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.

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

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

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

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.

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

Therefore

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

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

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

We compute

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

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

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

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

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

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.

Problem 2.

(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/blob/main/hw5.ipynb`

The Jacobian of f is

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

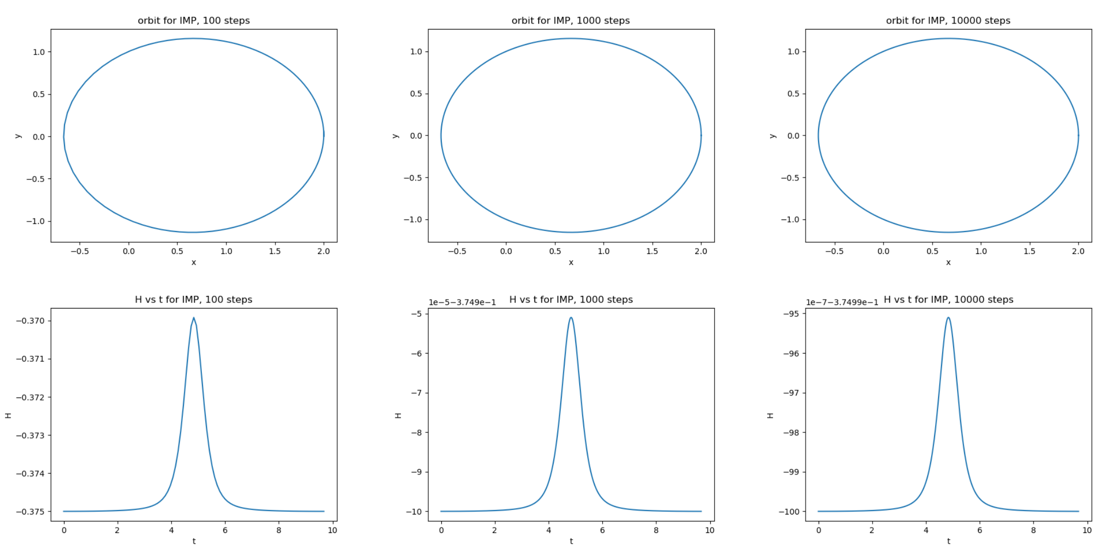
In the implicit midpoint rule (IMP), the initial approximation of k is given by

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

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

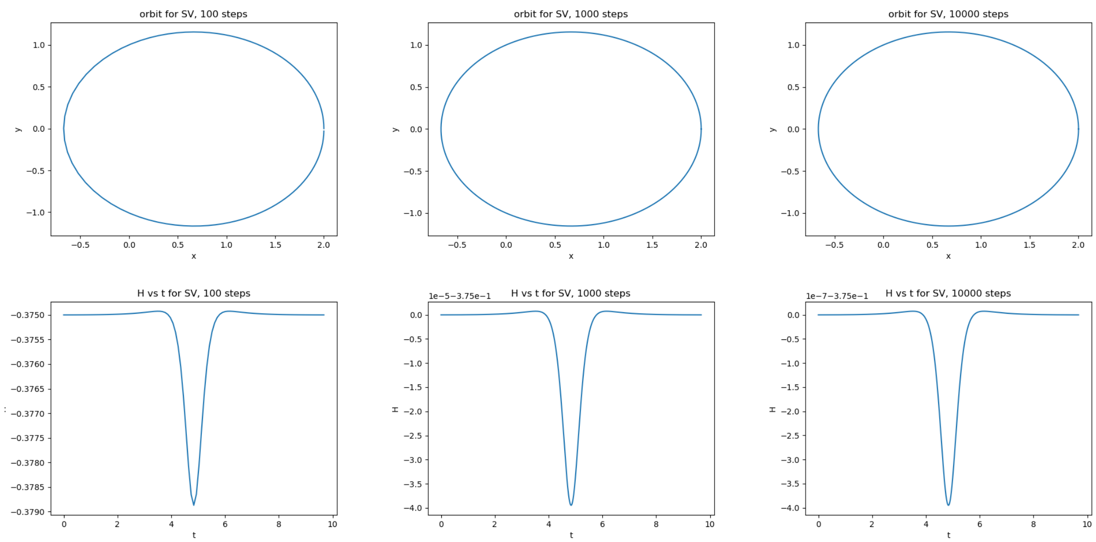
$$\partial_p H(p,q) = \nabla T(p) = \begin{bmatrix} u \\ v \end{bmatrix}, \quad \partial_q H(p,q) = \nabla U(q) = \begin{bmatrix} x(x^2+y^2)^{-3/2} \\ y(x^2+y^2)^{-3/2} \end{bmatrix}$$

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.



(d) To compare accuracy, we compare the differences in the maximum and minimum Hamiltonian, listed in the order corresponding to the number of steps taken per period: 100, 1000, 10000. The differences for IMP are:

$$0.005081464348190012, \quad 4.900006001706814 \cdot 10^{-5}, \quad 4.898265737462992 \cdot 10^{-7}$$

The differences for SV are:

$$0.0039456711144399415, \quad 4.022530826314208 \cdot 10^{-5}, \quad 4.0233147502455324 \cdot 10^{-7}$$

The differences for SV are smaller than those for IMP, so SV is more accurate than IMP.

Problem 3. Using $f(z) = \lambda z$,

$$k = f\left(z_n + \frac{1}{2}hk\right) = \lambda\left(z_n + \frac{1}{2}hk\right) = \lambda z_n + \frac{1}{2}h\lambda k \implies \left(1 - \frac{1}{2}h\lambda\right)k = \lambda z_n \implies k = \lambda\left(1 - \frac{1}{2}h\lambda\right)^{-1} z_n$$

$$\implies z_{n+1} = z_n + hk = z_n + h\lambda\left(1 - \frac{1}{2}h\lambda\right)^{-1} z_n = \left[1 + h\lambda\left(1 - \frac{1}{2}h\lambda\right)^{-1}\right] z_n$$

Set $w := h\lambda$, so

$$1 + h\lambda\left(1 - \frac{1}{2}h\lambda\right)^{-1} = 1 + w\left(1 - \frac{1}{2}w\right)^{-1} = 1 + w\left(\frac{2-w}{2}\right)^{-1} = 1 + \frac{2w}{2-w} = \frac{2-w+2w}{2-w} = \frac{w+2}{2-w}$$

$$\implies z_{n+1} = \frac{w+2}{2-w} z_n \implies z_n = \left(\frac{w+2}{2-w}\right)^n z_0$$

Now $w = x + iy$ where $x := \operatorname{Re} w$ and $y := \operatorname{Im} w$. Then

$$z_n \xrightarrow{n\to\infty} 0 \iff \left|\frac{w+2}{w-2}\right| < 1 \iff |w+2| < |w-2| \iff |w+2|^2 < |w-2|^2 \iff (x+2)^2 + y^2 < (x-2)^2 + y^2$$

$$\iff (x+2)^2 < (x-2)^2 \iff x^2 + 4 + 4x < x^2 + 4 - 4x \iff 4x < -4x \iff 8x < 0 \iff x < 0$$

Thus the RAS is $\{w \in \mathbb{C} : \operatorname{Re} w < 0\}$.