Study guide: Finite difference methods for vibration problems

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A simple vibration problem

$$u''(t) + \omega^2 u = 0$$
, $u(0) = I$, $u'(0) = 0$, $t \in (0, T]$

Exact solution:

$$u(t) = I\cos(\omega t)$$

u(t) oscillates with constant amplitude I and (angular) frequency ω . Period: $P=2\pi/\omega$.

A centered finite difference scheme; step 1 and 2

- Strategy: follow the four steps of the finite difference method.
- Step 1: Introduce a time mesh, here uniform on [0, T]: $t_n = n\Delta t$
- Step 2: Let the ODE be satisfied at each mesh point:

$$u''(t_n) + \omega^2 u(t_n) = 0, \quad n = 1, \dots, N_t$$

A centered finite difference scheme; step 3

Step 3: Approximate derivative(s) by finite difference approximation(s). Very common (standard!) formula for u'':

$$u''(t_n) \approx \frac{u^{n+1}-2u^n+u^{n-1}}{\Delta t^2}$$

Use this discrete initial condition together with the ODE at t=0 to eliminate u^{-1} :

$$\frac{u^{n+1}-2u^n+u^{n-1}}{\Lambda t^2}=-\omega^2 u^n$$

A centered finite difference scheme; step 4

Step 4: Formulate the computational algorithm. Assume u^{n-1} and u^n are known, solve for unknown u^{n+1} :

$$u^{n+1} = 2u^n - u^{n-1} - \Delta t^2 \omega^2 u^n$$

Nick names for this scheme: Störmer's method or Verlet integration.

Computing the first step

- The formula breaks down for u^1 because u^{-1} is unknown and outside the mesh!
- And: we have not used the initial condition u'(0) = 0.

Discretize u'(0) = 0 by a centered difference

$$\frac{u^1 - u^{-1}}{2\Delta t} = 0 \quad \Rightarrow \quad u^{-1} = u^1$$

Inserted in the scheme for n = 0 gives

$$u^1 = u^0 - \frac{1}{2} \Delta t^2 \omega^2 u^0$$

The computational algorithm

- $u^0 = I$
- \bigcirc compute u^1
- **3** for $n = 1, 2, \dots, N_t 1$:
 - $\mathbf{0}$ compute u^{n+1}

More precisly expressed in Python:

Note: w is consistently used for ω in my code.

Operator notation; ODE

With $[D_tD_tu]^n$ as the finite difference approximation to $u''(t_n)$ we can write

$$[D_t D_t u + \omega^2 u = 0]^n$$

 $[D_tD_tu]^n$ means applying a central difference with step $\Delta t/2$ twice:

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

which is written out as

$$\frac{1}{\Delta t} \left(\frac{u^{n+1} - u^n}{\Delta t} - \frac{u^n - u^{n-1}}{\Delta t} \right) = \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} \,.$$

Operator notation; initial condition

$$[u = I]^0$$
, $[D_{2t}u = 0]^0$

where $[D_{2t}u]^n$ is defined as

$$[D_{2t}u]^n = \frac{u^{n+1} - u^{n-1}}{2\Delta t}.$$

Computing u'

u is often displacement/position, u^{\prime} is velocity and can be computed by

$$u'(t_n) \approx \frac{u^{n+1} - u^{n-1}}{2 \wedge t} = [D_{2t}u]^n$$

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Core algorithm

```
import numpy as np
import matplotlib.pyplot as plt
def solver(I, w, dt, T):
    Solve u'' + w**2*u = 0 for t in (0,T], u(0)=I and u'(0)=0,
    by a central finite difference method with time step dt.
    n n n
    dt = float(dt)
    Nt = int(round(T/dt))
    u = np.zeros(Nt+1)
    t = np.linspace(0, Nt*dt, Nt+1)
    \mathbf{u}[0] = \mathbf{I}
    u[1] = u[0] - 0.5*dt**2*w**2*u[0]
    for n in range(1, Nt):
        u[n+1] = 2*u[n] - u[n-1] - dt**2*w**2*u[n]
    return u. t
def solver_adjust_w(I, w, dt, T, adjust_w=True):
    Solve u'' + w**2*u = 0 for t in (0,T], u(0)=I and u'(0)=0,
    by a central finite difference method with time step dt.
    11 11 11
    dt = float(dt)
    Nt = int(round(T/dt))
    u = np.zeros(Nt+1)
    t = nn linenace(0 Nt*dt Nt+1)
```

```
def u exact(t. I. w):
   return I*np.cos(w*t)
def visualize(u, t, I, w):
   plt.plot(t, u, 'r--o')
    t_fine = np.linspace(0, t[-1], 1001) # very fine mesh for u_e
   u_e = u_exact(t_fine, I, w)
   plt.hold('on')
   plt.plot(t_fine, u_e, 'b-')
   plt.legend(['numerical', 'exact'], loc='upper left')
   plt.xlabel('t')
   plt.ylabel('u')
   dt = t[1] - t[0]
   plt.title('dt=\%g' \% dt)
   umin = 1.2*u.min(); umax = -umin
   plt.axis([t[0], t[-1], umin, umax])
   plt.savefig('tmp1.png'); plt.savefig('tmp1.pdf')
```

Main program

```
I = 1
w = 2*pi
dt = 0.05
num_periods = 5
P = 2*pi/w # one period
T = P*num_periods
u, t = solver(I, w, dt, T)
visualize(u, t, I, w, dt)
```

User interface: command line

```
import argparse
parser = argparse.ArgumentParser()
parser.add_argument('--I', type=float, default=1.0)
parser.add_argument('--w', type=float, default=2*pi)
parser.add_argument('--dt', type=float, default=0.05)
parser.add_argument('--num_periods', type=int, default=5)
a = parser.parse_args()
I, w, dt, num_periods = a.I, a.w, a.dt, a.num_periods
```

Running the program

vib_undamped.py:

```
Terminal> python vib_undamped.py --dt 0.05 --num_periods 40
```

Generates frames tmp_vib%04d.png in files. Can make movie:

Terminal> ffmpeg -r 12 -i tmp_vib%04d.png -c:v flv movie.flv

Can use avconv instead of ffmpeg.

Format	Codec and filename
Flash	-c:v flv movie.flv
MP4	-c:v libx264 movie.mp4
Webm	-c:v libvpx movie.webm
Ogg	-c:v libtheora movie.ogg

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First steps for testing and debugging

- Testing very simple solutions: u = const or u = ct + d do not apply here (without a force term in the equation: $u'' + \omega^2 u = f$).
- Hand calculations: calculate u^1 and u^2 and compare with program.

Checking convergence rates

The next function estimates convergence rates, i.e., it

- performs m simulations with halved time steps: $2^{-k}\Delta t$, $k=0,\ldots,m-1$,
- ullet computes the L_2 norm of the error, $E=\sqrt{\Delta t_i\sum_{n=0}^{N_t-1}(u^n-u_{
 m e}(t_n))^2}$ in each case,
- estimates the rates r_i from two consecutive experiments $(\Delta t_{i-1}, E_{i-1})$ and $(\Delta t_i, E_i)$, assuming $E_i = C\Delta t_i^{r_i}$ and $E_{i-1} = C\Delta t_{i-1}^{r_i}$:

Implementational details

motume m

```
def convergence_rates(m, solver_function, num_periods=8):
    Return m-1 empirical estimates of the convergence rate
    based on m simulations, where the time step is halved
    for each simulation.
    solver\_function(I, w, dt, T) solves each problem, where T
    is based on simulation for num_periods periods.
    .. .. ..
   from math import pi
   w = 0.35: I = 0.3
                           # just chosen values
   P = 2*pi/w
                            # period
    dt = P/30
                            # 30 time step per period 2*pi/w
    T = P*num_periods
    dt values = []
   E values = []
    for i in range(m):
       u, t = solver_function(I, w, dt, T)
       u_e = u_exact(t, I, w)
       E = np.sqrt(dt*np.sum((u_e-u)**2))
        dt_values.append(dt)
       E_values.append(E)
        dt = dt/2
    r = [np.log(E_values[i-1]/E_values[i])/
         np.log(dt_values[i-1]/dt_values[i])
         for i in range(1, m, 1)]
```

Unit test for the convergence rate

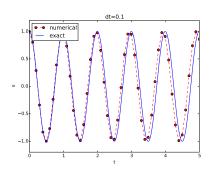
Use final r[-1] in a unit test:

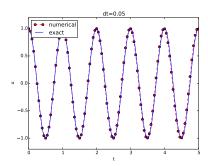
```
def test_convergence_rates():
    r = convergence_rates(m=5, solver_function=solver, num_periods=8)
    # Accept rate to 1 decimal place
    tol = 0.1
    assert abs(r[-1] - 2.0) < tol
    # Test that adjusted w obtains 4th order convergence
    r = convergence_rates(m=5, solver_function=solver_adjust_w, num_pe
    print 'adjust w rates:', r
    assert abs(r[-1] - 4.0) < tol</pre>
```

Complete code in vib_undamped.py.

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Effect of the time step on long simulations





- The numerical solution seems to have right amplitude.
- There is an angular frequency error (reduced by reducing the time step).
- The total angular frequency error seems to grow with time.

Using a moving plot window

- In long time simulations we need a plot window that follows the solution.
- Method 1: scitools.MovingPlotWindow.
- Method 2: scitools.avplotter (ASCII vertical plotter).

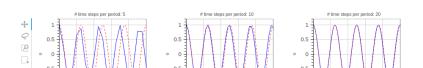
Example:

```
Terminal> python vib_undamped.py --dt 0.05 --num_periods 40
```

Movie of the moving plot window.

!splot

- Bokeh is a Python plotting library for fancy web graphics
- Example here: long time series with many coupled graphs that can move simultaneously



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Analysis of the numerical scheme

Can we understand the frequency error?





Movie of the angular frequency error

$$u'' + \omega^2 u = 0$$
, $u(0) = 1$, $u'(0) = 0$, $\omega = 2\pi$, $u_{\rm e}(t) = \cos(2\pi t)$, $\Delta t = 0.05$ (20 intervals per period)

Movie 1:

 ${\it mov-vib/vib_undamped_movie_dt0.05/movie.ogg}$

We can derive an exact solution of the discrete equations

- We have a linear, homogeneous, difference equation for u^n .
- Has solutions $u^n \sim IA^n$, where A is unknown (number).
- Here: $u_{\rm e}(t) = I\cos(\omega t) \sim I\exp{(i\omega t)} = I(e^{i\omega\Delta t})^n$
- Trick for simplifying the algebra: $u^n = IA^n$, with $A = \exp(i\tilde{\omega}\Delta t)$, then find $\tilde{\omega}$
- ullet $ilde{\omega}$: unknown *numerical frequency* (easier to calculate than A)
- ullet $\omega- ilde{\omega}$ is the angular frequency error
- Use the real part as the physical relevant part of a complex expression

Calculations of an exact solution of the discrete equations

$$u^n = IA^n = I \exp(\tilde{\omega}\Delta t n) = I \exp(\tilde{\omega}t) = I \cos(\tilde{\omega}t) + iI \sin(\tilde{\omega}t)$$
.

$$\begin{split} [D_t D_t u]^n &= \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} \\ &= I \frac{A^{n+1} - 2A^n + A^{n-1}}{\Delta t^2} \\ &= I \frac{\exp\left(i\tilde{\omega}(t + \Delta t)\right) - 2\exp\left(i\tilde{\omega}t\right) + \exp\left(i\tilde{\omega}(t - \Delta t)\right)}{\Delta t^2} \\ &= I \exp\left(i\tilde{\omega}t\right) \frac{1}{\Delta t^2} \left(\exp\left(i\tilde{\omega}(\Delta t)\right) + \exp\left(i\tilde{\omega}(-\Delta t)\right) - 2\right) \\ &= I \exp\left(i\tilde{\omega}t\right) \frac{2}{\Delta t^2} \left(\cosh(i\tilde{\omega}\Delta t) - 1\right) \\ &= I \exp\left(i\tilde{\omega}t\right) \frac{2}{\Delta t^2} \left(\cos(\tilde{\omega}\Delta t) - 1\right) \\ &= -I \exp\left(i\tilde{\omega}t\right) \frac{4}{\Delta t^2} \sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) \end{split}$$

Solving for the numerical frequency

The scheme with $u^n = I \exp(i\omega \hat{\Delta} t n)$ inserted gives

$$-I \exp{(i\tilde{\omega}t)} \frac{4}{\Delta t^2} \sin^2(\frac{\tilde{\omega}\Delta t}{2}) + \omega^2 I \exp{(i\tilde{\omega}t)} = 0$$

which after dividing by $I \exp(i\tilde{\omega}t)$ results in

$$\frac{4}{\Delta t^2} \sin^2(\frac{\tilde{\omega} \Delta t}{2}) = \omega^2$$

Solve for $\tilde{\omega}$:

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

- Frequency error because $\tilde{\omega} \neq \omega$.
- Note: dimensionless number $p=\omega\Delta t$ is the key parameter (i.e., no of time intervals per period is important, not Δt itself)
- ullet But how good is the approximation $ilde{\omega}$ to ω ?

Polynomial approximation of the frequency error

Taylor series expansion for small Δt gives a formula that is easier to understand:

```
>>> from sympy import *
>>> dt, w = symbols('dt w')
>>> w_tilde = asin(w*dt/2).series(dt, 0, 4)*2/dt
>>> print w_tilde
(dt*w + dt**3*w**3/24 + O(dt**4))/dt # note the final "/dt"
```

$$ilde{\omega} = \omega \left(1 + rac{1}{24} \omega^2 \Delta t^2
ight) + \mathcal{O}(\Delta t^3)$$

The numerical frequency is too large (to fast oscillations).

Plot of the frequency error



Recommendation: 25-30 points per period.

Exact discrete solution

$$u^n = I\cos\left(\tilde{\omega}n\Delta t\right), \quad \tilde{\omega} = \frac{2}{\Delta t}\sin^{-1}\left(\frac{\omega\Delta t}{2}\right)$$

The error mesh function,

$$e^{n} = u_{e}(t_{n}) - u^{n} = I \cos(\omega n \Delta t) - I \cos(\tilde{\omega} n \Delta t)$$

is ideal for verification and further analysis!

$$e^{n} = I \cos(\omega n \Delta t) - I \cos(\tilde{\omega} n \Delta t) = -2I \sin\left(t\frac{1}{2}(\omega - \tilde{\omega})\right) \sin\left(t\frac{1}{2}(\omega + \tilde{\omega})\right)$$

Convergence of the numerical scheme

Can easily show convergence:

$$e^n \rightarrow 0$$
 as $\Delta t \rightarrow 0$.

because

$$\lim_{\Delta t \to 0} \tilde{\omega} = \lim_{\Delta t \to 0} \frac{2}{\Delta t} \sin^{-1} \left(\frac{\omega \Delta t}{2} \right) = \omega,$$

by L'Hopital's rule or simply asking sympy: or WolframAlpha:

```
>>> import sympy as sym
>>> dt, w = sym.symbols('x w')
>>> sym.limit((2/dt)*sym.asin(w*dt/2), dt, 0, dir='+')
w
```

Stability

Observations:

- Numerical solution has constant amplitude (desired!), but an angular frequency error
- Constant amplitude requires $\sin^{-1}(\omega \Delta t/2)$ to be real-valued $\Rightarrow |\omega \Delta t/2| \leq 1$
- ullet sin $^{-1}(x)$ is complex if |x|>1, and then $ilde{\omega}$ becomes complex

What is the consequence of complex $\tilde{\omega}$?

- Set $\tilde{\omega} = \tilde{\omega}_r + i\tilde{\omega}_i$
- Since $\sin^{-1}(x)$ has a *negative* imaginary part for x>1, $\exp(i\omega\tilde{t})=\exp(-\tilde{\omega}_it)\exp(i\tilde{\omega}_rt)$ leads to exponential growth $e^{-\tilde{\omega}_it}$ when $-\tilde{\omega}_it>0$
- This is instability because the qualitative behavior is wrong

The stability criterion

Cannot tolerate growth and must therefore demand a *stability* criterion

$$rac{\omega \Delta t}{2} \leq 1 \quad \Rightarrow \quad \Delta t \leq rac{2}{\omega}$$

Try $\Delta t = \frac{2}{\omega} + 9.01 \cdot 10^{-5}$ (slightly too big!):



Summary of the analysis

We can draw three important conclusions:

- **①** The key parameter in the formulas is $p = \omega \Delta t$ (dimensionless)
 - Period of oscillations: $P=2\pi/\omega$
 - O Number of time steps per period: $N_P = P/\Delta t$

 - **1** The smallest possible N_P is $2 \Rightarrow p \in (0, \pi]$
- 2 For $p \le 2$ the amplitude of u^n is constant (stable solution)
- u^n has a relative frequency error $\tilde{\omega}/\omega \approx 1 + \frac{1}{24}p^2$, making numerical peaks occur too early

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Rewriting 2nd-order ODE as system of two 1st-order ODEs

The vast collection of ODE solvers (e.g., in Odespy) cannot be applied to

$$u'' + \omega^2 u = 0$$

unless we write this higher-order ODE as a system of 1st-order ODEs.

Introduce an auxiliary variable v = u':

$$u'=v, (1)$$

$$v' = -\omega^2 u. (2)$$

Initial conditions: u(0) = I and v(0) = 0.

The Forward Euler scheme

We apply the Forward Euler scheme to each component equation:

$$[D_t^+ u = v]^n,$$

$$[D_t^+ v = -\omega^2 u]^n,$$

or written out,

$$u^{n+1} = u^n + \Delta t v^n, \tag{3}$$

$$v^{n+1} = v^n - \Delta t \omega^2 u^n \,. \tag{4}$$

The Backward Euler scheme

We apply the Backward Euler scheme to each component equation:

$$[D_t^- u = v]^{n+1}, (5)$$

$$[D_t^- v = -\omega u]^{n+1}. (6)$$

Written out:

$$u^{n+1} - \Delta t v^{n+1} = u^n, \tag{7}$$

$$v^{n+1} + \Delta t \omega^2 u^{n+1} = v^n. \tag{8}$$

This is a *coupled* 2×2 system for the new values at $t = t_{n+1}$!

The Crank-Nicolson scheme

$$[D_t u = \overline{v}^t]^{n + \frac{1}{2}}, \tag{9}$$

$$[D_t v = -\omega \overline{u}^t]^{n+\frac{1}{2}}.$$
(10)

The result is also a coupled system:

$$u^{n+1} - \frac{1}{2}\Delta t v^{n+1} = u^n + \frac{1}{2}\Delta t v^n, \tag{11}$$

$$v^{n+1} + \frac{1}{2}\Delta t\omega^2 u^{n+1} = v^n - \frac{1}{2}\Delta t\omega^2 u^n.$$
 (12)

Comparison of schemes via Odespy

Can use Odespy to compare many methods for first-order schemes:

```
import odespy
import numpy as np
def f(u, t, w=1):
    # v, u numbering for EulerCromer to work well
    v, u = u # u is array of length 2 holding our [v, u]
   return [-w**2*u, v]
def run_solvers_and_plot(solvers, timesteps_per_period=20,
                         num_periods=1, I=1, w=2*np.pi):
   P = 2*np.pi/w # duration of one period
    dt = P/timesteps_per_period
   Nt = num_periods*timesteps_per_period
    T = Nt*dt
   t_mesh = np.linspace(0, T, Nt+1)
    legends = []
    for solver in solvers:
        solver.set(f_kwargs={'w': w})
        solver.set_initial_condition([0, I])
        u, t = solver.solve(t_mesh)
```

Forward and Backward Euler and Crank-Nicolson

```
solvers = [
   odespy.ForwardEuler(f),
   # Implicit methods must use Newton solver to converge
   odespy.BackwardEuler(f, nonlinear_solver='Newton'),
   odespy.CrankNicolson(f, nonlinear_solver='Newton'),
   ]
```

Two plot types:

- u(t) vs t
- Parameterized curve (u(t), v(t)) in phase space
- Exact curve is an ellipse: $(I\cos\omega t, -\omega I\sin\omega t)$, closed and periodic

Phase plane plot of the numerical solutions



Note: CrankNicolson in Odespy leads to the name MidpointImplicit in plots.

Plain solution curves



Figure: Comparison of classical schemes.

Observations from the figures

- Forward Euler has growing amplitude and outward (u, v) spiral pumps energy into the system.
- Backward Euler is opposite: decreasing amplitude, inward sprial, extracts energy.
- Forward and Backward Euler are useless for vibrations.
- Crank-Nicolson (MidpointImplicit) looks much better.

Runge-Kutta methods of order 2 and 4; short time series



Runge-Kutta methods of order 2 and 4; longer time series



Crank-Nicolson; longer time series



(MidpointImplicit means CrankNicolson in Odespy)

Observations of RK and CN methods

- ullet 4th-order Runge-Kutta is very accurate, also for large Δt .
- 2th-order Runge-Kutta is almost as bad as Forward and Backward Euler.
- Crank-Nicolson is accurate, but the amplitude is not as accurate as the difference scheme for $u'' + \omega^2 u = 0$.

Energy conservation property

The model

$$u'' + \omega^2 u = 0$$
, $u(0) = I$, $u'(0) = V$,

has the nice energy conservation property that

$$E(t) = \frac{1}{2}(u')^2 + \frac{1}{2}\omega^2 u^2 = \text{const}.$$

This can be used to check solutions.

Derivation of the energy conservation property

Multiply $u'' + \omega^2 u = 0$ by u' and integrate:

$$\int_0^T u''u'dt + \int_0^T \omega^2 uu'dt = 0.$$

Observing that

$$u''u' = \frac{d}{dt}\frac{1}{2}(u')^2, \quad uu' = \frac{d}{dt}\frac{1}{2}u^2,$$

we get

$$\int_0^T \left(\frac{d}{dt} \frac{1}{2} (u')^2 + \frac{d}{dt} \frac{1}{2} \omega^2 u^2\right) dt = E(T) - E(0),$$

where

$$E(t) = \frac{1}{2}(u')^2 + \frac{1}{2}\omega^2 u^2$$

Remark about E(t)

E(t) does not measure energy, energy per mass unit.

Starting with an ODE coming directly from Newton's 2nd law F=ma with a spring force F=-ku and ma=mu'' (a: acceleration, u: displacement), we have

$$mu'' + ku = 0$$

Integrating this equation gives a physical energy balance:

$$E(t) = \underbrace{\frac{1}{2}mv^2}_{\text{kinetic energy}} + \underbrace{\frac{1}{2}ku^2}_{\text{potential energy}} = E(0), \quad v = u'$$

Note: the balance is not valid if we add other terms to the ODE.

The Euler-Cromer method; idea

2x2 system for $u'' + \omega^2 u = 0$:

$$v' = -\omega^2 u$$
$$u' = v$$

Forward-backward discretization:

- Update v with Forward Euler
- ullet Update u with Backward Euler, using latest v

$$[D_t^+ v = -\omega^2 u]^n \tag{13}$$

$$[D_t^- u = v]^{n+1} (14)$$

The Euler-Cromer method; complete formulas

Written out:

$$u^0 = I, (15)$$

$$v^0 = 0, \tag{16}$$

$$v^{n+1} = v^n - \Delta t \omega^2 u^n \tag{17}$$

$$u^{n+1} = u^n + \Delta t v^{n+1} \tag{18}$$

Names: Forward-backward scheme, Semi-implicit Euler method, symplectic Euler, semi-explicit Euler, Newton-Stormer-Verlet, and *Euler-Cromer*.

Euler-Cromer is equivalent to the scheme for $u'' + \omega^2 u = 0$

- ullet Forward Euler and Backward Euler have error $\mathcal{O}(\Delta t)$
- ullet What about the overall scheme? Expect $\mathcal{O}(\Delta t)...$

We can eliminate v^n and v^{n+1} , resulting in

$$u^{n+1} = 2u^n - u^{n-1} - \Delta t^2 \omega^2 u^n$$

which is the centered finite difference scheme for $u'' + \omega^2 u = 0!$

The schemes are not equivalent wrt the initial conditions

$$u'=v=0 \Rightarrow v^0=0,$$

SO

$$v^1 = v^0 - \Delta t \omega^2 u^0 = -\Delta t \omega^2 u^0$$
 $u^1 = u^0 + \Delta t v^1 = u^0 - \Delta t \omega^2 u^0! = \underbrace{u^0 - \frac{1}{2} \Delta t \omega^2 u^0}_{\text{from } [D_t D_t u + \omega^2 u = 0]^n \text{ and } [D_{2t} u = 0]^0}$

The exact discrete solution derived earlier does not fit the Euler-Cromer scheme because of mismatch for u^1 .

- A simple vibration problem
- 2 Implementation
- 3 Verification
- 4 Long time simulations
 - Long time simulations visualized with aid of Bokeh: coupled panning of multiple graphs
 - How does Bokeh plotting code look like?
- 5 Analysis of the numerical scheme
- 6 Alternative schemes based on 1st-order equations
- Generalization: damping, nonlinear spring, and external excitation

Generalization: damping, nonlinear spring, and external excitation

$$mu'' + f(u') + s(u) = F(t), \quad u(0) = I, \ u'(0) = V, \ t \in (0, T]$$

Input data: m, f(u'), s(u), F(t), I, V, and T.

Typical choices of f and s:

- linear damping f(u') = bu, or
- quadratic damping f(u') = bu'|u'|
- linear spring s(u) = cu
- nonlinear spring $s(u) \sim \sin(u)$ (pendulum)

A centered scheme for linear damping

$$[mD_tD_tu + f(D_{2t}u) + s(u) = F]^n$$

Written out

$$m\frac{u^{n+1}-2u^n+u^{n-1}}{\Delta t^2}+f(\frac{u^{n+1}-u^{n-1}}{2\Delta t})+s(u^n)=F^n$$

Assume f(u') is linear in u' = v:

$$u^{n+1} = \left(2mu^n + (\frac{b}{2}\Delta t - m)u^{n-1} + \Delta t^2(F^n - s(u^n))\right)(m + \frac{b}{2}\Delta t)^{-1}$$

Initial conditions

$$u(0) = I, u'(0) = V$$
:

$$[u = I]^{0} \Rightarrow u^{0} = I$$
$$[D_{2t}u = V]^{0} \Rightarrow u^{-1} = u^{1} - 2\Delta tV$$

End result:

$$u^{1} = u^{0} + \Delta t V + \frac{\Delta t^{2}}{2m} (-bV - s(u^{0}) + F^{0})$$

Same formula for u^1 as when using a centered scheme for $u'' + \omega u = 0$.

Linearization via a geometric mean approximation

- f(u') = bu'|u'| leads to a quadratic equation for u^{n+1}
- Instead of solving the quadratic equation, we use a geometric mean approximation

In general, the geometric mean approximation reads

$$(w^2)^n \approx w^{n-\frac{1}{2}} w^{n+\frac{1}{2}}$$
.

For |u'|u' at t_n :

$$[u'|u'|]^n \approx u'(t_n+\frac{1}{2})|u'(t_n-\frac{1}{2})|.$$

For u' at $t_{n+1/2}$ we use centered difference:

$$u'(t_{n+1/2}) \approx [D_t u]^{n+\frac{1}{2}}, \quad u'(t_{n-1/2}) \approx [D_t u]^{n-\frac{1}{2}}$$

A centered scheme for quadratic damping

After some algebra:

$$u^{n+1} = (m+b|u^{n}-u^{n-1}|)^{-1} \times (2mu^{n}-mu^{n-1}+bu^{n}|u^{n}-u^{n-1}|+\Delta t^{2}(F^{n}-s(u^{n})))$$

Initial condition for quadratic damping

Simply use that u' = V in the scheme when t = 0 (n = 0):

$$[mD_tD_tu+bV|V|+s(u)=F]^0$$

which gives

$$u^{1} = u^{0} + \Delta t V + \frac{\Delta t^{2}}{2m} \left(-bV|V| - s(u^{0}) + F^{0} \right)$$

Algorithm

- $u^0 = I$
- \odot compute u^1 (formula depends on linear/quadratic damping)
- **3** for $n = 1, 2, ..., N_t 1$:
 - $oldsymbol{0}$ compute u^{n+1} from formula (depends on linear/quadratic damping)

Implementation

```
def solver(I, V, m, b, s, F, dt, T, damping='linear'):
   dt = float(dt); b = float(b); m = float(m) # avoid integer div.
   Nt = int(round(T/dt))
   u = zeros(Nt+1)
   t = linspace(0, Nt*dt, Nt+1)
   \mathbf{u}[0] = \mathbf{I}
   if damping == 'linear':
        u[1] = u[0] + dt*V + dt**2/(2*m)*(-b*V - s(u[0]) + F(t[0]))
    elif damping == 'quadratic':
        u[1] = u[0] + dt*V + 
               dt**2/(2*m)*(-b*V*abs(V) - s(u[0]) + F(t[0]))
   for n in range(1, Nt):
        if damping == 'linear':
            u[n+1] = (2*m*u[n] + (b*dt/2 - m)*u[n-1] +
                      dt**2*(F(t[n]) - s(u[n])))/(m + b*dt/2)
        elif damping == 'quadratic':
            u[n+1] = (2*m*u[n] - m*u[n-1] + b*u[n]*abs(u[n] - u[n-1])
                      + dt**2*(F(t[n]) - s(u[n])))/
                      (m + b*abs(u[n] - u[n-1]))
   return u, t
```

Verification

- Constant solution $u_e = I$ (V = 0) fulfills the ODE problem and the discrete equations. Ideal for debugging!
- Linear solution $u_e = Vt + I$ fulfills the ODE problem and the discrete equations.
- Quadratic solution $u_e = bt^2 + Vt + I$ fulfills the ODE problem and the discrete equations with linear damping, but not for quadratic damping. A special discrete source term can allow u_e to also fulfill the discrete equations with quadratic damping.

Demo program

vib.py supports input via the command line:

```
Terminal> python vib.py --s 'sin(u)' --F '3*cos(4*t)' --c 0.03
```

This results in a moving window following the function on the screen.



Euler-Cromer formulation

We rewrite

$$mu''+f(u')+s(u)=F(t),\quad u(0)=I,\ u'(0)=V,\ t\in(0,T]$$
 as a first-order ODE system

$$u' = v$$

 $v' = m^{-1} (F(t) - f(v) - s(u))$

Staggered grid

- u is unknown at t_n : u^n
- v is unknown at $t_{n+1/2}$: $v^{n+\frac{1}{2}}$
- All derivatives are approximated by centered differences

$$[D_t u = v]^{n-\frac{1}{2}}$$

$$[D_t v = m^{-1} (F(t) - f(v) - s(u))]^n$$

Written out,

$$\frac{u^{n} - u^{n-1}}{\Delta t} = v^{n-\frac{1}{2}}$$

$$\frac{v^{n+\frac{1}{2}} - v^{n-\frac{1}{2}}}{\Delta t} = m^{-1} \left(F^{n} - f(v^{n}) - s(u^{n}) \right)$$

Problem: $f(v^n)$

Linear damping

With f(v) = bv, we can use an arithmetic mean for bv^n a la Crank-Nicolson schemes.

$$u^{n} = u^{n-1} + \Delta t v^{n-\frac{1}{2}},$$

$$v^{n+\frac{1}{2}} = \left(1 + \frac{b}{2m} \Delta t\right)^{-1} \left(v^{n-\frac{1}{2}} + \Delta t m^{-1} \left(F^{n} - \frac{1}{2} f(v^{n-\frac{1}{2}}) - s(u^{n})\right)\right)$$

Quadratic damping

With f(v) = b|v|v, we can use a geometric mean

$$b|v^{n}|v^{n} \approx b|v^{n-\frac{1}{2}}|v^{n+\frac{1}{2}},$$

resulting in

$$u^{n} = u^{n-1} + \Delta t v^{n-\frac{1}{2}},$$

$$v^{n+\frac{1}{2}} = \left(1 + \frac{b}{m} |v^{n-\frac{1}{2}}| \Delta t\right)^{-1} \left(v^{n-\frac{1}{2}} + \Delta t m^{-1} \left(F^{n} - s(u^{n})\right)\right).$$

Initial conditions

$$u^{0} = I$$

$$v^{\frac{1}{2}} = V - \frac{1}{2} \Delta t \omega^{2} I$$