# Study Guide: Finite difference methods for wave motion

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# 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

$$
\begin{aligned}
\frac{\partial^2 u}{\partial t^2} &= c^2 \frac{\partial^2 u}{\partial x^2}, & x \in (0, L),\ t \in (0, T] \qquad (1)\\
u(x, 0) &= I(x), & x \in [0, L] \qquad (2)\\
\frac{\partial}{\partial t} u(x, 0) &= 0, & x \in [0, L] \qquad (3)\\
u(0, t) &= 0, & t \in (0, T] \qquad (4)\\
u(L, t) &= 0, & t \in (0, T] \qquad (5)
\end{aligned}
$$

# 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:

$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t-1} < t_{N_t} = T \qquad (6)$$

Mesh in space:

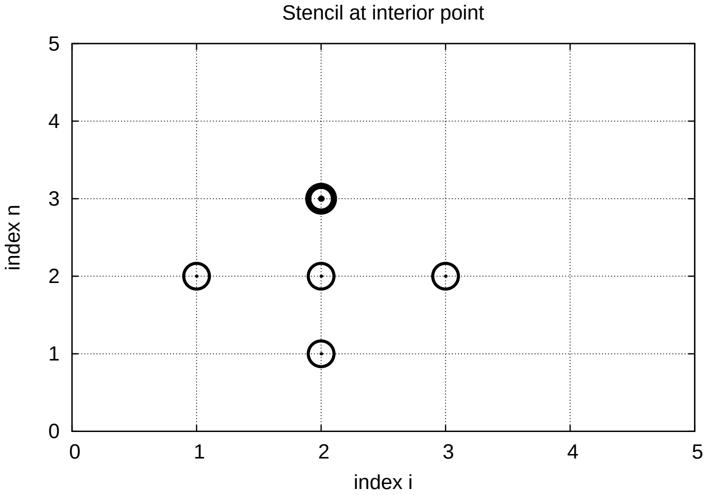
$$0 = x_0 < x_1 < x_2 < \cdots < x_{N_x-1} < x_{N_x} = L \qquad (7)$$

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

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

# The discrete solution

- The numerical solution is a mesh function: $u_i^n \approx u_{\mathrm{e}}(x_i, t_n)$
- 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 $i = 1, \ldots, N_x - 1$ and $n = 1, \ldots, N_t - 1$.
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 $u_t(x,0)$

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

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

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

# Step 4: Formulating a recursive algorithm

- Nature of the algorithm: compute $u$ in space at $t = \Delta t, 2\Delta t, 3\Delta t, \ldots$
- 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 $[D_tD_t u = c^2 D_x D_x]_i^n$ and solve for $u_i^{n+1}$,

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

# The Courant number

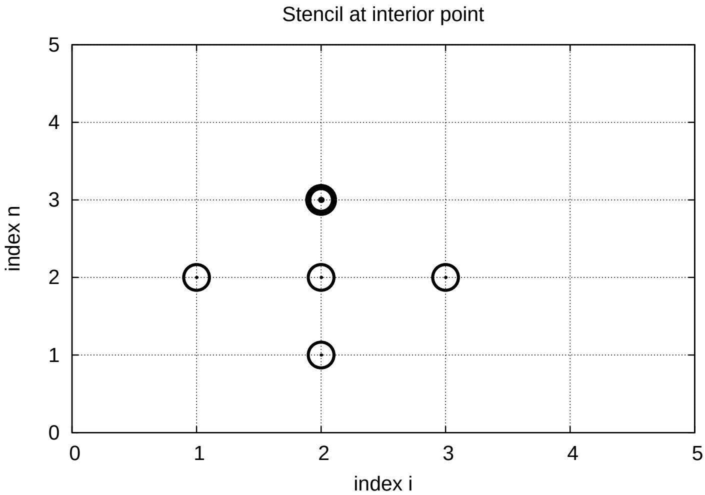
$$C = c\frac{\Delta t}{\Delta x}, \tag{13}$$

is known as the (dimensionless) *Courant number*

**Notice.**

There is only one parameter, $C$, in the discrete model: $C$ lumps mesh parameters with 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
- 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

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

# The algorithm

1. Compute $u_i^0 = I(x_i)$ for $i = 0, \ldots, N_x$
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 $n = 1, 2, \ldots, N_t - 1$
    1. apply (12) to find $u_i^{n+1}$ for $i = 1, \ldots, N_x - 1$
    2. 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:
  - `u[i]` stores $u_i^{n+1}$
  - `u_1[i]` stores $u_i^n$
  - `u_2[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):
    # Update all inner mesh points at time t[n+1]
    for i in range(1, Nx):
        u[i] = 2u_1[i] - u_2[i] - \
               C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])

    # Insert boundary conditions
    u[0] = 0;  u[Nx] = 0
```

# 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 $u_t(x,0)$:

$$\begin{aligned}
u_{tt} &= c^2 u_{xx} + f(x,t), & & (15)\\
u(x,0) &= I(x), & x \in [0,L] & \quad (16)\\
u_t(x,0) &= V(x), & x \in [0,L] & \quad (17)\\
u(0,t) &= 0, & t > 0, & \quad (18)\\
u(L,t) &= 0, & t > 0 & \quad (19)
\end{aligned}$$

# Discrete model for the generalized model problem

$$[D_tD_tu = c^2D_xD_x + f]^n_i \tag{20}$$

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

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

# Modified equation for the first time level

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

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

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

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

# Using an analytical solution of physical significance

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

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

- PDE data: $f = 0$, boundary conditions $u_e(0, t) = u_e(L, 0) = 0$, 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 $u_{\mathrm{e}}(x, t)$
  - Insert in PDE and fit $f$
  - Set boundary and initial conditions compatible with the chosen $u_{\mathrm{e}}(x, t)$

# Manufactured solution: example

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

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

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

Initial conditions become

$$\begin{aligned} u(x,0) &= I(x) = 0 \\ u_t(x,0) &= V(x) = (2 - x(L-x))\cos t \end{aligned}$$

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), $i = 0, \ldots, m$
- 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: $r_i \rightarrow 2$ 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 $u_{\mathrm{e}}$ also solves the discrete equations!
Useful preliminary result:

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

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

Hence,

$$[D_tD_t u_{\mathrm{e}}]^n_i = x_i(L-x_i)[D_tD_t(1+\frac{1}{2}t)]^n = x_i(L-x_i)\frac{1}{2}[D_tD_t t]^n = 0$$

# Analytical work with the discrete equations (1)

$$[D_xD_xu_e]^n_i = (1+\frac{1}{2}t_n)[D_xD_x(xL-x^2)]_i = (1+\frac{1}{2}t_n)[LD_xD_xx - D_xD_xx^2$$
$$= -2(1+\frac{1}{2}t_n)$$

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

$$[D_tD_tu_e - c^2D_xD_xu_e - f]^n_i = 0 - c^2(-1)2(1+\frac{1}{2}t_n + 2(1+\frac{1}{2}t_n)c^2 = 0$$

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

# Testing with the exact discrete solution

- We have established that $u_i^{n+1} = u_{\mathrm{e}}(x_i, t_{n+1}) = x_i(L - x_i)(1 + t_{n+1}/2)$
- Run *one* simulation with one choice of $c$, $\Delta t$, and $\Delta x$
- Check that $\max_i |u_i^{n+1} - u_{\mathrm{e}}(x_i, t_{n+1})| < \epsilon$, $\epsilon \sim 10^{-14}$ (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 $C = 1$ (!)

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# Implementation

# The algorithm

1. Compute $u_i^0 = I(x_i)$ for $i = 0, \ldots, N_x$
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 $n = 1, 2, \ldots, N_t - 1$
    1. apply (12) to find $u_i^{n+1}$ for $i = 1, \ldots, N_x - 1$
    2. 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)

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

```
def solver(I, V, f, c, L, Nx, C, T, user_action=None):
    ...
    # Special formula for first time step
    n = 0
    for i in range(1, Nx):
        u[i] = u_1[i] + dt*V(x[i]) + \
                  0.5*C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
                  0.5*dt**2*f(x[i], t[n])
    u[0] = 0;  u[Nx] = 0

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

    # Switch variables before next step
    u_2[:], u_1[:] = u_1, u


===== Making a solver function (3) =====

\begin{minted}[fontsize=\fontsize{9pt}{9pt},linenos=false,mathescap
def solver(I, V, f, c, L, Nx, C, T, user_action=None):
    ...
    # Time loop

    for n in range(1, Nt):
        # Update all inner points at time t[n+1]
        for i in range(1, Nx):
            u[i] = - u_2[i] + 2*u_1[i] + \
```

# Verification: exact quadratic solution

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

```
import nose.tools as nt

def test_quadratic():
    """Check that u(x,t)=x(L-x)(1+t/2) is exactly reproduced."""
    def exact_solution(x, t):
        return x*(L-x)*(1 + 0.5*t)

    def I(x):
        return exact_solution(x, 0)

    def V(x):
        return 0.5*exact_solution(x, 0)

    def f(x, t):
        return 2*(1 + 0.5*t)*c**2

    L = 2.5
    c = 1.5
    Nx = 3  # Very coarse mesh
    C = 0.75
    T = 18

    u, x, t, cpu = solver(I, V, f, c, L, Nx, C, T)
    u_e = exact_solution(x, t[-1])
    diff = abs(u - u_e).max()
```

# 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, Nx, C, T, umin, umax, animate=True):
    """Run solver and visualize u at each time level."""
    import scitools.std as plt
    import time, glob, os

    def plot_u(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

    # Clean up old movie frames
    for filename in glob.glob('frame_*.png'):
        os.remove(filename)

    user_action = plot_u if animate else None
    u, x, t, cpu = solver(I, V, f, c, L, Nx, C, T, user_action)

    # Make movie files
    fps = 4  # Frames per second
```

# 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 -vcodec flv       movie.flv
Terminal> avconv -r 4 -i frame_%04d.png -vcodec libtheora movie.ogg
Terminal> avconv -r 4 -i frame_%04d.png -vcodec libx264   movie.mp4
Terminal> avconv -r 4 -i frame_%04d.png -vcodec libtheora movie.ogg
Terminal> avconv -r 4 -i frame_%04d.png -vcodec 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)

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

Appropriate data:

- $L = 75$ cm, $x_0 = 0.8L$, $a = 5$ mm, $N_x = 50$, 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
    Nx = 50

    def I(x):
        return a*x/x0 if x < x0 else a/(L-x0)*(L-x)

    umin = -1.2*a;  umax = -umin
    cpu = viz(I, 0, 0, c, L, Nx, C, T, umin, umax, animate=True)
```

Program: `wave1D_u0_s.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 $N_x$)

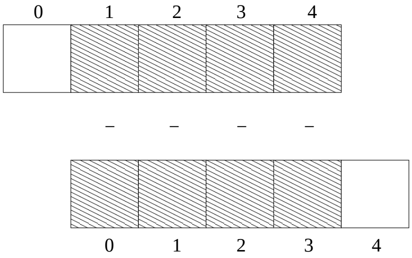
Next: vectorized loops

# 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 $d = (u_1, u_2, \ldots, u_n) - (u_0, u_1, \ldots, u_{n-1})$
- 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 `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:])
```

or

```
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_u0_sv.py`

# Verification of the vectorized version

```python
def test_quadratic():
    """
    Check the scalar and vectorized versions work 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
    exact_solution = lambda x, t: x*(L - x)*(1 + 0.5*t)
    I = lambda x: exact_solution(x, 0)
    V = lambda x: 0.5*exact_solution(x, 0)
    # f is a scalar (zeros_like(x) works for scalar x too)
    f = lambda x, t: zeros_like(x) + 2*c**2*(1 + 0.5*t)

    L = 2.5
    c = 1.5
    Nx = 3  # Very coarse mesh
    C = 1
    T = 18  # Long time integration

    def assert_no_error(u, x, t, n):
        u_e = exact_solution(x, t[n])
        diff = abs(u - u_e).max()
        nt.assert_almost_equal(diff, 0, places=13)

    solver(I, V, f, c, L, Nx, C, T,
           user_action=assert_no_error, version='scalar')
    solver(I, V, f, c, L, Nx, C, T,
           user_action=assert_no_error, version='vectorized')
```

# Efficiency measurements

- Run `wave1D_u0_sv.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

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

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 $u_t(x, 0)$
- Should use central difference for $u_x$ to preserve second order accuracy

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

# Discretization of derivatives at the boundary (2)

$$\frac{u^n_{-1} - u^n_1}{2\Delta x} = 0$$

- Problem: $u^n_{-1}$ is outside the mesh (fictitious value)
- Remedy: use the stencil at the boundary to eliminate $u^n_{-1}$; just replace $u^n_{-1}$ by $u^n_1$

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

# 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 $u^n_{i-1}$ by $u^n_{i+1}$ for $i = 0$
- Replace $u^n_{i+1}$ by $u^n_{i-1}$ 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 $n = 0, \ldots, N_t$
- 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 $i = 0, \ldots, N_x$
- Definition: $\mathcal{I}_x = \{0, \ldots, N_x\}$
- The first index: $i = \mathcal{I}_x^0$
- The last index: $i = \mathcal{I}_x^{-1}$
- All interior points: $i \in \mathcal{I}_x^i$, $\mathcal{I}_x^i = \{1, \ldots, N_x - 1\}$
- $\mathcal{I}_x^-$ 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:

$$\mathcal{I}_x = \{0, \ldots, N_x\}, \quad \mathcal{I}_t = \{0, \ldots, N_t\}, \tag{30}$$

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

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

Corresponding implementation:

```
for n in It[1:-1]:
    for i in Ix[1:-1]:
        u[i] = - u_2[i] + 2*u_1[i] + \
               C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
    i = Ix[0];  u[i] = 0
    i = Ix[-1]; u[i] = 0
```

Program `wave1D_dn.py`

# Alternative implementation via ghost cells

- 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 $u^n_{-1}$ and $u^n_{N_x+1}$ values are called *ghost values*
- Update ghost values as $u^n_{i-1} = u^n_{i+1}$ 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

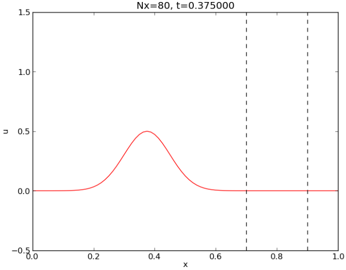
# Implementation of ghost cells (2)

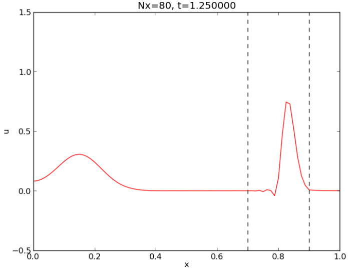
```
u = zeros(Nx+3)
Ix = range(1, u.shape[0]-1)

# 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]
i = Ix[-1]          # x=L boundary
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 $\phi$:

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

# Discretizing the variable coefficient (2)

Then discretize the inner operators:

$$\phi_{i+\frac{1}{2}} = q_{i+\frac{1}{2}} \left[\frac{\partial u}{\partial x}\right]^n_{i+\frac{1}{2}} \approx q_{i+\frac{1}{2}} \frac{u^n_{i+1} - u^n_i}{\Delta x} = [qD_x u]^n_{i+\frac{1}{2}}$$

Similarly,

$$\phi_{i-\frac{1}{2}} = q_{i-\frac{1}{2}} \left[\frac{\partial u}{\partial x}\right]^n_{i-\frac{1}{2}} \approx q_{i-\frac{1}{2}} \frac{u^n_{i} - u^n_{i-1}}{\Delta x} = [qD_x u]^n_{i-\frac{1}{2}}$$

# Discretizing the variable coefficient (3)

These intermediate results are now combined to

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

In operator notation:

$$\left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_i^n \approx [D_x q D_x u]_i^n \tag{33}$$

**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

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

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

$$q_{i+\frac{1}{2}} \approx \left(q_i q_{i+1}\right)^{1/2} \qquad \text{(geometric mean)} \tag{36}$$

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

# Discretization of variable-coefficient wave equation in operator notation

$$[D_tD_t u = D_x\overline{q}^x D_x u + f]^n_i \tag{37}$$

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

$$\begin{aligned}
u^{n+1}_i &= - u^{n-1}_i + 2u^n_i + \left(\frac{\Delta x}{\Delta t}\right)^2 \times \\
&\quad \left(\frac{1}{2}(q_{i} + q_{i+1})(u_{i+1}^n - u_{i}^n) - \frac{1}{2}(q_{i} + q_{i-1})(u_{i}^n - u_{i-1}^n)\right) + \\
&\quad \Delta t^2 f^n_i
\end{aligned} \tag{38}$$

# 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

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

(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

```
for i in range(1, Nx):
    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])
```

Here: C2=(dt/dx)**2

Vectorized version:

```
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])
```

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

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

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 $\varrho$, 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):

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

$b \geq 0$: prescribed damping coefficient.
Discretization via centered differences to ensure $\mathcal{O}(\Delta t^2)$ error:

$$[D_tD_tu + bD_{2t}u = c^2D_xD_xu + f]^n_i \tag{43}$$

Need special formula for $u^1_i$ + 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:

$$
\begin{aligned}
u_t &= (c^2(x)u_x)_x + f(x,t), && x \in (0,L),\ t \in (0,T] && (44)\\
u(x,0) &= I(x), && x \in [0,L] && (45)\\
u_t(x,0) &= V(t), && x \in [0,L] && (46)\\
u(0,t) &= U_0(t) \text{ or } u_x(0,t) = 0, && t \in (0,T] && (47)\\
u(L,t) &= U_L(t) \text{ or } u_x(L,t) = 0, && t \in (0,T] && (48)
\end{aligned}
$$

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 $c$:

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

Variable wave velocity:

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

# 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:

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

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

# 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. $u_t = V$.

# Mesh

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

# Discretization

$$[D_tD_t u = c^2(D_xD_x u + D_yD_y u) + f]^n_{i,j,k},$$

Written out in detail:

$$\frac{u^{n+1}_{i,j} - 2u^{n}_{i,j} + u^{n-1}_{i,j}}{\Delta t^2} = c^2\frac{u^{n}_{i+1,j} - 2u^{n}_{i,j} + u^{n}_{i-1,j}}{\Delta x^2} + \\ c^2\frac{u^{n}_{i,j+1} - 2u^{n}_{i,j} + u^{n}_{i,j-1}}{\Delta y^2} + f^n_{i,j},$$

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

$$u^{n+1}_{i,j} = 2u^n_{i,j} + u^{n-1}_{i,j} + c^2\Delta t^2[D_xD_x u + D_yD_y u]^n_{i,j}$$

# Special stencil for the first time step

- The stencil for $u^1_{i,j}$ ($n=0$) involves $u^{-1}_{i,j}$ 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)

$$[D_{2t}u = V]^0_{i,j} \quad \Rightarrow \quad u^{-1}_{i,j} = u^1_{i,j} - 2\Delta t V_{i,j}$$

$$u^{n+1}_{i,j} = u^n_{i,j} - 2\Delta V_{i,j} + \frac{1}{2}c^2\Delta t^2[D_xD_xu + D_yD_yu]^n_{i,j}$$

# 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:

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

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

## Variable coefficients (2)

Written out:

$$\begin{aligned}
u^{n+1}_{i,j,k} &= -u^{n-1}_{i,j,k} + 2u^{n}_{i,j,k} + \\
&= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i+1,j,k})(u^{n}_{i+1,j,k} - u^{n}_{i,j,k}) - \\
&\qquad \frac{1}{2}(q_{i-1,j,k} + q_{i,j,k})(u^{n}_{i,j,k} - u^{n}_{i-1,j,k})) + \\
&= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i,j+1,k})(u^{n}_{i,j+1,k} - u^{n}_{i,j,k}) - \\
&\qquad \frac{1}{2}(q_{i,j-1,k} + q_{i,j,k})(u^{n}_{i,j,k} - u^{n}_{i,j-1,k})) + \\
&= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i,j,k+1})(u^{n}_{i,j,k+1} - u^{n}_{i,j,k}) - \\
&\qquad \frac{1}{2}(q_{i,j,k-1} + q_{i,j,k})(u^{n}_{i,j,k} - u^{n}_{i,j,k-1})) + \\
+ &\qquad \Delta t^2 f^{n}_{i,j,k}
\end{aligned}$$

# 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:

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

Insert $u^n_{i,-1} = u^n_{i,1}$ in the stencil for $u^{n+1}_{i,j=0}$ 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

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

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

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

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

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

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

# Algorithm

1. Set initial condition $u^0_{i,j} = I(x_i, y_j)$
2. Compute $u^1_{i,j} = \cdots$ for $i \in \mathcal{I}^i_x$ and $j \in \mathcal{I}^i_y$
3. Set $u^1_{i,j} = 0$ for the boundaries $i = 0, N_x$, $j = 0, N_y$
4. For $n = 1, 2, \ldots, N_t$:
    1. Find $u^{n+1}_{i,j} = \cdots$ for $i \in \mathcal{I}^i_x$ and $j \in \mathcal{I}^i_y$
    2. Set $u^{n+1}_{i,j} = 0$ for the boundaries $i = 0, N_x$, $j = 0, N_y$

# Scalar computations: mesh

Program: `wave2D_u0.py`

```
def solver(I, V, f, c, Lx, Ly, Nx, Ny, dt, T,
           user_action=None, version='scalar'):
```

Mesh:

```
x = linspace(0, Lx, Nx+1)                   # mesh points in x dir
y = linspace(0, Ly, Ny+1)                   # mesh points in y dir
dx = x[1] - x[0]
dy = y[1] - y[0]
Nt = int(round(T/float(dt)))
t = linspace(0, N*dt, N+1)                  # mesh points in time
Cx2 = (c*dt/dx)**2;  Cy2 = (c*dt/dy)**2     # help variables
dt2 = dt**2
```

## 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, dt,
                   V=None, step1=False):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    dt2 = dt**2
    if step1:
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2
        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
```

# 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, dt,
                       V=None, step1=False):
    dt2 = dt**2
    if step1:
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 1
    u_xx = 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:

$$u_{\mathrm{e}}(x, y, t) = x(L_x - x)y(L_y - y)(1 + \frac{1}{2}t) \tag{59}$$

Requires $f = 2c^2(1 + \frac{1}{2}t)(y(L_y - y) + x(L_x - x))$.
This $u_{\mathrm{e}}$ is ideal because it also solves the discrete equations!

# Verification: quadratic solution (2)

- $[D_tD_t1]^n = 0$
- $[D_tD_tt]^n = 0$
- $[D_tD_tt^2] = 2$
- $D_tD_t$ is a linear operator:
  $[D_tD_t(au+bv)]^n = a[D_tD_tu]^n + b[D_tD_tv]^n$

$$
\begin{aligned}
[D_xD_xu_{\rm e}]^n_{i,j} &= [y(L_y-y)(1+\frac{1}{2}t)D_xD_xx(L_x-x)]^n_{i,j}\\
&= y_j(L_y-y_j)(1+\frac{1}{2}t_n)2
\end{aligned}
$$

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

# Migrating loops to Cython

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

# Declaring variables and annotating the code

Pure Python code:

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

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

# Cython version of the functions

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

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

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

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

# Visual inspection of the C translation

See how effective Cython can translate this code to C:

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

Load `wave2D_u0_loop_cy.html` in a browser (white: pure C, yellow: still Python):

Raw output: wave2D_u0_loop_cy.c

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

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

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

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

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

# Building the extension module

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

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

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

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

# Calling the Cython function from Python

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

Efficiency:

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

# Migrating loops to Fortran

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

# The Fortran subroutine

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

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

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

# Building the Fortran module with f2py

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

`f2py` changes the argument list (!)

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

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

# How to avoid array copying

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

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

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

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

# Efficiency of translating to Fortran

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

# Migrating loops to C via Cython

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

# The C code

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

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

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

# The Cython interface file

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

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

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

# Building the extension module

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

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

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

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

In Python:

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

# Migrating loops to C via f2py

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

# The C code and the Fortran interface file

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

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

```
      subroutine advance(u, u_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
```

# Building the extension module

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

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

The compile and build step must list the C files:

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

# Migrating loops to C++ via f2py

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

# 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:

$$u(x,t) = g_R(x - ct) + g_L(x + ct), \tag{60}$$

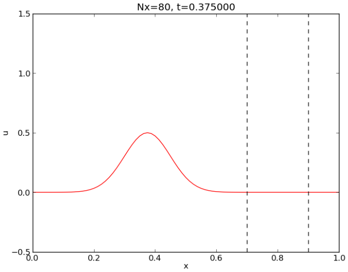
If $u(x,0) = I(x)$ and $u_t(x,0) = 0$:

$$u(x,t) = \frac{1}{2}I(x - ct) + \frac{1}{2}I(x + ct) \tag{61}$$

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

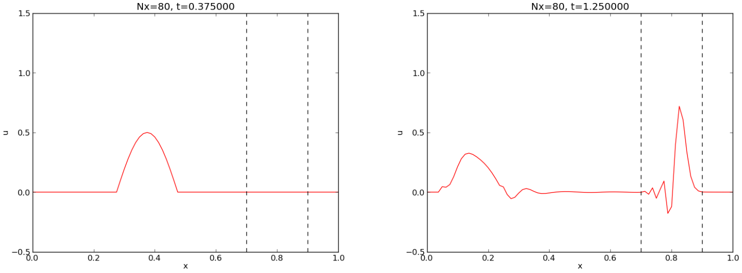
# Effect of variable wave velocity

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



# What happens here?

We have just changed the initial condition...



# Representation of waves as sum of sine/cosine waves

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

$$I(x) \approx \sum_{k \in K} b_k e^{ikx} \tag{62}$$

- $k$ is the frequency of a component ($\lambda = 2\pi/k$ corresponding wave length)
- $K$ is some set of all $k$ needed to approximate $I(x)$ well
- $b_k$ must be computed (Fourier coefficients)

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

$$u(x,t) = \frac{1}{2}\sum_{k \in K} b_k e^{ik(x-ct)} + \frac{1}{2}\sum_{k \in K} b_k e^{ik(x+ct)} \tag{63}$$

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

# Analysis of the finite difference scheme

A similar discrete $u_q^n = e^{i(kx_q - \tilde{\omega} t_n)}$ solves

$$[D_t D_t u = c^2 D_x D_x u]_q^n \tag{64}$$

Note: different frequency $\tilde{\omega} \neq \omega$

- How accurate is $\tilde{\omega}$ compared to $\omega$?
- What about the wave amplitude?

# 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 $\omega \rightarrow k,\ t \rightarrow x,\ n \rightarrow q$) it follows that

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

# Numerical wave propagation (1)

Inserting a basic wave component $u = e^{i(kx_q - \tilde{\omega} t_n)}$ in the scheme (64) requires computation of

$$
\begin{aligned}
\lbrack D_tD_t e^{ikx}e^{-i\tilde{\omega} t}\rbrack^n_q &= \lbrack D_tD_t e^{-i\tilde{\omega} t}\rbrack^n e^{ikq\Delta x}\\
&= -\frac{4}{\Delta t^2}\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) e^{-i\tilde{\omega} n\Delta t}e^{ikq\Delta x} \qquad (65)\\
\lbrack D_xD_x e^{ikx}e^{-i\tilde{\omega} t}\rbrack^n_q &= \lbrack D_xD_x e^{ikx}\rbrack_q e^{-i\tilde{\omega} n\Delta t}\\
&= -\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right) e^{ikq\Delta x}e^{-i\tilde{\omega} n\Delta t} \qquad (66)
\end{aligned}
$$

## Numerical wave propagation (2)

The complete scheme,

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

leads to an equation for $\tilde{\omega}$:

$$\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C^2 \sin^2\left(\frac{k\Delta x}{2}\right), \tag{67}$$

where $C = \frac{c\Delta t}{\Delta x}$ is the Courant number

# Numerical wave propagation (3)

Taking the square root of (67):

$$\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C\sin\left(\frac{k\Delta x}{2}\right), \tag{68}$$

- Exact $\omega$ is real
- Look for a real solution $\tilde{\omega}$ of (68)
- Then the sine functions are in $[-1, 1]$
- Lef-hand side in $[-1, 1]$ requires $C \leq 1$

Stability criterion

$$C = \frac{c\Delta t}{\Delta x} \leq 1 \tag{69}$$

# Why $C \leq 1$ is a stability criterion

Assume $C > 1$. Then

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

- $|\sin x| > 1$ 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

# Numerical dispersion relation

- How close is $\tilde{\omega}$ to $\omega$?
- Can solve for an explicit formula for $\tilde{\omega}$

$$\tilde{\omega} = \frac{2}{\Delta t}\sin^{-1}\left(C\sin\left(\frac{k\Delta x}{2}\right)\right) \tag{70}$$

- $\omega = kc$ is the *analytical dispersion relation*
- $\tilde{\omega} = \tilde{\omega}(k, c, \Delta x, \Delta t)$ is the *numerical dispersion relation*
- Speed of waves: $c = \omega/k$, $\tilde{c} = \tilde{\omega}/k$
- The numerical wave component has a wrong, mesh-dependent speed

# The special case $C = 1$

- For $C = 1$, $\tilde{\omega} = \omega$
- The numerical solution is exact (at the mesh points)!
- The only requirement is constant $c$

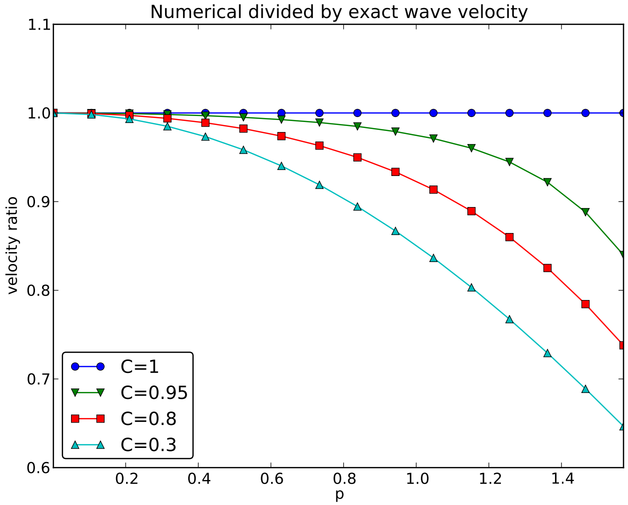
# Computing the error in wave velocity

- Introduce $p = k\Delta x/2$
- $p$ measures no of mesh points in space per wave length in space
- Study error in wave velocity through $\tilde{c}/c$ as function of $p$

$$r(C,p) = \frac{\tilde{c}}{c} = \frac{1}{Cp}\sin^{-1}\left(C\sin p\right), \quad C \in (0,1],\ p \in (0,\pi/2]$$

# Visualizing the error in wave velocity

```
def r(C, p):
    return 2/(C*p)*asin(C*sin(p))
```



# Taylor expanding the error in wave velocity

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

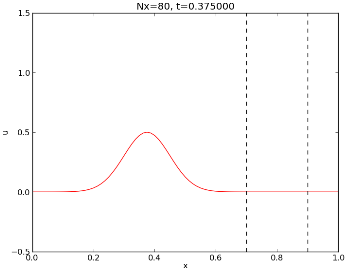
```
>>> C, p = symbols('C p')
>>> rs = r(C, p).series(p, 0, 7)
>>> print rs
1 - p**2/6 + p**4/120 - p**6/5040 + C**2*p**2/6 -
C**2*p**4/12 + 13*C**2*p**6/720 + 3*C**4*p**4/40 -
C**4*p**6/16 + 5*C**6*p**6/112 + O(p**7)

>>> # Factorize each term and drop the remainder O(...) term
>>> rs_factored = [factor(term) for term in rs.lseries(p)]
>>> rs_factored = sum(rs_factored)
>>> print rs_factored
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
```

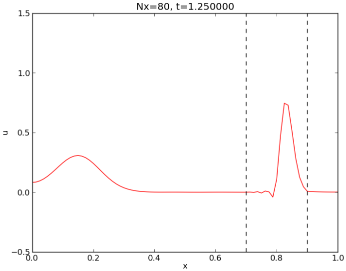
Leading error term is $\frac{1}{6}(C^2 - 1)p^2$ or

$$\frac{1}{6}\left(\frac{k\Delta x}{2}\right)^2 (C^2 - 1) = \frac{k^2}{24}\left(c^2\Delta t^2 - \Delta x^2\right) = \mathcal{O}(\Delta t^2, \Delta x^2) \quad (71)$$

# Example on effect of wrong wave velocity (1)

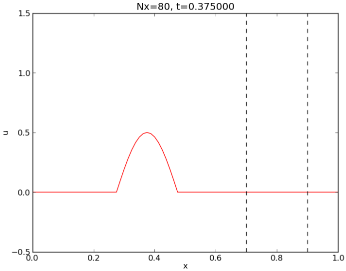
Smooth wave, few short waves (large $k$) in $I(x)$:



# Example on effect of wrong wave velocity (1)

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



# 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

$$[D_tD_tu = c^2(D_xD_xu + D_yD_yu)]^n_{q,r} \tag{72}$$

This equation admits a Fourier component

$$u^n_{q,r} = e^{i(k_xq\Delta x + k_yr\Delta y - \tilde\omega n\Delta t)} \tag{73}$$

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

$$\sin^2\left(\frac{\tilde\omega\Delta t}{2}\right) = C_x^2\sin^2 p_x + C_y^2\sin^2 p_y, \tag{74}$$

where

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

# Stability criterion in 2D

Rreal-valued $\tilde{\omega}$ requires

$$C_x^2 + C_y^2 \leq 1 \tag{75}$$

or

$$\Delta t \leq \frac{1}{c}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)^{-1/2} \tag{76}$$

# Stability criterion in 3D

$$\Delta t \leq \frac{1}{c}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right)^{-1/2} \tag{77}$$

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

$$\Delta t \leq \beta\frac{1}{\bar{c}}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right)^{-1/2} \tag{78}$$

# 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 $\theta$:

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

Also: $\Delta x = \Delta y = h$. Then $C_x = C_y = c\Delta t/h \equiv C$.
Now $\tilde{\omega}$ depends on

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

# Numerical dispersion relation in 2D (2)

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

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)