Scientific Computing HW 5

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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.

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

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

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

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.

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

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

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

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

Therefore

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

2. 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. e