Scientific Computing HW 5

Ryan Chen

March 4, 2023

Problem 1.

1. From $H(p,q) = T(p) + U(q)$,

$$\partial_p H(p,q) = T'(p), \quad \partial_q H(p,q) = U'(q)$$

Plug into the Stoermer–Verlet method.

$$p_{n+1/2} = p_n - \frac{1}{2}hU'(q_n)$$

$$q_{n+1} = q_n + \frac{1}{2}h[T'(p_{n+1/2}) + T'(p_{n+1/2})] = q_n + hT'\left(p_n - \frac{1}{2}hU'(q_n)\right)$$

$$p_{n+1} = p_n - \frac{1}{2}hU'(q_n) - \frac{1}{2}hU'(q_{n+1}) = p_n - \frac{1}{2}h\left[U'(q_n) + U'\left(q_n + hT'\left(p_n - \frac{1}{2}hU'(q_n)\right)\right)\right]$$

The RHS quantities are independent of p_{n+1}, q_{n+1}, so the method is explicit.

The Hamiltonian for the 1D simple harmonic oscillator is

$$H(p,q) = T(p) + U(q), \quad T(p) := \frac{p^2}{2m}, \quad U(q) := \frac{m\omega^2 q^2}{2}$$

First compute

$$T'(p) = \frac{p}{m}, \quad U'(q) = m\omega^2 q$$

Plug into the method.

$$q_{n+1} = q_n + hT'\left(p_n - \frac{1}{2}hm\omega^2 q_n\right) = q_n + \frac{h}{m}\left[p_n - \frac{1}{2}h\omega^2 q_n\right] = \frac{h}{m}p_n + \left(1 - \frac{1}{2}h^2\omega^2\right)q_n$$

$$p_{n+1} = p_n - \frac{1}{2}h\left[m\omega^2 q_n + m\omega^2\left(q_n + \frac{h}{m}\left(p_n - \frac{1}{2}hm\omega^2 q_n\right)\right)\right]$$

In the above expression, collect coefficients of the following terms.

$$p_n: \quad 1 - \frac{1}{2}hm\omega^2\frac{h}{m} = 1 - \frac{1}{2}h^2\omega^2$$

$$q_n: \quad -\frac{1}{2}h\left[m\omega^2 + m\omega^2\left(1 + \frac{h}{m}\left(-\frac{1}{2}hm\omega^2\right)\right)\right] = -\frac{1}{2}hm\omega^2\left(2 - \frac{1}{2}h^2\omega^2\right) = hm\omega^2\left(\frac{1}{4}h^2\omega^2 - 1\right)$$

Therefore

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = A\begin{bmatrix} p_n \\ q_n \end{bmatrix}, \quad A := \begin{bmatrix} a & b \\ c & a \end{bmatrix}, \quad a := 1 - \frac{1}{2}h^2\omega^2, \quad b := hm\omega^2\left(\frac{1}{4}h^2\omega^2 - 1\right), \quad c := \frac{h}{m}$$

2. **Pf.** We compute

$$JA = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ c & a \end{bmatrix} = \begin{bmatrix} c & a \\ -a & -b \end{bmatrix}$$

$$\implies A^T JA = \begin{bmatrix} a & c \\ b & a \end{bmatrix} \begin{bmatrix} c & a \\ -a & -b \end{bmatrix} = \begin{bmatrix} ac - ca & a^2 - bc \\ bc - a^2 & ba - ab \end{bmatrix} = \begin{bmatrix} 0 & a^2 - bc \\ -(a^2 - bc) & 0 \end{bmatrix}$$

$$a^2 - bc = 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2 - h^2\omega^2 \left(\frac{1}{4}h^2\omega^2 - 1\right) = 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2 - \frac{1}{4}h^4\omega^4 + h^2\omega^2 = 1$$

$$\implies A^T JA = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = J$$

3. **Pf.** The shadow Hamiltonian is

$$H^*(p_n, q_n) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \left[1 - \frac{1}{4}h^2\omega^2\right] = \begin{bmatrix} p_n \\ q_n \end{bmatrix}^T S \begin{bmatrix} p_n \\ q_n \end{bmatrix}, \quad S := \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix}, \quad d := \frac{1}{2m}, \quad e := \frac{1}{2}m\omega^2 \left[1 - \frac{1}{4}h^2\omega^2\right]$$

We compute

$$SA = \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix} \begin{bmatrix} a & b \\ c & a \end{bmatrix} = \begin{bmatrix} da & db \\ ec & ea \end{bmatrix}$$

$$A^T SA = \begin{bmatrix} a & c \\ b & a \end{bmatrix} \begin{bmatrix} da & db \\ ec & ea \end{bmatrix} = \begin{bmatrix} da^2 + ec^2 & dba + eac \\ bda + aec & db^2 + ea^2 \end{bmatrix} = \begin{bmatrix} da^2 + ec^2 & a(bd + ec) \\ a(bd + ec) & db^2 + ea^2 \end{bmatrix}$$

$$\begin{aligned} da^2 + ec^2 &= \frac{1}{2m}\left[1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2\right] + \frac{1}{2}m\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right]\frac{h^2}{m^2} \\ &= \frac{1}{2m}\left[1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2 + h^2\omega^2 - \frac{1}{4}h^4\omega^4\right] \\ &= \frac{1}{2m} \\ &= d \end{aligned}$$

$$bd + ec = \frac{1}{2}h\omega^2\left[\frac{1}{4}h^2\omega^2 - 1\right] + \frac{1}{2}h\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right] = 0$$

$$\begin{aligned} db^2 + ea^2 &= \frac{1}{2m}h^2m^2\omega^4\left[\frac{1}{4}h^2\omega^2 - 1\right]^2 + \frac{1}{2}m\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right]\left[1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2\right] \\ &= \frac{1}{2}m\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right]\left[h^2\omega^2\left(1 - \frac{1}{4}h^2\omega^2\right) + 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2\right] \\ &= \frac{1}{2}m\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right]\left[h^2\omega^2 - \frac{1}{4}h^4\omega^4 + 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2\right] \\ &= \frac{1}{2}m\omega^2\left[1 - \frac{1}{4}h^2\omega^2\right] \\ &= e \end{aligned}$$

Put together,

$$A^T SA = \begin{bmatrix} d & a \cdot 0 \\ a \cdot 0 & e \end{bmatrix} = \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix} = S$$

$$\implies H^*(p_{n+1}, q_{n+1}) = \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix}^T S \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} p_n \\ q_n \end{bmatrix}^T A^T SA \begin{bmatrix} p_n \\ q_n \end{bmatrix} = \begin{bmatrix} p_n \\ q_n \end{bmatrix}^T S \begin{bmatrix} p_n \\ q_n \end{bmatrix} = H^*(p_n, q_n)$$

Thus H^* is conserved.