Numerical Programming 2 (CSE) 2015

Worksheet 1

Exercise 1

The divergence of a vector field $f(x) : \mathbb{R}^n \to \mathbb{R}^n$ is defined as

$$\text{div} f = \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_i}.$$

The Liouville theorem[1] says that the flow of a vector field with divergence equal to zero preserves the volume in phase space.

- By defining $z = (p, q)$ show that the Hamiltonian flow has divergence equal to zero
$$\text{div}[\Omega \nabla_z H](z) = 0, \qquad \Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$
and therefore is volume preserving
- The symplectic condition can also be used to show that the Hamiltonian flow preserves volume in phase space. Can you show how?
- Find an example of a vector field that is volume preserving but that does not satisfies the symplectic condition

Exercise 2

The Hamiltonian of the "Fermi-Pasta-Ulam" problem is defined as

$$\begin{cases} H(q,p) = \dfrac{1}{2m} \displaystyle\sum_{i=1}^{N-1} p_i^2 + \dfrac{\kappa}{2} \displaystyle\sum_{i=0}^{N-1} (q_{i+1} - q_i)^2 + \dfrac{\lambda}{3} \displaystyle\sum_{i=0}^{N-1} (q_{i+1} - q_i)^3 \\ q_0 = q_N = p_0 = p_N = 0 \end{cases}$$

and represents a one-dimensional chain of N non-linear oscillators. The constant κ is Hooke's elastic constant while λ is a small, positive parameter. Set $N = 32$, $\kappa = m = 1$, $\lambda = 1/4$ and use the following initial condition

$$q_j(t=0) = \left(\frac{2}{N}\right)^{1/2} \sin\left(\frac{j\pi}{N}\right), \qquad p_j(t=0) = 0 \text{ with } j = 1, ..., N-1$$

to simulate the system over the time interval $[0, t_f]$, $t_f = 200(\frac{2\pi}{\omega})$ with $\omega = 2\sin\left(\frac{\pi}{2N}\right)$.

[1] If time allows we will prove this theorem during the tutorial class

Implement both the Euler-B method

$$\begin{cases} q^{n+1} = q^n + h\nabla_p H(q^n, p^{n+1}) \\ p^{n+1} = p^n - h\nabla_q H(q^n, p^{n+1}) \end{cases}$$

and the Störmer-Verlet method on the Fermi-Pasta-Ulam problem.

Monitor the Hamiltonian $H(p, q)$ and the harmonic energy

$$E = \frac{1}{2m}\sum_{i=1}^{N-1} p_i^2 + \frac{\kappa}{2}\sum_{i=0}^{N-1}(q_i - q_{i-1})^2$$

for increasing values of λ. What do you notice?

Exercise 3

Given the Hamiltonian ODE $z' = \Omega^{-1}\nabla H(z)$ the implicit midpoint rule:

$$z^{n+1} = z^n + hf\left(t_n + \frac{h}{2}, \frac{1}{2}(z^n + z^{n+1})\right)$$

1. Prove that
$$\frac{\partial z^{n+1}}{\partial z^n} = (id - \Omega A)(id + \Omega A)^{-1}$$
where $A = \frac{h}{2}D^2 H\left(\frac{z^{n+1}+z^n}{2}\right)$ and $\Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

2. Let $X = \frac{\partial z^{n+1}}{\partial z^n}$ and show that X can be rewritten as
$$X = \Omega(A + \Omega)(A - \Omega)^{-1}\Omega \qquad \text{and} \qquad X = -(A - \Omega)^{-1}(A + \Omega)$$
*Hint:*Use the fact that $(id - \Omega A)^{-1}$ $(id + \Omega A)$ commute.

3. Using the two representations of X described above show that
$$X^T \Omega X = \Omega.$$