Scientific Computing HW 5

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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

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

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

$$\begin{aligned} O(1) &: \quad 1 + \alpha_0 + \alpha_1 = 0 \text{ (already true by part (a))} \\ O(h) &: \quad 2 + \alpha_0 - \beta_{-1} - \beta_0 - \beta_1 = 0 \text{ (already true by part (a))} \\ O(h^2) &: 2 + \frac{\alpha_0}{2} - 2\beta_{-1} - \beta_0 = 0 \iff 2 + \frac{\alpha_0}{2} = 2\beta_{-1} + \beta_0 \\ O(h^3) &: \frac{4}{3} + \frac{\alpha_0}{6} - 2\beta_{-1} - \frac{\beta_0}{2} = 0 \iff \frac{4}{3} + \frac{\alpha_0}{6} = 2\beta_{-1} + \frac{\beta_0}{2} \end{aligned}$$

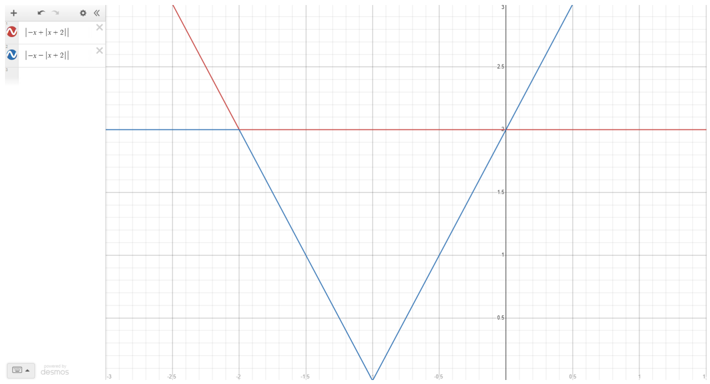
(c) Restricting to consistent methods, so that $\alpha_1 = -1 - a_0$, the roots of $\rho(z)$ are

$$z_\pm = \frac{-\alpha_0 \pm \sqrt{\alpha_0^2 - 4\alpha_1}}{2} = \frac{-\alpha_0 \pm \sqrt{a_0^2 + 4a_0 + 4}}{2} = \frac{-\alpha_0 \pm |a_0 + 2|}{2}$$

Checking one of the root conditions,

$$|z_\pm| \le 1 \iff |-a_0 \pm |a_0 + 2|| \le 2$$

Below is a plot of the functions $x \mapsto |-x \pm |x + 2||$.



We see that $|z_\pm| \le 1$ iff $-2 \le \alpha_0 \le 0$. To fulfill the other root condition (roots with modulus 1 have multiplicity 1), we exclude the case $\alpha_0 = -2$. Thus the method is consistent iff $-2 < \alpha_0 \le 0$.

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.

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

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

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

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.

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

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

Therefore

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

(b) We compute

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

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

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

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

(c) The shadow Hamiltonian is

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

where we define

$$S := \begin{bmatrix} d & 0 \\ 0 & e \end{bmatrix}, \quad d := \frac{1}{2m}, \quad e := \frac{1}{2}m\omega^2 \left[1 - \frac{1}{4}h^2\omega^2\right]$$

We compute

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

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

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

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

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

Put together,

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

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

Thus H^* is conserved.

3. (a) The Hamiltonian equations of motion are

$$\begin{aligned} \dot{u} &= -\partial_x H(u, v, x, y) = -x(x^2 + y^2)^{-3/2} \\ \dot{v} &= -\partial_y H(u, v, x, y) = -y(x^2 + y^2)^{-3/2} \\ \dot{x} &= -\partial_u H(u, v, x, y) = u \\ \dot{y} &= -\partial_v H(u, v, x, y) = v \end{aligned}$$

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

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

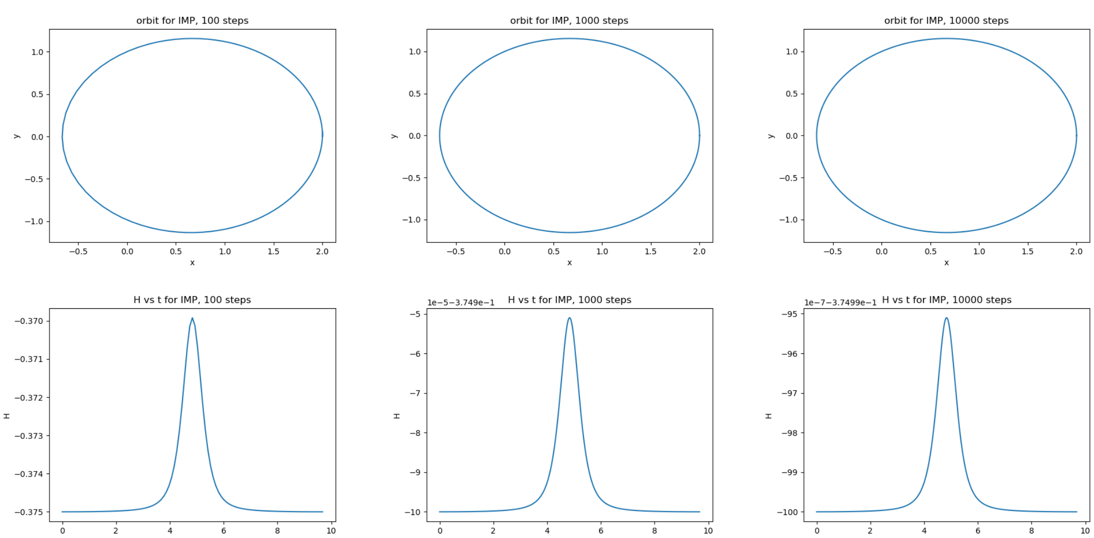
In the implicit midpoint rule (IMP), the initial approximation of k is given by

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

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

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

In the method derived in problem 1, replace T' and U' by $\boldsymbol{\nabla} T$ and $\boldsymbol{\nabla} U$.

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

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

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