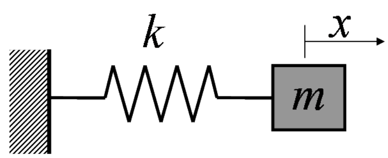
ISC 5315
Applied Computational Science 1

Symplectic Integrators

1 Introduction

Consider a simple mass-spring system shown below. When the mass is stretched away from its equilibrium position, the spring tries to pull it back. This is well-studied example of a harmonic oscillator.



Harmonic oscillators are ubiquitous in physics: they occur in mechanical systems such as pendulums, acoustical systems, RLC circuits in electrical engineering, molecular vibrations in quantum mechanics, models of flexibility in macromolecules etc. The wikipedia entry on harmonic oscillators goes one step further in claiming: "They are the source of virtually all sinusoidal vibrations and waves."

In this lab, we are going to use a simple mass-spring harmonic oscillator to study what happens to conserved quantities such as total energy in **long time numerical integration** of ODEs. What makes some integrators better than others, for such types of problems?

2 Scope

We will first lay down the appropriate differential equations, simplify them, and theoretically analyze their properties.

Next, we will then consider a bunch of different IVP integrators,

(a) forward Euler

(b) backward Euler

(c) implicit trapezoidal, and

(d) leap-frog

to numerically solve the problem, and compare their performance with the expected theoretical response. In particular, we are interested in how effectively these integrators conserve the total energy.

3 Simplified Model

One can write Newton's second law to describe the mass-spring system:

$$m \frac{d^2x}{dt^2} = -kx.$$

In this lab we will set $m = k = 1$ for simplicity, and use the shorthand notation $x'(t)$ and $x''(t)$ to represent the first and second time derivatives of x, respectively. Furthermore, we recognize that $v(t) = x'(t)$ is simply the velocity of the particle at any time.

Under these simplifications, the differential equation reduces to,

$$x''(t) + x(t) = 0. \tag{1}$$

Suppose, we are given the initial conditions $x(0)$ and $v(0) = x'(0)$. It can be shown that the solution to this IVP problem is given by,

$$x(t) = x(0) \cos t + v(0) \sin t. \tag{2}$$

Task 1: Verify that $x(t)$ satisfies the IVP.

From thermodynamics, we know that the total energy is conserved. The total energy is the sum of the potential and kinetic energies:

$$E(t) = \frac{1}{2} k x^2(t) + \frac{1}{2} m v^2(t).$$

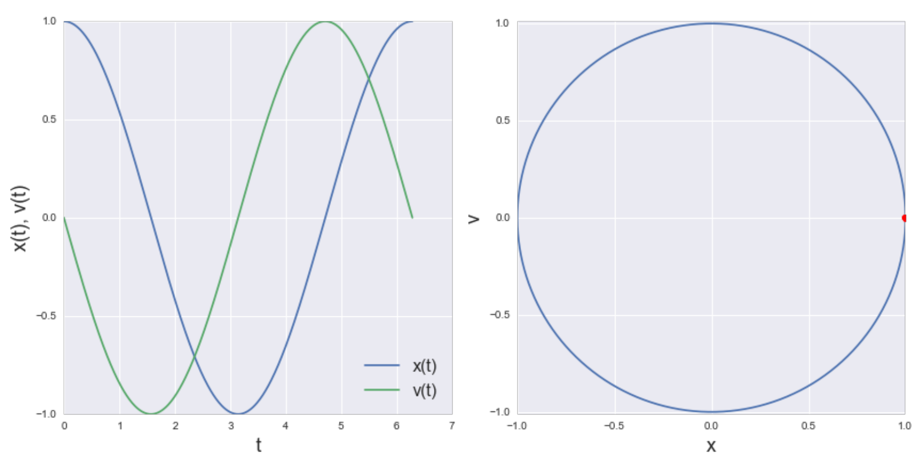
Since the energy is conserved:

$$E(t) = \frac{1}{2}\left[x^2(t) + v^2(t)\right] = E(0) = \frac{1}{2}\left[x^2(0) + v^2(0)\right].$$

Task 2: Verify that $x(t)$ from eqn. 2 is consistent with a constant $E(t)$.

For specificity, we will assume $x(0) = 1$ and $v(0) = 0$, in the rest of this lab. Note that in this particular case, the solution becomes $x(t) = \cos t$, $v(t) = -\sin t$, and the total energy is $E(t) = 1/2(\cos^2 t + \sin^2 t) = 1/2$.

We can plot the x versus v trajectory on a 2D phase-plot, as shown below.



On the phase-plot, the motion of the oscillator is described by a circle. Since there is no friction or dissipation in the model, once the mass is set into motion, it oscillates perpetually. It stays on the circle in the phase plot for eternity.

4 Integrators

Now let us consider four different integrators for the equation $x''(t) + x = 0$. First, we split our second order equation into two first order equations as

$$x' = v \tag{3}$$
$$v' = -x \tag{4}$$

We use a simple right difference formula to discretize the first derivatives, with stepsize h. The four integrators differ in how they account for the RHS.

- Forward Euler:

$$X_{n+1} = X_n + hV_n \tag{5}$$
$$V_{n+1} = V_n - hX_n \tag{6}$$

- Backward Euler

$$X_{n+1} = X_n + hV_{n+1} \tag{7}$$
$$V_{n+1} = V_n - hX_{n+1} \tag{8}$$

- Implicit Trapezoidal

$$X_{n+1} = X_n + \frac{h}{2}(V_n + V_{n+1}) \tag{9}$$
$$V_{n+1} = V_n - \frac{h}{2}(X_n + X_{n+1}) \tag{10}$$

- Leap-Frog

$$X_{n+1} = X_n + hV_n \tag{11}$$
$$V_{n+1} = V_n - hX_{n+1} \tag{12}$$

If we represent $U = [X, V]^T$, we can write these methods in a form $U_{n+1} = GU_n$. For the implicit trapezoidal method, for instance,

$$G_{IT} = \begin{bmatrix} 1 & -h/2 \\ h/2 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 & h/2 \\ -h/2 & 1 \end{bmatrix}.$$

Task 3: Write the corresponding matrices G_{FE}, G_{BE}, and G_{LF}, for the other three methods.

5 Programming Tasks

Consider a step size $h = 2\pi/32$, and a time interval, $T = [0, 10\pi]$.

(i) For each of the four methods:

- Write code to implement the method
- Plot $x(t)$, $v(t)$, a phase diagram x versus v, and the total energy $E(t)$. Compare it with the exact solution in each case.

(ii) Methods for which the energy doesn't monotonically drift upwards or downwards are called symplectic methods. Which two methods are symplectic? Which two are not?

(iii) We can gain additional insight into the numerical methods, by realizing that our time integration can be thought of as:

$$U_n = G^n U_0,$$

This might remind you of the Power method. The magnitude of the eigenvalues $|\lambda|$ of G tells us something about whether the solution grows, decays, or remains bounded.

- Find the eigenvalues for the four methods. Try to find the eigenvalues symbolically (as a function of h), either by hand, or by using software.
- Can you make sense of the behavior of the four methods, by considering their eigenvalues?

(iv) Compare and contrast the two symplectic methods: in particular, mention one specific practical advantage of each.