Numerical Simulation LA50600
(ISAPS/Physics)
Week3 : March 08

- Solve a system of ODE.
- Review charged particle motion in inhomogeneous magnetic field.
- Symplectic integrator: good energy conservation.
- Take nonlinear pendulum problem for example and compare (1) Euler, (2) Improved Euler, and (3) Symplectic integrator.
With magnetic inhomogeneity we see $\nabla B$ drift

- With the magnetic moment $\mu = mv_{\perp}^2/2B$, we obtain the $\nabla B$ drift velocity,

$$v_d = \frac{\mathbf{B} \times \mu \nabla B}{qB^2} = \frac{\mathbf{B} \times mv_{\perp}^2 \nabla B}{2qB^3}$$

- After normalization by $\Omega_c = qB/m$ and scale length $L$,

$$\bar{v}_d = \text{sign}(q)\frac{\mathbf{B} \times \bar{v}_{\perp}^2 \nabla \bar{B}}{2\bar{B}^3} = \pm \frac{\mathbf{B} \times \mu \nabla \bar{B}}{\bar{B}^2}$$

For the guiding center approximation to be appropriate, $\rho \ll a$.

$$B_z(x, y) = x^2 + y^2 - a^2 = r^2 - a^2$$

$$\nabla B = \partial_r B_z(x, y) = 2rr\hat{r} = 2\sqrt{x^2 + y^2}\hat{r}$$

Therefore

$$\bar{v}_d = \pm \frac{\mu \hat{z} \times 2r\hat{r}}{r^2 - a^2} = \pm \frac{2\mu r}{r^2 - a^2} \hat{\theta}$$

Here $+$ for ions $-$ for the electrons.
Let us revisit a system (from 3/5)

- So far we only dealt with a first order ODE \( \frac{dx}{dt} = -x \). Let us try solving a system of ODE (simultaneous ODE).
- A second order equation

\[
\frac{d^2q}{dt^2} = -\sin(q),
\]

can be separated into two first order ODE

\[
\frac{dp}{dt} = -\sin(q)
\]

\[
\frac{dq}{dt} = p.
\]

- In Euler, this reads

\[
p_0 = p
\]

\[
q_0 = q
\]

\[
p = p_0 - h \cdot \sin(q_0)
\]
\[ q = q_0 + h \cdot p_0 \]

- In improved Euler this reads

\[
\begin{align*}
\text{do } & \text{i }= 1, n \\
p_0 & = p \\
q_0 & = q \\
p_{mid} & = p_0 - (h/2.0) \cdot \sin(q_0) \\
q_{mid} & = q_0 + (h/2.0) \cdot p_0 \\
p & = p_0 - h \cdot \sin(q_{mid}) \\
q & = q_0 + h \cdot p_{mid} \\
\text{enddo}
\end{align*}
\]

- Note that the order in advancing \( q \) and \( p \) does not matter in the example above.
Hamiltonian disc is useful in energy conserving sys

- Let us consider nonlinear pendulum motion in usual way along the azimuthal ($\theta$) direction. The equation of motion is given by
  \[ ml\ddot{\theta} = mg \sin \theta \quad \text{(or) \quad l\ddot{\theta} = g \sin \theta) \]

- Note that if we use \( \sin (\theta) \simeq \theta \) we resume harmonic oscillator.
• We can use Hamiltonian to derive the equation of motion:
• Hamiltonian is equivalent to total energy

\[ H(p, q, t) \equiv \sum p \cdot \dot{q} - L = \frac{p^2}{2m} + mgl \,(1 - \cos q) \]

where we have momentum \( p = mlv_\theta = ml^2\dot{\theta} \) (angular momentum) and a conjugate coordinate \( q = \theta \). Note we use \((q, p)\) as independent variables.
• With the Hamiltonian, we obtain the equation of motion\(^a\)

\[ \dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial q} = -mgl \sin q. \]

\(^a\)A system equivalent to \( \dot{x} = v, \dot{v} = -\sin x \) as we just did.
The phase space trajectory in \((q, p)\) space provides us with intuitive understanding.

- Libration and rotation separated by the island separatrix.
- We can check if Hamiltonian (or total energy) is conserved at each time step.
A symplectic integrator advances kinetic energy and potential energy part separately

- An alternative name is leap-frog:

\[
q \leftarrow q(0) \\
p \leftarrow p(0) \\
\text{for } k = 1 \text{ to } n \text{ do} \\
\hspace{1cm} q = q + 0.50 \times dt \times p \\
\hspace{1cm} p = p - dt \times \sin(q) \\
\hspace{1cm} q = q + 0.50 \times dt \times p \\
\hspace{1cm} \text{printf } q, p \\
\text{end for}
\]
Energy conservation for the three methods, are compared

- (1) Euler (black), (2) Improved Euler (red), and (3) Symplectic integrator (green).
Symplectic integrator can be understood in terms of differential operator

- Canonical equation reads

\[
\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = D \begin{pmatrix} p \\ q \end{pmatrix}
\]

- Compared to the scalar equation

\[
\frac{dx}{dt} = kx \quad \Rightarrow \quad x = \exp(kt)x(0),
\]

we can write

\[
\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \exp(tD) \begin{pmatrix} p(0) \\ q(0) \end{pmatrix}
\]
One important feature of chaotic motion is an exponential divergence of initial condition.

- **Lyapunov exponent**: Provided $\delta_0$ to be a small distance between two particles at $t = 0$, and the distance after time interval $t$ diverges exponentially as $d_2(t) = d_1 \exp(ht)$, the coefficient $h$ is called the Lyapunov exponent.
• However, if one takes the logarithm of \( h = (1/t) \log \left[ \delta(t)/\delta_0 \right] \), one sees numerical errors.

• To reduce this error, we follow two particles, an objective particle and a test one, and repeated replacing the test one. By this replacement, the test particle always stays nearby retaining the information of the latter. Also by replacing; the position of the test particle is adjusted in the direction of an eigenvector.

• Provided \( \mathbf{R}_j \) and \( \mathbf{r}_j \) are the position of the objective particle and the test one respectively, we replace the position of the test one to

\[
\mathbf{r}_{j+1} = \mathbf{R}_{j+1} + \delta_0 \frac{\mathbf{R}_j - \mathbf{r}_j}{|\mathbf{R}_j - \mathbf{r}_j|},
\]

where the integer \( j \) denotes the numerical time step. Thus, KS-entropy \( h \) is computed by

\[
h = \lim_{N \to \infty} \frac{1}{N \Delta t} \sum_{j=1}^{N} \log \left( \frac{|\mathbf{r}_{j+1} - \mathbf{R}_{j+1}|}{\delta_0} \right).
\]
Summary of this week’s discussions

- System of ODE and improved Euler (2nd order) method.
- Single charged particle motion in electromagnetic field (and grad-B). Guiding center simulation.
- Symplectic system → energy conserving leap-frog method.
- 3/12, higher order Runge-Kutta-Gill method.
- Estimating instability parameter Lyapunov exponent.
- Shooting method as an application of ODE.