

Study guide: Finite difference methods for vibration problems

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A simple vibration problem

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

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} :

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

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

1. $u^0 = I$
2. compute u^1
3. for $n = 1, 2, \dots, N_t - 1$:
 - (a) compute u^{n+1}

More precisely expressed in Python:

```

t = linspace(0, T, Nt+1) # mesh points in time
dt = t[1] - t[0]         # constant time step.
u = zeros(Nt+1)          # solution

u[0] = 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]

```

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

Operator notation; ODE

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

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

$[D_t D_t u]^n$ 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

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

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' is velocity and can be computed by

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

Implementation

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  $dt$ .
    """
    dt = float(dt)
    Nt = int(round(T/dt))
    u = np.zeros(Nt+1)
    t = np.linspace(0, Nt*dt, Nt+1)

    u[0] = 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  $dt$ .
    """
    dt = float(dt)
    Nt = int(round(T/dt))
    u = np.zeros(Nt+1)
    t = np.linspace(0, Nt*dt, Nt+1)
    w_adj = w*(1 - w**2*dt**2/24.) if adjust_w else w

    u[0] = I
    u[1] = u[0] - 0.5*dt**2*w_adj**2*u[0]
    for n in range(1, Nt):
        u[n+1] = 2*u[n] - u[n-1] - dt**2*w_adj**2*u[n]
    return u, t

```

Plotting

```

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	<code>-c:v flv movie.flv</code>
MP4	<code>-c:v libx264 movie.mp4</code>
Webm	<code>-c:v libvpx movie.webm</code>
Ogg	<code>-c:v libtheora movie.ogg</code>

Verification

First steps for testing and debugging

- **Testing very simple solutions:** $u = \text{const}$ 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: $2^{-k}\Delta t$, $k = 0, \dots, m-1$,
- computes the L_2 norm of the error, $E = \sqrt{\Delta t_i \sum_{n=0}^{N_t-1} (u^n - u_e(t_n))^2}$ 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

```

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)]
    return r

```

Result: `r` contains values equal to 2.00 - as expected!

Unit test for the convergence rate

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

```

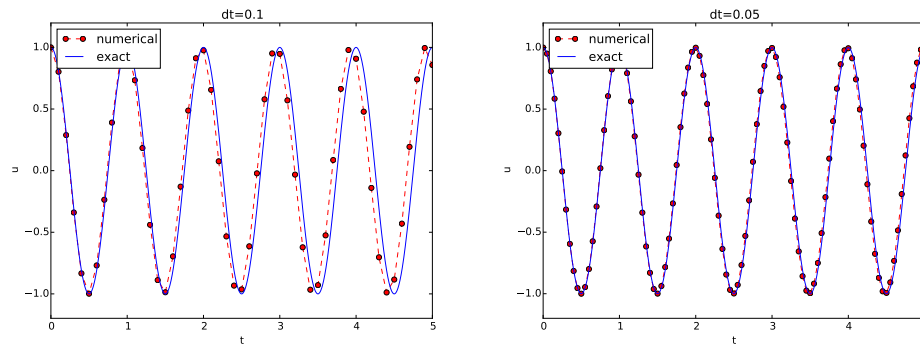
def test_convergence_rates():
    r = convergence_rates(m=5, solver_function=solver, num_periods=8)
    # Accept rate to 1 decimal place
    tol = 0.1
    assert abs(r[-1] - 2.0) < tol
    # Test that adjusted w obtains 4th order convergence
    r = convergence_rates(m=5, solver_function=solver_adjust_w,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

```

Complete code in [vib_undamped.py](#).

Long time simulations

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).

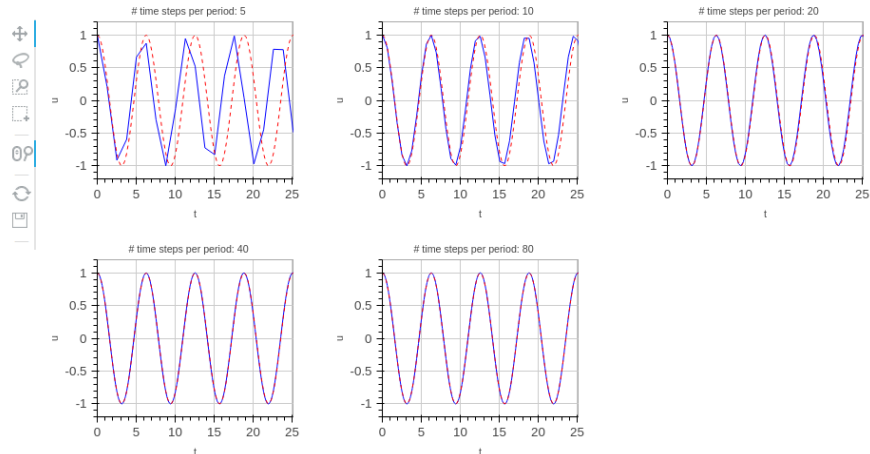
Example:

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

Movie of the moving plot window.
`!splot`

Long time simulations visualized with aid of Bokeh: coupled panning of multiple graphs

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



!splot

How does Bokeh plotting code look like?

```
def bokeh_plot(u, t, legends, I, w, t_range, filename):
    """
    Make plots for u vs t using the Bokeh library.
    u and t are lists (several experiments can be compared).
    legends contain legend strings for the various u,t pairs.
    """
    if not isinstance(u, (list,tuple)):
        u = [u] # wrap in list
    if not isinstance(t, (list,tuple)):
        t = [t] # wrap in list
    if not isinstance(legends, (list,tuple)):
        legends = [legends] # wrap in list

    import bokeh.plotting as plt
    plt.output_file(filename, mode='cdn', title='Comparison')
    # Assume that all t arrays have the same range
    t_fine = np.linspace(0, t[0][-1], 1001) # fine mesh for u_e
    tools = 'pan,wheel_zoom,box_zoom,reset,'\
            'save,box_select,lasso_select'
    u_range = [-1.2*I, 1.2*I]
    font_size = '8pt'
    p = [] # list of plot objects
    # Make the first figure
    p_ = plt.figure(
        width=300, plot_height=250, title=legends[0],
        x_axis_label='t', y_axis_label='u',
        x_range=t_range, y_range=u_range, tools=tools,
```

```

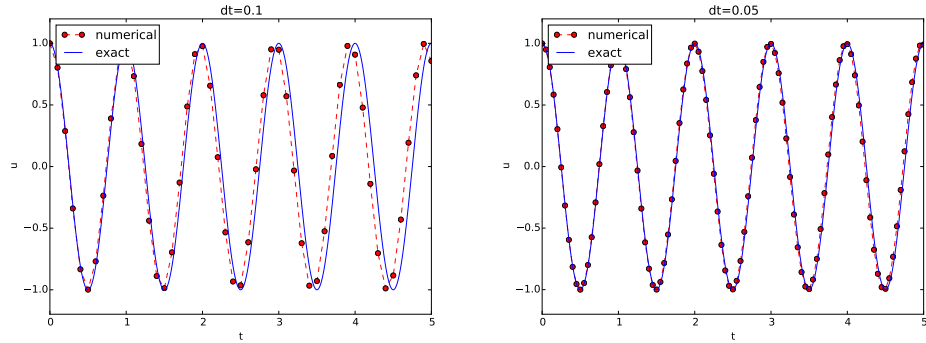
        title_text_font_size=font_size)
p_.axis(axis_label_text_font_size=font_size)
p_.axis(axis_label_text_font_size=font_size)
p_.line(t[0], u[0], line_color='blue')
# Add exact solution
u_e = u_exact(t_fine, I, w)
p_.line(t_fine, u_e, line_color='red', line_dash='4 4')
p_.append(p_)
# Make the rest of the figures and attach their axes to
# the first figure's axes
for i in range(1, len(t)):
    p_ = plt.figure(
        width=300, plot_height=250, title=legends[i],
        x_axis_label='t', y_axis_label='u',
        x_range=p[0].x_range, y_range=p[0].y_range, tools=tools,
        title_text_font_size=font_size)
    p_.axis(axis_label_text_font_size = font_size)
    p_.axis(axis_label_text_font_size = font_size)
    p_.line(t[i], u[i], line_color='blue')
    p_.line(t_fine, u_e, line_color='red', line_dash='4 4')
    p_.append(p_)

# Arrange all plots in a grid with 3 plots per row
grid = [[]]
for i, p_ in enumerate(p):
    grid[-1].append(p_)
    if (i+1) % 3 == 0:
        # New row
        grid.append([])
plot = plt.gridplot(grid, toolbar_location='left')
plt.savefig('plot.png')
plt.show(plot)

```

Analysis of the numerical scheme

Can we understand the frequency error?



Movie of the angular frequency error

$u'' + \omega^2 u = 0$, $u(0) = 1$, $u'(0) = 0$, $\omega = 2\pi$, $u_e(t) = \cos(2\pi t)$, $\Delta t = 0.05$ (20 intervals per period)

Movie 1: `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 $u^n \sim I A^n$, where A is unknown (number).
- Here: $u_e(t) = I \cos(\omega t) \sim I \exp(i\omega t) = I(e^{i\omega\Delta t})^n$
- Trick for simplifying the algebra: $u^n = I A^n$, with $A = \exp(i\tilde{\omega}\Delta t)$, then find $\tilde{\omega}$
- $\tilde{\omega}$: unknown *numerical frequency* (easier to calculate than A)
- $\omega - \tilde{\omega}$ 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

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

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

Solving for the numerical frequency

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

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

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

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

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)
- But how good is the approximation $\tilde{\omega}$ to ω ?

Polynomial approximation of the frequency error

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

```

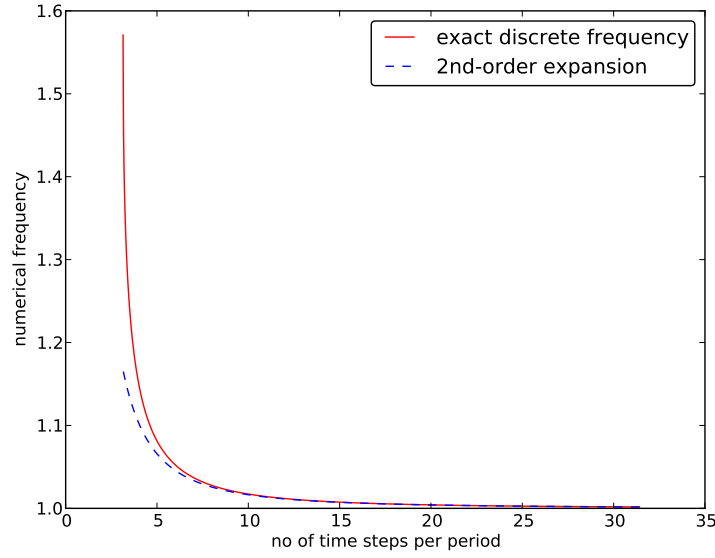
>>> from sympy import *
>>> dt, w = symbols('dt w')
>>> w_tilde = asin(w*dt/2).series(dt, 0, 4)*2/dt
>>> print w_tilde
(dt*w + dt**3*w**3/24 + 0(dt**4))/dt # note the final "/dt"

```

$$\tilde{\omega} = \omega \left(1 + \frac{1}{24} \omega^2 \Delta t^2 \right) + \mathcal{O}(\Delta t^3)$$

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

Plot of the frequency error



Recommendation: 25-30 points per period.

Exact discrete solution

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

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*:

$$e^n \rightarrow 0 \text{ as } \Delta t \rightarrow 0,$$

because

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

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 $\Rightarrow |\omega \Delta t / 2| \leq 1$
- $\sin^{-1}(x)$ is complex if $|x| > 1$, and then $\tilde{\omega}$ becomes complex

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

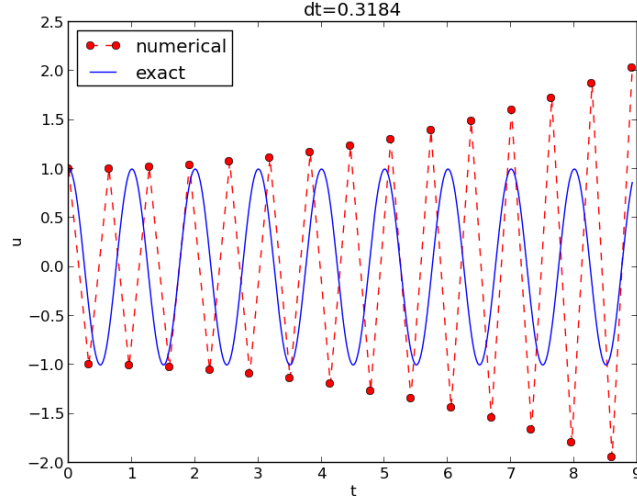
- Set $\tilde{\omega} = \tilde{\omega}_r + i\tilde{\omega}_i$
- Since $\sin^{-1}(x)$ has a ***negative* imaginary part** for $x > 1$, $\exp(i\omega \tilde{t}) = \exp(-\tilde{\omega}_i t) \exp(i\tilde{\omega}_r t)$ leads to exponential growth $e^{-\tilde{\omega}_i t}$ when $-\tilde{\omega}_i t > 0$
-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

The stability criterion

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

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

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)
 - (a) Period of oscillations: $P = 2\pi/\omega$
 - (b) Number of time steps per period: $N_P = P/\Delta t$
 - (c) $\Rightarrow p = \omega\Delta t = 2\pi/N_P \sim 1/N_P$
 - (d) The smallest possible N_P is 2 $\Rightarrow p \in (0, \pi]$
2. For $p \leq 2$ the amplitude of u^n is constant (stable solution)
3. u^n has a relative frequency error $\tilde{\omega}/\omega \approx 1 + \frac{1}{24}p^2$, making numerical peaks occur too early

Alternative schemes based on 1st-order equations

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 $v = u'$:

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

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

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

The Forward Euler scheme

We apply the Forward Euler scheme to each component equation:

$$\begin{aligned} [D_t^+ u = v]^n, \\ [D_t^+ v = -\omega^2 u]^n, \end{aligned}$$

or written out,

$$u^{n+1} = u^n + \Delta t v^n, \quad (3)$$

$$v^{n+1} = v^n - \Delta t \omega^2 u^n. \quad (4)$$

The Backward Euler scheme

We apply the Backward Euler scheme to each component equation:

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

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

Written out:

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

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

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

The Crank-Nicolson scheme

$$[D_t u = \bar{v}^t]^{n+\frac{1}{2}}, \quad (9)$$

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

The result is also a coupled system:

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

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

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)
```

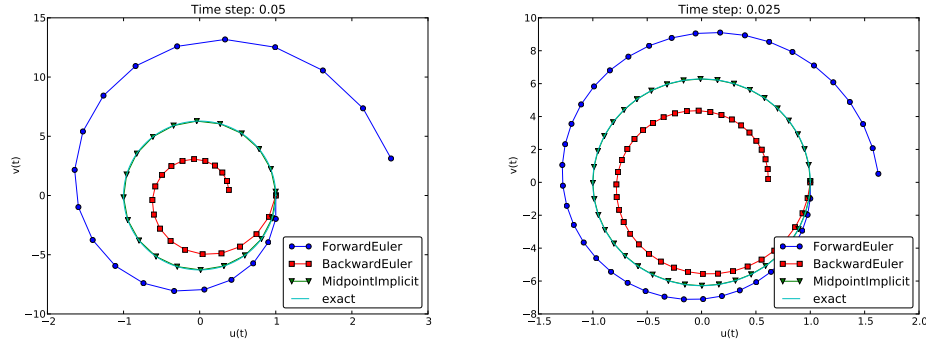
Forward and Backward Euler and Crank-Nicolson

```
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

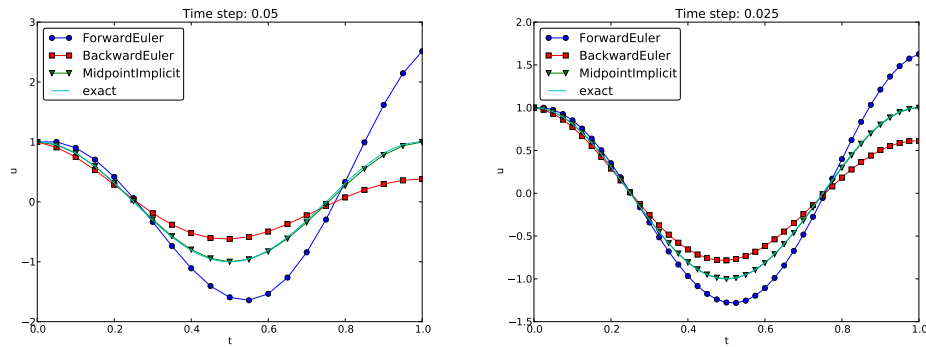
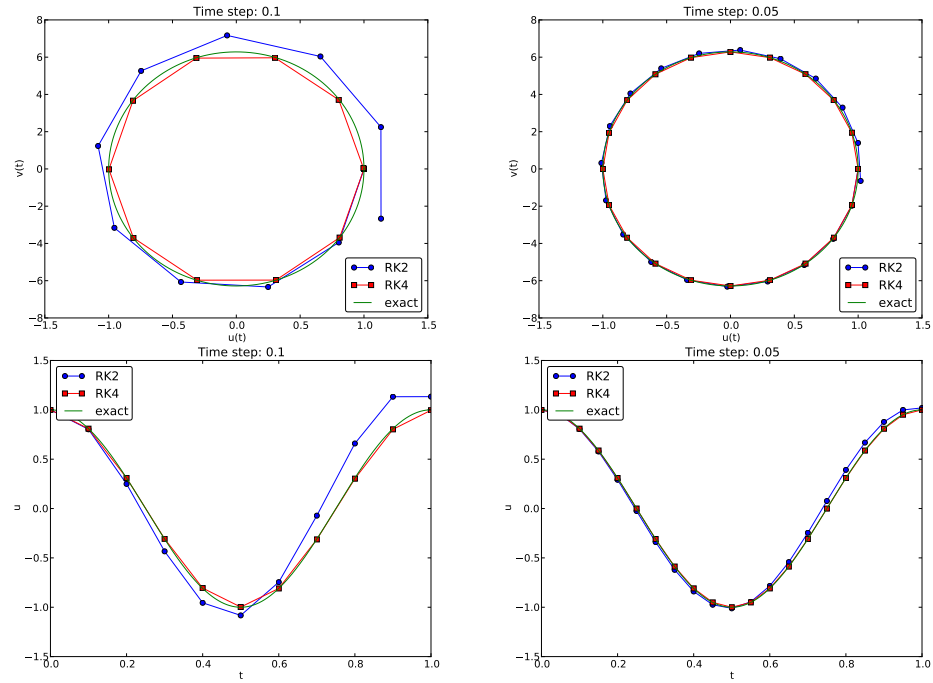


Figure 1: Comparison of classical schemes.

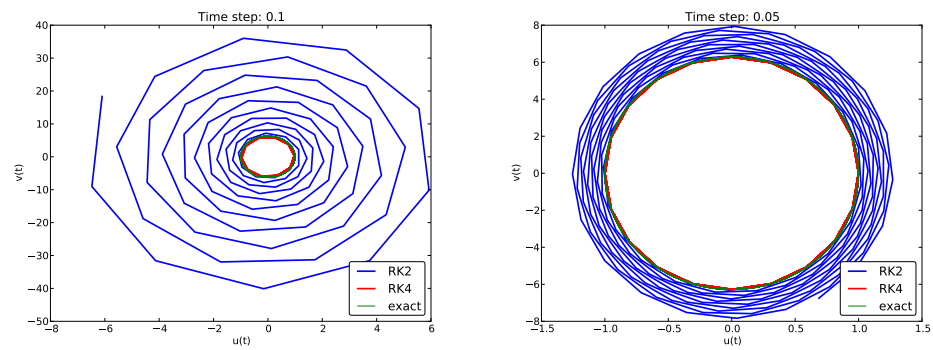
Observations from the figures

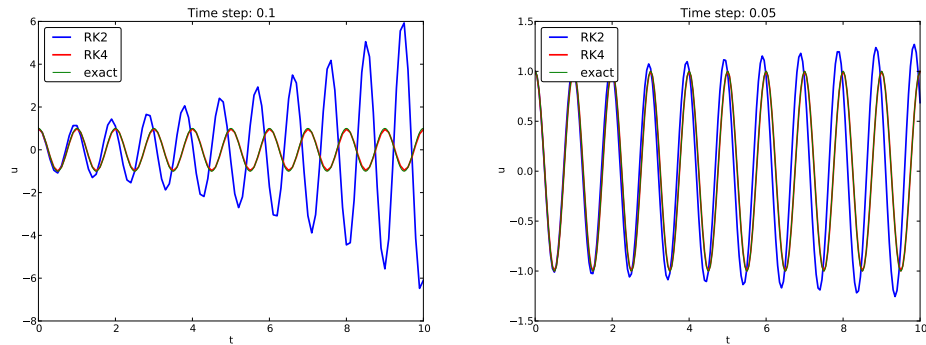
- Forward Euler has growing amplitude and outward (u, v) spiral - pumps energy into the system.
- Backward Euler is opposite: decreasing amplitude, inward spiral, extracts energy.
- **Forward and Backward Euler are useless for vibrations.**
- Crank-Nicolson (MidpointImplicit) looks much better.

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

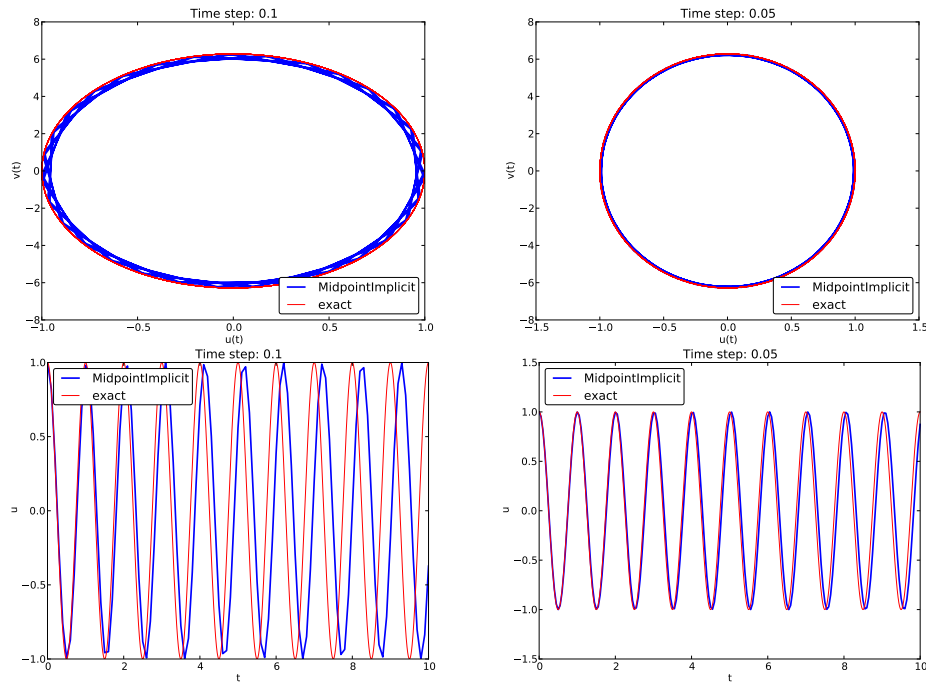


Runge-Kutta methods of order 2 and 4; longer time series





Crank-Nicolson; longer time series



(MidpointImplicit means CrankNicolson in Odespy)

Observations of RK and CN methods

- 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

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

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:

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

Observing that

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

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

$$\begin{aligned}v' &= -\omega^2 u \\ u' &= v\end{aligned}$$

Forward-backward discretization:

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

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

$$[D_t^- u = v]^{n+1} \tag{14}$$

The Euler-Cromer method; complete formulas

Written out:

$$u^0 = I, \tag{15}$$

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

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

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

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

- Forward Euler and Backward Euler have error $\mathcal{O}(\Delta t)$
- 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

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

so

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

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

Generalization: damping, nonlinear spring, and external excitation

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

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

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

Written out

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

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

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

Initial conditions

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

$$\begin{aligned} [u = I]^0 &\Rightarrow u^0 = I \\ [D_{2t}u = V]^0 &\Rightarrow u^{-1} = u^1 - 2\Delta t V \end{aligned}$$

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 $t_{n\pm 1/2}$ 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:

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

Initial condition for quadratic damping

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

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

which gives

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

Algorithm

1. $u^0 = I$
2. compute u^1 (formula depends on linear/quadratic damping)
3. for $n = 1, 2, \dots, N_t - 1$:
 - (a) 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)

    u[0] = 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

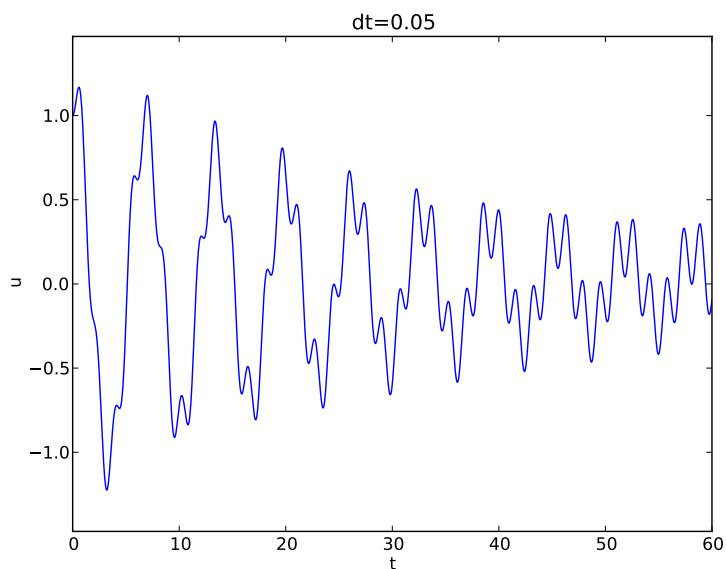
- Constant solution $u_e = I$ ($V = 0$) fulfills the ODE problem and the discrete equations. Ideal for debugging!
- Linear solution $u_e = Vt + I$ fulfills the ODE problem and the discrete equations.
- Quadratic solution $u_e = bt^2 + Vt + I$ fulfills the ODE problem and the discrete equations with linear 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

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

as a first-order ODE system

$$\begin{aligned} u' &= v \\ v' &= m^{-1} (F(t) - f(v) - s(u)) \end{aligned}$$

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

$$\begin{aligned} [D_t u = v]^{n-\frac{1}{2}} \\ [D_t v = m^{-1} (F(t) - f(v) - s(u))]^n \end{aligned}$$

Written out,

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

Problem: $f(v^n)$

Linear damping

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

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

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

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

Initial conditions

$$\begin{aligned} u^0 &= I \\ v^{\frac{1}{2}} &= V - \frac{1}{2} \Delta t \omega^2 I \end{aligned}$$