# Computational Methods in Plasma Physics. Lecture I

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# Goal: Modern Computational Techniques for Plasma Physics

Vast majority of plasma physics in contained in the Vlasov-Maxwell equations that describe self-consistent evolution of distribution function $f(\mathbf{x}, \mathbf{v}, t)$ and electromagnetic fields:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = \left(\frac{\partial f_s}{\partial t}\right)_c$$

where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The EM fields are determined from Maxwell equations

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \sum_s q_s \int_{-\infty}^{\infty} v f_s \, d\mathbf{v}^3$$

Highly nonlinear: fields tell particles how to move. Particle motion generates fields. This is a very difficult system of equations to solve! Theoretical and computational plasma physics consists of making approximations and solving these equations in specific situations.

# Why is solving Vlasov-Maxwell equations directly so hard?

Despite being the fundamental equation in plasma physics the VM equations remain highly challenging to solve.

- Highly nonlinear with the coupling between fields and particles via currents and Lorentz force. Collisions can further complicate things due to long-range forces in a plasma; dominated by small-angle collisions
- High dimensionality and multiple species with large mass ratios: 6D phase-space, $m_e/m_p = 1/1836$ and possibly dozens of species.
- Enormous scales in the system: light speed and electron plasma oscillations; cyclotron motion of electrons and ions; fluid-like evolution on intermediate scales; resistive slow evolution of near-equilibrium states; transport scale evolution in tokamak discharges. 14 orders of magnitude of physics in these equations!

# Many approximations developed over the decades

Modern computational plasma physics consists of making justified approximations to the VM system and then coming up with efficient schemes to solve them.

- Major recent theoretical development in plasma physics is the discovery of gyrokinetic equations, an asymptotic approximation for plasmas in strong magnetic fields. Reduces dimensionality to 5D (from 6D) and eliminates cyclotron frequency and gyroradius from the system. Very active area of research.
- Many fluid approximations have been developed to treat plasma via low-order moments: extended MHD models; multimoment models; various reduced MHD equations
- Numerical methods for these equations have undergone renaissance in recent years: emphasis on *memetic* schemes that preserve conservation laws and some geometric features of the continuous equations. Based on Lagrangian and Hamiltonian formulation of basic equations. Very active area of research.

With advent of large scale computing much research is now focused on schemes that scale well on thousands (millions) of CPU/GPU cores.

# Goal of this course is to look at some key schemes and study their properties

Computational plasma physics is vast: we can only cover a (very) small fraction of interesting methods. In this class we will focus on

- Solving the Vlasov-Maxwell equations using particles, the "Particle-in-cell" method; methods to solve Maxwell equations. This is probably the most widely used method that yields reasonable results for many kinetic problems
- Shock-capturing methods for plasma fluid equations. These are particularly relevant to astrophysical problems in which flows can be supersonic or super-Alfvenic. A brief look at fluid solvers for use in fusion machines (tokamaks, stellarators) in which dynamics is much slower.
- Directly discretizing the Vlasov-Maxwell equations as a PDE in 5D/6D. This is an emerging area of active research and may open up study of turbulence in fusion machines and also exploring fundamental plasma physics in phase-space.

# Conservation properties of Vlasov-Maxwell equations

It is important to design methods that preserve at least some properties of continuous Vlasov-Maxwell system. Define the moment operator for any function $\varphi(\mathbf{v})$ as

$$\langle \varphi(\mathbf{v}) \rangle_s \equiv \int_{-\infty}^{\infty} \varphi(\mathbf{v}) f_s(t, \mathbf{x}, \mathbf{v}) \, d^3\mathbf{v}.$$

The Vlasov-Maxwell system conserves particles:

$$\frac{d}{dt} \int_\Omega \sum_s \langle 1 \rangle_s \, d^3\mathbf{x} = 0.$$

The Vlasov-Maxwell system conserves total (particles plus field) momentum.

$$\frac{d}{dt} \int_\Omega \left( \sum_s \langle m_s \mathbf{v} \rangle_s + \epsilon_0 \mathbf{E} \times \mathbf{B} \right) \, d^3\mathbf{x} = 0.$$

The Vlasov-Maxwell system conserves total (particles plus field) energy.

$$\frac{d}{dt} \int_\Omega \left( \sum_s \langle \frac{1}{2} m_s |\mathbf{v}|^2 \rangle_s + \frac{\epsilon_0}{2} |\mathbf{E}|^2 + \frac{1}{2\mu_0} |\mathbf{B}|^2 \right) \, d^3\mathbf{x} = 0.$$

# Conservation properties of Vlasov-Maxwell equations

Besides the fundamental conservation laws, in the *absence of collisions* we can also show that

$$\frac{d}{dt}\int_K \frac{1}{2} f_s^2 \, d\mathbf{z} = 0,$$

where the integration is taken over the complete phase-space. Also, the entropy is a *non-decreasing* function of time

$$\frac{d}{dt}\int_K -f_s \ln(f_s) \, d\mathbf{z} \geq 0.$$

For collisionless system the entropy remains *constant*. (Prove these properties as homework/classwork problems).

- It is not always possible to ensure all these properties are preserved numerically. For example: usually one can either ensure momentum *or* energy conservation but not both; it is very hard to ensure $f(t, \mathbf{x}, \mathbf{v}) > 0$.
- Much of modern computational plasma physics research is aimed towards constructing schemes that preserve these properties.

# 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

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

- 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:

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

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 $\sigma$ 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 $\Delta t$.

# 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.