Lecture #23 Numerical Simulation of Plasmas

I. Numerical Solution vs. Simulation:

A. The computer can be used to solve a wide variety of plasma physics problems. There are two primary ways we use the computer:

1. Numerical Solution of an equation, or system of equations.

Examples: a. Solving for normal mode frequencies and damping rates

b. Calculating an equilibrium state of a plasma system.

2. Simulation of the evolution of a plasma in time, starting from initial conditions, represents a major branch of plasma physics research.

a. Determine the stability or instability of an equilibrium

b. Determine the transport of mass, momentum, and energy via the dynamics of the plasma.

II. Numerical Simulation

A. The Goal of Numerical Simulation

1. The goal is numerical simulation is NOT to run the code, but to improve our understanding of plasma behavior.
2. The ideal result is to refine our understanding of the plasma behavior so that we do not need to run the code to predict what will occur.
3. We would like to develop relatively simple analytical models that accurately describe the behavior of the tremendously more complex nonlinear numerical simulations.
4. In the present climate of plasmas effort focused on numerical simulation, it is easy to forget that simulation codes are a means, not an end!

II. (Continued)

B. Roadmap to Progress Using Numerical Simulation

1. Define the problem in precise mathematical terms
2. Develop multiple, independent algorithms and simulation codes
3. Benchmark codes in simple analytical limits and against each other.
4. Use simulations to
   a. Study cases of immediate interest
   b. Developing an analytical understanding of the physical processes
5. "Turn off" the computer.

C. Major Choices in Numerical Simulation

We will focus on this ⇒ 1. Physical Model: Fluid vs. Kinetic, immobile vs. dynamics ions, etc.

These are common to any scientific computational approach.

2. Numerical Algorithms For Evolution of Equations in time: Eulerian (grid) vs. Lagrangian (particle), explicit vs. implicit, etc.
3. Implementation of Numerical Method: Adaptive vs. Fixed resolution, serial vs. parallel, etc.

III. Physical Models and Relevant Numerical Approaches

1. There are nearly as wide a variety of numerical approaches, and slight variants thereof, as there are problems to study.
2. I will not give an exhaustive list of all the methods in use to study plasmas, but merely hope to list some of the more widely used techniques and give some sense of how to use these approaches.

Lecture #23 (Continued)

III. (Continued)

A. Kinetic Plasma Physics

System: $$\frac{\partial f_s}{\partial t} + \underset{\sim}{v}\cdot\nabla f_s + \frac{q_s}{m_s}(\underset{\sim}{E}+\underset{\sim}{v}\times\underset{\sim}{B})\cdot\frac{\partial f_s}{\partial \underset{\sim}{x}} = \left(\frac{\partial f_s}{\partial t}\right)_{coll}$$

$f_s(\underset{\sim}{x},\underset{\sim}{v},t)$

$\underset{\sim}{E}(\underset{\sim}{x},t)$

$\underset{\sim}{B}(\underset{\sim}{x},t)$

$$\nabla\cdot\underset{\sim}{E} = \frac{\rho_q}{\epsilon_0}$$

$$\nabla\times\underset{\sim}{E} = -\frac{\partial \underset{\sim}{B}}{\partial t}$$

$$\nabla\times\underset{\sim}{B} = \mu_0\underset{\sim}{j} + \mu_0\epsilon_0\frac{\partial \underset{\sim}{E}}{\partial t}$$

$$\nabla\cdot\underset{\sim}{B} = 0$$

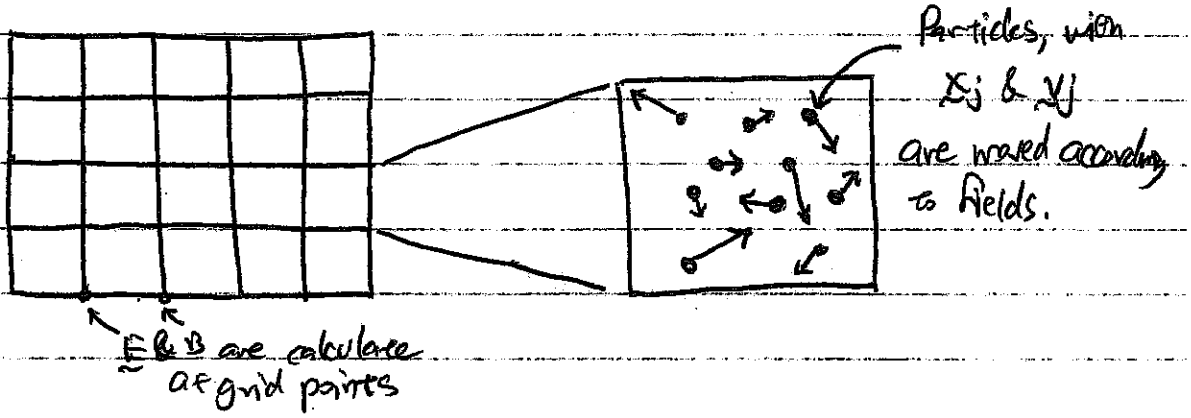
$$\rho_q = \sum_s \int d^3\underset{\sim}{v}\, q_s f_s$$

$$\underset{\sim}{j} = \sum_s \int d^3\underset{\sim}{v}\, q_s \underset{\sim}{v} f_s$$

1. Particle-in-Cell (PIC):

a. $\underset{\sim}{E}(\underset{\sim}{x},t)$ & $\underset{\sim}{B}(\underset{\sim}{x},t)$ are solved on a mesh in space

b. Velocity space in $f_s(\underset{\sim}{x},\underset{\sim}{v},t)$ is sampled by a statistical ensemble of Lagrangian tracer particles.



c. General Flow of PIC Simulation

① Pick initial conditions at $t=0$: $f_s(\underset{\sim}{x},\underset{\sim}{v})$, $\underset{\sim}{E}(\underset{\sim}{x})$, $\underset{\sim}{B}(\underset{\sim}{x})$

② Load a random distribution of particles consistent with $f_s(\underset{\sim}{x},\underset{\sim}{v})$

③ Push particles Δt forward in time: $\frac{d\underset{\sim}{v}}{dt} = \frac{q_s}{m_s}(\underset{\sim}{E}+\underset{\sim}{v}\times\underset{\sim}{B})$, $\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{v}$

④ Compute new charge and current densities, $\rho_q(\underset{\sim}{x},t)$, $\underset{\sim}{j}(\underset{\sim}{x},t)$

⑤ Compute new fields $\underset{\sim}{E}(\underset{\sim}{x},t)$, $\underset{\sim}{B}(\underset{\sim}{x},t)$

Repeat ③–⑤

III. A. 1. (Continued)

d. NOTE: An important point is that the "particles" do not represent real charged particles. Instead, they are "super-particles" that are best thought of as representing small chunks of phase space $(\underset{\sim}{x}, \underset{\sim}{v})$. Within that small volume of phase space are many "real" particles of the physical system.

e. Collisions can be incorporated using a Monte Carlo method, i.e., choosing a random number to determine if a particle has suffered a collision.

2. Vlasov or Fokker-Planck Codes (Continuum codes)

a. In this approach, both real space and velocity space are determined on a grid.

Thus $f(\underset{\sim}{x}, \underset{\sim}{v}, t)$ is defined on a 6-D grid, while $\underset{\sim}{E}(\underset{\sim}{x}, t)$ and $\underset{\sim}{B}(\underset{\sim}{x}, t)$ are on a 3-D grid as usual.

b. Vlasov methods have $\left(\frac{\partial f_s}{\partial t}\right)_{coll} = 0$

while Fokker-Planck codes employ a Fokker-Planck collision operator $\left(\frac{\partial f_s}{\partial t}\right)_{coll} = -\frac{\partial}{\partial \underset{\sim}{v}} \cdot \left[\left\langle \frac{\Delta \underset{\sim}{v}}{\Delta t} \right\rangle_s f_s\right] + \frac{1}{2}\left(\frac{\partial}{\partial \underset{\sim}{v}}\frac{\partial}{\partial \underset{\sim}{v}}\right) : \left[\left\langle \frac{\Delta \underset{\sim}{v}\Delta \underset{\sim}{v}}{\Delta t} \right\rangle_s f_s\right]$

(tensors)

[See GB Sec 11.3 for details]

c. These methods tend to be restricted to fewer than 3-D in real space due to the very high computational cost of full 6-D simulations.

III. A. (Continued)

3. Gyrokinetics:

a. Gyrokinetics is a rigorous limit of kinetic theory in the limit of low-frequency, $\omega \ll \omega_{cs}$.

b. In this limit, we can exploit the invariance of the magnetic moment μ (the First Adiabatic Invariant) to eliminate one of the dimensions of velocity space.

1. Consider a cylindrical velocity space $(v_\parallel, v_\perp, \phi)$ (where $\parallel$ & $\perp$ refer to directions relative to mean field $\mathbf{B}_0$).

2. Integrate over the gyrophase ϕ to yield a system of equations that are dependent only on $(v_\parallel, v_\perp)$ in velocity space

Gyrokinetic Equation

$$\frac{\partial h_s}{\partial t} + v_\parallel \hat{\mathbf{z}} \cdot \frac{\partial h_s}{\partial \mathbf{R}_s} + \frac{c}{B_0}\left[\langle \chi \rangle_{\mathbf{R}_s}, h_s\right] - q_s \frac{\partial \langle \chi \rangle_{\mathbf{R}_s}}{\partial t} \frac{F_{0s}}{T_{0s}} = \left(\frac{\partial h_s}{\partial t}\right)_{coll}$$

where the full distribution function $f_s = F_{0s} e^{-\frac{q_s \phi(\mathbf{x},t)}{T_{0s}}} + h_s(\mathbf{R}_s, v_\parallel, v_\perp, t)$

(F_{0s}: Maxwellian; h_s: Guiding Center of gyroaverage)

NOTE: These equations are in cgs, not SI, units!

and gyroaveraged, low frequency Maxwell's Equations

Poisson's Eq: $\sum_s \frac{q_s^2 n_{0s}}{T_{0s}} \phi = q_s \int d^3\mathbf{v} \langle h_s \rangle_{\mathbf{r}}$

Parallel Component of Ampere's Law: $-\nabla_\perp^2 A_\parallel = \sum_s \frac{4\pi}{c} q_s \int d^3\mathbf{v}\, v_\parallel \langle h_s \rangle_{\mathbf{r}}$

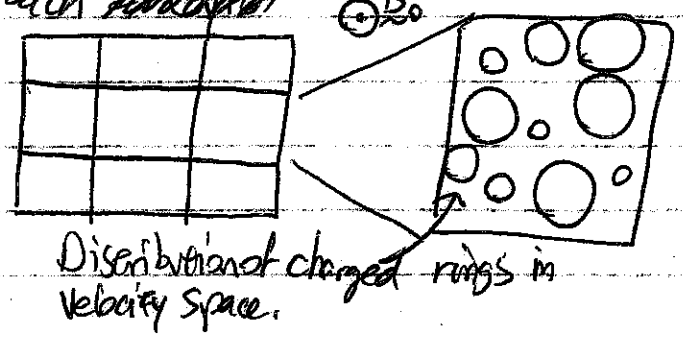
Perpendicular Component of Ampere's Law: $\nabla_\perp \delta B_\parallel = \sum_s \frac{4\pi}{c} q_s \int d^3\mathbf{v} \langle (\hat{\mathbf{z}} \times \mathbf{v}_\perp) h_s \rangle_{\mathbf{r}}$

where $\langle\ \rangle$ defines a gyroaverage taken at either position $\mathbf{r}$ or guiding center $\mathbf{R}_s$

III. A. 3. (Continued)

c. Velocity-space in Gyrokinetics may be handled either by a particle or continuum approach

1. Particle ⇒ Gyro-PIC



Distribution of charged rings in velocity space.

2. Continuum: Handle velocity-space using a grid. This often uses grid points in a polar coordinate system. For example, energy $\mathcal{E} = v_\perp^2 + v_\parallel^2$ (radius) and pitch angle $\xi = \frac{v_\parallel}{v}$.

d. Although the gyro-averaging procedure eliminates cyclotron frequency effects, such as cyclotron damping, gyrokinetics includes all collisionless damping by the Landau resonance and all finite Larmor radius effects (FLR).

e. Gyrokinetics requires the plasma to be magnetized, $\rho_i / L \ll 1$, where L is the length scale of equilibrium gradients in the system. Thus, it is a very useful approximation relevant to magnetic fusion research.

f. Since one dimension of velocity space has been eliminated, the gyrokinetic distribution function $h_s(x, y, z, v_\perp, v_\parallel, t)$ is a function in 5-dimensions and time.

⇒ This just allows simulations of turbulence in fusion and astrophysical plasmas, allowing a full, low-frequency kinetic determination of the transport of mass, momentum, and energy.

4. Molecular Dynamics:

a. Simulations of atoms and molecules and their interactions in time.

II. A. 4. (Continued)

b. Interactions between atoms are modelled by potentials of varying physical realism
   1. Simplified potential
   2. Full quantum mechanical orbitals (electron clouds are assumed – electrons move on a much shorter timescale & adjust instantaneously)

c. Used often in condensed matter — for crystal structure and nanostructure properties — and in biophysics for protein structure

d. In plasma physics, it is relevant to strongly-coupled plasmas.
   * Here, the plasma parameter $N_D \ll 1$.
   2. Interactions between nearby particles are very strong, where collective effects (ie, all particles in Debye sphere interacting) are weak.

e. This regime is relevant to dusty plasmas (See Prof. Carter's research).

B. Mixed Fluid and Kinetic

1. Hybrid codes:

a. For many applications, it is helpful to treat ions kinetically and electrons as a fluid

b. Since the timescale for electron dynamics is often much faster than the dynamics of interest, they can adjust to a Boltzmann distribution rapidly. In this case, a fluid treatment is a good approximation

c. Often, ions are treated by PIC method, while the electron fluid is solved on the same grid as the $\underline{E}$ & $\underline{B}$ fields.

III. (Continued)

C. Fluid

Ex: MHD:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \underset{\sim}{U}\cdot\nabla\rho = -\rho\nabla\cdot\underset{\sim}{U}$$

$$\frac{d\underset{\sim}{U}}{dt} = \frac{\partial \underset{\sim}{U}}{\partial t} + \underset{\sim}{U}\cdot\nabla\underset{\sim}{U} = -\frac{1}{\rho}\nabla p + \frac{(\nabla\times\underset{\sim}{B})\times\underset{\sim}{B}}{\mu_0\rho}$$

$$\frac{d\underset{\sim}{B}}{dt} = \frac{\partial \underset{\sim}{B}}{\partial t} + \underset{\sim}{U}\cdot\nabla\underset{\sim}{B} = \nabla\times(\underset{\sim}{U}\times\underset{\sim}{B}) + \underset{\sim}{U}\cdot\nabla\underset{\sim}{B}$$

$$\frac{dp}{dt} = \frac{\partial p}{\partial t} + \underset{\sim}{U}\cdot\nabla p = -\gamma p\nabla\cdot\underset{\sim}{U}$$

1. MHD (Ideal)

a. Certainly the most widely used plasma description, chosen often more for its simplicity than its formal validity.

b. Generally, the evolution of the fluid variables $(\rho, \underset{\sim}{U}, \underset{\sim}{B}, p)$ are solved on a grid. This is the Eulerian approach, where the time evolution at a fixed point in space is $\frac{\partial}{\partial t}$.

c. Fluid equations may also be solved using a Lagrangian approach, following the evolution of fluid elements along their path of flow. In this case, the change in time of a variable in a fluid element is given by the convective derivative $\frac{\partial}{\partial t} + \underset{\sim}{U}\cdot\nabla \equiv \frac{d}{dt}$. Here the grid points move, and can be treated as particles in the numerical implementation.

d. 1. Lagrangian approaches typically are less dissipative, but conservation properties may not be exact.

2. Eulerian approaches are more dissipative, but often have superior conservation properties (conservation of mass, momentum, and energy).

e. There exist mixed Lagrangian/Eulerian approaches — for example, ALE for Arbitrary Lagrangian/Eulerian.

III. C. 1. (Continued)

f. Magnetic Divergence, maintained $\nabla \cdot \underset{\sim}{B} = 0$ everywhere and at all times, is one of the key challenges for MHD simulation.

g. As with all fluid approaches, cannot describe collisionless (kinetic) damping.

2. Gyrofluid

a. This approach uses an analytical approximation to the Plasma Dispersion Function $Z(\zeta)$ to calculate the damping rate for each wave mode (or growth).

b. This attempts to model kinetic effects (collisionless damping) in a lower-dimensional fluid treatment (3-D in real space rather than 6-D phase space).

c. Implementation is much more complicated than MHD but far less computationally costly than a true kinetic treatment.

3. Two-Fluid

a. In this case, the ions and electrons are modelled as separate fluids that can respond to electromagnetic fields differently (for example, due to finite Larmor radius averaging for the ions).

b. Again, limited by the lack of collisionless kinetic effects.

4. Hall MHD, Electron MHD (eMHD), Reduced MHD (RMHD), Extended MHD

a. These are a wide variety of fluid approach that attempt to alleviate the restrictions of the MHD approximation or to include additional effects such as radiation transfer

b. Few of these "patches" to MHD are formally rigorous limits of the kinetic plasma physics, but they can give a feel for how various effects, such as Finite Larmor Radius, influence the plasma dynamics.