Finite difference methods for vibration problems

Hans Petter Langtangen[1,2]

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

Nov 12, 2014

Note: **PRELIMINARY VERSION** (expect typos)

Contents

List of Exercises and Problems

Vibration problems lead to differential equations with solutions that oscillate in time, typically in a damped or undamped sinusoidal fashion. Such solutions put certain demands on the numerical methods compared to other phenomena whose solutions are monotone. Both the frequency and amplitude of the oscillations need to be accurately handled by the numerical schemes. Most of the reasoning and specific building blocks introduced in the fortcoming text can be reused to construct sound methods for partial differential equations of wave nature in multiple spatial dimensions.

1 Finite difference discretization

Much of the numerical challenges with computing oscillatory solutions in ODEs and PDEs can be captured by the very simple ODE $u'' + u = 0$ and this is therefore the starting point for method development, implementation, and analysis.

1.1 A basic model for vibrations

A system that vibrates without damping and external forcing can be described by ODE problem

$$u'' + \omega^2 u = 0, \quad u(0) = I,\ u'(0) = 0,\ t \in (0, T]\,. \tag{1}$$

Here, ω and I are given constants. The exact solution of (1) is

$$u(t) = I\cos(\omega t)\,. \tag{2}$$

That is, u oscillates with constant amplitude I and angular frequency ω. The corresponding period of oscillations (i.e., the time between two neighboring peaks in the cosine function) is $P = 2\pi/\omega$. The number of periods per second is $f = \omega/(2\pi)$ and measured in the unit Hz. Both f and ω are referred to as frequency, but ω may be more precisely named angular frequency, measured in rad/s.

In vibrating mechanical systems modeled by (1), $u(t)$ very often represents a position or a displacement of a particular point in the system. The derivative $u'(t)$ then has the interpretation of the point's velocity, and $u''(t)$ is the associated acceleration. The model (1) is not only applicable to vibrating mechanical systems, but also to oscillations in electrical circuits.

1.2 A centered finite difference scheme

To formulate a finite difference method for the model problem (1) we follow the four steps from Section **??**in [1].

Step 1: Discretizing the domain. The domain is discretized by introducing a uniformly partitioned time mesh in the present problem. The points in the mesh are hence $t_n = n\Delta t$, $n = 0, 1, \ldots, N_t$, where $\Delta t = T/N_t$ is the constant length of the time steps. We introduce a mesh function u^n for $n = 0, 1, \ldots, N_t$, which approximates the exact solution at the mesh points. The mesh function will be computed from algebraic equations derived from the differential equation problem.

Step 2: Fulfilling the equation at discrete time points. The ODE is to be satisfied at each mesh point:

$$u''(t_n) + \omega^2 u(t_n) = 0, \quad n = 1, \ldots, N_t\,. \tag{3}$$

Step 3: Replacing derivatives by finite differences. The derivative $u''(t_n)$ is to be replaced by a finite difference approximation. A common second-order accurate approximation to the second-order derivative is

$$u''(t_n) \approx \frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2}\,. \tag{4}$$

Inserting (4) in (3) yields

$$\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} = -\omega^2 u^n\,. \tag{5}$$

We also need to replace the derivative in the initial condition by a finite difference. Here we choose a centered difference, whose accuracy is similar to the centered difference we used for u'':

$$\frac{u^1 - u^{-1}}{2\Delta t} = 0\,. \tag{6}$$

Step 4: Formulating a recursive algorithm. To formulate the computational algorithm, we assume that we have already computed u^{n-1} and u^n such that u^{n+1} is the unknown value, which we can readily solve for:

$$u^{n+1} = 2u^n - u^{n-1} - \Delta t^2\omega^2 u^n\,. \tag{7}$$

The computational algorithm is simply to apply (7) successively for $n = 1, 2, \ldots, N_t - 1$. This numerical scheme sometimes goes under the name Störmer's method or Verlet integration[1].

Computing the first step. We observe that (7) cannot be used for $n = 0$ since the computation of u^1 then involves the undefined value u^{-1} at $t = -\Delta t$. The discretization of the initial condition then come to rescue: (6) implies $u^{-1} = u^1$ and this relation can be combined with (7) for $n = 1$ to yield a value for u^1:

$$u^1 = 2u^0 - u^1 - \Delta t^2\omega^2 u^0,$$

which reduces to

$$u^1 = u^0 - \frac{1}{2}\Delta t^2\omega^2 u^0\,. \tag{8}$$

Exercise 5 asks you to perform an alternative derivation and also to generalize the initial condition to $u'(0) = V \neq 0$.

The computational algorithm. The steps for solving (1) becomes

1. $u^0 = I$
2. compute u^1 from (8)
3. for $n = 1, 2, \ldots, N_t - 1$:
   (a) compute u^{n+1} from (7)

The algorithm is more precisely expressed directly in Python:

[1] `http://en.wikipedia.org/wiki/Verlet_integration`

```
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]
```

Remark.

In the code, we use `w` as the symbol for ω. The reason is that this author prefers `w` for readability and comparison with the mathematical ω instead of the full word `omega` as variable name.

Operator notation. We may write the scheme using the compact difference notation (see Section **??**in [1]). The difference (4) has the operator notation $[D_tD_tu]^n$ such that we can write:

$$[D_tD_tu + \omega^2 u = 0]^n \,. \tag{9}$$

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

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

which is written out as

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

The discretization of initial conditions can in the operator notation be expressed as

$$[u = I]^0, \quad [D_{2t}u = 0]^0, \tag{10}$$

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

$$[D_{2t}u]^n = \frac{u^{n+1} - u^{n-1}}{2\Delta t}\,. \tag{11}$$

2 Implementation

2.1 Making a solver function

The algorithm from the previous section is readily translated to a complete Python function for computing (returning) $u^0, u^1, \ldots, u^{N_t}$ and $t_0, t_1, \ldots, t_{N_t}$, given the input I, ω, Δt, and T:

```
from numpy import *
from matplotlib.pyplot import *
from vib_empirical_analysis import minmax, periods, amplitudes

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 = zeros(Nt+1)
    t = 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
```

A function for plotting the numerical and the exact solution is also convenient to have:

```
def u_exact(t, I, w):
    return I*cos(w*t)

def visualize(u, t, I, w):
    plot(t, u, 'r--o')
    t_fine = linspace(0, t[-1], 1001)  # very fine mesh for u_e
    u_e = u_exact(t_fine, I, w)
    hold('on')
    plot(t_fine, u_e, 'b-')
    legend(['numerical', 'exact'], loc='upper left')
    xlabel('t')
    ylabel('u')
    dt = t[1] - t[0]
    title('dt=%g' % dt)
    umin = 1.2*u.min();  umax = -umin
    axis([t[0], t[-1], umin, umax])
    savefig('vib1.png')
    savefig('vib1.pdf')
```

A corresponding main program calling these functions for a simulation of a given number of periods (`num_periods`) may take the form

```
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)
```

Adjusting some of the input parameters on the command line can be handy. Here is a code segment using the `ArgumentParser` tool in the `argparse` module to define option value (`-option value`) pairs on the 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
```

A typical execution goes like

```
Terminal> python vib_undamped.py --num_periods 20 --dt 0.1
```

Computing u'. In mechanical vibration applications one is often interested in computing the velocity $v(t) = u'(t)$ after $u(t)$ has been computed. This can be done by a central difference,

$$v(t_n) = u'(t_n) \approx v^n = \frac{u^{n+1} - u^{n-1}}{2\Delta t} = [D_{2t}u]^n \,. \tag{12}$$

This formula applies for all inner mesh points, $n = 1, \ldots, N_t - 1$. For $n = 0$ we have that $v(0)$ is given by the initial condition on $u'(0)$, and for $n = N_t$ we can use a one-sided, backward difference: $v^n = [D_t^- u]^n$.

Appropriate vectorized Python code becomes

```
v = np.zeros_like(u)
v[1:-1] = (u[2:] - u[:-2])/(2*dt)  # internal mesh points
v[0] = V                           # Given boundary condition u'(0)
v[-1] = (u[-1] - u[-2])/dt         # backward difference
```

2.2 Verification

Manual calculation. The simplest type of verification, which is also instructive for understanding the algorithm, is to compute u^1, u^2, and u^3 with the aid of a calculator and make a function for comparing these results with those from the `solver` function. We refer to the `test_three_steps` function in the file `vib_undamped.py`[2] for details.

Testing very simple solutions. Constructing test problems where the exact solution is constant or linear helps initial debugging and verification as one expects any reasonable numerical method to reproduce such solutions to machine precision. Second-order accurate methods will often also reproduce a quadratic solution. Here $[D_t D_t t^2]^n = 2$, which is the exact result. A solution $u = t^2$ leads to $u'' + \omega^2 u = 2 + (\omega t)^2 \neq 0$. We must therefore add a source in the equation: $u'' + \omega^2 u = f$ to allow a solution $u = t^2$ for $f = (\omega t)^2$. By simple insertion we can show that the mesh function $u^n = t_n^2$ is also a solution of the discrete equations. Problem 1 asks you to carry out all details with showing that linear and quadratic solutions are solutions of the discrete equations. Such results are very useful for debugging and verification.

Checking convergence rates. Empirical computation of convergence rates, as explained in Section **??**in [1], yields a good method for verification. The function below

- performs m simulations with halved time steps: $2^{-i}\Delta t$, $i = 0, \ldots, m-1$,
- computes the L^2 norm of the error, $E = \sqrt{2^{-i}\Delta t \sum_{n=0}^{N_t-1}(u^n - u_{\mathrm{e}}(t_n))^2}$ in each case,
- estimates the convergence rates r_i based on 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 $E_{i-1} = C\Delta t_{i-1}^{r_i}$. From these equations it follows that $r_{i-1} = \ln(E_{i-1}/E_i)/\ln(\Delta t_{i-1}/\Delta t_i)$, for $i = 1, \ldots, m-1$.

All the implementational details appear below.

[2] `http://tinyurl.com/nm5587k/vib/vib_undamped.py`

```
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.
    """
    w = 0.35; I = 0.3
    dt = 2*pi/w/30  # 30 time step per period 2*pi/w
    T = 2*pi/w*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 = sqrt(dt*sum((u_e-u)**2))
        dt_values.append(dt)
        E_values.append(E)
        dt = dt/2

    r = [log(E_values[i-1]/E_values[i])/
         log(dt_values[i-1]/dt_values[i])
         for i in range(1, m, 1)]
    return r
```

The returned `r` list has its values equal to 2.00, which is in excellent agreement with what is expected from the second-order finite difference approximation $[D_tD_tu]^n$ and other theoretical measures of the error in the numerical method. The final `r[-1]` value is a good candidate for a unit test:

```
def test_convergence_rates():
    r = convergence_rates(m=5, solver_function=solver, num_periods=8)
    # Accept rate to 1 decimal place
    nt.assert_almost_equal(r[-1], 2.0, places=1)
```

The complete code appears in the file `vib_undamped.py`.

3 Long time simulations

Figure 1 shows a comparison of the exact and numerical solution for $\Delta t = 0.1, 0.05$ and $w = 2\pi$. From the plot we make the following observations:

- The numerical solution seems to have correct amplitude.
- There is a phase error which is reduced by reducing the time step.
- The total phase error grows with time.

By phase error we mean that the peaks of the numerical solution have incorrect positions compared with the peaks of the exact cosine solution. This effect can be understood as if also the numerical solution is on the form $I\cos\tilde{\omega}t$, but where $\tilde{\omega}$ is not exactly equal to ω. Later, we shall mathematically quantify this numerical frequency $\tilde{\omega}$.

3.1 Using a moving plot window

In vibration problems it is often of interest to investigate the system's behavior over long time intervals. Errors in the phase may then show up as crucial. Let us investigate long time

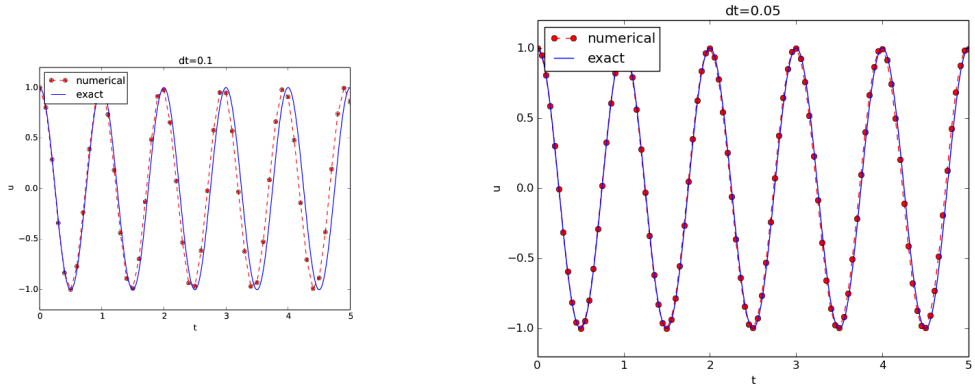

Figure 1: Effect of halving the time step.

series by introducing a moving plot window that can move along with the p most recently computed periods of the solution. The SciTools[3] package contains a convenient tool for this: `MovingPlotWindow`. Typing `pydoc scitools.MovingPlotWindow` shows a demo and description of usage. The function below illustrates the usage and is invoked in the `vib_undamped.py` code if the number of periods in the simulation exceeds 10:

```
def visualize_front(u, t, I, w, savefig=False):
    """
    Visualize u and the exact solution vs t, using a
    moving plot window and continuous drawing of the
    curves as they evolve in time.
    Makes it easy to plot very long time series.
    """
    import scitools.std as st
    from scitools.MovingPlotWindow import MovingPlotWindow

    P = 2*pi/w  # one period
    umin = 1.2*u.min();  umax = -umin
    plot_manager = MovingPlotWindow(
        window_width=8*P,
        dt=t[1]-t[0],
        yaxis=[umin, umax],
        mode='continuous drawing')
    for n in range(1,len(u)):
        if plot_manager.plot(n):
            s = plot_manager.first_index_in_plot
            st.plot(t[s:n+1], u[s:n+1], 'r-1',
                    t[s:n+1], I*cos(w*t)[s:n+1], 'b-1',
                    title='t=%6.3f' % t[n],
                    axis=plot_manager.axis(),
                    show=not savefig) # drop window if savefig
            if savefig:
                filename = 'tmp_vib%04d.png' % n
                st.savefig(filename)
                print 'making plot file', filename, 'at t=%g' % t[n]
        plot_manager.update(n)
```

Running

[3] `http://code.google.com/p/scitools`

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

makes the simulation last for 40 periods of the cosine function. With the moving plot window we can follow the numerical and exact solution as time progresses, and we see from this demo that the phase error is small in the beginning, but then becomes more prominent with time. Running `vib_undamped.py` with $\Delta t = 0.1$ clearly shows that the phase errors become significant even earlier in the time series and destroys the solution.

3.2 Making a video

The `visualize_front` function stores all the plots in files whose names are numbered: `tmp_vib0000.png`, `tmp_vib0001.png`, `tmp_vib0002.png`, and so on. From these files we may make a movie. The Flash format is popular,

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

The `avconv` program can be replaced by the `ffmpeg` program in the above command if desired. The `-r` option should come first and describes the number of frames per second in the movie. The `-i` option describes the name of the plot files. Other formats can be generated by changing the video codec and equipping the video file with the right extension:

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`

The video file can be played by some video player like `vlc`, `mplayer`, `gxine`, or `totem`, e.g.,

```
Terminal> vlc movie.webm
```

A web page can also be used to play the movie. Today's standard is to use the HTML5 `video` tag:

```
<video autoplay loop controls
       width='640' height='365' preload='none'>
<source src='movie.webm'  type='video/webm; codecs="vp8, vorbis"'>
</video>
```

Caution: number the plot files correctly.

To ensure that the individual plot frames are shown in correct order, it is important to number the files with zero-padded numbers (0000, 0001, 0002, etc.). The printf format `%04d` specifies an integer in a field of width 4, padded with zeros from the left. A simple Unix wildcard file specification like `tmp_vib*.png` will then list the frames in the right order.

If the numbers in the filenames were not zero-padded, the frame `tmp_vib11.png` would appear before `tmp_vib2.png` in the movie.

3.3 Using a line-by-line ascii plotter

Plotting functions vertically, line by line, in the terminal window using ascii characters only is a simple, fast, and convenient visualization technique for long time series (the time arrow points downward). The tool `scitools.avplotter.Plotter` makes it easy to create such plots:

```
def visualize_front_ascii(u, t, I, w, fps=10):
    """
    Plot u and the exact solution vs t line by line in a
    terminal window (only using ascii characters).
    Makes it easy to plot very long time series.
    """
    from scitools.avplotter import Plotter
    import time
    P = 2*pi/w
    umin = 1.2*u.min();  umax = -umin

    p = Plotter(ymin=umin, ymax=umax, width=60, symbols='+o')
    for n in range(len(u)):
        print p.plot(t[n], u[n], I*cos(w*t[n])), \
              '%.1f' % (t[n]/P)
        time.sleep(1/float(fps))

if __name__ == '__main__':
    main()
    raw_input()
```

The call `p.plot` returns a line of text, with the t axis marked and a symbol `+` for the first function (`u`) and `o` for the second function (the exact solution). Here we append this text a time counter reflecting how many periods the current time point corresponds to. A typical output ($\omega = 2\pi$, $\Delta t = 0.05$) looks like this:

```
                                |                       o+      14.0
                                |                      + o      14.0
                                |                   +    o      14.1
                                |              +     o          14.1
                                |     +         o               14.2
                               +|       o                      14.2
                      +         |                              14.2
              +       o         |                              14.3
          +     o               |                              14.4
        +   o                   |                              14.4
       +o                       |                              14.5
       o +                      |                              14.5
        o    +                  |                              14.6
            o      +            |                              14.6
                 o        +     |                              14.7
                        o       | +                            14.7
                                |       +                      14.8
                                |       o       +              14.8
                                |               o     +        14.9
                                |                     o   +    14.9
                                |                         o+   15.0
```

3.4 Empirical analysis of the solution

For oscillating functions like those in Figure 1 we may compute the amplitude and frequency (or period) empirically. That is, we run through the discrete solution points (t_n, u_n) and find all

maxima and minima points. The distance between two consecutive maxima (or minima) points can be used as estimate of the local period, while half the difference between the u value at a maximum and a nearby minimum gives an estimate of the local amplitude.

The local maxima are the points where

$$u^{n-1} < u^n > u^{n+1}, \quad n = 1, \ldots, N_t - 1, \tag{13}$$

and the local minima are recognized by

$$u^{n-1} > u^n < u^{n+1}, \quad n = 1, \ldots, N_t - 1\,. \tag{14}$$

In computer code this becomes

```
def minmax(t, u):
    minima = []; maxima = []
    for n in range(1, len(u)-1, 1):
        if u[n-1] > u[n] < u[n+1]:
            minima.append((t[n], u[n]))
        if u[n-1] < u[n] > u[n+1]:
            maxima.append((t[n], u[n]))
    return minima, maxima
```

Note that the returned objects are list of tuples.

Let (t_i, e_i), $i = 0, \ldots, M-1$, be the sequence of all the M maxima points, where t_i is the time value and e_i the corresponding u value. The local period can be defined as $p_i = t_{i+1} - t_i$. With Python syntax this reads

```
def periods(maxima):
    p = [extrema[n][0] - maxima[n-1][0]
         for n in range(1, len(maxima))]
    return np.array(p)
```

The list `p` created by a list comprehension is converted to an array since we probably want to compute with it, e.g., find the corresponding frequencies `2*pi/p`.

Having the minima and the maxima, the local amplitude can be calculated as the difference between two neighboring minimum and maximum points:

```
def amplitudes(minima, maxima):
    a = [(abs(maxima[n][1] - minima[n][1]))/2.0
         for n in range(min(len(minima),len(maxima)))]
    return np.array(a)
```

The code segments are found in the file `vib_empirical_analysis.py`[4].

Visualization of the periods `p` or the amplitudes `a` it is most conveniently done with just a counter on the horizontal axis, since `a[i]` and `p[i]` correspond to the i-th amplitude estimate and the i-th period estimate, respectively. There is no unique time point associated with either of these estimate since values at two different time points were used in the computations.

In the analysis of very long time series, it is advantageous to compute and plot `p` and `a` instead of u to get an impression of the development of the oscillations.

[4] `http://tinyurl.com/nm5587k/vib/vib_empirical_analysis.py`

4 Analysis of the numerical scheme

4.1 Deriving a solution of the numerical scheme

After having seen the phase error grow with time in the previous section, we shall now quantify this error through mathematical analysis. The key tool in the analysis will be to establish an exact solution of the discrete equations. The difference equation (7) has constant coefficients and is homogeneous. The solution is then $u^n = CA^n$, where A is some number to be determined from the differential equation and C is determined from the initial condition ($C = I$). Recall that n in u^n is a superscript labeling the time level, while n in A^n is an exponent. With oscillating functions as solutions, the algebra will be considerably simplified if we seek an A on the form

$$A = e^{i\tilde{\omega}\Delta t},$$

and solve for the numerical frequency $\tilde{\omega}$ rather than A. Note that $i = \sqrt{-1}$ is the imaginary unit. (Using a complex exponential function gives simpler arithmetics than working with a sine or cosine function.) We have

$$A^n = e^{i\tilde{\omega}\Delta t\, n} = e^{i\tilde{\omega}t} = \cos(\tilde{\omega}t) + i\sin(\tilde{\omega}t)\,.$$

The physically relevant numerical solution can be taken as the real part of this complex expression.

The calculations goes as

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

The last line follows from the relation $\cos x - 1 = -2\sin^2(x/2)$ (try `cos(x)-1` in wolframalpha.com[5] to see the formula).

The scheme (7) with $u^n = Ie^{i\omega\tilde{\Delta}t\, n}$ inserted now gives

$$-Ie^{i\tilde{\omega}t}\frac{4}{\Delta t^2}\sin^2(\frac{\tilde{\omega}\Delta t}{2}) + \omega^2 Ie^{i\tilde{\omega}t} = 0, \tag{15}$$

which after dividing by $Ie^{i\tilde{\omega}t}$ results in

$$\frac{4}{\Delta t^2}\sin^2(\frac{\tilde{\omega}\Delta t}{2}) = \omega^2\,. \tag{16}$$

[5] `http://www.wolframalpha.com`

The first step in solving for the unknown $\tilde{\omega}$ is

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

Then, taking the square root, applying the inverse sine function, and multiplying by $2/\Delta t$, results in

$$\tilde{\omega} = \pm\frac{2}{\Delta t}\sin^{-1}\left(\frac{\omega\Delta t}{2}\right) . \tag{17}$$

The first observation of (17) tells that there is a phase error since the numerical frequency $\tilde{\omega}$ never equals the exact frequency ω. But how good is the approximation (17)? That is, what is the error $\omega - \tilde{\omega}$ or $\tilde{\omega}/\omega$? Taylor series expansion for small Δt may give an expression that is easier to understand than the complicated function in (17):

```
>>> from sympy import *
>>> dt, w = symbols('dt w')
>>> w_tilde_e = 2/dt*asin(w*dt/2)
>>> w_tilde_series = w_tilde_e.series(dt, 0, 4)
>>> print w_tilde_series
w + dt**2*w**3/24 + O(dt**4)
```

This means that

$$\tilde{\omega} = \omega\left(1 + \frac{1}{24}\omega^2\Delta t^2\right) + \mathcal{O}(\Delta t^4) . \tag{18}$$

The error in the numerical frequency is of second-order in Δt, and the error vanishes as $\Delta t \to 0$. We see that $\tilde{\omega} > \omega$ since the term $\omega^3\Delta t^2/24 > 0$ and this is by far the biggest term in the series expansion for small $\omega\Delta t$. A numerical frequency that is too large gives an oscillating curve that oscillates too fast and therefore "lags behind" the exact oscillations, a feature that can be seen in the plots.

Figure 2 plots the discrete frequency (17) and its approximation (18) for $\omega = 1$ (based on the program `vib_plot_freq.py`[6]). Although $\tilde{\omega}$ is a function of Δt in (18), it is misleading to think of Δt as the important discretization parameter. It is the product $\omega\Delta t$ that is the key discretization parameter. This quantity reflects the *number of time steps per period* of the oscillations. To see this, we set $P = N_P\Delta t$, where P is the length of a period, and N_P is the number of time steps during a period. Since P and ω are related by $P = 2\pi/\omega$, we get that $\omega\Delta t = 2\pi/N_P$, which shows that $\omega\Delta t$ is directly related to N_P.

The plot shows that at least $N_P \sim 25 - 30$ points per period are necessary for reasonable accuracy, but this depends on the length of the simulation (T) as the total phase error due to the frequency error grows linearly with time (see Exercise 2).

4.2 Exact discrete solution

Perhaps more important than the $\tilde{\omega} = \omega + \mathcal{O}(\Delta t^2)$ result found above is the fact that we have an exact discrete solution of the problem:

$$u^n = I\cos\left(\tilde{\omega}n\Delta t\right), \quad \tilde{\omega} = \frac{2}{\Delta t}\sin^{-1}\left(\frac{\omega\Delta t}{2}\right) . \tag{19}$$

We can then compute the error mesh function

[6] `http://tinyurl.com/nm5587k/vib/vib_plot_freq.py`

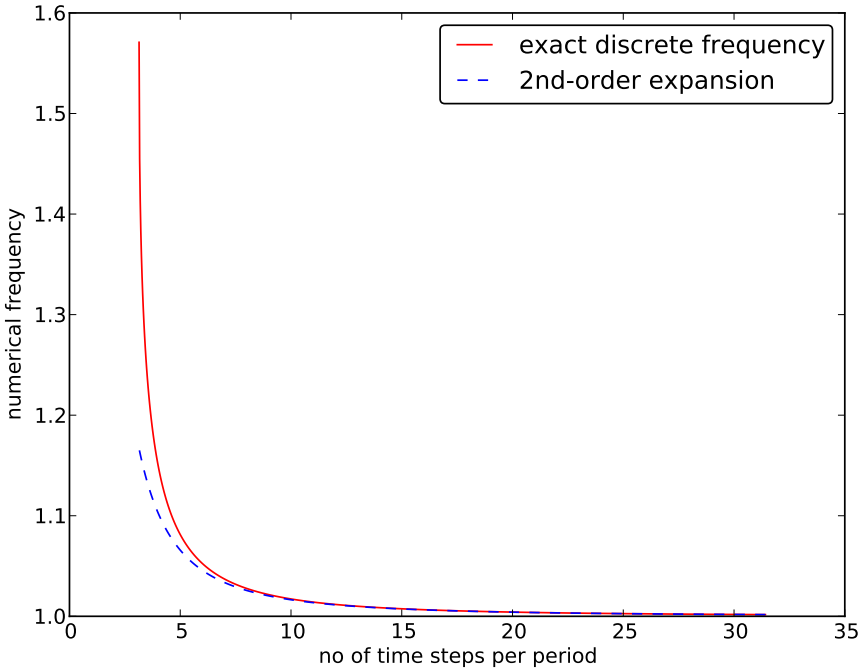

Figure 2: Exact discrete frequency and its second-order series expansion.

$$e^n = u_{\mathrm{e}}(t_n) - u^n = I\cos\left(\omega n\Delta t\right) - I\cos\left(\tilde{\omega} n\Delta t\right)\ . \tag{20}$$

From the formula $\cos 2x - \cos 2y = -2\sin(x-y)\sin(x+y)$ we can rewrite e^n so the expression is easier to interpret:

$$e^n = -2I\sin\left(t\frac{1}{2}\left(\omega - \tilde{\omega}\right)\right)\sin\left(t\frac{1}{2}\left(\omega + \tilde{\omega}\right)\right)\ . \tag{21}$$

In particular, we can use (21) to show *convergence* of the numerical scheme, i.e., $e^n \to 0$ as $\Delta t \to 0$. We have that

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

by L'Hopital's rule or simply asking `sympy` or WolframAlpha[7] about the limit:

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

Therefore, $\tilde{\omega} \to \omega$ and obviously $e^n \to 0$.

The error mesh function is ideal for verification purposes and you are strongly encouraged to make a test based on (19) by doing Exercise 10.

[7] `http://www.wolframalpha.com/input/?i=%282%2Fx%29*asin%28w*x%2F2%29+as+x-%3E0`

4.3 The global error

To achieve more analytical insight into the nature of the global error, we can Taylor expand the error mesh function. Since $\tilde{\omega}$ contains Δt in the denominator we use the series expansion for $\tilde{\omega}$ inside the cosine function:

```
>>> dt, w, t = symbols('dt w t')
>>> w_tilde_e = 2/dt*asin(w*dt/2)
>>> w_tilde_series = w_tilde_e.series(dt, 0, 4)
>>> # Get rid of O() term
>>> w_tilde_series = sum(w_tilde_series.as_ordered_terms()[:-1])
>>> w_tilde_series
dt**2*w**3/24 + w
>>> error = cos(w*t) - cos(w_tilde_series*t)
>>> error.series(dt, 0, 6)
dt**2*t*w**3*sin(t*w)/24 + dt**4*t**2*w**6*cos(t*w)/1152 + O(dt**6)
>>> error.series(dt, 0, 6).as_leading_term(dt)
dt**2*t*w**3*sin(t*w)/24
```

This means that the leading order global (true) error at a point t is proportional to $\omega^3 t\Delta t^2$. Setting $t = n\Delta t$ and replacing $\sin(\omega t)$ by its maximum value 1, we have the analytical leading-order expression

$$e^n = \frac{1}{24} n\omega^3 \Delta t^3,$$

and the ℓ^2 norm of this error can be computed as

$$||e^n||_{\ell^2}^2 = \Delta t \sum_{n=0}^{N_t} \frac{1}{24^2} n^2 \omega^6 \Delta t^6 = \frac{1}{24^2} \omega^6 \Delta t^7 \sum_{n=0}^{N_t} n^2 \,.$$

The sum $\sum_{n=0}^{N_t} n^2$ is approximately equal to $\frac{1}{3}N_t^3$. Replacing N_t by $T/\Delta t$ and taking the square root gives the expression

$$||e^n||_{\ell^2} = \frac{1}{24}\sqrt{\frac{T^3}{3}}\omega^3 \Delta t^2,$$

which shows that also the integrated error is proportional to Δt^2.

4.4 Stability

Looking at (19), it appears that the numerical solution has constant and correct amplitude, but an error in the frequency (phase error). However, there is another error that is more serious, namely an unstable growing amplitude that can occur of Δt is too large.

We realize that a constant amplitude demands $\tilde{\omega}$ to be a real number. A complex $\tilde{\omega}$ is indeed possible if the argument x of $\sin^{-1}(x)$ has magnitude larger than unity: $|x| > 1$ (type `asin(x)` in wolframalpha.com[8] to see basic properties of $\sin^{-1}(x)$). A complex $\tilde{\omega}$ can be written $\tilde{\omega} = \tilde{\omega}_r + i\tilde{\omega}_i$. Since $\sin^{-1}(x)$ has a *negative* imaginary part for $x > 1$, $\tilde{\omega}_i < 0$, it means that $\exp\left(i\omega\tilde{t}\right) = \exp\left(-\tilde{\omega}_i t\right)\exp\left(i\tilde{\omega}_r t\right)$ will lead to exponential growth in time because $\exp\left(-\tilde{\omega}_i t\right)$ with $\tilde{\omega}_i < 0$ has a positive exponent.

We do not tolerate growth in the amplitude and we therefore have a *stability criterion* arising from requiring the argument $\omega\Delta t/2$ in the inverse sine function to be less than one:

$$\frac{\omega\Delta t}{2} \leq 1 \quad \Rightarrow \quad \Delta t \leq \frac{2}{\omega}\,. \tag{22}$$

[8] `http://www.wolframalpha.com`

With $\omega = 2\pi$, $\Delta t > \pi^{-1} = 0.3183098861837907$ will give growing solutions. Figure 3 displays what happens when $\Delta t = 0.3184$, which is slightly above the critical value: $\Delta t = \pi^{-1} + 9.01 \cdot 10^{-5}$.

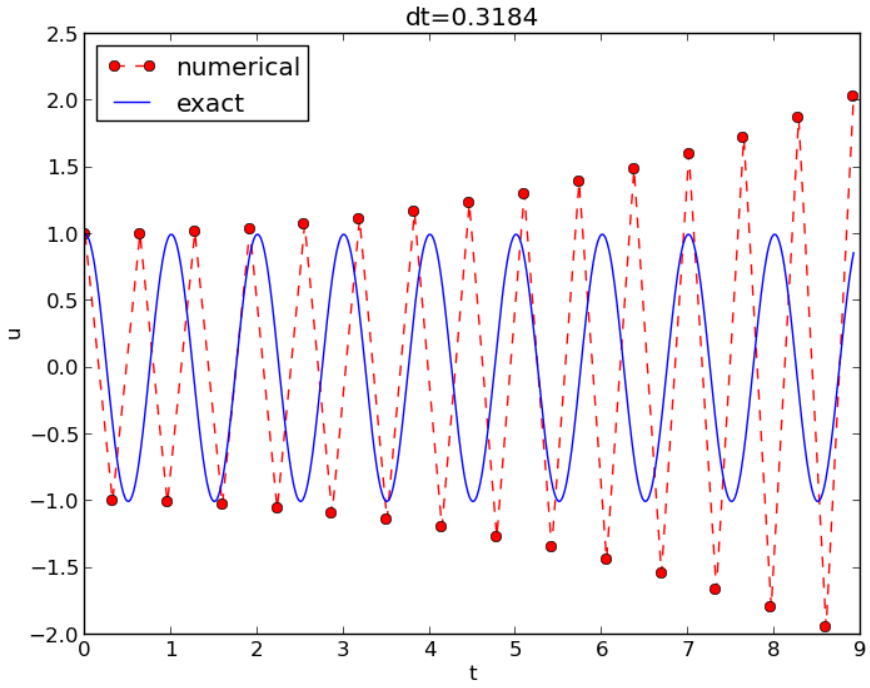

Figure 3: Growing, unstable solution because of a time step slightly beyond the stability limit.

4.5 About the accuracy at the stability limit

An interesting question is whether the stability condition $\Delta t < 2/\omega$ is unfortunate, or more precisely: would it be meaningful to take larger time steps to speed up computations? The answer is a clear no. At the stability limit, we have that $\sin^{-1} \omega\Delta t/2 = \sin^{-1} 1 = \pi/2$, and therefore $\tilde{\omega} = \pi/\Delta t$. (Note that the approximate formula (18) is very inaccurate for this value of Δt as it predicts $\tilde{\omega} = 2.34/pi$, which is a 25 percent reduction.) The corresponding period of the numerical solution is $\tilde{P} = 2\pi/\tilde{\omega} = 2\Delta t$, which means that there is just one time step Δt between a peak and a through in the numerical solution. This is the shortest possible wave that can be represented in the mesh. In other words, it is not meaningful to use a larger time step than the stability limit.

Also, the phase error when $\Delta t = 2/\omega$ is severe: Figure 4 shows a comparison of the numerical and analytical solution with $\omega = 2\pi$ and $\Delta t = 2/\omega = \pi^{-1}$. Already after one period, the numerical solution has a through while the exact solution has a peak (!). The error in frequency when Δt is at the stability limit becomes $\omega - \tilde{\omega} = \omega(1 - \pi/2) \approx -0.57\omega$. The corresponding error in the period is $P - \tilde{P} \approx 0.36P$. The error after m periods is then $0.36mP$. This error has reach half a period when $m = 1/(2 \cdot 0.36) \approx 1.38$, which theoretically confirms the observations in Figure 4 that the numerical solution is a through ahead of a peak already after one and a half period.

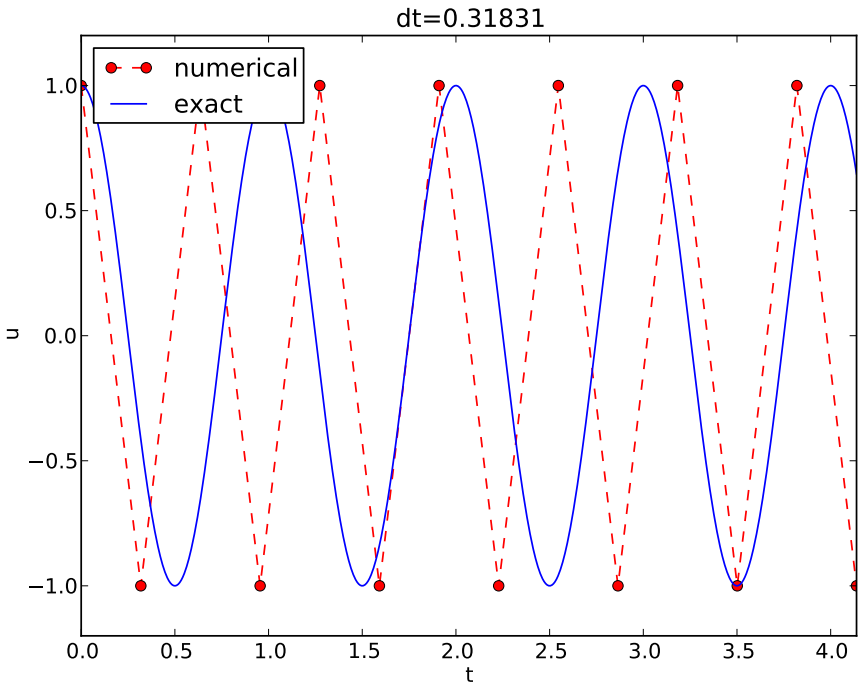

Figure 4: Numerical solution with Δt exactly at the stability limit.

Summary.

From the accuracy and stability analysis we can draw three important conclusions:

1. The key parameter in the formulas is $p = \omega\Delta t$. The period of oscillations is $P = 2\pi/\omega$, and the number of time steps per period is $N_P = P/\Delta t$. Therefore, $p = \omega\Delta t = 2\pi N_P$, showing that the critical parameter is the number of time steps per period. The smallest possible N_P is 2, showing that $p \in (0, \pi]$.
2. Provided $p \leq 2$, the amplitude of the numerical solution is constant.
3. The numerical solution exhibits a relative phase error $\tilde{\omega}/\omega \approx 1 + \frac{1}{24}p^2$. This error leads to wrongly displaced peaks of the numerical solution, and the error in peak location grows linearly with time (see Exercise 2).

5 Alternative schemes based on 1st-order equations

A standard technique for solving second-order ODEs is to rewrite them as a system of first-order ODEs and then apply the vast collection of methods for first-order ODE systems. Given the

second-order ODE problem

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

we introduce the auxiliary variable $v = u'$ and express the ODE problem in terms of first-order derivatives of u and v:

$$u' = v, \tag{23}$$
$$v' = -\omega^2 u\,. \tag{24}$$

The initial conditions become $u(0) = I$ and $v(0) = 0$.

6 Standard methods for 1st-order ODE systems

6.1 The Forward Euler scheme

A Forward Euler approximation to our 2×2 system of ODEs (23)-(24) becomes

$$[D_t^+ u = v]^n, [D_t^+ v = -\omega^2 u]^n, \tag{25}$$

or written out,

$$u^{n+1} = u^n + \Delta t v^n, \tag{26}$$
$$v^{n+1} = v^n - \Delta t \omega^2 u^n\,. \tag{27}$$

Let us briefly compare this Forward Euler method with the centered difference scheme for the second-order differential equation. We have from (26) and (27) applied at levels n and $n-1$ that

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

Since from (26)

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

it follows that

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

which is very close to the centered difference scheme, but the last term is evaluated at t_{n-1} instead of t_n. Dividing by Δt^2, the left-hand side is an approximation to u'' at t_n, while the right-hand side is sampled at t_{n-1}. This inconsistency in the scheme turns out to be rather crucial for the accuracy of the Forward Euler method applied to vibration problems.

6.2 The Backward Euler scheme

A Backward Euler approximation the ODE system is equally easy to write up in the operator notation:

$$[D_t^- u = v]^{n+1}, \tag{28}$$
$$[D_t^- v = -\omega u]^{n+1}\,. \tag{29}$$

This becomes a coupled system for u^{n+1} and v^{n+1}:

$$u^{n+1} - \Delta t v^{n+1} = u^n, \tag{30}$$
$$v^{n+1} + \Delta t\omega^2 u^{n+1} = v^n\,. \tag{31}$$

We can compare (30)-(31) with central the scheme for the second-order differential equation. To this end, we eliminate v^{n+1} in (30) using (31) solved with respect to v^{n+1}. Thereafter, we eliminate v^n using (30) solved with respect to v^{n+1} and replacing $n+1$ by n. The resulting equation involving only u^{n+1}, u^n, and u^{n-1} can be ordered as

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

which has almost the same form as the centered scheme for the second-order differential equation, but the right-hand side is evaluated at u^{n+1} and not u^n. This obvious inconsistency has a dramatic effect on the numerical solution.

6.3 The Crank-Nicolson scheme

The Crank-Nicolson scheme takes this form in the operator notation:

$$[D_t u = \overline{v}^t]^{n+\frac{1}{2}}, \tag{32}$$
$$[D_t v = -\omega\overline{u}^t]^{n+\frac{1}{2}}\,. \tag{33}$$

Writing the equations out shows that this is also a coupled system:

$$u^{n+1} - \frac{1}{2}\Delta t v^{n+1} = u^n + \frac{1}{2}\Delta t v^n, \tag{34}$$
$$v^{n+1} + \frac{1}{2}\Delta t\omega^2 u^{n+1} = v^n - \frac{1}{2}\Delta t\omega^2 u^n\,. \tag{35}$$

6.4 Comparison of schemes

We can easily compare methods like the ones above (and many more!) with the aid of the Odespy[9] package. Below is a sketch of the code.

```
import odespy
import numpy as np

def f(u, t, w=1):
    u, v = u  # u is array of length 2 holding our [u, v]
    return [v, -w**2*u]

def run_solvers_and_plot(solvers, timesteps_per_period=20,
```

[9] https://github.com/hplgit/odespy

```
                          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([I, 0])
        u, t = solver.solve(t_mesh)
```

There is quite some more code dealing with plots also, and we refer to the source file `vib_undamped_odespy.py`[10] for details. Observe that keyword arguments in `f(u,t,w=1)` can be supplied through a solver parameter `f_kwargs` (dictionary of additional keyword arguments to `f`).

Specification of the Forward Euler, Backward Euler, and Crank-Nicolson schemes is done like this:

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

The `vib_undamped_odespy.py` program makes two plots of the computed solutions with the various methods in the `solvers` list: one plot with $u(t)$ versus t, and one *phase plane plot* where v is plotted against u. That is, the phase plane plot is the curve $(u(t), v(t))$ parameterized by t. Analytically, $u = I\cos(\omega t)$ and $v = u' = -\omega I\sin(\omega t)$. The exact curve $(u(t), v(t))$ is therefore an ellipse, which often looks like a circle in a plot if the axes are automatically scaled. The important feature, however, is that exact curve $(u(t), v(t))$ is closed and repeats itself for every period. Not all numerical schemes are capable to do that, meaning that the amplitude instead shrinks or grows with time.

The Forward Euler scheme in Figure 5 has a pronounced spiral curve, pointing to the fact that the amplitude steadily grows, which is also evident in Figure 6. The Backward Euler scheme has a similar feature, except that the spriral goes inward and the amplitude is significantly damped. The changing amplitude and the sprial form decreases with decreasing time step. The Crank-Nicolson scheme looks much more accurate. In fact, these plots tell that the Forward and Backward Euler schemes are not suitable for solving our ODEs with oscillating solutions.

6.5 Runge-Kutta methods

We may run two popular standard methods for first-order ODEs, the 2nd- and 4th-order Runge-Kutta methods, to see how they perform. Figures 7 and 8 show the solutions with larger Δt values than what was used in the previous two plots.

The visual impression is that the 4th-order Runge-Kutta method is very accurate, under all circumstances in these tests, and the 2nd-order scheme suffer from amplitude errors unless the time step is very small.

The corresponding results for the Crank-Nicolson scheme are shown in Figures 9 and 10. It is clear that the Crank-Nicolson scheme outperforms the 2nd-order Runge-Kutta method. Both schemes have the same order of accuracy $\mathcal{O}(\Delta t^2)$, but their differences in the accuracy that

[10] `http://tinyurl.com/nm5587k/vib/vib_undamped_odespy.py`

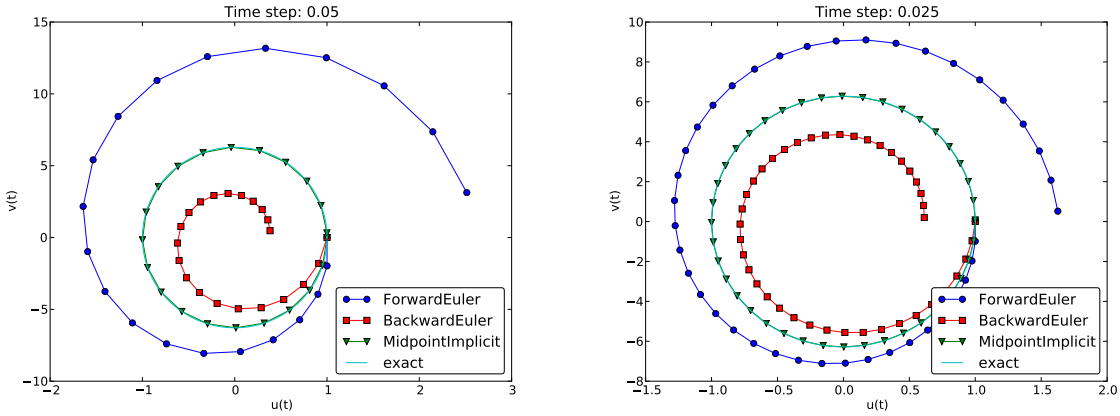

Figure 5: Comparison of classical schemes in the phase plane.

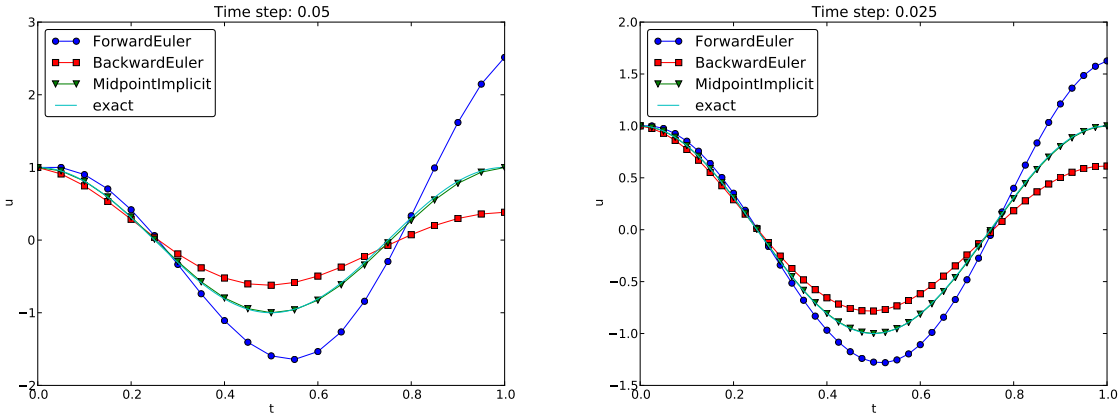

Figure 6: Comparison of classical schemes.

matters in a real physical application is very clearly pronounced in this example. Exercise 12 invites you to investigate how

6.6 Analysis of the Forward Euler scheme

We may try to find exact solutions of the discrete equations in the Forward Euler method. An "ansatz" is

$$u^n = IA^n,$$
$$v^n = qIA^n,$$

where q and A are unknown numbers. We could have used a complex exponential form $\exp(i\tilde{\omega}n\Delta t)$ since we get oscillatory form, but the oscillations grow in the Forward Euler method, so the numerical frequency $\tilde{\omega}$ will be complex anyway (to produce an exponentially growing amplitude), so it is easier to just work with potentially complex A and q as introduced above.

The Forward Euler scheme leads to

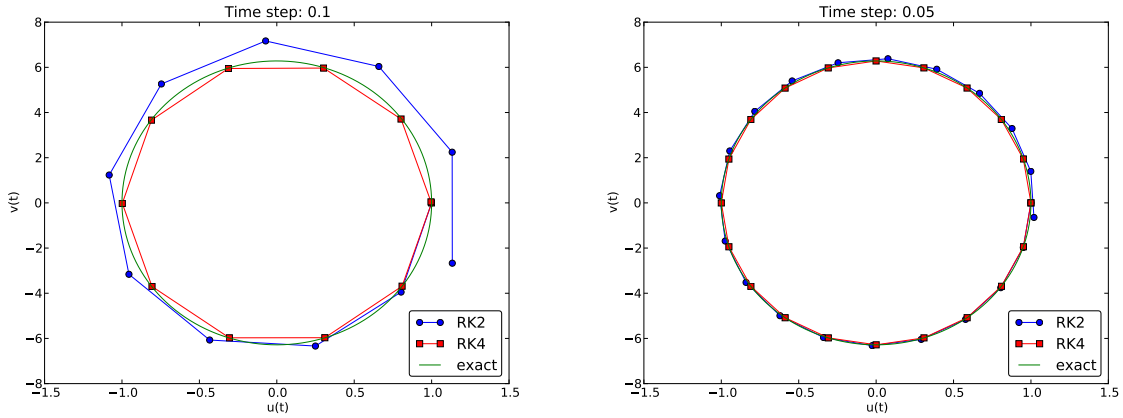

Figure 7: Comparison of Runge-Kutta schemes in the phase plane.

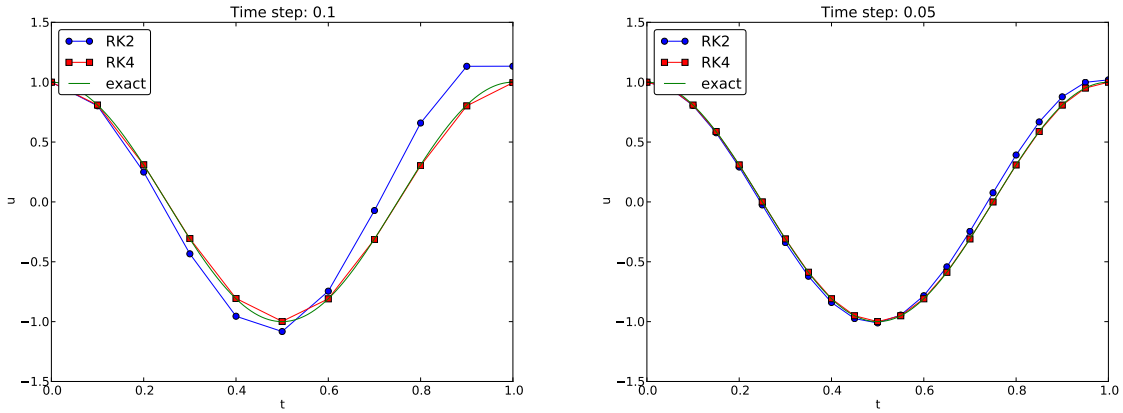

Figure 8: Comparison of Runge-Kutta schemes.

$$A = 1 + \Delta t q,$$
$$A = 1 - \Delta t \omega^2 q^{-1}\,.$$

We can easily eliminate A, get $q^2 + \omega^2 = 0$, and solve for

$$q = \pm i\omega,$$

which gives

$$A = 1 \pm \Delta t i\omega\,.$$

We shall take the real part of A^n as the solution. The two values of A are complex conjugates, and the real part of A^n will be the same for the two roots. This is easy to realize if we rewrite the complex numbers in polar form ($re^{i\theta}$), which is also convenient for further analysis and understanding. The polar form of the two values for A become

$$1 \pm \Delta t i\omega = \sqrt{1 + \omega^2 \Delta t^2} e^{\pm i \tan^{-1}(\omega \Delta t)}\,.$$

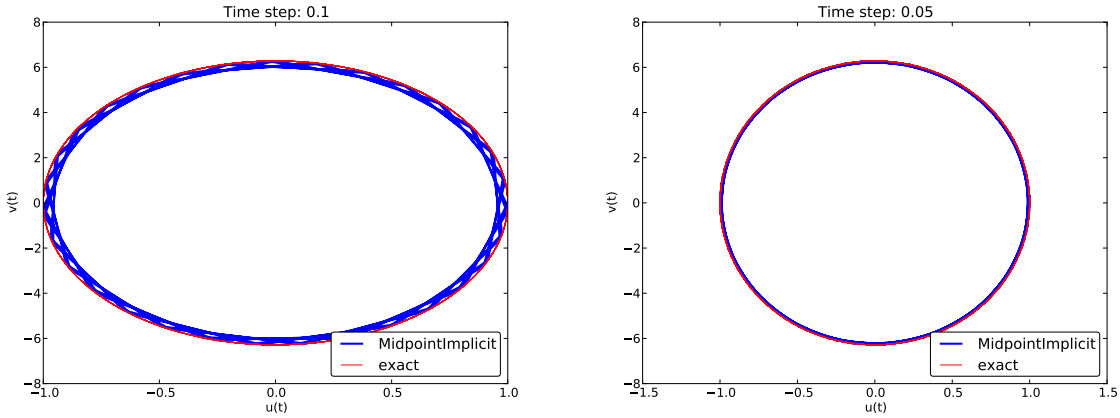

Figure 9: Long-time behavior of the Crank-Nicolson scheme in the phase plane.

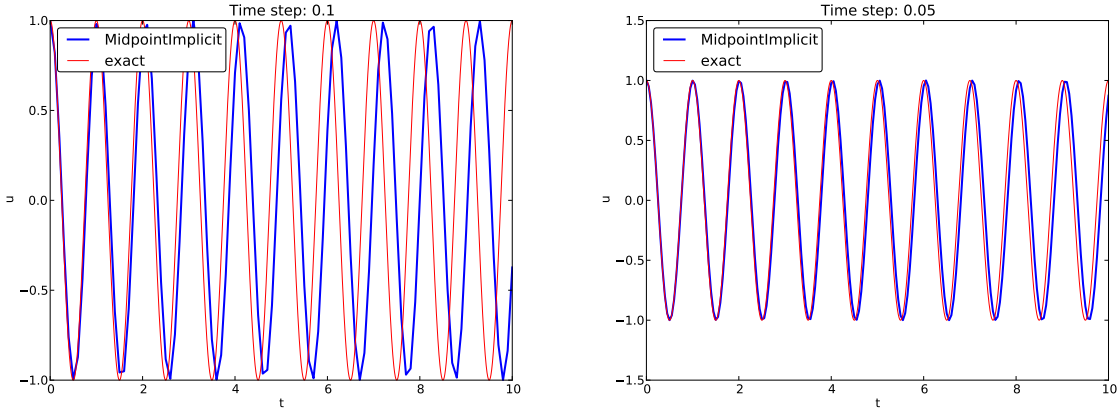

Figure 10: Long-time behavior of the Crank-Nicolson scheme.

Now,

$$(1 \pm \Delta t i\omega)^n = (1 + \omega^2 \Delta t^2) n/2 e^{\pm ni \tan^{-1}(\omega \Delta t)} .$$

Since $\cos(\theta n) = \cos(-\theta n)$, the real part of the two numbers become the same. We therefore continue with the solution that has the plus sign.

The general solution is $u^n = CA^n$, where C is a constant. This is determined from the initial condition: $u^0 = C = I$. Then also $v^n = qIA^n$. The final solutions consist of the real part of the expressions in polar form:

$$u^n = I(1 + \omega^2 \Delta t^2) n/2 \cos(n \tan^{-1}(\omega \Delta t)), \quad v^n = -\omega I(1 + \omega^2 \Delta t^2) n/2 \sin(n \tan^{-1}(\omega \Delta t)) .$$

The expression $(1 + \omega^2 \Delta t^2) n/2$ causes growth of the amplitude, since a number greater than one is raised to an integer power. By expanding first the square root, $\sqrt{1 + x^2} \approx 1 + \frac{1}{2} x^2$, we realize that raising the approximation to any integer power, will give rise to a polynomial with leading terms $1 + x^2$, or with $x = \omega \Delta$ as in our case, the amplitude in the Forward Euler scheme grows as $1 + \omega^2 \Delta t^2$.

7 Energy considerations

The observations of various methods in the previous section can be better interpreted if we compute an quantity reflecting the total *energy of the system*. It turns out that this quantity,

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

is *constant* for all t. Checking that $E(t)$ really remains constant brings evidence that the numerical computations are sound. Such energy measures, when they exist, are much used to check numerical simulations.

7.1 Derivation of the energy expression

We starting multiplying

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

by u' and integrating from 0 to T:

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

Observing that

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

we get

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

where we have introduced the energy measure $E(t)$

$$E(t) = \frac{1}{2}(u')^2 + \frac{1}{2}\omega^2 u^2\,. \tag{36}$$

The important result from this derivation is that the total energy is constant:

$$E(t) = E(0)\,.$$

Warning.

The quantity $E(t)$ derived above is physically not the energy of a vibrating mechanical system, but the energy per unit mass. To see this, we start with Newton's second law $F = ma$ (F is the sum of forces, m is the mass of the system, and a is the acceleration). The displacement u is related to a through $a = u''$. With a spring force as the only force we have $F = -ku$, where k is a spring constant measuring the stiffness of the spring. Newton's second law then implies the differential equation

$$-ku = mu'' \quad \Rightarrow mu'' + ku = 0\,.$$

This equation of motion can be turned into an energy balance equation by finding the work done by each term during a time interval $[0, T]$. To this end, we multiply the equation by $du = u'dt$ and integrate:

$$\int_0^T muu'dt + \int_0^T kuu'dt = 0\,.$$

The result is

$$E(t) = E_k(t) + E_p(t) = 0,$$

where

$$E_k(t) = \frac{1}{-}2mv^2, \quad v = u', \tag{37}$$

is the *kinetic energy* of the system,

$$E_p(t) = \frac{1}{2}ku^2 \tag{38}$$

is the *potential energy*, and the sum $E(t)$ is the total energy. The derivation demonstrates the famous energy principle that any change in the kinetic energy is due to a change in potential energy and vice versa.

The equation $mu'' + ku = 0$ can be divided by m and written as $u'' + \omega^2 u = 0$ for $\omega = \sqrt{k/m}$. The energy expression $E(t) = \frac{1}{2}(u')^2 + \frac{1}{2}\omega^2 u^2$ derived earlier is then simply the true physical total energy $\frac{1}{2}m(u')^2 + \frac{1}{2}k^2u^2$ divided by m, i.e., total energy per unit mass.

Energy of the exact solution. Analytically, we have $u(t) = I\cos\omega t$, if $u(0) = I$ and $u'(0) = 0$, so we can easily check that the evolution of the energy $E(t)$ is constant:

$$E(t) = \frac{1}{2}I^2(-\omega\sin\omega t)^2 + \frac{1}{2}\omega^2 I^2\cos^2\omega t = \frac{1}{2}\omega^2(\sin^2\omega t + \cos^2\omega t) = \frac{1}{2}\omega^2\,.$$

7.2 An error measure based on total energy

The error in total energy, as a mesh function, can be computed by

$$e_E^n = \frac{1}{2}\left(\frac{u^{n+1} - u^{n-1}}{2\Delta t}\right)^2 + \frac{1}{2}\omega^2(u^n)^2 - E(0), \quad n = 1, \ldots, N_t - 1, \tag{39}$$

where

$$E(0) = \frac{1}{2}V^2 + \frac{1}{2}\omega^2 I^2,$$

if $u(0) = I$ and $u'(0) = V$. A useful norm can be the maximum absolute value of e_E^n:

$$||e_E^n||_{\ell^\infty} = \max_{1\leq n<N_t} |e_E^n|\,.$$

The corresponding Python implementation takes the form

```
# import numpy as np and compute u, t
dt = t[1]-t[0]
E = 0.5*((u[2:] - u[:-2])/(2*dt))**2 + 0.5*w**2*u[1:-1]**2
E0 = 0.5*V**2 + 0.5**w**2*I**2
e_E = E - E0
e_E_norm = np.abs(e_E).max()
```

The convergence rates of the quantity `e_E_norm` can be used for verification. The value of `e_E_norm` is also useful for comparing schemes through their ability to preserve energy. Below is a table demonstrating the error in total energy for various schemes. We clearly see that the Crank-Nicolson and 4th-order Runge-Kutta schemes are superior to the 2nd-order Runge-Kutta method and even more superior to the Forward and Backward Euler schemes.

Method	T	Δt	$\max \lvert e_E^n \rvert$
Forward Euler	1	0.05	$1.113 \cdot 10^{2}$
Forward Euler	1	0.025	$3.312 \cdot 10^{1}$
Backward Euler	1	0.05	$1.683 \cdot 10^{1}$
Backward Euler	1	0.025	$1.231 \cdot 10^{1}$
Runge-Kutta 2nd-order	1	0.1	8.401
Runge-Kutta 2nd-order	1	0.05	$9.637 \cdot 10^{-1}$
Crank-Nicolson	1	0.05	$9.389 \cdot 10^{-1}$
Crank-Nicolson	1	0.025	$2.411 \cdot 10^{-1}$
Runge-Kutta 4th-order	1	0.1	2.387
Runge-Kutta 4th-order	1	0.05	$6.476 \cdot 10^{-1}$
Crank-Nicolson	10	0.1	3.389
Crank-Nicolson	10	0.05	$9.389 \cdot 10^{-1}$
Runge-Kutta 4th-order	10	0.1	3.686
Runge-Kutta 4th-order	10	0.05	$6.928 \cdot 10^{-1}$

8 The Euler-Cromer method

While the 4th-order Runge-Kutta method and the a centered Crank-Nicolson scheme work well for the first-order formulation of the vibration model, both were inferior to the straightforward centered difference scheme for the second-order equation $u'' + \omega^2 u = 0$. However, there is a similarly successful scheme available for the first-order system $u' = v$, $v' = -\omega^2 u$, to be presented next.

8.1 Forward-backward discretization

The idea is to apply a Forward Euler discretization to the first equation and a Backward Euler discretization to the second. In operator notation this is stated as

$$[D_t^+ u = v]^n, \tag{40}$$

$$[D_t^- v = -\omega u]^{n+1}\,. \tag{41}$$

We can write out the formulas and collect the unknowns on the left-hand side:

$$u^{n+1} = u^n + \Delta t v^n, \tag{42}$$

$$v^{n+1} = v^n - \Delta t \omega^2 u^{n+1}\,. \tag{43}$$

We realize that u^{n+1} can be computed from (42) and then v^{n+1} from (43) using the recently computed value u^{n+1} on the right-hand side.

In physics, it is more common to update the v equation first, with a forward difference, and thereafter the u equation, with a backward difference that applies the most recently computed v value:

$$v^{n+1} = v^n - \Delta t \omega^2 u^n, \tag{44}$$

$$u^{n+1} = u^n + \Delta t v^{n+1}\,. \tag{45}$$

The advantage of this sequence of the first-order ODEs becomes evident when we turn to more complicated models. A typical vibration ODE can in general be written as

$$\ddot{u} + g(u, u', t) = 0,$$

which results in the system

$$v' = -g(u, v, t),$$
$$u' = v,$$

and the scheme

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

We realize that the first update works well with any g since old values u^n and v^n are used. Switching the equations would demand $u^n{+}1$ and v^{n+1} values in g.

The scheme (45)-(44) goes under several names: Forward-backward scheme, Semi-implicit Euler method[11], symplectic Euler, semi-explicit Euler, Newton-Störmer-Verlet, and Euler-Cromer. We shall stick to the latter name. Since both time discretizations are based on first-order difference approximation, one may think that the scheme is only of first-order, but this is not true: the use of a forward and then a backward difference make errors cancel so that the overall error in the scheme is $\mathcal{O}(\Delta t^2)$. This is explaned below.

8.2 Equivalence with the scheme for the second-order ODE

We may eliminate the v^n variable from (42)-(43) or (45)-(44). The v^{n+1} term in (44) can be eliminated from (45):

$$u^{n+1} = u^n + \Delta t(v^n - \omega^2 \Delta t^2 u^n)\,. \tag{46}$$

The v^n quantity can be expressed by u^n and u^{n-1} using (45):

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

and when this is inserted in (46) we get

$$u^{n+1} = 2u^n - u^{n-1} - \Delta t^2 \omega^2 u^n, \tag{47}$$

[11] `http://en.wikipedia.org/wiki/Semi-implicit_Euler_method`

which is nothing but the centered scheme (7)! Therefore, the previous analysis of (7) also applies to the Euler-Cromer method. In particular, the amplitude is constant, given that the stability criterion is fulfilled, but there is always a phase error (18). Exercise 20 gives guidance on how to derive the exact discrete solution of the two equations in the Euler-Cromer method.

The initial condition $u' = 0$ means $u' = v = 0$. From (45) we get $v^1 = -\omega^2 u^0$ and $u^1 = u^0 - \omega^2 \Delta t^2 u^0$, which is not exactly the same u^1 value as obtained by a centered approximation of $v'(0) = 0$ and combined with the discretization (7) of the second-order ODE: a factor $\frac{1}{2}$ is missing in the second term. In fact, if we approximate $u'(0) = 0$ by a backward difference, $(u^0 - u^{-1})/\Delta t = 0$, we get $u^{-1} = u^0$, and when combined with (7), it results in $u^1 = u^0 - \omega^2 \Delta t^2 u^0$. That is, the Euler-Cromer method based on (45)-(44) corresponds to using only a first-order approximation to the initial condition in the method from Section 1.2.

Correspondingly, using the formulation (42)-(43) with $v^n = 0$ leads to $u^1 = u^0$, which can be interpreted as using a forward difference approximation for the initial condition $u'(0) = 0$. Both Euler-Cromer formulations lead to slightly different values for u^1 compared to the method in Section 1.2. The error is $\frac{1}{2}\omega^2 \Delta t^2 u^0$ and of the same order as the overall scheme.

8.3 Implementation

The function below, found in `vib_EulerCromer.py`[12] implements the Euler-Cromer scheme (45)-(44):

```
from numpy import zeros, linspace

def solver(I, w, dt, T):
    """
    Solve v' = - w**2*u, u'=v for t in (0,T], u(0)=I and v(0)=0,
    by an Euler-Cromer method.
    """
    dt = float(dt)
    Nt = int(round(T/dt))
    u = zeros(Nt+1)
    v = zeros(Nt+1)
    t = linspace(0, Nt*dt, Nt+1)

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

Since the Euler-Cromer scheme is equivalent to the finite difference method for the second-order ODE $u'' + \omega^2 u = 0$ (see Section 8.2), the performance of the above `solver` function is the same as for the `solver` function in Section 2. The only difference is the formula for the first time step, as discussed above. This deviation in the Euler-Cromer scheme means that the discrete solution listed in Section 4.2 is not a solution of the Euler-Cromer scheme. To verify the implementation of the Euler-Cromer method we can adjust `v[1]` so that the computer-generated values can be compared formula from in Section 4.2. This adjustment is done in an alternative solver function, `solver_ic_fix` in `vib_EulerCromer.py`, and combined with a nose test in the function `test_solver` that checks equality of computed values with the exact discrete solution to machine precision. Another function, `demo`, visualizes the difference between Euler-Cromer scheme and the scheme for the second-oder ODE, arising from the mismatch in the first time level.

[12] `http://tinyurl.com/nm5587k/vib/vib_EulerCromer.py`

8.4 The velocity Verlet algorithm

Another very popular algorithm for vibration problems $u'' + \omega^2 u = 0$ can be derived as follows. First, we step u forward from t_n to t_{n+1} using a three-term Taylor series,

$$u(t_{n+1}) = u(t_n) + u'(t_n)\Delta t + \frac{1}{2}u''(t_n)\Delta t^2 .$$

Using $u' = v$ and $u'' = -\omega^2 u$, we get the updating formula

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

Second, the first-order equation for v,

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

is discretized by a centered difference in a Crank-Nicolson fashion at $t_{n+\frac{1}{2}}$:

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

or in operator form that explicitly demonstrates the thinking:

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

To summarize, we have the scheme

$$u^{n+1} = u^n + v^n\Delta t - \frac{1}{2}\Delta^2\omega^2 u^n \tag{48}$$

$$v^{n+1} = v^n - \frac{1}{2}\Delta t\omega^2(u^n + u^{n+1}), \tag{49}$$

known as the *velocity Verlet* algorithm. Observe that this scheme is explicit since u^{n+1} in (49) is already computed from (48).

The algorithm can be straightforwardly implemented as shown below.

```
from vib_undamped import (
    zeros, linspace,
    convergence_rates,
    main)

def solver(I, w, dt, T, return_v=False):
    """
    Solve u'=v, v'=-w**2*u for t in (0,T], u(0)=I and v(0)=0,
    by the velocity Verlet method with time step dt.
    """
    dt = float(dt)
    Nt = int(round(T/dt))
    u = zeros(Nt+1)
    v = zeros(Nt+1)
    t = linspace(0, Nt*dt, Nt+1)

    u[0] = I
    v[0] = 0
    for n in range(Nt):
        u[n+1] = u[n] + v[n]*dt - 0.5*dt**2*w**2*u[n]
        v[n+1] = v[n] - 0.5*dt*w**2*(u[n] + u[n+1])
    if return_v:
```

```
        return u, v, t
    else:
        # Return just u and t as in the vib_undamped.py's solver
        return u, t
```

We provide the option that this `solver` function returns the same data as the `solver` function from Section 2.1 (if `return_v` is `False`), but we may return `v` along with `u` and `t`.

The error in the Taylor series expansion behind (48) is $\mathcal{O}(\Delta t^3)$, while the error in the central difference for v is $\mathcal{O}(\Delta t^2)$. The overall error is then no better than $\mathcal{O}(\Delta t^2)$, which can be verified empirically using the `convergence_rates` function from 2.2:

```
>>> import vib_undamped_velocity_Verlet as m
>>> m.convergence_rates(4, solver_function=m.solver)
[2.0036366687367346, 2.0009497328124835, 2.000240105995295]
```

9 Generalization: damping, nonlinear spring, and external excitation

We shall now generalize the simple model problem from Section 1 to include a possibly nonlinear damping term $f(u')$, a possibly nonlinear spring (or restoring) force $s(u)$, and some external excitation $F(t)$:

$$mu'' + f(u') + s(u) = F(t), \quad u(0) = I,\ u'(0) = V,\ t \in (0, T]\,. \tag{50}$$

We have also included a possibly nonzero initial value of $u'(0)$. The parameters m, $f(u')$, $s(u)$, $F(t)$, I, V, and T are input data.

There are two main types of damping (friction) forces: linear $f(u') = bu$, or quadratic $f(u') = bu'|u'|$. Spring systems often feature linear damping, while air resistance usually gives rise to quadratic damping. Spring forces are often linear: $s(u) = cu$, but nonlinear versions are also common, the most famous is the gravity force on a pendulum that acts as a spring with $s(u) \sim \sin(u)$.

9.1 A centered scheme for linear damping

Sampling (50) at a mesh point t_n, replacing $u''(t_n)$ by $[D_tD_tu]^n$, and $u'(t_n)$ by $[D_{2t}u]^n$ results in the discretization

$$[mD_tD_tu + f(D_{2t}u) + s(u) = F]^n, \tag{51}$$

which written out means

$$m\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} + f(\frac{u^{n+1} - u^{n-1}}{2\Delta t}) + s(u^n) = F^n, \tag{52}$$

where F^n as usual means $F(t)$ evaluated at $t = t_n$. Solving (52) with respect to the unknown u^{n+1} gives a problem: the u^{n+1} inside the f function makes the equation *nonlinear* unless $f(u')$ is a linear function, $f(u') = bu'$. For now we shall assume that f is linear in u'. Then

$$m\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} + b\frac{u^{n+1} - u^{n-1}}{2\Delta t} + s(u^n) = F^n, \tag{53}$$

which gives an explicit formula for u at each new time level:

$$u^{n+1} = (2mu^n + (\frac{b}{2}\Delta t - m)u^{n-1} + \Delta t^2(F^n - s(u^n)))(m + \frac{b}{2}\Delta t)^{-1}\,. \tag{54}$$

For the first time step we need to discretize $u'(0) = V$ as $[D_{2t}u = V]^0$ and combine with (54) for $n = 0$. The discretized initial condition leads to

$$u^{-1} = u^1 - 2\Delta t V, \tag{55}$$

which inserted in (54) for $n = 0$ gives an equation that can be solved for u^1:

$$u^1 = u^0 + \Delta t\, V + \frac{\Delta t^2}{2m}(-bV - s(u^0) + F^0)\,. \tag{56}$$

9.2 A centered scheme for quadratic damping

When $f(u') = bu'|u'|$, we get a quadratic equation for u^{n+1} in (52). This equation can straightforwardly be solved, but we can also avoid the nonlinearity by performing an approximation that is within other numerical errors that we have already committed by replacing derivatives with finite differences.

The idea is to reconsider (50) and only replace u'' by D_tD_tu, giving

$$[mD_tD_tu + bu'|u'| + s(u) = F]^n, \tag{57}$$

Here, $u'|u'|$ is to be computed at time t_n. We can introduce a *geometric mean*, defined by

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

for some quantity w depending on time. The error in the geometric mean approximation is $\mathcal{O}(\Delta t^2)$, the same as in the approximation $u'' \approx D_tD_tu$. With $w = u'$ it follows that

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

The next step is to approximate u' at $t_{n\pm1/2}$, but here a centered difference can be used:

$$u'(t_{n+1/2}) \approx [D_tu]^{n+\frac{1}{2}}, \quad u'(t_{n-1/2}) \approx [D_tu]^{n-\frac{1}{2}}\,. \tag{58}$$

We then get

$$[u'|u'|]^n \approx [D_tu]^{n+\frac{1}{2}}|[D_tu]^{n-\frac{1}{2}}| = \frac{u^{n+1} - u^n}{\Delta t}\frac{|u^n - u^{n-1}|}{\Delta t}\,. \tag{59}$$

The counterpart to (52) is then

$$m\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} + b\frac{u^{n+1} - u^n}{\Delta t}\frac{|u^n - u^{n-1}|}{\Delta t} + s(u^n) = F^n, \tag{60}$$

which is linear in u^{n+1}. Therefore, we can easily solve with respect to u^{n+1} and achieve the explicit updating formula

$$u^{n+1} = \big(m + b|u^n - u^{n-1}|\big)^{-1} \times \\ \big(2mu^n - mu^{n-1} + bu^n|u^n - u^{n-1}| + \Delta t^2(F^n - s(u^n))\big)\,. \tag{61}$$

In the derivation of a special equation for the first time step we run into some trouble: inserting (55) in (61) for $n = 0$ results in a complicated nonlinear equation for u^1. By thinking differently about the problem we can easily get away with the nonlinearity again. We have for $n = 0$ that $b[u'|u'|]^0 = bV|V|$. Using this value in (57) gives

$$[mD_tD_tu + bV|V| + s(u) = F]^0 \,. \tag{62}$$

Writing this equation out and using (55) results in the special equation for the first time step:

$$u^1 = u^0 + \Delta t V + \frac{\Delta t^2}{2m}\left(-bV|V| - s(u^0) + F^0\right) \,. \tag{63}$$

9.3 A forward-backward discretization of the quadratic damping term

The previous section first proposed to discretize the quadratic damping term $|u'|u'$ using centered differences: $[|D_{2t}|D_{2t}u]^n$. As this gives rise to a nonlinearity in u^{n+1}, it was instead proposed to use a geometric mean combined with centered differences. But there are other alternatives. To get rid of the nonlinearity in $[|D_{2t}|D_{2t}u]^n$, one can think differently: apply a backward difference to $|u'|$, such that the term involves known values, and apply a forward difference to u' to make the term linear in the unknown u^{n+1}. With mathematics,

$$[\beta|u'|u']^n \approx \beta|[D_t^- u]^n|[D_t^+ u]^n = \beta\left|\frac{u^- u^{n-1}}{\Delta t}\right|\frac{u^{n+1}-u^n}{\Delta t} \,.$$

The forward and backward differences have both an error proportional to Δt so one may think the discretization above leads to a first-order scheme. However, by looking at the formulas, we realize that the forward-backward differences result in exactly the same scheme as when we used a geometric mean and centered differences. Therefore, the forward-backward differences act in a symmetric way and actually produce a second-order accurate discretization of the quadratic damping term.

9.4 Implementation

The algorithm arising from the methods in Sections 9.1 and 9.2 is very similar to the undamped case in Section 1.2. The difference is basically a question of different formulas for u^1 and u^{n+1}. This is actually quite remarkable. The equation (50) is normally impossible to solve by pen and paper, but possible for some special choices of F, s, and f. On the contrary, the complexity of the nonlinear generalized model (50) versus the simple undamped model is not a big deal when we solve the problem numerically!

The computational algorithm takes the form

1. $u^0 = I$
2. compute u^1 from (56) if linear damping or (63) if quadratic damping
3. for $n = 1, 2, \ldots, N_t - 1$:
   (a) compute u^{n+1} from (54) if linear damping or (61) if quadratic damping

Modifying the `solver` function for the undamped case is fairly easy, the big difference being many more terms and if tests on the type of damping:

```
def solver(I, V, m, b, s, F, dt, T, damping='linear'):
    """
    Solve m*u'' + f(u') + s(u) = F(t) for t in (0,T],
    u(0)=I and u'(0)=V,
    by a central finite difference method with time step dt.
    If damping is 'linear', f(u')=b*u, while if damping is
    'quadratic', f(u')=b*u'*abs(u').
    F(t) and s(u) are Python functions.
    """
    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
```

The complete code resides in the file `vib.py`[13].

9.5 Verification

Constant solution. For debugging and initial verification, a constant solution is often very useful. We choose $u_{\mathrm{e}}(t) = I$, which implies $V = 0$. Inserted in the ODE, we get $F(t) = s(I)$ for any choice of f. Since the discrete derivative of a constant vanishes (in particular, $[D_{2t}I]^n = 0$, $[D_tI]^n = 0$, and $[D_tD_tI]^n = 0$), the constant solution also fulfills the discrete equations. The constant should therefore be reproduced to machine precision.

Linear solution. Now we choose a linear solution: $u_{\mathrm{e}} = ct + d$. The initial condition $u(0) = I$ implies $d = I$, and $u'(0) = V$ forces c to be V. Inserting $u_{\mathrm{e}} = Vt + I$ in the ODE with linear damping results in

$$0 + bV + s(Vt + I) = F(t),$$

while quadratic damping requires the source term

$$0 + b|V|V + s(Vt + I) = F(t)\,.$$

Since the finite difference approximations used to compute u' all are exact for a linear function, it turns out that the linear u_{e} is also a solution of the discrete equations. Exercise 9 asks you to carry out all the details.

[13] `http://tinyurl.com/nm5587k/vib/vib.py`

Quadratic solution. Choosing $u_e = bt^2 + Vt + I$, with b arbitrary, fulfills the initial conditions and fits the ODE if F is adjusted properly. The solution also solves the discrete equations with linear damping. However, this quadratic polynomial in t does not fulfill the discrete equations in case of quadratic damping, because the geometric mean used in the approximation of this term introduces an error. Doing Exercise 9 will reveal the details. One can fit F^n in the discrete equations such that the quadratic polynomial is reproduced by the numerical method (to machine precision).

9.6 Visualization

The functions for visualizations differ significantly from those in the undamped case in the `vib_undamped.py` program because we in the present general case do not have an exact solution to include in the plots. Moreover, we have no good estimate of the periods of the oscillations as there will be one period determined by the system parameters, essentially the approximate frequency $\sqrt{s'(0)/m}$ for linear s and small damping, and one period dictated by $F(t)$ in case the excitation is periodic. This is, however, nothing that the program can depend on or make use of. Therefore, the user has to specify T and the window width in case of a plot that moves with the graph and shows the most recent parts of it in long time simulations.

The `vib.py` code contains several functions for analyzing the time series signal and for visualizing the solutions.

9.7 User interface

The `main` function has substantial changes from the `vib_undamped.py` code since we need to specify the new data c, $s(u)$, and $F(t)$. In addition, we must set T and the plot window width (instead of the number of periods we want to simulate as in `vib_undamped.py`). To figure out whether we can use one plot for the whole time series or if we should follow the most recent part of u, we can use the `plot_empricial_freq_and_amplitude` function's estimate of the number of local maxima. This number is now returned from the function and used in `main` to decide on the visualization technique.

```
def main():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument('--I', type=float, default=1.0)
    parser.add_argument('--V', type=float, default=0.0)
    parser.add_argument('--m', type=float, default=1.0)
    parser.add_argument('--c', type=float, default=0.0)
    parser.add_argument('--s', type=str, default='u')
    parser.add_argument('--F', type=str, default='0')
    parser.add_argument('--dt', type=float, default=0.05)
    parser.add_argument('--T', type=float, default=140)
    parser.add_argument('--damping', type=str, default='linear')
    parser.add_argument('--window_width', type=float, default=30)
    parser.add_argument('--savefig', action='store_true')
    a = parser.parse_args()
    from scitools.std import StringFunction
    s = StringFunction(a.s, independent_variable='u')
    F = StringFunction(a.F, independent_variable='t')
    I, V, m, c, dt, T, window_width, savefig, damping = \
       a.I, a.V, a.m, a.c, a.dt, a.T, a.window_width, a.savefig, \
       a.damping

    u, t = solver(I, V, m, c, s, F, dt, T)
    num_periods = empirical_freq_and_amplitude(u, t)
```

```
    if num_periods <= 15:
        figure()
        visualize(u, t)
    else:
        visualize_front(u, t, window_width, savefig)
    show()
```

The program `vib.py` contains the above code snippets and can solve the model problem (50). As a demo of `vib.py`, we consider the case $I = 1$, $V = 0$, $m = 1$, $c = 0.03$, $s(u) = \sin(u)$, $F(t) = 3\cos(4t)$, $\Delta t = 0.05$, and $T = 140$. The relevant command to run is

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

This results in a moving window following the function[14] on the screen. Figure 11 shows a part of the time series.

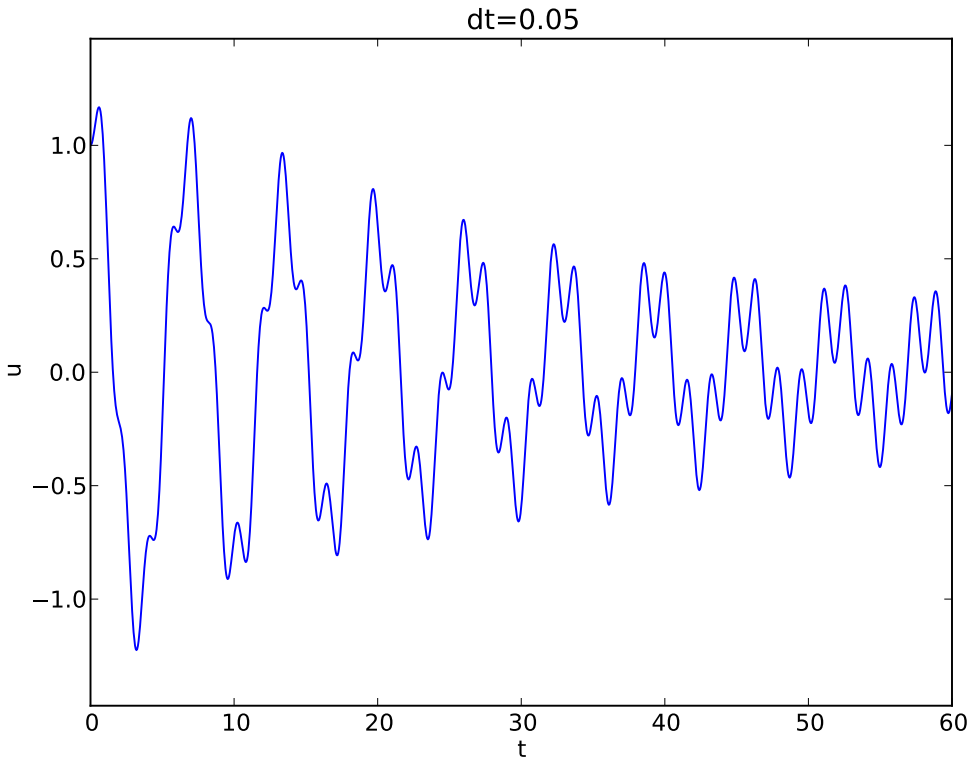

Figure 11: Damped oscillator excited by a sinusoidal function.

[14] `http://tinyurl.com/opdfafk/pub/mov-vib/vib_generalized_dt0.05/index.html`

9.8 The Euler-Cromer scheme for the generalized model

The ideas of the Euler-Cromer method from Section 8 carry over to the generalized model. We write (50) as two equations for u and $v = u'$. The first equation is taken as the one with v' on the left-hand side:

$$v' = \frac{1}{m}(F(t) - s(u) - f(v)), \tag{64}$$

$$u' = v\,. \tag{65}$$

The idea is to step (64) forward using a standard Forward Euler method, while we update u from (65) with a Backward Euler method, utilizing the recent, computed v^{n+1} value. In detail,

$$\frac{v^{n+1} - v^n}{\Delta t} = \frac{1}{m}(F(t_n) - s(u^n) - f(v^n)), \tag{66}$$

$$\frac{u^{n+1} - u^n}{\Delta t} = v^{n+1}, \tag{67}$$

resulting in the explicit scheme

$$v^{n+1} = v^n + \Delta t\frac{1}{m}(F(t_n) - s(u^n) - f(v^n)), \tag{68}$$

$$u^{n+1} = u^n + \Delta t\, v^{n+1}\,. \tag{69}$$

We immediately note one very favorable feature of this scheme: all the nonlinearities in $s(u)$ and $f(v)$ are evaluated at a previous time level. This makes the Euler-Cromer method easier to apply and hence much more convenient than the centered scheme for the second-order ODE (50).

The initial conditions are trivially set as

$$v^0 = V, \tag{70}$$

$$u^0 = I\,. \tag{71}$$

10 Exercises and Problems

Problem 1: Use linear/quadratic functions for verification

Consider the ODE problem

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

Discretize this equation according to $[D_tD_tu + \omega^2 u = f]^n$.

a) Derive the equation for the first time step (u^1).

b) For verification purposes, we use the method of manufactured solutions (MMS) with the choice of $u_{\mathrm{e}}(x,t) = ct + d$. Find restrictions on c and d from the initial conditions. Compute the corresponding source term f by term. Show that $[D_tD_tt]^n = 0$ and use the fact that the D_tD_t operator is linear, $[D_tD_t(ct + d)]^n = c[D_tD_tt]^n + [D_tD_td]^n = 0$, to show that u_{e} is also a perfect solution of the discrete equations.

c) Use `sympy` to do the symbolic calculations above. Here is a sketch of the program `vib_undamped_verify_mms.py`:

```
import sympy as sp
V, t, I, w, dt = sp.symbols('V t I w dt')  # global symbols
f = None  # global variable for the source term in the ODE

def ode_source_term(u):
    """Return the terms in the ODE that the source term
    must balance, here u'' + w**2*u.
    u is symbolic Python function of t."""
    return sp.diff(u(t), t, t) + w**2*u(t)

def residual_discrete_eq(u):
    """Return the residual of the discrete eq. with u inserted."""
    R = ...
    return sp.simplify(R)

def residual_discrete_eq_step1(u):
    """Return the residual of the discrete eq. at the first
    step with u inserted."""
    R = ...
    return sp.simplify(R)

def DtDt(u, dt):
    """Return 2nd-order finite difference for u_tt.
    u is a symbolic Python function of t.
    """
    return ...

def main(u):
    """
    Given some chosen solution u (as a function of t, implemented
    as a Python function), use the method of manufactured solutions
    to compute the source term f, and check if u also solves
    the discrete equations.
    """
    print '=== Testing exact solution: %s ===' % u
    print "Initial conditions u(0)=%s, u'(0)=%s:" % \
          (u(t).subs(t, 0), sp.diff(u(t), t).subs(t, 0))

    # Method of manufactured solution requires fitting f
    global f  # source term in the ODE
    f = sp.simplify(ode_lhs(u))

    # Residual in discrete equations (should be 0)
    print 'residual step1:', residual_discrete_eq_step1(u)
    print 'residual:', residual_discrete_eq(u)

def linear():
    main(lambda t: V*t + I)

if __name__ == '__main__':
    linear()
```

Fill in the various functions such that the calls in the `main` function works.

d) The purpose now is to choose a quadratic function $u_{\mathrm{e}} = bt^2 + ct + d$ as exact solution. Extend the `sympy` code above with a function `quadratic` for fitting `f` and checking if the discrete equations are fulfilled. (The function is very similar to `linear`.)

e) Will a polynomial of degree three fulfill the discrete equations?

f) Implement a `solver` function for computing the numerical solution of this problem.

g) Write a nose test for checking that the quadratic solution is computed to correctly (too machine precision, but the round-off errors accumulate and increase with T) by the `solver` function.
Filenames: `vib_undamped_verify_mms.pdf`, `vib_undamped_verify_mms.py`.

Exercise 2: Show linear growth of the phase with time

Consider an exact solution $I\cos(\omega t)$ and an approximation $I\cos(\tilde{\omega}t)$. Define the phase error as time lag between the peak I in the exact solution and the corresponding peak in the approximation after m periods of oscillations. Show that this phase error is linear in m. Filename: `vib_phase_error_growth.pdf`.

Exercise 3: Improve the accuracy by adjusting the frequency

According to (18), the numerical frequency deviates from the exact frequency by a (dominating) amount $\omega^3\Delta t^2/24 > 0$. Replace the `w` parameter in the algorithm in the `solver` function in `vib_undamped.py` by `w*(1 - (1./24)*w**2*dt**2` and test how this adjustment in the numerical algorithm improves the accuracy (use $\Delta t = 0.1$ and simulate for 80 periods, with and without adjustment of ω). Filename: `vib_adjust_w.py`.

Exercise 4: See if adaptive methods improve the phase error

Adaptive methods for solving ODEs aim at adjusting Δt such that the error is within a user-prescribed tolerance. Implement the equation $u'' + u = 0$ in the Odespy[15] software. Use the example from Section **??**in [1]. Run the scheme with a very low tolerance (say 10^{-14}) and for a long time, check the number of time points in the solver's mesh (`len(solver.t_all)`), and compare the phase error with that produced by the simple finite difference method from Section 1.2 with the same number of (equally spaced) mesh points. The question is whether it pays off to use an adaptive solver or if equally many points with a simple method gives about the same accuracy. Filename: `vib_undamped_adaptive.py`.

Exercise 5: Use a Taylor polynomial to compute u^1

As an alternative to the derivation of (8) for computing u^1, one can use a Taylor polynomial with three terms for u^1:

$$u(t_1) \approx u(0) + u'(0)\Delta t + \frac{1}{2}u''(0)\Delta t^2$$

With $u'' = -\omega^2 u$ and $u'(0) = 0$, show that this method also leads to (8). Generalize the condition on $u'(0)$ to be $u'(0) = V$ and compute u^1 in this case with both methods. Filename: `vib_first_step.pdf`.

Exercise 6: Find the minimal resolution of an oscillatory function

Sketch the function on a given mesh which has the highest possible frequency. That is, this oscillatory "cos-like" function has its maxima and minima at every two grid points. Find an expression for the frequency of this function, and use the result to find the largest relevant value of $\omega\Delta t$ when ω is the frequency of an oscillating function and Δt is the mesh spacing. Filename: `vib_largest_wdt.pdf`.

[15] `https://github.com/hplgit/odespy`

Exercise 7: Visualize the accuracy of finite differences for a cosine function

We introduce the error fraction

$$E = \frac{[D_t D_t u]^n}{u''(t_n)}$$

to measure the error in the finite difference approximation $D_t D_t u$ to u''. Compute E for the specific choice of a cosine/sine function of the form $u = \exp(i\omega t)$ and show that

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

Plot E as a function of $p = \omega\Delta t$. The relevant values of p are $[0, \pi]$ (see Exercise 6 for why $p > \pi$ does not make sense). The deviation of the curve from unity visualizes the error in the approximation. Also expand E as a Taylor polynomial in p up to fourth degree (use, e.g., `sympy`). Filename: `vib_plot_fd_exp_error.py`.

Exercise 8: Verify convergence rates of the error in energy

We consider the ODE problem $u'' + \omega^2 u = 0$, $u(0) = I$, $u'(0) = V$, for $t \in (0, T]$. The total energy of the solution $E(t) = \frac{1}{2}(u')^2 + \frac{1}{2}\omega^2 u^2$ should stay constant. The error in energy can be computed as explained in Section 7.

Make a nose test in a file `test_error_conv.py`, where code from `vib_undamped.py` is imported, but the `convergence_rates` and `test_convergence_rates` functions are copied and modified to also incorporate computations of the error in energy and the convergence rate of this error. The expected rate is 2. Filename: `test_error_conv.py`.

Exercise 9: Use linear/quadratic functions for verification

This exercise is a generalization of Problem 1 to the extended model problem (50) where the damping term is either linear or quadratic. Solve the various subproblems and see how the results and problem settings change with the generalized ODE in case of linear or quadratic damping. By modifying the code from Problem 1, `sympy` will do most of the work required to analyze the generalized problem. Filename: `vib_verify_mms.py`.

Exercise 10: Use an exact discrete solution for verification

Write a nose test function in a separate file that employs the exact discrete solution (19) to verify the implementation of the `solver` function in the file `vib_undamped.py`. Filename: `test_vib_undamped_exact_discrete_sol.py`.

Exercise 11: Use analytical solution for convergence rate tests

The purpose of this exercise is to perform convergence tests of the problem (50) when $s(u) = \omega^2 u$ and $F(t) = A\sin\phi t$. Find the complete analytical solution to the problem in this case (most textbooks on mechanics or ordinary differential equations list the various elements you need to write down the exact solution). Modify the `convergence_rate` function from the `vib_undamped.py` program to perform experiments with the extended model. Verify that the error is of order Δt^2. Filename: `vib_conv_rate.py`.

Exercise 12: Investigate the amplitude errors of many solvers

Use the program `vib_undamped_odespy.py` from Section 6 and the amplitude estimation from the `amplitudes` function in the `vib_undamped.py` file (see Section 3.4) to investigate how well famous methods for 1st-order ODEs can preserve the amplitude of u in undamped oscillations. Test, for example, the 3rd- and 4th-order Runge-Kutta methods (`RK3`, `RK4`), the Crank-Nicolson method (`CrankNicolson`), the 2nd- and 3rd-order Adams-Bashforth methods (`AdamsBashforth2`, `AdamsBashforth3`), and a 2nd-order Backwards scheme (`Backward2Step`). The relevant governing equations are listed in Section 23. Filename: `vib_amplitude_errors.py`.

Exercise 13: Minimize memory usage of a vibration solver

The program `vib.py`[16] store the complete solution $u^0, u^1, \ldots, u^{N_t}$ in memory, which is convenient for later plotting. Make a memory minimizing version of this program where only the last three u^{n+1}, u^n, and u^{n-1} values are stored in memory. Write each computed (t_{n+1}, u^{n+1}) pair to file. Visualize the data in the file (a cool solution is to read one line at a time and plot the u value using the line-by-line plotter in the `visualize_front_ascii` function - this technique makes it trivial to visualize very long time simulations). Filename: `vib_memsave.py`.

Exercise 14: Implement the solver via classes

Reimplement the `vib.py` program using a class `Problem` to hold all the physical parameters of the problem, a class `Solver` to hold the numerical parameters and compute the solution, and a class `Visualizer` to display the solution.

Hint. Use the ideas and examples from Section **??** and **??**in [1]. More specifically, make a superclass `Problem` for holding the scalar physical parameters of a problem and let subclasses implement the $s(u)$ and $F(t)$ functions as methods. Try to call up as much existing functionality in `vib.py` as possible.
Filename: `vib_class.py`.

Exercise 15: Interpret $[D_tD_tu]^n$ as a forward-backward difference

Show that the difference $[D_tD_tu]^n$ is equal to $[D_t^+D_t^-u]^n$ and $D_t^-D_t^+u]^n$. That is, instead of applying a centered difference twice one can alternatively apply a mixture forward and backward differences. Filename: `vib_DtDt_fw_bw.pdf`.

Exercise 16: Use the forward-backward scheme with quadratic damping

We consider the generalized model with quadratic damping, expressed as a system of two first-order equations as in Section **??**:

$$
\begin{aligned}
u' &= v, \\
v' &= \frac{1}{m}\left(F(t) - \beta|v|v - s(u)\right) .
\end{aligned}
$$

However, contrary to what is done in Section **??**, we want to apply the idea of the forward-backward discretization in Section 8. Express the idea in operator notation and write out the

[16] `http://tinyurl.com/nm5587k/vib/vib.py`

scheme. Unfortunately, the backward difference for the v equation creates a nonlinearity $|v^{n+1}|v^n$. To linearize this nonlinearity, use the known value v^n inside the absolute value factor, i.e., $|v^{n+1}|v^n \approx |v^n|v^{n+1}$. Show that the resulting scheme is equivalent to the one in Section **??** for some time level $n \geq 1$.

What we learn from this exercise is that the first-order differences and the linearization trick play together in "the right way" such that the scheme is as good as when we (in Section **??**) carefully apply centered differences and a geometric mean on a staggered mesh to achieve second-order accuracy. There is a difference in the handling of the initial conditions, though, as explained at the end of Section 8. Filename: `vib_gen_bwdamping.pdf`.

Exercise 17: Use a backward difference for the damping term

As an alternative to discretizing the damping terms $\beta u'$ and $\beta|u'|u'$ by centered differences, we may apply backward differences:

$$
\begin{aligned}
[u']^n &\approx [D_t^- u]^n, \\
[|u'|u']^n &\approx [|D_t^- u| D_t^- u]^n = |[D_t^- u]^n| [D_t^- u]^n \,.
\end{aligned}
$$

The advantage of the backward difference is that the damping term is evaluated using known values u^n and u^{n-1} only. Extend the `vib.py`[17] code with a scheme based on using backward differences in the damping terms. Add statements to compare the original approach with centered difference and the new idea launched in this exercise. Perform numerical experiments to investigate how much accuracy that is lost by using the backward differences. Filename: `vib_gen_bwdamping.pdf`.

Exercise 18: Simulate a bouncing ball

A bouncing ball is a body in free vertically fall until it impacts the ground. During the impact, some kinetic energy is lost, and a new motion upwards with reduced velocity starts. At some point the velocity close to the ground is so small that the ball is considered to be finally at rest.

The motion of the ball falling in air is governed by Newton's second law $F = ma$, where a is the acceleration of the body, m is the mass, and F is the sum of all forces. Here, we neglect the air resistance so that gravity $-mg$ is the only force. The height of the ball is denoted by h and v is the velocity. The relations between h, v, and a,

$$
h'(t) = v(t), \quad v'(t) = a(t),
$$

combined with Newton's second law gives the ODE model

$$
h''(t) = -g, \tag{72}
$$

or expressed alternatively as a system of first-order equations:

$$
v'(t) = -g, \tag{73}
$$

$$
h'(t) = v(t) \,. \tag{74}
$$

These equations govern the motion as long as the ball is away from the ground by a small distance $\epsilon_h > 0$. When $h < \epsilon_h$, we have two cases.

[17] `http://tinyurl.com/nm5587k/vib/vib.py`

1. The ball impacts the ground, recognized by a sufficiently large negative velocity ($v < -\epsilon_v$). The velocity then changes sign and is reduced by a factor C_R, known as the coefficient of restitution[18]. For plotting purposes, one may set $h = 0$.

2. The motion stops, recognized by a sufficiently small velocity ($|v| < \epsilon_v$) close to the ground.

Choose one of the models, (72) or (73)-(74), and simulate a bouncing ball. Plot $h(t)$. Think about how to plot $v(t)$.

Hint. A naive implementation may get stuck in repeated impacts for large time step sizes. To avoid this situation, one can introduce a state variable that holds the mode of the motion: free fall, impact, or rest. Two consecutive impacts imply that the motion has stopped.
Filename: `bouncing_ball.py`.

Exercise 19: Simulate an elastic pendulum

Consider an elastic pendulum fixed to the point $\boldsymbol{r}_0 = (0, L_0)$. The length of the pendulum wire when not stretched is L_0. The wire is massless and always straight. At the end point $\boldsymbol{r}$, we have a mass m. Stretching the elastic wire a distance s gives rise to a spring force ks in the opposite direction of the stretching. Let $\boldsymbol{n}$ be a unit normal vector along the wire:

$$\boldsymbol{n} = \frac{\boldsymbol{r} - \boldsymbol{r}_0}{||\boldsymbol{r} - \boldsymbol{r}_0||}\,.$$

The stretch s in the wire is the current length $||\boldsymbol{r} - \boldsymbol{r}_0||$ at some time t minus the original length L_0:

$$s = ||\boldsymbol{r} - \boldsymbol{r}_0|| - L_0\,.$$

The force in the wire is then $\boldsymbol{F}_w = -ks\boldsymbol{n}$. Newton's second law of motion applied to the mass results in

$$m\ddot{\boldsymbol{r}} = -ks\boldsymbol{n} - mg\boldsymbol{j}, \tag{75}$$

where $\boldsymbol{j}$ is a unit vector in the upward vertical direction. Let $\boldsymbol{r} = (x, y)$ and $\boldsymbol{n} = (n_x, n_y)$. The two components of (75) then becomes

$$\ddot{x} = -m^{-1}ksn_x, \tag{76}$$

$$\tag{77}$$

$$\ddot{y} = -m^{-1}ksn_y - g\,. \tag{78}$$

The mass point (x, y) will undergo a two-dimensional motion, but if the wire is stiff (large k), the elastic pendulum will approach the classical one where the mass point moves along a circle. However, the elastic pendulum is modeled by a direct application of Newton's second law, because the force in the wire is known (as a function of the motion), while the classical pendulum involves constrained motion, which requires elimination of an unknown via the constraint (by invoking polar coordinates).

In equilibrium, the mass hangs in the position $(0, y_0)$ determined by

[18] `http://en.wikipedia.org/wiki/Coefficient_of_restitution`

$$0 = -m^{-1}ksn_y - g = m^{-1}k(y_0 - L_0) - g \quad \Rightarrow \quad y_0 = L_0 + mg/k = L\,.$$

We then displace the mass an angle θ_0 to the right. The initial position $(x(0), y(0))$ then becomes

$$x(0) = L\sin\theta_0, \quad y(0) = L_0 - L\cos\theta_0\,.$$

The velocity is zero, $x'(0) = y'(0) = 0$.

a) Write a code that can simulate such an elastic pendulum. Plot y against x in a plot with the same length scale on the axis such that we get a correct picture of the motion. Also plot the angle the pendulum: $\theta = \tan^{-1} x/(L_0 - y)$.

A possible set of parameters is $L_0 = 9.81$ m, $m = 1$ kg, $theta_0 = 30$ degrees.

Hint 1. The associated classical pendulum, for large k, has an equation $\ddot{\theta} + g/L_0\theta = 0$. With $g = L_0$, the period is 2π: $\theta(t) = \theta_0\cos(t)$. One can compare in a plot the angle of the elastic solution ($\theta = \tan^{-1} x/(L_0 - y)$) with the solution of the classical pendulum problem.

Hint 2. The equation of motion is subject to round-off errors for large k, because s is then small such that ks is a product of a large and a small number. Moreover, in this stiff case, $m^{-1}ksn_y$ is close to g such that we also subtract two almost equal numbers in the force term in the equation. For the given parameters, $k = 150$ is a large value and gives a solution close to the motion of a perfect classical pendulum. Much larger values gives unstable solutions.

b) Air resistance is a force $\frac{1}{2}\varrho C_D A||bmv||\boldsymbol{v}$, where C_D is a drag coefficient (0.2 for a sphere), ϱ is the density of air (1.2 kg m^{-3}), A is the cross section area ($A = \pi R^2$ for a sphere, where R is the radius), and $\boldsymbol{v}$ is the velocity: $\boldsymbol{v} = \dot{\boldsymbol{r}}$. Include air resistance in the model and show plots comparing the motion with and without air resistance.
Filename: `elastic_pendulum.py`.

Exercise 20: Analysis of the Euler-Cromer scheme

The Euler-Cromer scheme for the model problem $u'' + \omega^2 u = 0$, $u(0) = I$, $u'(0) = 0$, is given in (45)-(44). Find the exact discrete solutions of this scheme and show that the solution for u^n coincides with that found in Section 4.

Hint. Use an "ansatz" $u^n = I\exp(i\tilde{\omega}\Delta t\, n)$ and $v^{=}qu^n$, where $\tilde{\omega}$ and q are unknown parameters. The formula

$$\exp(i\tilde{\omega}(\Delta t)) + \exp(i\tilde{\omega}(-\Delta t)) - 2 = 2\left(\cosh(i\tilde{\omega}\Delta t) - 1\right) = -4\sin^2(\frac{\tilde{\omega}\Delta t}{2}),$$

becomes handy.

References

[1] H. P. Langtangen. Introduction to computing with finite difference methods. Web document, Simula Research Laboratory and University of Oslo, 2013.

Index