Computational Methods in Plasma Physics. Lecture II

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PPPL Graduate Summer School, 2020

Single particle motion in an electromagnetic field

- In the *Particle-in-cell* (PIC) method the Vlasov-Maxwell equation is solved in the *Lagrangian frame* in which 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

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

- We will first focus on solving the equations-of-motion for the macro-particles, leaving solution of Maxwell equations and coupling to particles for Lecture 2.

Simple harmonic oscillator

Consider first the simple harmonic oscillator

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

This has exact solution $z = a\cos(\omega t) + b\sin(\omega t)$, where a and b are arbitrary constants. How to solve this numerically? Write as a system of first-order ODEs

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

Note that the coordinates (z, v) label the *phase-space* of the harmonic oscillator. Multiply the second equation by v and use the first equation to get

$$\frac{d}{dt}\left(\frac{1}{2}v^2 + \frac{1}{2}\omega^2 z^2\right) = 0.$$

This is the *energy* and is *conserved*.
Question: how to solve the ODE such that the energy is conserved by the discrete scheme?

Harmonic oscillator: Forward Euler Scheme

First attempt: use the simplest possible scheme, replace derivatives with difference approximations

$$\frac{z^{n+1} - z^n}{\Delta t} = v^n; \quad \frac{v^{n+1} - v^n}{\Delta t} = -\omega^2 z^n$$

or

$$z^{n+1} = z^n + \Delta t v^n; \quad v^{n+1} = v^n - \Delta t \omega^2 z^n$$

This is the *forward Euler* scheme. Lets check if the discrete scheme conserves energy:

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

The presence of the $\omega^2 \Delta t^2$ in the bracket spoils the conservation. So the forward Euler scheme *does not* conserve energy. Also, note that the energy, in fact, is *increasing*!

Harmonic oscillator: Forward Euler Scheme

Closer look: write as a matrix equation

$$\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \Delta t \\ -\omega^2 \Delta t & 1 \end{bmatrix}}_{\text{Jacobian, } J} \begin{bmatrix} z^n \\ v^n \end{bmatrix}.$$

Observe that the determinant of the Jacobian is $\det(J) = (1 + \omega^2 \Delta t^2)$ which is the same factor as appears in the energy relation. One may reasonably conjecture that when this determinant is one, then perhaps energy is conserved.

Volume Preserving Scheme

We will call say a scheme preserves *phase-space* volume if the determinant of the Jacobian is $\det(J) = 1$.

Harmonic oscillator: Mid-point Scheme

Perhaps a better approximation will be obtained if we use *averaged* values of z, v on the RHS of the discrete equation:

$$
\begin{aligned}
\frac{z^{n+1} - z^n}{\Delta t} &= \frac{v^n + v^{n+1}}{2} \\
\frac{v^{n+1} - v^n}{\Delta t} &= -\omega^2 \frac{z^n + z^{n+1}}{2}
\end{aligned}
$$

This is an *implicit* method as the solution at the next time-step depends on the old as well as the next time-step values. In this simple case we can explicitly write the update in a matrix form as

$$
\begin{bmatrix} z^{n+1} \\ v^{n+1} \end{bmatrix} = \frac{1}{1+\omega^2\Delta t^2/4} \begin{bmatrix} 1-\omega^2\Delta t^2/4 & \Delta t \\ -\omega^2\Delta t & 1-\omega^2\Delta t^2/4 \end{bmatrix} \begin{bmatrix} z^n \\ v^n \end{bmatrix}.
$$

For this scheme $\det(J) = 1$. So the mid-point scheme conserves phase-space volume! Some algebra also shows that

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

showing that energy is also conserved by the mid-point scheme.

Harmonic oscillator: Mid-point Scheme is symplectic

A more stringent constraint on a scheme for the simple harmonic oscillator is that it be *symplectic*. To check if a scheme is symplectic one checks to see if

$$J^T \sigma J = \sigma$$

where σ is the *unit symplectic matrix*

$$\sigma = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

Turns out that the mid-point scheme for the harmonic oscillator is also symplectic. Note that if a scheme conserves phase-space volume, it *need not* be symplectic.

Accuracy and Stability

To study the stability, accuracy and convergence of a scheme one usually looks at the first order ODE

$$\frac{dz}{dt} = -\gamma z$$

where $\gamma = \lambda + i\omega$ is the complex frequency. The exact solution to this equation is $z(t) = z_0 e^{-\gamma t}$. The solution has damped/growing modes ($\lambda > 0$ or $\lambda < 0$) as well as oscillating modes.

- The forward Euler scheme for this equation is

$$z^{n+1} = z^n - \Delta t \gamma z^n = (1 - \Delta t \gamma) z^n.$$

- The mid-point scheme for this equation is

$$z^{n+1} = \left(\frac{1 - \gamma \Delta t/2}{1 + \gamma \Delta t/2} \right) z^n$$

Accuracy and Stability

We can determine how *accurate* the scheme is by looking at how many terms the scheme matches the Taylor series expansion of the exact solution:

$$z(t^{n+1}) = z(t^n)\left(1 - \gamma\Delta t + \frac{1}{2}\gamma^2\Delta t^2 - \frac{1}{6}\gamma^3\Delta t^3 + \dots\right)$$

- The forward Euler scheme matches the *first two terms*

$$z^{n+1} = z^n(1 - \Delta t\gamma)$$

- The mid-point scheme matches the *first three terms*

$$z^{n+1} = z^n\left(1 - \Delta t\gamma - \frac{1}{2}\gamma^2\Delta t^2 - \frac{1}{4}\gamma^3\Delta t^3 + \dots\right)$$

Accuracy and Stability

We can determine if the scheme is *stable* by looking at the amplification factor $|z^{n+1}/z^n|$. Note that for damped modes $(\lambda > 0)$ this quantity *decays* in time, while for purely oscillating modes $(\lambda = 0)$ this quantity remains *constant*.

- The amplification factor for the forward Euler scheme in the absence of damping is $1 + \omega^2 \Delta t^2 > 1$, hence this scheme is *unconditionally unstable*.
- The amplification factor for the mid-point scheme in the absence of damping is exactly 1, showing that the mid-point scheme is *unconditionally stable*, that is, one can take as large time-step one wants without the scheme "blowing up". Of course, the errors will increase with larger Δt.

Runge-Kutta schemes

- Even though the forward Euler scheme is unconditionally unstable, we can use it to construct other schemes that *are* stable and are also more accurate (than first order).
- For example, a class of Runge-Kutta schemes can be written as a combination of forward Euler updates. In particular, the *strong stability preserving* schemes are important when solving hyperbolic equations. Note that these RK schemes will *not* conserve energy for the harmonic oscillator, but *decay* it.
- Other multi-stage Runge-Kutta schemes can be constructed that allow very large time-steps for diffusive processes, for example, that come about when time-stepping diffusion equations.

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

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\begin{aligned}
\frac{d\mathbf{x}}{dt} &= \mathbf{v} \\
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\end{aligned}
$$

- 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.

The Boris algorithm for the staggered scheme

How to do the rotation? The Boris algorithm does this in several steps:

- Compute the $\mathbf{t}$ and $\mathbf{s}$ vectors as follows

$$\mathbf{t} = \tan\left(\frac{qB}{m}\frac{\Delta t}{2}\right)\frac{\mathbf{B}}{B} \approx \frac{q\mathbf{B}}{m}\frac{\Delta t}{2}$$
$$\mathbf{s} = \frac{2\mathbf{t}}{1+|\mathbf{t}|^2}$$

- Compute $\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$ and finally $\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$.

See Birdsall and Langdon text book Section 4-3 and 4-4 and figure 4-4a. Easily extended to relativistic case. Note that using the approxiate form in computing $\mathbf{t}$ will lead to *an error in the gyroangle*.

Note that in the absence of an electric field the Boris algorithm conserves kinetic energy.

Why is the Boris algorithm so good? Can one do better?

See paper by Qin at. al. Phys. Plasmas, **20**, 084503 (2013) in which it is shown that the Boris algorithm *conserves phase-space volume*. However, they also show that the Boris algorithm is *not* symplectic.

- The relativistic Boris algorithm does not properly compute the $\mathbf{E}\times\mathbf{B}$ velocity. This can be corrected. For example Vay, Phys. Plasmas, **15**, 056701 (2008). The Vay algorithm however, breaks the phase-space volume preserving property of the Boris algorithm.
- Higuera and Cary, Phys. Plasmas, **24**, 052104 (2017) showed how to compute the correct $\mathbf{E}\times\mathbf{B}$ drift velocity and restore volume preserving property. Seems this is probably the current-best algorithm for updating Lorentz equations.
- The saga for better particle push algorithms is not over! For example, an active area of research is to discover good algorithms for *asymptotic* systems, for example, when gyroradius is much smaller than gradient length-scales or gyrofrequency is much higher than other time-scales in the system. Common in most magnetized plasmas.

Appendix: Find $\mathbf{A}$ if $\mathbf{A} = \mathbf{R} + \mathbf{A} \times \mathbf{B}$

Take the cross-product with $\mathbf{B}$:

$$\mathbf{A} \times \mathbf{B} = \mathbf{R} \times \mathbf{B} + (\mathbf{A} \times \mathbf{B}) \times \mathbf{B}$$

Use $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{C} \times \mathbf{B}) \times \mathbf{A} = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$ to write

$$(\mathbf{A} \times \mathbf{B}) \times \mathbf{B} = (\mathbf{B} \cdot \mathbf{A})\mathbf{B} - B^2\mathbf{A}$$

to get

$$\mathbf{A} \times \mathbf{B} = \mathbf{R} \times \mathbf{B} + (\mathbf{B} \cdot \mathbf{A})\mathbf{B} - B^2\mathbf{A}.$$

From the original equation we have $\mathbf{A} \times \mathbf{B} = \mathbf{A} - \mathbf{R}$ and $\mathbf{B} \cdot \mathbf{A} = \mathbf{B} \cdot \mathbf{R}$. Plugging these into the last expression we finally get

$$\mathbf{A} = \frac{\mathbf{R} + \mathbf{R} \times \mathbf{B} + (\mathbf{B} \cdot \mathbf{R})\mathbf{B}}{1 + B^2}.$$

One can use this to find an explicit expression for the velocity update in the Boris scheme.