Supplementary Note 9.2

Why Verlet Methods Behave So Well

Energy, Time Reversibility, and Symplectic Integration

Chapter 9 of the textbook

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1 A question about numerical accuracy

In Section 9.14 of the textbook, we found that Verlet and velocity Verlet are particularly good choices for particle dynamics. But there is a puzzle. Velocity Verlet is only second-order accurate, while the familiar fourth-order Runge–Kutta method (RK4) has a smaller error per step when the time step is sufficiently small. Why, then, might we prefer Verlet for a simulation that runs through thousands or millions of time steps?

The answer is not that Verlet calculates each individual position more accurately. Instead, it respects some of the structure of Newton's equations. That structure becomes especially important when we follow a system for a long time. Let us examine three related ideas: conservation of energy, time reversibility, and symplectic integration.

Throughout the note we consider a particle moving in a time-independent potential $U(x)$, so that

$$m\ddot{x} = F(x) = -\frac{dU}{dx}, \qquad v = \dot{x}.$$

The mechanical energy is

$$E = \frac{1}{2}mv^2 + U(x). \tag{1}$$

For the exact motion, $dE/dt = 0$. To see why, differentiate Eq. (1):

$$\frac{dE}{dt} = mv\dot{v} + \frac{dU}{dx}\dot{x} = v\left(m\dot{v} + \frac{dU}{dx}\right) = 0.$$

A numerical method does not automatically inherit this conservation law.

2 A simple test: the harmonic oscillator

We will use an oscillator because we know exactly what its motion should be:

$$\ddot{x} = -\omega^2 x, \qquad E = \frac{m}{2}\left(v^2 + \omega^2 x^2\right). \tag{2}$$

Its energy is constant, and its trajectory in the $(x, v/\omega)$ plane is an ellipse (a circle if the two axes are scaled equally). Our numerical solution should follow this closed path without spiraling away from it or toward the origin.

2.1 What happens with forward Euler?

The forward Euler equations are

$$x_{n+1} = x_n + hv_n, \qquad v_{n+1} = v_n - h\omega^2 x_n. \tag{3}$$

Instead of guessing what happens to the energy, let us calculate it. Substituting Eq. (3) into Eq. (2) and expanding gives

$$\begin{aligned} \frac{2E_{n+1}}{m} &= \left(v_n - h\omega^2 x_n\right)^2 + \omega^2\left(x_n + hv_n\right)^2 \\ &= \left(1 + h^2\omega^2\right)\left(v_n^2 + \omega^2 x_n^2\right). \end{aligned}$$

Thus

$$\boxed{E_{n+1} = (1 + h^2\omega^2)E_n.} \tag{4}$$

Every step increases the energy, however small h may be. Making h smaller reduces the rate of growth, but does not remove the systematic drift. The resulting orbit spirals outward.

3 Velocity Verlet: a different way to look at the algorithm

In Note 9.1, we derived velocity Verlet using Taylor expansions:

$$x_{n+1} = x_n + hv_n + \frac{h^2}{2}a(x_n), \tag{5}$$

$$v_{n+1} = v_n + \frac{h}{2}[a(x_n) + a(x_{n+1})]. \tag{6}$$

These equations tell us how to calculate the new position and velocity. But there is another way to organize the very same calculation. It will help us understand why Verlet has some unusual properties.

Suppose we divide one time step into three operations.

First, update the velocity by half a step.

$$v_{n+1/2} = v_n + \frac{h}{2}a(x_n). \tag{7}$$

The position is held fixed while the velocity changes. We can think of this as giving the particle a small *kick*.

Next, update the position for a full step.

$$x_{n+1} = x_n + hv_{n+1/2}. \tag{8}$$

Here the intermediate velocity is kept fixed while the particle moves. We call this a *drift*.

Finally, complete the velocity update. At the new position we calculate $a(x_{n+1})$ and perform another half kick:

$$v_{n+1} = v_{n+1/2} + \frac{h}{2}a(x_{n+1}).$$

Have we invented a different method? No. Substitute Eq. (7) into Eq. (8) and we recover Eq. (5). Likewise, adding the two half kicks gives Eq. (6). It is exactly the same velocity Verlet step, written as *half kick–full drift–half kick*.

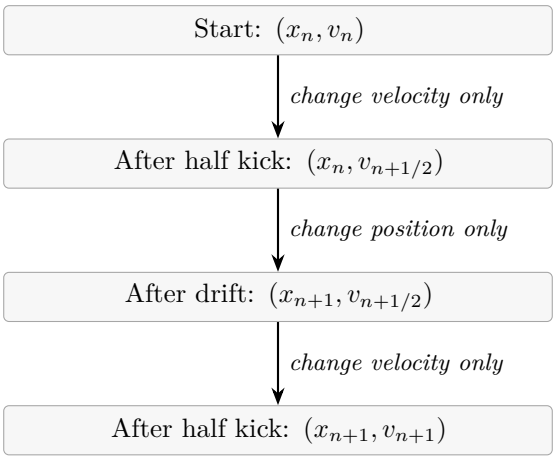


Figure 1: One velocity Verlet time step. The position changes during the drift; the velocity changes during the two kicks. After the drift, we calculate the new acceleration for the final half kick.

Why bother with this rearrangement? Each operation is remarkably simple: one changes only velocity, while the other changes only position. In the following sections we will see what this arrangement tells us about reversing a time step and preserving the geometry of the motion.

4 Time reversibility

Newton's equations have an interesting property. If we know the position and velocity of a particle, we can calculate the motion forward or backward in time. Suppose we start at (x_n, v_n), move forward by a time step h, and obtain (x_{n+1}, v_{n+1}). Integrating backward by the same amount should bring us back to where we started.

For the exact solution this is possible, but a numerical method does not necessarily return to its starting point. Let us check velocity Verlet rather than assume that it does.

For a forward step, our three operations are

$$v_{n+1/2} = v_n + \frac{h}{2}a(x_n),$$

$$x_{n+1} = x_n + hv_{n+1/2},$$
$$v_{n+1} = v_{n+1/2} + \frac{h}{2}a(x_{n+1}).$$

Now suppose we are given the final values and repeat the method with the *negative* time step $-h$.

Undo the last half kick.

$$v_{n+1/2} = v_{n+1} - \frac{h}{2}a(x_{n+1}).$$

This recovers precisely the intermediate velocity used in the forward step.

Undo the drift.

$$x_n = x_{n+1} - hv_{n+1/2}.$$

We have recovered the original position.

Undo the first half kick.

$$v_n = v_{n+1/2} - \frac{h}{2}a(x_n).$$

And now we have recovered the original velocity as well:

$$\boxed{(x_n, v_n) \xrightarrow{h} (x_{n+1}, v_{n+1}) \xrightarrow{-h} (x_n, v_n).}$$

The same numerical algorithm with a negative step undoes a positive step, in exact arithmetic. This is what we mean here by *time reversibility* of the numerical method. The result applies to the position-dependent acceleration assumed throughout this note. Floating-point rounding will, of course, prevent perfect cancellation on a computer.

This symmetry means that the method does not favor one direction of time over the other. It is one part of the explanation for Verlet's good long-time behavior. But we should not jump to the conclusion that a time-reversible method must conserve energy. It need not. There is another property worth investigating.

5 What does *symplectic* mean?

5.1 From particle motion to phase space

So far, we have described a particle using its position x and velocity v. We could instead use position and momentum $p = mv$. Imagine a graph with x along the horizontal axis and p along the vertical axis. We call this *phase space*. At any instant the particle corresponds to one point (x, p); as time passes, that point traces out a curve.

For the harmonic oscillator,

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

Because the exact energy is constant, the curve in the (x, p) plane is an ellipse. In this picture we are following the motion of a point around a closed curve, rather than plotting x against time.

5.2 What happens to nearby trajectories?

Now imagine not one particle but a large collection of *possible* initial conditions, each with a slightly different position and momentum. These are not interacting particles: each point corresponds to a separate solution of the same equations.

Suppose the points initially fill a small rectangle in phase space. As they evolve, the rectangle can stretch, tilt, or bend. The remarkable property of Hamiltonian motion is that its area is preserved, even though its shape can change.

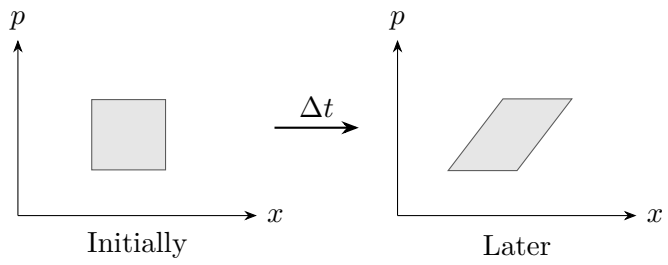


Figure 2: A schematic picture of phase-space area preservation. A small region of initial conditions may change shape as it evolves, but its area remains the same. The shapes are illustrative, not calculated harmonic-oscillator trajectories.

Why should we care about this? Preserving area means that the exact motion does not artificially squeeze a little patch of possible initial conditions into a smaller area or spread it into a larger one. For a system with one position and one momentum coordinate, a numerical method that preserves this phase-space area is called *symplectic*. With more degrees of freedom the full symplectic condition is stronger than merely preserving phase-space volume.

5.3 How can we check whether a numerical step preserves area?

Recall that velocity Verlet is made of kicks and drifts. Let us examine these operations separately, writing the equations in terms of momentum $p = mv$.

A kick. During a kick the position stays fixed, but the momentum changes:

$$x_{\text{new}} = x_{\text{old}},$$
$$p_{\text{new}} = p_{\text{old}} + \Delta t\, F(x_{\text{old}}).$$

Here Δt is the duration of this operation ($h/2$ for either half kick). To find what happens to a small region, consider how a small change in the old coordinates affects the new ones. We need

four partial derivatives:

$$\frac{\partial x_{\text{new}}}{\partial x_{\text{old}}} = 1, \qquad \frac{\partial x_{\text{new}}}{\partial p_{\text{old}}} = 0,$$
$$\frac{\partial p_{\text{new}}}{\partial x_{\text{old}}} = \Delta t \, \frac{dF}{dx}, \qquad \frac{\partial p_{\text{new}}}{\partial p_{\text{old}}} = 1.$$

Putting them in a 2×2 matrix gives the *Jacobian*:

$$J_{\text{kick}} = \begin{pmatrix} 1 & 0 \\ \Delta t \, dF/dx & 1 \end{pmatrix}.$$

Its determinant is

$$\boxed{\det J_{\text{kick}} = 1.}$$

The absolute value of a Jacobian determinant gives the factor by which a small area changes under the transformation. A determinant of one therefore means that the kick preserves area.

A drift. During a drift, momentum stays fixed while position changes:

$$x_{\text{new}} = x_{\text{old}} + \frac{\Delta t}{m} p_{\text{old}},$$
$$p_{\text{new}} = p_{\text{old}}.$$

The corresponding Jacobian is

$$J_{\text{drift}} = \begin{pmatrix} 1 & \Delta t/m \\ 0 & 1 \end{pmatrix},$$

so once again

$$\boxed{\det J_{\text{drift}} = 1.}$$

A drift also preserves phase-space area.

5.4 Putting the three steps together

A complete velocity Verlet step is a half kick, a full drift, and another half kick. The Jacobian of successive transformations is the product of the individual Jacobians; the determinant of a product is the product of their determinants. Therefore

$$\det J_{\text{Verlet}} = \det J_{\text{kick}} \, \det J_{\text{drift}} \, \det J_{\text{kick}} = 1. \tag{9}$$

Thus velocity Verlet preserves phase-space area. For our one-dimensional particle this establishes that the method is symplectic. Notice that we never used a special formula for $F(x)$: this property comes from how the algorithm is organized.

> **An important distinction.** A symplectic method does *not* usually conserve the exact mechanical energy at each step. It preserves a geometric property of Hamiltonian motion.

> Under suitable conditions, that property helps explain why the energy often has small, bounded oscillations instead of a steady drift.

6 Energy conservation for the harmonic oscillator

We have established that velocity Verlet is symplectic. But we have also emphasized that symplecticity is not the same as exact energy conservation. What, then, does Verlet do to the energy of the harmonic oscillator? Here we can find an exact answer.

6.1 Applying velocity Verlet to the oscillator

Consider again

$$\ddot{x} = -\omega^2 x.$$

For simplicity, in this and the next section we take $m = 1$. The physical energy, calculated from the position and velocity, is

$$E_n = \frac{1}{2}v_n^2 + \frac{1}{2}\omega^2 x_n^2. \tag{10}$$

For the exact motion it would remain constant. We will use the symbol E_n even when x_n and v_n come from a numerical solution.

The velocity Verlet position update is

$$x_{n+1} = x_n + hv_n - \frac{h^2\omega^2}{2}x_n.$$

Before going on, let us introduce a shorthand that has a useful physical meaning:

$$q = h\omega = 2\pi\frac{h}{T}, \qquad T = \frac{2\pi}{\omega}.$$

Here h is the numerical time step and T is the period of one oscillation. Thus q tells us how large the time step is compared with the oscillation period. For example, if we use 100 steps per period, then $q = 2\pi/100 \approx 0.063$. A smaller value of q means more steps per oscillation.

With this notation, the two velocity Verlet equations become

$$x_{n+1} = \left(1 - \frac{q^2}{2}\right) x_n + hv_n, \tag{11}$$

$$v_{n+1} = \left(1 - \frac{q^2}{2}\right) v_n - h\omega^2 \left(1 - \frac{q^2}{4}\right) x_n. \tag{12}$$

The second equation follows by substituting the first into $v_{n+1} = v_n - h\omega^2(x_n + x_{n+1})/2$.

6.2 Can we find an energy-like quantity that stays constant?

We know the physical energy involves x^2 and v^2. Perhaps the numerical method conserves a *slightly different* combination of these same quantities. Let us find out, rather than guess.

Look for a quantity of the form

$$\widetilde{E}_n = \frac{1}{2}v_n^2 + \frac{1}{2}Kx_n^2,$$

where K is a constant that we have yet to determine. The tilde is just a reminder that $\widetilde{E}_n$ need not equal the physical energy E_n. We want to choose K so that $\widetilde{E}_{n+1} = \widetilde{E}_n$.

To keep the algebra manageable, write

$$A = 1 - \frac{q^2}{2}, \qquad B = \omega^2\left(1 - \frac{q^2}{4}\right).$$

Equations (11)–(12) are then simply

$$x_{n+1} = Ax_n + hv_n, \qquad v_{n+1} = Av_n - hBx_n.$$

Now substitute them into the trial expression for the new energy:

$$\begin{aligned} 2\widetilde{E}_{n+1} &= (Av_n - hBx_n)^2 + K(Ax_n + hv_n)^2 \\ &= (A^2 + Kh^2)v_n^2 + (h^2B^2 + KA^2)x_n^2 + 2Ah(K - B)x_nv_n. \end{aligned}$$

For this to equal $2\widetilde{E}_n = v_n^2 + Kx_n^2$ for arbitrary position and velocity, the mixed term must disappear. It does so if $K = B$. With this choice, notice that

$$A^2 + h^2B = \left(1 - \frac{q^2}{2}\right)^2 + q^2\left(1 - \frac{q^2}{4}\right) = 1.$$

Therefore the coefficients of v_n^2 and x_n^2 also match. We have found the conserved quantity:

$$\boxed{\widetilde{E}_n = \frac{1}{2}v_n^2 + \frac{1}{2}\omega^2\left(1 - \frac{h^2\omega^2}{4}\right)x_n^2.} \tag{13}$$

For this particular oscillator, velocity Verlet gives

$$\boxed{\widetilde{E}_{n+1} = \widetilde{E}_n}$$

exactly in mathematical arithmetic. We did not assume this result: we found the coefficient that makes it true.

6.3 What is the difference between the two energies?

The ordinary energy is still Eq. (10). Subtracting the modified energy, Eq. (13), gives

$$\begin{aligned} E_n - \widetilde{E}_n &= \frac{1}{2}\omega^2 x_n^2 - \frac{1}{2}\omega^2 \left(1 - \frac{h^2\omega^2}{4}\right) x_n^2 \\ &= \frac{h^2\omega^4}{8} x_n^2. \end{aligned}$$

Hence

$$\boxed{E_n = \widetilde{E}_n + \frac{h^2\omega^4}{8} x_n^2.} \tag{14}$$

The modified energy stays constant, while the difference between it and the physical energy changes with x_n^2. For bounded oscillator motion, x_n oscillates, so the energy error also oscillates instead of accumulating as a steady drift. The difference is proportional to h^2, which also tells us why decreasing the step improves the energy accuracy.

6.4 Why must the step satisfy a restriction?

Does velocity Verlet give bounded oscillations for any h? No. Look again at the modified energy in Eq. (13). For it to be a positive sum of a velocity term and a position term, we need

$$1 - \frac{h^2\omega^2}{4} > 0.$$

Since $h > 0$ and $\omega > 0$, this is equivalent to

$$\boxed{h\omega < 2.} \tag{15}$$

In this range the conserved modified energy bounds both x_n and v_n. If $h\omega > 2$, the method is unstable. At $h\omega = 2$, the position term vanishes: for generic initial conditions the position can grow linearly with the number of steps, so the boundary is not generally stable either.

Since $h\omega = 2\pi h/T$, the condition can also be written

$$\frac{h}{T} < \frac{1}{\pi}.$$

That is more than about 3.14 steps per period. This is a *stability* limit, not a recommendation for accuracy: in practice we usually need many more steps per oscillation.

7 What happens when we use RK4?

Velocity Verlet conserves a modified energy for this oscillator. Does a higher-order method, such as fourth-order Runge–Kutta (RK4), necessarily behave better over very long times? Let us find out.

7.1 Applying RK4 to the harmonic oscillator

We again start with

$$\frac{dx}{dt} = v, \qquad \frac{dv}{dt} = -\omega^2 x.$$

RK4 combines four estimates of the derivatives during each step. Each estimate now has two components, one for x and one for v:

$$\begin{aligned}
k_{1x} &= v_n, & k_{1v} &= -\omega^2 x_n, \\
k_{2x} &= v_n + \frac{h}{2}k_{1v}, & k_{2v} &= -\omega^2\left(x_n + \frac{h}{2}k_{1x}\right), \\
k_{3x} &= v_n + \frac{h}{2}k_{2v}, & k_{3v} &= -\omega^2\left(x_n + \frac{h}{2}k_{2x}\right), \\
k_{4x} &= v_n + hk_{3v}, & k_{4v} &= -\omega^2\left(x_n + hk_{3x}\right).
\end{aligned}$$

We then combine them in the familiar way:

$$\begin{aligned}
x_{n+1} &= x_n + \frac{h}{6}(k_{1x} + 2k_{2x} + 2k_{3x} + k_{4x}), \\
v_{n+1} &= v_n + \frac{h}{6}(k_{1v} + 2k_{2v} + 2k_{3v} + k_{4v}).
\end{aligned}$$

Because our oscillator equations are linear, we can substitute the four stages and collect terms in x_n and v_n. For example, the position increments simplify to

$$k_{1x} + 2k_{2x} + 2k_{3x} + k_{4x} = \left(6 - \omega^2 h^2\right) v_n + \left(-3h\omega^2 + \frac{h^3\omega^4}{4}\right) x_n.$$

The resulting updates can be written compactly as

$$x_{n+1} = Cx_n + \frac{D}{\omega}v_n, \tag{16}$$

$$v_{n+1} = Cv_n - \omega D x_n, \tag{17}$$

where

$$C = 1 - \frac{q^2}{2} + \frac{q^4}{24}, \qquad D = q - \frac{q^3}{6}, \qquad q = h\omega. \tag{18}$$

We introduced $q = 2\pi h/T$ in Section 6 to compare the time step with the oscillator period. The symbols C and D are simply short names for the coefficients produced by an ordinary RK4 step.

7.2 How does the energy change?

At the end of the step, the physical energy calculated from the numerical values is

$$E_{n+1} = \frac{1}{2}v_{n+1}^2 + \frac{1}{2}\omega^2 x_{n+1}^2.$$

Substitute Eqs. (16)–(17):

$$\begin{aligned} 2E_{n+1} &= (Cv_n - \omega D x_n)^2 + \omega^2 \left(C x_n + \frac{D}{\omega} v_n \right)^2 \\ &= (C^2 + D^2)(v_n^2 + \omega^2 x_n^2). \end{aligned}$$

The cross terms cancel. Since the last parentheses equals $2E_n$, we have a particularly simple result:

$$E_{n+1} = (C^2 + D^2) E_n.$$

Now use the coefficients in Eq. (18):

$$\begin{aligned} C^2 + D^2 &= \left(1 - \frac{q^2}{2} + \frac{q^4}{24} \right)^2 + \left(q - \frac{q^3}{6} \right)^2 \\ &= 1 - \frac{q^6}{72} + \frac{q^8}{576}. \end{aligned}$$

Thus

$$\boxed{E_{n+1} = \left(1 - \frac{q^6}{72} + \frac{q^8}{576} \right) E_n.} \tag{19}$$

We can now see the energy behavior directly from the RK4 algorithm, without introducing a new stability-function notation.

7.3 Does RK4 conserve energy?

Rewrite the factor in Eq. (19) as

$$r = 1 - \frac{q^6}{576}(8 - q^2).$$

For a positive step with $0 < q < \sqrt{8}$, this factor is slightly less than one (and positive). Therefore $E_{n+1} = rE_n < E_n$: RK4 loses a small amount of energy at each step of this oscillator. With a constant step, the same factor is applied repeatedly, so after n steps

$$\boxed{E_n = r^n E_0.} \tag{20}$$

Even a tiny loss per step can become noticeable when we take many steps. This looks like damping of the oscillator, but there is no physical damping force; the effect comes from the integration method. For small q the fractional change in one step is approximately

$$\frac{E_{n+1} - E_n}{E_n} \approx -\frac{q^6}{72}.$$

A smaller step reduces this error rapidly. RK4 can therefore be very accurate over a finite interval, despite its slow systematic energy loss over long integrations.

7.4 What should we learn from this comparison?

For the stable harmonic oscillator, Verlet's physical energy oscillates around a nearby constant value because the method exactly conserves a modified energy. Standard RK4, for the small steps just considered, gives a systematic energy decrease. This does *not* mean that velocity Verlet is always more accurate. RK4 has fourth-order global accuracy, compared with second order for velocity Verlet, and may give a much more accurate trajectory over a fixed time interval.

The point is that *accuracy over a fixed interval* and *behavior over a very long time* are not the same question. That distinction matters whenever we simulate conservative motion for many oscillations.

8 A numerical comparison

Figure 3 compares the three methods on the same problem. For each run we start at $x_0 = 1$, $v_0 = 0$, and set $m = \omega = 1$. We choose $h = 0.5$ deliberately so that the differences are visible. The figure was generated directly from the update equations, without correcting the numerical energies afterward.

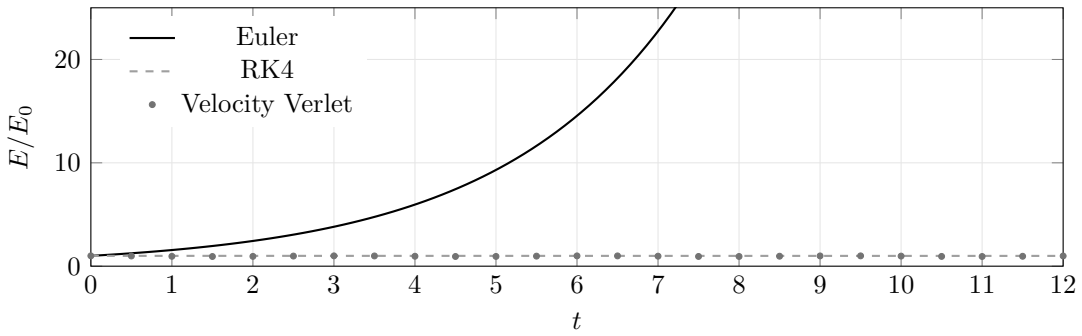


Figure 3: Short-time comparison for the harmonic oscillator. Euler's energy increases rapidly. RK4 and velocity Verlet remain much closer to the correct energy, so the next plot is needed to distinguish them.

9 What should we conclude?

The lesson is not that Verlet is always better than RK4. For a short integration requiring high pointwise accuracy, RK4 can be a very good choice. For long simulations of conservative particle systems, however, the structure of the numerical method matters as well as its order of accuracy.

Velocity Verlet combines three useful properties: it is second-order accurate, it is time-reversible for autonomous position-dependent forces, and it is symplectic. For the harmonic

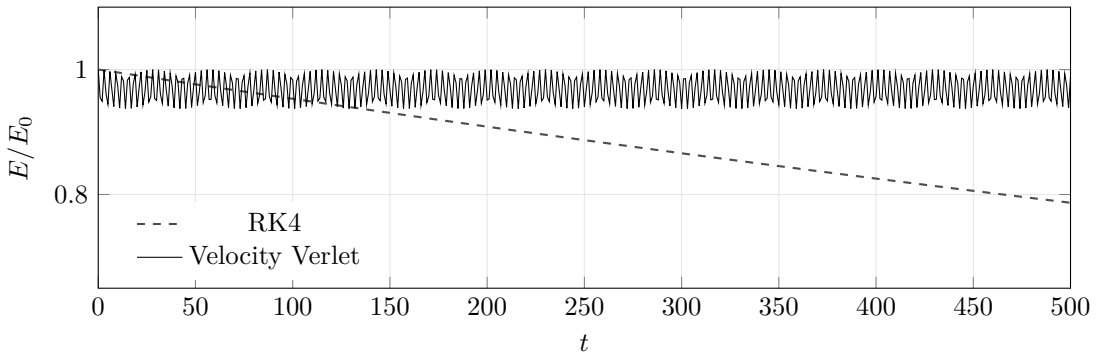


Figure 4: Long-time energy behavior for the same oscillator and time step. RK4 loses energy slowly but systematically, while the energy error of velocity Verlet oscillates without a sustained drift. Euler is omitted because its energy has already grown far beyond the plotted range.

oscillator we went one step further: we found an exactly conserved modified energy. For more general smooth Hamiltonian systems, related long-time energy behavior can often be understood through modified Hamiltonians, although exact conservation of a simple expression like Eq. (13) is no longer guaranteed. Strong nonlinear effects, resonance, changing time steps, thermostats, and other modifications may also change the picture.

> **The main point.** When we simulate a physical system, we should ask two questions: *How accurate is each numerical step?* and *Which properties of the physical motion does the method respect?* For molecular dynamics, both questions are important.

10 Try it yourself

A useful experiment is to repeat Figure 4 for $h = 0.2$, 0.5, and 1.0, holding the physical end time fixed. Plot both the energy error $E_n/E_0 - 1$ and the trajectory in the $(x, v/\omega)$ phase plane. Which method gives the smallest energy error over a short interval? What changes when the simulation is extended? Finally, increase h toward $2/\omega$ and compare what you see with Eq. (15).