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

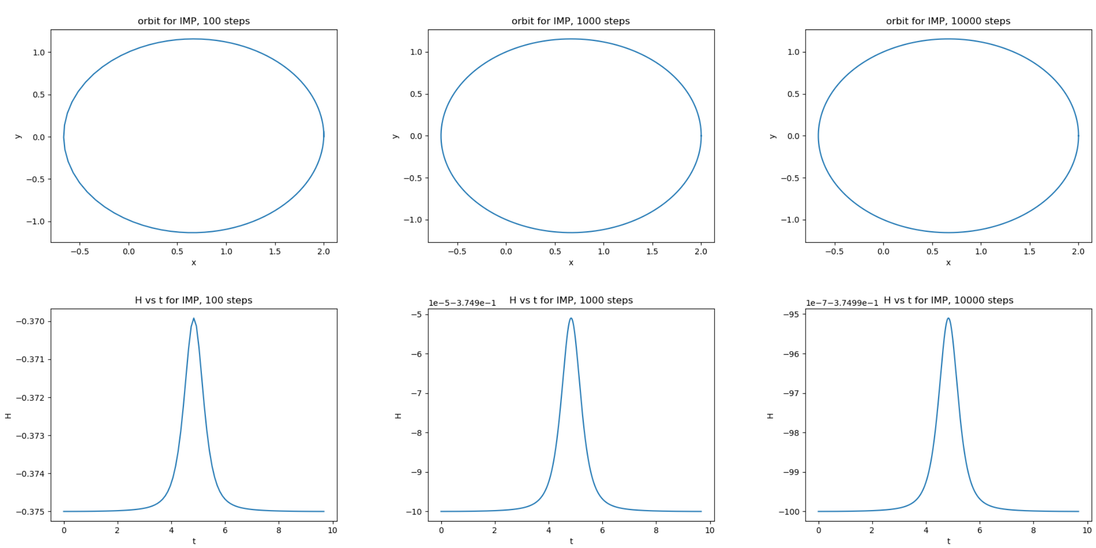
$$Df(u, v, x, y) = \begin{bmatrix} 0 & 0 & (2x^2 - y^2)(x^2 + y^2)^{-5/2} & 3xy(x^2 + y^2)^{-5/2} \\ 0 & 0 & 3xy(x^2 + y^2)^{-5/2} & (2y^2 - x^2)(x^2 + y^2)^{-5/2} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

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 $F(k) := k - f(z_n + \frac{1}{2}hk)$,

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



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

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

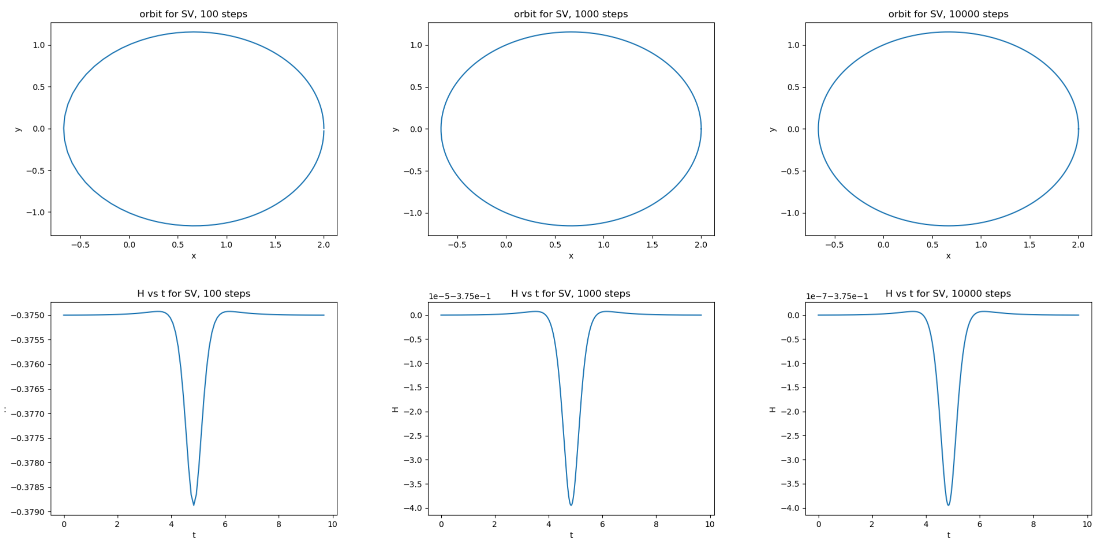
so that

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

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

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

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



(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 $\{w \in \mathbb{C} : \operatorname{Re} w < 0\}$.