Lior Silberman's Math 428: Problem Set 4

Symplectic integrators

In this problem set we work to the standard phase space $M = \mathbb{R}^d \times \left(\mathbb{R}^d\right)^*$ equipped with the standard symplectic structure $J = \begin{pmatrix} & I_d \\ -I_d & \end{pmatrix}$ and take a standard Hamiltonian $H(x,p) = \frac{p^2}{2m} + V(x)$ on $\mathbb{R}^d \times \left(\mathbb{R}^d\right)^*$. The Hamiltonian flow is then

$$\begin{cases} \dot{x} = \frac{1}{m}p \\ \dot{p} = -dV \end{cases}.$$

Suppose that V is a smooth convex function (e.g. x^2). For greater generality you may consider $H = T(p) + V(x)$ where T, V are both smooth and convex.

1. Verify that H is conserved by the motion.

2. Consider the Euler Scheme from PS1: fixing a timestep h, it is

$$\begin{cases} x_{k+1} &= x_k + h\frac{1}{m}p_k \\ p_{k+1} &= p_k - hdV(x_k) \end{cases}.$$

   (a) Show that $H(x_{k+1}, p_{k+1}) - H(x_k, p_k) = Ch^2 + O(h^3)$ where $C > 0$.
   (b*) Suppose V is radial. What happens to the angular momentum of the system?
   (c) Show that $F(x,p) = \left(x + \frac{h}{m}p, p - hdV(x)\right)$ does not preserve volume (i.e. its Jacobian determinant is not 1), violating Liouville's Theorem
   (d) Show that F is not even a symplectomorphism.

3*. (For those who have experiment with numerical methods) Consider instead the Implicit Euler Scheme, where (x_{k+1}, p_{k+1}) is defined by

$$\begin{cases} x_{k+1} &= x_k + h\frac{1}{m}p_{k+1} \\ p_{k+1} &= p_k - hdV(x_{k+1}) \end{cases}.$$

   (note that this is a nonlinear system of equations for x_{k+1}, y_{k+1}).
   (a) Show that now $H(x_{k+1}, p_{k+1}) < H(x_k, p_k)$.
   (b) What happens to the angular momentum in the radial case?

4. Now consider instead the "buggy Euler scheme"

$$\begin{cases} x_{k+1} &= x_k + h\frac{1}{m}p_k \\ p_{k+1} &= p_k - hdV(x_{k+1}) \end{cases}$$

   (observe the use of the updated x_{k+1} value in the second equation)
   (a) Show that in the limit $h \to 0$ this scheme still solves the ODE. Similarly if we first compute p_{k+1} and then set $x_{k+1} = x_k + \frac{h}{m}p_{k+1}$.
   (b) Under what conditions on the matrix $A \in M_d(\mathbb{R})$, is the *transvection* $\tilde{A} = \begin{pmatrix} I_d & \\ A & I_d \end{pmatrix} \in M_{2d}(\mathbb{R})$ a symplectomorphism (in that $\tilde{A}^T J \tilde{A} = J$)?
   (c) Show that any transformation $F(x,p) = (x + dT(p), p)$ and $G(x,p) = (x, p - dV(x))$ of M is a symplectomorphism. Apply this to the numerical scheme under consideration.

5**. (The Shadow Hamiltonian)

(a) Show that the maps $\varphi_h^{(1)}(x,p) = (x + hdT(p), p) = \exp(hX_T)$ and $\varphi_h^{(2)}(x,p) = \exp(hX_V)$ are the exact time-h Hamiltonian flows for the Hamiltonians T,V.

(b) Applying the Baker–Campbell–Hausdorff formula, conclude that $\varphi_h^{(2)}(x,p)\varphi_h^{(1)}(x,p) = \exp(hX)$ where $X = X_T + X_V + \cdots$ where all higher-order terms are commutators of X_T, X_V.

(c) Applying the formula $[X_A, X_B] = X_{\{A,B\}}$ show that $X = X_{\tilde{H}}$ for a *shadow Hamiltonian* $\tilde{H} = T + V + O(h)$.

(d) Show that $\tilde{H}$ is conserved exactly by the numerical scheme.

6**. Consider now the *Vernet integrator* $\varphi_{h/2}^{(1)}(x,p)\varphi_h^{(2)}(x,p)\varphi_{h/2}^{(1)}(x,p)$

(a) Repeat 4(a), showing that this is now a second-order scheme.

(b) Repeat 4(c), showing that this scheme is symplectic.

(c) Repeat problem 5, obtaining a shadow Hamiltonian here as well.