Homework 5. Due March 12

Please upload a single pdf file on ELMS. Link your codes to your pdf (i.e., put your codes to dropbox, Github, google drive, etc. and place links to them in your pdf file with your solutions.

1. **(16 pts)**

   (a) The Stoermer-Verlet method for integration of Hamiltonian systems of the form

   $$\frac{dp}{dt} = -\nabla_q H(p,q), \quad \frac{dq}{dt} = \nabla_p H(p,q) \text{ or, equivalently, } \frac{d}{dt}\begin{bmatrix} p \\ q \end{bmatrix} = J^{-1}\nabla H(p,q)$$

   is given by

   $$p_{n+1/2} = p_n - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_n), \tag{1}$$
   $$q_{n+1} = q_n + \frac{h}{2}\left(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1})\right), \tag{2}$$
   $$p_{n+1} = p_{n+1/2} - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_{n+1}). \tag{3}$$

   Rewrite this scheme for the case of a separable Hamiltonian, i.e., a Hamiltonian of the form $H(p,q) = T(p) + U(q)$. Show that it is an explicit scheme in this case. This scheme is also known as *velocity Verlet*. Apply the obtained scheme to the simple harmonic oscillator in 1D with the Hamiltonian

   $$H(p,q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}. \tag{4}$$

   Rewrite the resulting equations in the form

   $$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = A \begin{bmatrix} p_n \\ q_n \end{bmatrix},$$

   where A is a 2×2 matrix that you need to find.

   (b) Show that the linear map given by the found matrix A is symplectic, i.e., $A^\top J A = J$.

   (c) The velocity Verlet scheme does not conserve the Hamiltonian given by Eq. (4). Prove that it conserves the so called *shadow Hamiltonian* given by

   $$H^* = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\left(1 - \left(\frac{\omega h}{2}\right)^2\right). \tag{5}$$

   (d) Consider the motion in the gravitational field with the Hamiltonian

   $$H(u,v,x,y) = \frac{1}{2}u^2 + \frac{1}{2}v^2 - \frac{1}{\sqrt{x^2+y^2}}, \tag{6}$$

   where $x,\ y$ are the coordinates and $u,\ v$ are the momenta in the reduced units. Write the Hamiltonian equations of motion. Set the initial conditions to $u(0) =$

$0,\ v(0) = \frac{1}{2},\ x(0) = 2,\ y(0) = 0$. Check that the total energy is negative, hence the motion will follow an elliptic trajectory.

The exact motion according to these Hamiltonian equations with the initial conditions $u(0) = 0,\ v(0) = \frac{1}{2},\ x(0) = 2,\ y(0) = 0$ occurs by the elliptical orbit with one focus at the origin, the major semiaxis $a = 4/3$, eccentricity $e = 1/2$, and the exact period of revolution $T = 2\pi a^{3/2} = 9.673596609249161$. Hence, for the exact orbit, $x_{\max} = a(1+e) = 2$, and $x_{\min} = -a(1-e) = -2/3$.

Integrate the system for 10 revolutions using the Stoermer-Verlet method. Use time step size $0.01T$. Plot x and y components of your numerical solutions on the same xy-plane. Plot the Hamiltonian versus time for your numerical solution.

2. **(6 pts)** Consider the matrix A arising in the finite difference discretization of the Poisson equation in the square domain $\Omega = [0,1]^2$ with mesh step $h = 1/J$ and homogeneous Dirichlet boundary conditions. This matrix is of size $(J-1)^2 \times (J-1)^2$ and has a block form with $(J-1) \times (J-1)$ blocks:

$$A = \frac{1}{h^2}\begin{bmatrix} T & I & & \\ I & T & I & \\ & \ddots & \ddots & \ddots \\ & & I & T \end{bmatrix}, \quad \text{where} \quad T = \begin{bmatrix} -4 & 1 & & \\ 1 & -4 & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & -4 \end{bmatrix}, \tag{7}$$

and I is the $(J-1) \times (J-1)$ identity matrix.

(a) Check that a mesh function of the form

$$v_{k_x,k_y}(x,y) = \sin(k_x x)\sin(k_y y), \quad \text{where} \quad k_x, k_y \in \{\pi, 2\pi, \dots, (J-1)\pi\}, \tag{8}$$

is an eigenvector of A with the corresponding eigenvalue

$$\lambda_{k_x,k_y} = \frac{2}{h^2}\left(\cos(k_x h) + \cos(k_y h) - 2\right) = -\frac{4}{h^2}\sin^2\left(\frac{k_x h}{2}\right)\sin^2\left(\frac{k_x h}{2}\right), \tag{9}$$

i.e., $Av_{k_x,k_y} = \lambda_{k_x,k_y} v_{k_x,k_y}$. *Hint: Plug $v_{k_x,k_y}(x,y)$ into the scheme*

$$\frac{1}{h^2}\left(U_N + U_S + U_W + U_E - 4U_P\right) \tag{10}$$

and obtain $[\lambda_{k_x,k_y} v_{k_x,k_y}]_P$.

(b) What are the smallest and the largest eigenvalues, and what are the corresponding eigenvectors? Plot eigenvectors for $J = 10$ corresponding to corresponding to $k_x = k_y = \pi$, $k_x = \pi,\ k_y = 2\pi$, and $k_x = k_y = (J-1)\pi$.