

Scientific Computing HW 5

Ryan Chen

March 4, 2024

1. (a) Consider the polynomials

$$\rho(z) := z^2 + \alpha_0 z + \alpha_1, \quad \sigma(z) := \beta_{-1} z^2 + \beta_0 z + \beta_1$$

Compute $\rho'(z) = 2z + \alpha_0$. By theorem 7 in the notes,

$$\text{method consistent} \iff \rho(1) = 0, \rho'(1) = \sigma(1) \iff 1 + \alpha_0 + \alpha_1 = 0, 2 + \alpha_0 = \beta_{-1} + \beta_0 + \beta_1$$

- (b) First compute

$$\begin{aligned} \rho(e^h) - h\sigma(e^h) &= e^{2h} + \alpha_0 e^h + \alpha_1 - h [\beta_{-1} e^{2h} + \beta_0 e^h + \beta_1] \\ &= 1 + 2h + \frac{4}{2}h^2 + \frac{8}{6}h^3 + O(h^4) \\ &\quad + \alpha_0 \left[1 + h + \frac{1}{2}h^2 + \frac{1}{6}h^3 + O(h^4) \right] + \alpha_1 \\ &\quad - h \left[\beta_{-1} \left[1 + 2h + \frac{4}{2}h^2 + O(h^3) \right] + \beta_0 \left[1 + h + \frac{1}{2}h^2 + O(h^3) \right] + \beta_1 \right] \end{aligned}$$

The method is consistent of order 3 iff $\rho(e^h) - h\sigma(e^h) = O(h^4)$ as $h \rightarrow 0$, which holds iff the following hold:

$$O(1) : 1 + \alpha_0 + \alpha_1 = 0 \text{ (already true by part (a))}$$

$$O(h) : 2 + \alpha_0 - \beta_{-1} - \beta_0 - \beta_1 = 0 \text{ (already true by part (a))}$$

$$O(h^2) : 2 + \frac{\alpha_0}{2} - 2\beta_{-1} - \beta_0 = 0 \iff 2 + \frac{\alpha_0}{2} = 2\beta_{-1} + \beta_0$$

$$O(h^3) : \frac{4}{3} + \frac{\alpha_0}{6} - 2\beta_{-1} - \frac{\beta_0}{2} = 0 \iff \frac{4}{3} + \frac{\alpha_0}{6} = 2\beta_{-1} + \frac{\beta_0}{2}$$

(c)

(d)

(e)

2. (a) 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.

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

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

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

(b) We compute

$$\begin{aligned} JA &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ c & a \end{bmatrix} = \begin{bmatrix} c & a \\ -a & -b \end{bmatrix} \\ \implies A^T JA &= \begin{bmatrix} a & c \\ b & a \end{bmatrix} \begin{bmatrix} c & a \\ -a & -b \end{bmatrix} = \begin{bmatrix} ac - ca & a^2 - bc \\ bc - a^2 & ba - ab \end{bmatrix} = \begin{bmatrix} 0 & a^2 - bc \\ -(a^2 - bc) & 0 \end{bmatrix} \\ a^2 - bc &= 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2 - h^2\omega^2 \left(\frac{1}{4}h^2\omega^2 - 1 \right) = 1 + \frac{1}{4}h^4\omega^4 - h^2\omega^2 - \frac{1}{4}h^4\omega^4 + h^2\omega^2 = 1 \\ \implies A^T JA &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = J \end{aligned}$$

(c) The shadow Hamiltonian is

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

We compute

$$\begin{aligned} SA &= \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix} \begin{bmatrix} a & b \\ c & a \end{bmatrix} = \begin{bmatrix} da & db \\ ec & ea \end{bmatrix} \\ \implies A^T SA &= \begin{bmatrix} a & c \\ b & a \end{bmatrix} \begin{bmatrix} da & db \\ ec & ea \end{bmatrix} = \begin{bmatrix} da^2 + ec^2 & dba + eac \\ bda + aec & db^2 + ea^2 \end{bmatrix} = \begin{bmatrix} da^2 + ec^2 & a(bd + ec) \\ a(bd + ec) & db^2 + ea^2 \end{bmatrix} \end{aligned}$$

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

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

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

Put together,

$$\begin{aligned} A^T S A &= \begin{bmatrix} d & a \cdot 0 \\ a \cdot 0 & e \end{bmatrix} = \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix} = S \\ \implies H^*(p_{n+1}, q_{n+1}) &= \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix}^T S \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} p_n \\ q_n \end{bmatrix}^T A^T S A \begin{bmatrix} p_n \\ q_n \end{bmatrix} = \begin{bmatrix} p_n \\ q_n \end{bmatrix}^T S \begin{bmatrix} p_n \\ q_n \end{bmatrix} = H^*(p_n, q_n) \end{aligned}$$

Thus H^* is conserved.

3. (a) The Hamiltonian equations of motion are

$$\dot{u} = -\partial_x H(u, v, x, y) = -x(x^2 + y^2)^{-3/2}$$

$$\dot{v} = -\partial_y H(u, v, x, y) = -y(x^2 + y^2)^{-3/2}$$

$$\dot{x} = -\partial_u H(u, v, x, y) = u$$

$$\dot{y} = -\partial_v H(u, v, x, y) = v$$

From the initial conditions, the total energy is

$$H \Big|_{t=0} = \frac{1}{2}0^2 + \frac{1}{2} \left(\frac{1}{2} \right)^2 - \frac{1}{(2^2 + 0^2)^{1/2}} = \frac{1}{8} - \frac{1}{2} = -\frac{3}{8} < 0$$

- (b) Code: <https://github.com/RokettoJanpu/scientific-computing-2-redux/blob/main/hw5p3.ipynb>

The Jacobian of f is

$$Df(u, v, x, y) = \begin{bmatrix} 0 & 0 & (2x^2 - y^2)(x^2 + y^2)^{-5/2} & 3xy(x^2 + y^2)^{-5/2} \\ 0 & 0 & 3xy(x^2 + y^2)^{-5/2} & (2y^2 - x^2)(x^2 + y^2)^{-5/2} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

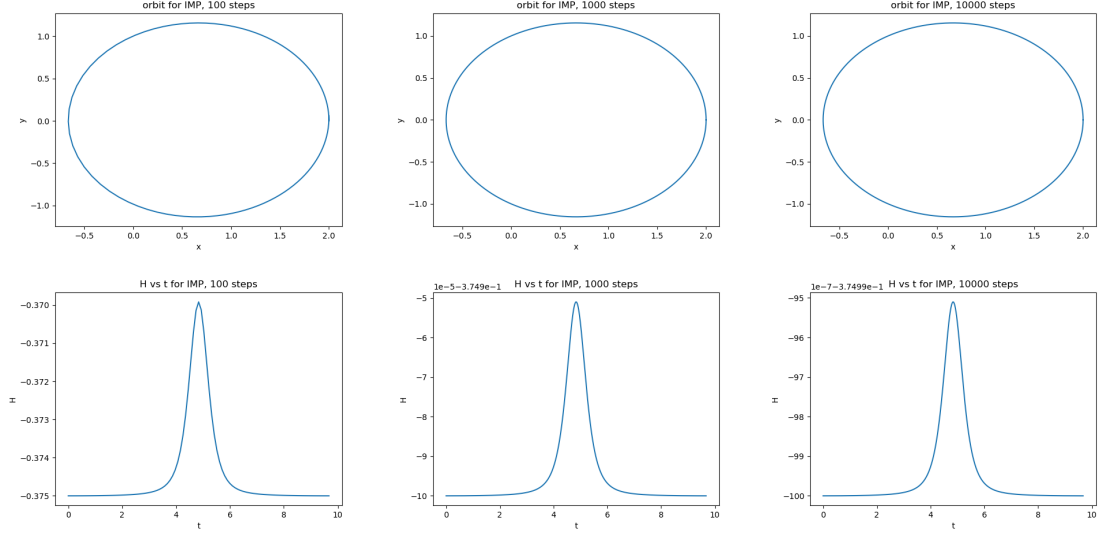
In the implicit midpoint rule (IMP), the initial approximation of k is given by

$$k = f(z_n) + \frac{1}{2}hDf(z_n)k \implies \left[I - \frac{1}{2}hDf(z_n) \right] k = f(z_n) \implies k = \left[I - \frac{1}{2}hDf(z_n) \right]^{-1} f(z_n)$$

Newton's iteration for approximating k uses the Jacobian of $F(k) := k - f(z_n + \frac{1}{2}hk)$,

$$DF(k) = I - Df\left(z_n + \frac{1}{2}hk\right) \frac{1}{2}hI = I - \frac{1}{2}hDf\left(z_n + \frac{1}{2}hk\right)$$

Below are the orbits using IMP for 100, 1000, and 10000 steps per period, and the corresponding Hamiltonian vs time graphs.



(c) In the Stoermer–Verlet method (SV), set $p := (u, v)$ and $q := (x, y)$. The Hamiltonian is

$$H(p, q) = T(p) + U(q), \quad T(p) := \frac{1}{2}u^2 + \frac{1}{2}v^2, \quad U(q) := -(x^2 + y^2)^{-1/2}$$

so that

$$\partial_p H(p, q) = \nabla T(p) = \begin{bmatrix} u \\ v \end{bmatrix}, \quad \partial_q H(p, q) = \nabla U(q) = \begin{bmatrix} x(x^2 + y^2)^{-3/2} \\ y(x^2 + y^2)^{-3/2} \end{bmatrix}$$

In the method derived in problem 1, replace T' and U' by ∇T and ∇U .

$$q_{n+1} = q_n + h\nabla T\left(p_n - \frac{1}{2}hU'(q_n)\right)$$

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

Below are the same plots as in part (b) but using SV instead.

