (3)

