Computational Methods in Plasma Physics. Lecture II

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Simple harmonic oscillator

We looked at

$$\frac{d^2 z}{dt^2} = -\omega^2 z$$

and wrote it as system of first-order ODEs

$$\frac{dz}{dt} = v; \quad \frac{dv}{dt} = -\omega^2 z$$

Now introduce energy-angle coordinates

$$\omega z = E \sin\theta; \quad v = E\cos\theta$$

then $E^2 = \omega^2 z^2 + v^2 \equiv E_0^2$ is a constant as we showed before. Using these expressions we get the very simple ODE $\dot{\theta} = \omega$. This shows that in phase-space $(v, \omega z)$ the motion is with uniform angular speed along a circle.

Simple harmonic oscillator: Phase-errors

The mid-point scheme had

$$(v^{n+1})^2 + \omega^2 (z^{n+1})^2 = (v^n)^2 + \omega^2 (z^n)^2 = E_0^2$$

which means that the mid-point scheme gets the energy coordinate *exactly* correct. However, we have

$$\tan\theta^{n+1} = \frac{\omega z^{n+1}}{v^{n+1}}.$$

Using the expressions for the scheme and Taylor expanding in Δt we get

$$\tan\theta^{n+1} = \tan\theta^n + \frac{\omega E_0^2}{(v^n)^2}\Delta t + \frac{\omega^3 z^n E_0^2}{(v^n)^3}\Delta t^2 + O(\Delta t^3)$$

The first three terms match the Taylor expansion of the exact solution $\tan(\theta^n + \omega\Delta t)$ and the last term is the *phase-error*.

Single particle motion in an electromagnetic field

- In PIC method the Vlasov-Maxwell equation is solved in the *Lagrangian frame*: the phase-space is represented by *finite-sized* "macro-particles".
- In the Lagrangian frame the distribution function remains constants along *characteristics* in phase-space.
- These characteristics satisfy the ODE of particles moving under Lorentz force law

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$
$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}(\mathbf{E}(\mathbf{x},t) + \mathbf{v} \times \mathbf{B}(\mathbf{x},t))$$

- In the absence of an electric field, the kinetic energy must be conserved

$$\frac{1}{2}|\mathbf{v}|^2 = \text{constant}.$$

  This is independent of the spatial or time dependence of the magnetic field. Geometrically this means that in the absence of an electric field the velocity vector rotates and its tip always lies on a sphere.

Single particle motion in an electromagnetic field

- A mid-point scheme for this equation system would look like

$$\frac{\mathbf{x}^{n+1}-\mathbf{x}^{n}}{\Delta t}=\frac{\mathbf{v}^{n+1}+\mathbf{v}^{n}}{2}$$
$$\frac{\mathbf{v}^{n+1}-\mathbf{v}^{n}}{\Delta t}=\frac{q}{m}\left(\overline{\mathbf{E}}(\mathbf{x},t)+\frac{\mathbf{v}^{n+1}+\mathbf{v}^{n}}{2}\times\overline{\mathbf{B}}(\mathbf{x},t)\right)$$

  The overbars indicate some averaged electric and magnetic fields evaluated from the new and old positions. In general, this would make the scheme nonlinear!

- Instead, we will use a *staggered* scheme in which the position and velocity are staggered by half a time-step.

$$\frac{\mathbf{x}^{n+1}-\mathbf{x}^{n}}{\Delta t}=\mathbf{v}^{n+1/2}$$
$$\frac{\mathbf{v}^{n+1/2}-\mathbf{v}^{n-1/2}}{\Delta t}=\frac{q}{m}\left(\mathbf{E}(\mathbf{x}^{n},t^{n})+\frac{\mathbf{v}^{n+1/2}+\mathbf{v}^{n-1/2}}{2}\times\mathbf{B}(\mathbf{x}^{n},t^{n})\right)$$

The Boris algorithm for the staggered scheme

The velocity update formula is

$$\frac{\mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}(\mathbf{x}^n, t^n) + \frac{\mathbf{v}^{n+1/2} + \mathbf{v}^{n-1/2}}{2} \times \mathbf{B}(\mathbf{x}^n, t^n)\right)$$

This appears like an implicit method: most obvious is to construct a linear 3×3 system of equations and invert them to determine $\mathbf{v}^{n+1}$. Puzzle to test your vector-identity foo: find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$.
The Boris algorithm updates this equation in three steps:

$$\begin{aligned}
\mathbf{v}^- &= \mathbf{v}^{n-1/2} + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2} \\
\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} &= \frac{q}{2m}(\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}^n \\
\mathbf{v}^{n+1/2} &= \mathbf{v}^+ + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2}
\end{aligned}$$

Convince yourself that this is indeed equivalent to the staggered expression above. So we have two electric field updates with half time-steps and a rotation due to the magnetic field. Once the updated velocity is computed, we can trivially compute the updated positions.