Week 4

Symplectic Integrators for Hamiltonian Dynamics

1 What happens with higher-order derivatives?

In physical problems, one often encounters higher than first-order systems of differential equations. This might seem like a problem since the numerical methods we've learned thus far such as Runge-Kutta methods are designed to solve first-order systems. Newton's Second Law for classical systems of particles is an example of a dynamical law states that yields a higher-than-first order system of ordinary differential equations. For a given force function $\mathbf{F}(t, \mathbf{r}(t), \dot{\mathbf{r}}(t))$ that may depend on time, position, and velocity, the acceleration of the system satisfies

$$\ddot{\mathbf{r}}(t) = \frac{1}{m}\mathbf{F}(t, \mathbf{r}(t), \dot{\mathbf{r}}(t)). \tag{1}$$

This is a second-order system of differential equations. It turns out that one has no problem applying the methods we've developed thus far to higher-order systems of differential equations because

> Any system of n ODEs of order m can be converted into a system of $n \times m$ first-order ODEs.

Can you see one simple way to do this in general? There is actually often more than one way to perform this reduction of order and convert a higher-order system into a first-order system, but in these notes, we will concentrate on one such method. The dynamics of many systems, especially those in classical mechanics, can be modeled as **Hamiltonian Systems**. Hamilton's equations, the equations that govern the dynamics of Hamiltonian systems, are a

first-order system of ordinary differential equations, so they are automatically amenable by solution to numerical methods that solve first-order systems.

2 A light-speed review of Hamiltonian dynamics

Hamiltonian systems are a special kind of dynamical system whose dynamics are governed by a function called the **Hamiltonian** of the system. The Hamiltonian H is generally a function $H(t, q, p)$ of time, t, **generalized coordinates**

$$q = (q^1, q^2, \ldots, q^d), \tag{2}$$

and their corresponding **canonical momenta**

$$p = (p_1, p_2, \ldots, p_d). \tag{3}$$

The corresponding dynamical equations, often called **Hamilton's equations**, are

$$\dot{q}^k = \frac{\partial H}{\partial p_k}, \qquad \dot{p}_k = -\frac{\partial H}{\partial q^k} \tag{4}$$

for all k in the range $1, 2, \ldots d$. The form of the equations given above is actually a bit of an abuse of notation. The equations really say that at each time t and for each k,

$$\dot{q}^k(t) = \frac{\partial H}{\partial p_k}(t, q(t), p(t)), \qquad \dot{p}_k(t) = -\frac{\partial H}{\partial q^k}(t, q(t), p(t)) \tag{5}$$

Using the more general terminology and notation for dynamical systems introduced in the last set of notes, we find that the state of a hamiltonian system is the $(2d)$-tuple of generalized positions and corresponding canonical momenta:

$$s = (q^1, q^2, \ldots q^d, p_1, p_2, \ldots, p_d), \tag{6}$$

so the phase space of the system has dimension $D = 2d$. In particular, the phase space of a Hamiltonian system is also even-dimensional. If we want, we can now write Hamilton's equations in the following extremely compact form:

$$\dot{s}(t) = f(t, s(t)) \tag{7}$$

provided we define

$$f = \left(\frac{\partial H}{\partial p_1}, \ldots, \frac{\partial H}{\partial p_d}, -\frac{\partial H}{\partial q^1}, \ldots, -\frac{\partial H}{\partial q^d} \right). \tag{8}$$

When the Hamiltonian is evaluated along a solution $(q(t), p(t))$ of the equations of motion, one finds that

$$\frac{d}{dt} H(t, q(t), p(t)) = \frac{\partial H}{\partial t} + \sum_{k=1}^{d} \left[\frac{\partial H}{\partial q^k} \dot{q}^k + \frac{\partial H}{\partial p_k} \dot{p}_k \right] \tag{9}$$

$$= \frac{\partial H}{\partial t} + \sum_{k=1}^{d} \left[\frac{\partial H}{\partial q^k} \left(\frac{\partial H}{\partial p_k} \right) + \frac{\partial H}{\partial p_k} \left(-\frac{\partial H}{\partial q^k} \right) \right] \tag{10}$$

$$= \frac{\partial H}{\partial t} \tag{11}$$

The first equality is the chain rule, and the second invokes Hamilton's equations (4). For the sake of notational compactness in the above computation, we have suppressed the fact the partial derivatives of H are being evaluated on the solution $(t, q(t), p(t))$ in all terms, and we have suppressed the fact that $\dot{q}^k$ and $\dot{p}_k$ are being evaluated at the same time t wherever they appear.

It follows from this computation that if H has no dependence on its first argument, time t, then its partial derivative with respect to t will vanish and its time derivative along solutions to the equations of motion will vanish. In other words

> *If the Hamiltonian doesn't depend explicitly on time, then it is conserved along any solution to the equations of motion.*

For the remainder of these notes, we restrict our attention to Hamiltonians with no explicit time dependence. In cases where the Hamiltonian can be interpreted as the total energy of the system, this statement is simply the statement of energy conservation for the system. This fact allows us to think of the phase space trajectories in an interesting, geometric way. When the Hamiltonian has no explicit time dependence, the system moves along the level sets of the Hamiltonian, sets of points in phase space who all share the same value of the Hamiltonian. Level sets of the Hamiltonian will be surfaces of dimension $D-1$ consisting of all points (q, p) in phase space satisfying the equation

$$H(q, p) = H_0, \tag{12}$$

where H_0 is the initial value of the Hamiltonian. As we will now see, there are special classes of numerical methods constructed to simulate the dynamics of Hamiltonian systems. These methods generally perform better than Runge-Kutta methods when applied to Hamiltonian dynamics. This does not mean that Runge-Kutta methods can't be used – they can be. It's simply that they get badly outperformed by certain other methods in a certain sense we'll demonstrate. In the next section, we discover one such method by examining a concrete example of a Hamiltonian system.

3 The classical harmonic oscillator - motivating a new, interesting class of numerical methods

A simple example of a Hamiltonian system is the one-dimensional, classical harmonic oscillator of mass m and angular frequency ω. In Cartesian coordinates, its Hamiltonian is

$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{13}$$

The corresponding Hamilton's equations are

$$\dot{x} = p/m \tag{14}$$

$$\dot{p} = -m\omega^2 x. \tag{15}$$

If t_0 is some initial time, and if we specify the position $x_0 = x(t_0)$ and the momentum $p_0 = p(t_0)$ at the initial time, then this system of equations can be solved analytically with the following result:

$$x(t) = x_0 \cos(\omega(t - t_0)) + \frac{p_0}{m\omega} \sin(\omega(t - t_0)) \tag{16}$$

$$p(t) = -m\omega x_0 \sin(\omega(t - t_0)) + p_0 \cos(\omega(t - t_0)). \tag{17}$$

Since the Hamiltonian of this system doesn't depend explicitly on time, the solution should march along the level sets of the Hamiltonian which, in this case, are ellipses:

Since the true solution to the equations of motion conserves the Hamiltonian, a good numerical method should approximately do the same. Does the Euler method approximately conserve the energy of the oscillator? Let's investigate. For this system, Euler's

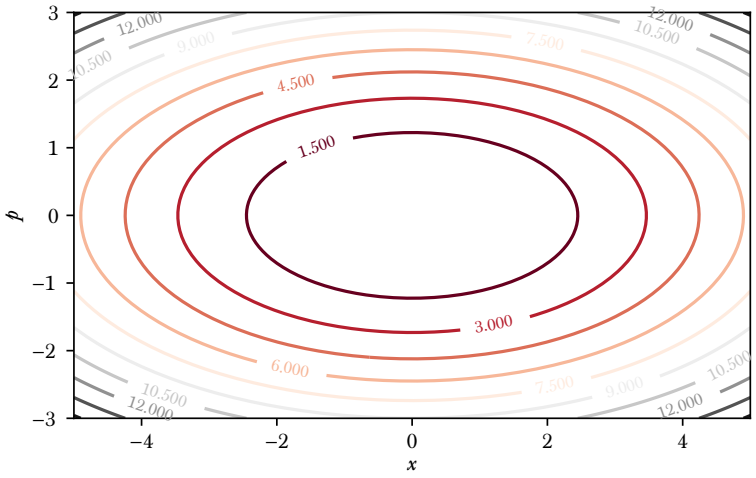

Figure 1: Plot of the level curves of the harmonic oscillator hamiltonian for $m = 0.5$, $\omega = 1.0$.

method is as follows:

$$x_{n+1} = x_n + h\frac{p_n}{m} \tag{18}$$

$$p_{n+1} = p_n - hm\omega^2 x_n. \tag{19}$$

If we define $H_n = H(x_n, p_n)$, which is simply the value of the Hamiltonian at time step n, then with some algebra, one can show that

$$H_{n+1} = (1 + (h\omega)^2)H_n. \tag{20}$$

Euler's method *increases* the Hamiltonian by a quantity second order in the step size. This may not seem so bad at first glance because it seems that by making the step size sufficiently small, we can reduce this artificial increase in energy as much as we'd like. However, notice that the Hamiltonian at step $n+1$ is generated by multiplying the Hamiltonian at step n by a positive number $1 + (h\omega)^2)$, so no matter how small the step size is, if one takes enough steps, the Hamiltonian will grow large. More explicitly, notice that starting from the initial time and taking N steps yields

$$H_N = (1 + (\omega h)^2)^N H_0, \tag{21}$$

so for a given step size, the value of the Hamiltonian at the end of N steps has increased relative to its initial value by a function that is exponential in N. This means that no matter how small we choose the step size, if we run the simulation for long enough, the

energy of the numerical solution will always exponentially diverge from the initial energy. This is a sad state of affairs because it seriously limits the usefulness of Euler's method when applied to simulating the dynamics of even this simple system for long times. Euler's method is **unstable** for any size time step when applied to the classical harmonic oscillator.

4 A clever modification of Euler's method

Euler's method performs badly on the harmonic oscillator, but all is not lost! Humans are very clever, and some very dedicated people discovered an amazing thing that I want to now show you. Let me draw your attention for a moment to a very slight modification of Euler's method:

$$x_{n+1} = x_n + h\frac{p_n}{m} \tag{22}$$

$$p_{n+1} = p_n - hm\omega^2 x_{n+1}. \tag{23}$$

Can you see how this is different than Euler's method? The modification is so small that perhaps not. If you look hard enough, you will find that in the second line, the momentum update equation (23), the *updated* value of the position x_{n+1} is used to compute the updated value of the momentum. This is not what Euler's method does. Euler's method uses the *un-updated* position x_n to update the momentum.

It might appear that this slight change will have a negligible affect on the performance of the method – let's see if that's the case. To test this, we run both Euler's method and this new method, which we call "method X" for the moment, and see how they compare in their performance for an amount of time corresponding to one period of oscillation and for a time step equal to one-20$^{\text{th}}$ of that period (see figure 2).

Notice that while Euler's method diverges from the level set of the Hamiltonian on which it started, the new method we've introduced seems to remain bounded. The new method still isn't exact – it has some error related to the step size, but it is at least much more stable than Euler's method for this problem. This leads to a few interesting questions:

1. Will our new method X remain bounded even if we run the simulation for many periods?

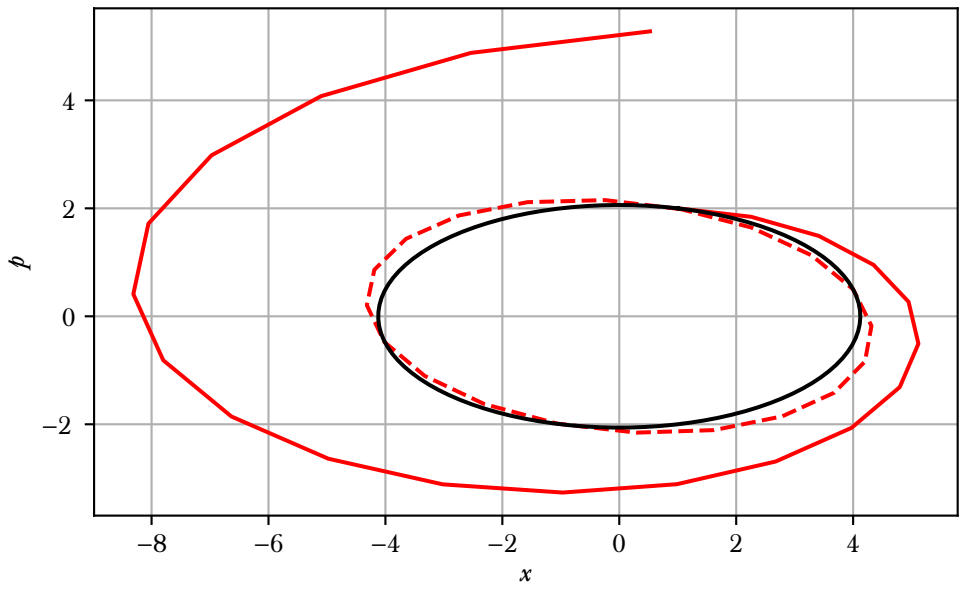

Figure 2: Plot of exact harmonic oscillator solution (black) versus Euler's method (solid red) versus "Method X" (dotted red) for $m = 0.5$, $\omega = 1.0$, $N = 20$, and $h = 2\pi/(N\omega)$

2. If so, is there some deeper reason for this?
3. How does the performance of method X depend on the step size?

The answer to the third question is something you will discover in the project for the week. Amazingly, the answers to the first two of these questions turn out to be yes! To get some intuition for why, it helps to run method X for various initial values of the Hamiltonian and see what the corresponding trajectories look like (see figure 3). Doesn't it kind of look like this method evolves the system along the level sets of some different Hamiltonian whose level sets look like ellipses that are a bit deformed relative to the true level sets? It turns out that this is actually precisely what's happening. In fact, if for each step size h we define a **modified Hamiltonian** $\bar{H}_h$ as follows:

$$\bar{H}_h(x, p) = H(x, p) + h\frac{\omega^2 x p}{2}, \tag{24}$$

then one can show that the new method exactly conserves the modified Hamiltonian at every time step:

$$\bar{H}_{h,n+1} = \bar{H}_{h,n}. \tag{25}$$

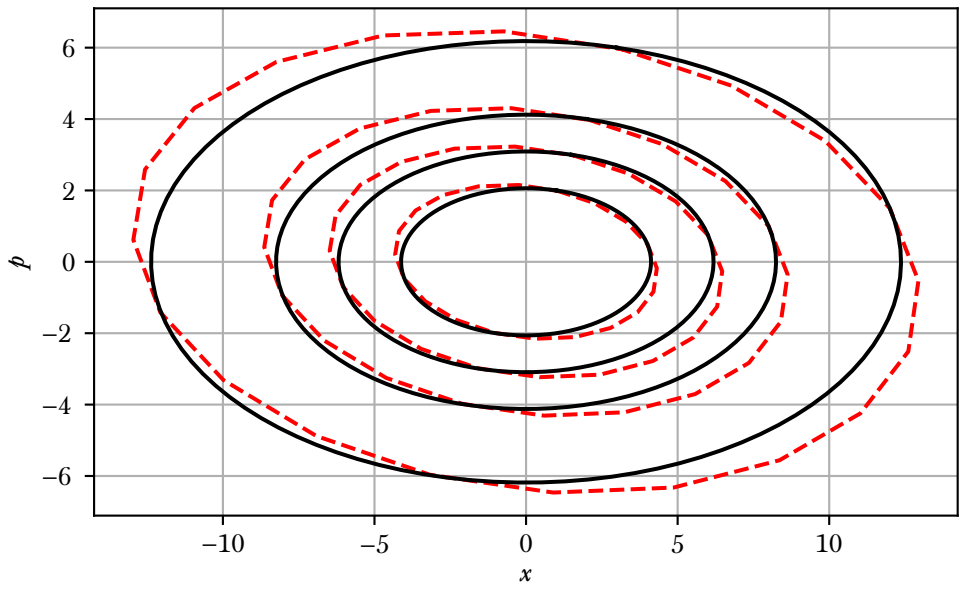

Figure 3: Plot of exact harmonic oscillator solution (black) versus versus "Method X" (dotted red) for $m = 0.5$, $\omega = 1.0$, $N = 20$, $h = 2\pi/(N\omega)$, and various initial energies.

This is really cool! It means that the new method we've proposed moves along the level curves of this modified Hamiltonian, so by plotting its level sets, we can get a nice geometric picture of what the method is doing. Notice, in particular, that since the modified Hamiltonian differs from the true Hamiltonian by only a term of order h, we can make its level curves as close to the level curves of the true Hamiltonian as we wish simply by making the step size sufficiently small. In particular, this shows why the new proposed method is so stable! The new method we proposed here, method X, is actually called the **symplectic Euler** method or the **Euler-Cromer** method.

5 The two most famous symplectic integrators

The really amazing thing is that there is a whole class of numerical methods that provably behave essentially in this way for a large class of Hamiltonian systems. These are the so-called **symplectic integrators**. The word "symplectic" has a specific technical meaning that is at the heart of what's responsible for these methods working in this way, but we'd be going beyond the scope of the class in exploring that issue. The interested reader is encouraged to learn

more about this in the scholarly literature.

Many systems in classical mechanics can be described as Hamiltonian systems with Hamiltonians of the form

$$H(q, p) = T(p) + U(q), \tag{26}$$

where T can be thought of as the system's kinetic energy and U as the system's potential energy. In particular, notice that the first term of such a hamiltonian depends only on momentum p, and the second term depends only on position q. For the algorithms that follow, we restrict our attention to Hamiltonians of this form. The simplest symplectic method is **symplectic Euler** which we abbreviate as **SE**:

$$q^k_{n+1} = q^k_n + h \cdot \frac{\partial H}{\partial p_k}(q_n, p_n) \tag{27}$$

$$p_{k,n+1} = p_{k,n} - h \cdot \frac{\partial H}{\partial q^k}(q_{n+1}, p_n) \tag{28}$$

This is precisely the same as Euler's method *except* for one minute change: the updated positions q_{n+1} are used instead of the old positions q_n to compute the updated momenta p_{n+1}. A more accurate method than symplectic Euler is the famous **Stormer-Verlet** method which we abbreviate as **SV**:

$$p_{k,n+\frac{1}{2}} = p_{k,n} - \frac{h}{2} \cdot \frac{\partial H}{\partial q^k}(q_n, p_n) \tag{29}$$

$$q^k_{n+1} = q^k_n + h \cdot \frac{\partial H}{\partial p_k}(q_n, p_{n+\frac{1}{2}}) \tag{30}$$

$$p_{k,n+1} = p_{k,n+\frac{1}{2}} - \frac{h}{2} \cdot \frac{\partial H}{\partial q^k}(q_{n+1}, p_n) \tag{31}$$

6 The two-body (Kepler) problem

It's possible to show that the motion of a pair of masses m_1 and m_2 moving under only their mutual Newtonian gravitational attraction but otherwise isolated from all other matter will be restricted to a plane, which we take to be the x-y plane without loss of generality. It is possible to further show that the dynamics of this system can be reduced to the the dynamics of a single mathematical point having

position $\mathbf{r} = (x, y)$ and **reduced mass** μ attracted to the origin by an inverse square law force with "strength" k:

$$\mu\ddot{\mathbf{r}} = -k\frac{\mathbf{r}}{|\mathbf{r}|^3}, \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}, \qquad k = G m_1 m_2 \tag{32}$$

where G is Newton's gravitational constant. The positions $\mathbf{r}_1$ and $\mathbf{r}_2$ of the two masses in the original two-body problem are related to the position $\mathbf{r}$ as follows:

$$\mathbf{r}_1 = \frac{m_2}{m_1 + m_2}\mathbf{r}, \quad \mathbf{r}_2 = -\frac{m_1}{m_1 + m_2}\mathbf{r}. \tag{33}$$

Once one has solved the reduced one-body problem, one can use these formulas to generate the trajectories of the original two bodies. The Hamiltonian that generates the correct dynamics for this reduced problem is

$$H(x, y, p_x, p_y) = \frac{1}{2\mu}(p_x^2 + p_y^2) - \frac{k}{(x^2 + y^2)^{1/2}}. \tag{34}$$

This reduced, one-body problem is often called the **Kepler problem**. The solutions to the Kepler problem famously move along conic sections in the x-y plane.

6.1 Conserved quantities

For the Kepler problem, there are interesting conserved quantities beyond the Hamiltonian: the angular momentum J given by

$$J = x p_y - y p_x, \tag{35}$$

and the Laplace-Runge-Lenz vector whose components A_x and A_y are given by

$$A_x = p_y J - \mu k \frac{x}{(x^2 + y^2)^{1/2}} \tag{36}$$

$$A_y = -p_x J - \mu k \frac{y}{(x^2 + y^2)^{1/2}}. \tag{37}$$

7 Let's take stock of what we've learned

Here is a summary of the general procedure for numerically simulating the dynamics of a system that is to be modeled via differential equations

1. Write down the system of differential equations satisfied by the system.

2. Convert the system to a first-order system. This might mean reformulating the problem as a Hamiltonian system and writing down Hamilton's equations.

3. Choose an appropriate numerical method to generate an approximate solution to system of equations. If the system is not Hamiltonian, RK4 is a reasonable default choice. If the system is Hamiltonian of the form $H(q, p) = T(p) + U(q)$, then SV is a reasonable default choice.