**Lecture 5: Introduction to Plasma Simulation Codes**

## 5.1. How to Choose a Suitable Simulation Code for Your Problem

Plasma consists of positive charged ions and negative charged electrons. Since $m_i >> m_e$, there are many intrinsic time scales in a plasma system even in a uniform background environment. For time scale less than the intrinsic time scales, it is hard for the plasma to reach a thermal dynamic equilibrium state. As a result, the kinetic effect might become important for time scale less than the intrinsic time scales of the plasma.

Present plasma simulation codes can be classified based on their phase space resolutions as listed in Table 5.1. Note that the so-called *particle-code simulation* is indeed a *multiple-fluid simulation*. A *simulation particle* in the particle-code simulation is indeed a *fluid element* in the phase space ($\mathbf{x},\mathbf{v}$).

**Table 5.1.** Classification of Plasma Simulation Codes

| | Simulation Code | Phenomena scale length $\lambda$ | Assuming thermal dynamic equilibrium? | | |
|---|---|---|---|---|---|
| | | | e-e | i-i | e-i |
| Fluid Simulations | MHD code | $\lambda \geq 10^3 \lambda_i$ | yes | yes | yes |
| | Two-Fuild code | $10^3 \lambda_i \geq \lambda \geq 10\lambda_i$ | yes | yes | no |
| Kinetic Simulations | Hybrid code *fluid electrons & kinetic ions* | $10\lambda_i \geq \lambda \geq \lambda_i$ | yes | no | no |
| | Full particle code | $\lambda_i \geq \lambda \geq \lambda_e$ | no | no | no |
| | Test particle code | Strong magnetic field | n/a | n/a | n/a |
| | Vlasov Code | $\lambda_i \geq \lambda \geq \lambda_e$ | no | no | no |

The kinetic effect becomes important when the non-uniformity scale length of the system is comparable to the characteristic scale length of a species (ions and/or electrons), or *when the wave speed observed in the center of mass frame of a species is approximately equal or less than the thermal speed of that species*. When the kinetic effect is important, we have to use a kinetic simulation code to study the nonlinear evolutions of wave-particle interactions in the phase space. On the other hand, a fluid simulation code can provide reasonable and quick simulation results when the kinetic effects are unimportant. The governing equations of simulations at different time scales are given in Tables 5.2-5.8.

**Table 5.2.** Governing equations of the MHD-time-scale simulation

| |
|---|
| $$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{V})$$ |
| $$\frac{\partial}{\partial t}(\rho \mathbf{V}) = -\nabla \cdot [\rho \mathbf{V}\mathbf{V} + (p + \frac{B^2}{2\mu_0})\mathbf{1} - \frac{\mathbf{B}\mathbf{B}}{\mu_0}] + \eta_V \rho \nabla^2 \mathbf{V}$$ |
| $$\frac{\partial}{\partial t}(\frac{1}{2}\rho V^2 + \frac{3}{2}p + \frac{B^2}{2\mu_0}) = -\nabla \cdot [(\frac{1}{2}\rho V^2 + \frac{5}{2}p + \frac{B^2}{\mu_0})\mathbf{V} - \frac{\mathbf{B}\mathbf{B}}{\mu_0} \cdot \mathbf{V}] + \eta_T \rho \nabla^2 (\frac{p}{\rho})$$ |
| $$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{V} \times \mathbf{B}) + \eta_B \nabla^2 \mathbf{B}$$ |
| $$\mathbf{E} = -\mathbf{V} \times \mathbf{B}$$ $$\mathbf{J} = \frac{\nabla \times \mathbf{B}}{\mu_0}$$ Initial condition: $$\nabla \cdot \mathbf{B} = 0$$ |

**Table 5.3.** Governing equations of the electron-time-scale two-fluid simulation.

| |
|---|
| $$\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \mathbf{V}_i)$$ |
| $$\frac{\partial n_e}{\partial t} = -\nabla \cdot (n_e \mathbf{V}_e)$$ |
| $$\frac{\partial}{\partial t}(\mathbf{V}_i) = -\mathbf{V}_i \cdot \nabla \mathbf{V}_i + \frac{e}{m_i}(\mathbf{E} + \mathbf{V}_i \times \mathbf{B}) - \frac{\nabla p_i}{m_i n_i} + \eta_{V_i} \nabla^2 \mathbf{V}_i$$ |
| $$\frac{\partial}{\partial t}(\mathbf{V}_e) = -\mathbf{V}_e \cdot \nabla \mathbf{V}_e - \frac{e}{m_e}(\mathbf{E} + \mathbf{V}_e \times \mathbf{B}) - \frac{\nabla p_e}{m_e n_e} + \eta_{V_e} \nabla^2 \mathbf{V}_e$$ |
| $$\frac{\partial}{\partial t}(p_i) \approx -\nabla \cdot (p_i \mathbf{V}_i) - \frac{2}{3} p_i (\nabla \cdot \mathbf{V}_i) + \eta_{T_i} n_i \nabla^2 (\frac{p_i}{n_i})$$ |
| $$\frac{\partial}{\partial t}(p_e) \approx -\nabla \cdot (p_e \mathbf{V}_e) - \frac{2}{3} p_e (\nabla \cdot \mathbf{V}_e) + \eta_{T_e} n_e \nabla^2 (\frac{p_e}{n_e})$$ |
| $$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \eta_B \nabla^2 \mathbf{B}$$ |
| $$\frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \frac{e}{\varepsilon_0}(n_i \mathbf{V}_i - n_e \mathbf{V}_e)$$ |
| Initial conditions<br>$$\nabla \cdot \mathbf{B} = 0$$<br>$$\nabla \cdot \mathbf{E} = \frac{e}{\varepsilon_0}(n_i - n_e)$$ |

**Table 5.4.** Governing equations of ion-time-scale two-fluid simulation.

| |
|---|
| $\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \eta_B \nabla^2 \mathbf{B}$ |
| $\frac{\partial n_i}{\partial t} = -\nabla \cdot (n_i \mathbf{V}_i)$ |
| $\frac{\partial \mathbf{V}_i}{\partial t} = +\frac{e}{m_i}\mathbf{V}_i \times \mathbf{B} + \frac{e}{m_i}\mathbf{E} - \frac{\nabla p_i}{m_i n_i} - \mathbf{V}_i \cdot \nabla \mathbf{V}_i + \eta_{V_i} \nabla^2 \mathbf{V}_i$ |
| $\frac{\partial p_i}{\partial t} = -\nabla \cdot (p_i \mathbf{V}_i) - \frac{2}{3} p_i (\nabla \cdot \mathbf{V}_i) + \eta_{T_i} n_i \nabla^2 (\frac{p_i}{n_i})$ |
| $\frac{\partial p_e}{\partial t} = -\nabla \cdot (p_e \mathbf{V}_e) - \frac{2}{3} p_e (\nabla \cdot \mathbf{V}_e) + \eta_{T_e} n_e \nabla^2 (\frac{p_e}{n_e})$ |
| $\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \eta_B \nabla^2 \mathbf{B}$ |
| $n_e \approx n_i$<br>$\mathbf{J} = \frac{\nabla \times \mathbf{B}}{\mu_0}$<br>$\mathbf{V}_e = \mathbf{V}_i - \frac{\mathbf{J}}{e n_i}$<br>$\mathbf{E} = -\mathbf{V}_e \times \mathbf{B} - \frac{\nabla p_e}{e n_i} - \frac{m_e}{e}\mathbf{V}_e \cdot \nabla \mathbf{V}_e + \frac{c^2}{\omega_{pe}^2}\nabla^2 \mathbf{E}$<br>Initial condition:<br>$\nabla \cdot \mathbf{B} = 0$ |

**Table 5.5.** Governing equations of non-relativistic electrostatic full-particle code simulation

| |
|---|
| $\dfrac{d\mathbf{x}_k(t)}{dt} = \mathbf{v}_k(t)$ |
| $\dfrac{d\mathbf{v}_k(t)}{dt} = \dfrac{e_k}{m_k}\int [\mathbf{E}(\mathbf{x},t) + \mathbf{v}_k(t)\times\mathbf{B}(\mathbf{x},t)]S[\mathbf{x}-\mathbf{x}_k(t)]d\mathbf{x}$ |
| $\nabla\cdot\mathbf{E}(\mathbf{x},t) = \int\sum_k \dfrac{e_k}{\varepsilon_0}\delta[\mathbf{x}'-\mathbf{x}_k(t)]S(\mathbf{x}-\mathbf{x}')d\mathbf{x}'$ |

where $S$ denotes the shape function of the finite-size simulation particle (fluid element)

**Table 5.6a.** Governing equations of relativistic electromagnetic full-particle code simulation

| |
|---|
| $\dfrac{d\mathbf{x}_k(t)}{dt} = \mathbf{v}_k(t)$ |
| $\dfrac{d\mathbf{u}_k(t)}{dt} = \dfrac{e_k}{m_k}\int [\mathbf{E}(\mathbf{x},t) + \mathbf{v}_k(t)\times\mathbf{B}(\mathbf{x},t)]\delta[\mathbf{x}'-\mathbf{x}_k(t)]S(\mathbf{x}-\mathbf{x}')d\mathbf{x}$ |
| $\dfrac{\partial\mathbf{B}(\mathbf{x},t)}{\partial t} = -\nabla\times\mathbf{E}(\mathbf{x},t)$ |
| $\dfrac{\partial\mathbf{E}(\mathbf{x},t)}{\partial t} = c^2\nabla\times\mathbf{B}(\mathbf{x},t) - \dfrac{1}{\varepsilon_0}\int\sum_k e_k\mathbf{v}_k(t)\delta[\mathbf{x}'-\mathbf{x}_k(t)]S(\mathbf{x}-\mathbf{x}')d\mathbf{x}'$ |
| $\mathbf{v}_k(t) = \dfrac{\mathbf{u}_k(t)}{\sqrt{1+[u_k(t)/c]^2}}$ <br> Initial condition: <br> $\nabla\cdot\mathbf{B} = 0$ <br> $\nabla\cdot\mathbf{E}(\mathbf{x},t) = \int\sum_k \dfrac{e_k}{\varepsilon_0}\delta(\mathbf{x}'-\mathbf{x}_k(t))S(\mathbf{x}-\mathbf{x}')d\mathbf{x}'$ |

where $S$ denotes the shape function of the finite-size simulation particle (fluid element)

**Table 5.6b.** Governing equations of 1-D relativistic electromagnetic full-particle simulation

| |
|---|
| $$\frac{dx_k(t)}{dt} = v_{xk}(t)$$ |
| $$\frac{d\mathbf{u}_k(t)}{dt} = \frac{e_k}{m_k}\int [\mathbf{E}(x,t)+\mathbf{v}_k(t)\times\mathbf{B}(x,t)]\delta[x'-x_k(t)]S(x-x')dx$$ |
| $$\frac{\partial E_x(x,t)}{\partial x} = \int \sum_k \frac{e_k}{\varepsilon_0}\delta(x'-x_k(t))S(x-x')dx'$$ |
| $$\frac{\partial B_y(x,t)}{\partial t} = +\frac{\partial E_z(x,t)}{\partial x}$$ $$\frac{\partial B_z(x,t)}{\partial t} = -\frac{\partial E_y(x,t)}{\partial x}$$ |
| $$\frac{\partial E_y(x,t)}{\partial t} = -c^2\frac{\partial B_z(x,t)}{\partial x} - \frac{1}{\varepsilon_0}\int \sum_k e_k v_{yk}\delta[x'-x_k(t)]S(x-x')dx'$$ $$\frac{\partial E_z(x,t)}{\partial t} = +c^2\frac{\partial B_y(x,t)}{\partial x} - \frac{1}{\varepsilon_0}\int \sum_k e_k v_{zk}(t)\delta[x'-x_k(t)]S(x-x')dx'$$ |
| $$\mathbf{v}_k(t) = \frac{\mathbf{u}_k(t)}{\sqrt{1+[u_k(t)/c]^2}}$$ $$B_x = \text{constant}$$ |

where $S$ denotes the shape function of the finite-size simulation particle (fluid element)

**Table 5.7a.** Governing equations of a non-relativistic test particle simulation

| |
|---|
| $\frac{d\mathbf{x}_\alpha(t)}{dt} = \mathbf{v}_\alpha(t)$ |
| $\frac{d\mathbf{v}_\alpha(t)}{dt} = \frac{e_\alpha}{m_\alpha}[\mathbf{E}(\mathbf{x},t)+\mathbf{v}_\alpha(t)\times\mathbf{B}(\mathbf{x},t)]\delta[\mathbf{x}-\mathbf{x}_\alpha(t)]$ |

where test particle is characterized by mass $m_\alpha$ charge $e_\alpha$, and moving in the background electric field $\mathbf{E}(\mathbf{x},t)$ and magnetic field $\mathbf{B}(\mathbf{x},t)$

**Table 5.7b.** Governing equations of a non-relativistic test particle simulation

| |
|---|
| $\frac{d\mathbf{x}_\alpha(t)}{dt} = \frac{\mathbf{u}_\alpha(t)}{\sqrt{1+[u_\alpha(t)/c]^2}}$ |
| $\frac{d\mathbf{u}_\alpha(t)}{dt} = \frac{e_\alpha}{m_\alpha}[\mathbf{E}(\mathbf{x},t)+\frac{\mathbf{u}_\alpha(t)}{\sqrt{1+[u_\alpha(t)/c]^2}}\times\mathbf{B}(\mathbf{x},t)]\delta[\mathbf{x}-\mathbf{x}_\alpha(t)]$ |

where test particle is characterized by mass $m_\alpha$ charge $e_\alpha$, and moving in the background electric field $\mathbf{E}(\mathbf{x},t)$ and magnetic field $\mathbf{B}(\mathbf{x},t)$

**Table 5.8.** Governing equations of electromagnetic relativistic Vlasov simulation

| |
|---|
| $\frac{\partial f_e}{\partial t} = -\frac{\mathbf{u}}{\sqrt{1+(u/c)^2}}\cdot\frac{\partial f_e}{\partial \mathbf{x}} + \frac{e}{m_e}(\mathbf{E}+\frac{\mathbf{u}}{\sqrt{1+(u/c)^2}}\times\mathbf{B})\cdot\frac{\partial f_e}{\partial \mathbf{u}}$ |
| $\frac{\partial f_i}{\partial t} = -\frac{\mathbf{u}}{\sqrt{1+(u/c)^2}}\cdot\frac{\partial f_i}{\partial \mathbf{x}} - \frac{e}{m_i}(\mathbf{E}+\frac{\mathbf{u}}{\sqrt{1+(u/c)^2}}\times\mathbf{B})\cdot\frac{\partial f_i}{\partial \mathbf{u}}$ |
| $\frac{\partial \mathbf{B}}{\partial t} = -\nabla\times\mathbf{E}$ |
| $\frac{\partial \mathbf{E}}{\partial t} = c^2\nabla\times\mathbf{B} - \frac{e}{\varepsilon_0}[\iiint \frac{\mathbf{u}}{\sqrt{1+(u/c)^2}} f_i d^3u - \iiint \frac{\mathbf{u}}{\sqrt{1+(u/c)^2}} f_e d^3u]$ |
| Initial conditions<br>$\nabla\cdot\mathbf{B}=0$<br>$\nabla\cdot\mathbf{E} = \frac{e}{\varepsilon_0}[\iiint f_i d^3u - \iiint f_e d^3u]$ |

## 5.2. Diagnostics of Simulation Results

We need to make a good diagnostics to understand detail nonlinear evolution processes and to determine the complicated cause-and-result relationships from the simulation results. Making good diagnostics is as important as choosing a good simulation scheme.

Guideline for making a *correct* simulation and good diagnostics:

**Check your simulation results:**

Check and make sure the total energy is conserved.

Check and make sure that your simulation results satisfy the *Courant condition*. That is, the maximum speed $v$ (which is equal to the largest possible wave speed plus the maximum flow speed or particle speed) multiplying one time step $\Delta t$ is less than one grid size $\Delta_x$. Indeed, we recommend that $v\Delta t < 0.1\Delta_x$.

Check and make sure that your simulation results are almost unchanged when the simulation system length is doubled, or when the simulation time step is reduced in half, or when the simulation grid size is reduced in half, or when the number of simulation particles is doubled, or when the real ion-electron mass ratio is used.

**Always use double precision in your simulation**.

**Display your simulation results:**

Use Excel, Matlab, or IDL to display your simulation results.

**Analysis your simulation results:**

Carefully trace the time evolution of all fluid variables in the simulation.

Carefully trace the phase-space trajectory of a *group* of simulation particles.

Finally, it is generally believed that a test particle simulation might help you to understand your simulation results.

## 5.3. Summary and Discussion

If you want to use numerical simulation to study nonlinear plasma phenomena, you should

(a) choose a right simulation code for your problem,

(b) do your best to save CPU time (simulation scheme) and real time (I/O),

(c) *always keep a macroscopic vision and a microscopic alert in your mind*,

(d) make a good diagnostics for your simulation results.

Prospective of Numerical Simulations

To form a good simulation research group, we need good hardwares, good softwares, and *scientists* with good experiences in doing different types of plasma simulations.

Beethoven can compose a symphony after he lost his hearing ability.

A simulation expert can predict simulation results even without a computer.

**References**

Hildebrand, F. B., *Advanced Calculus for Applications, 2nd edition,* Prentice-Hall, Inc., Englewood, Cliffs, New Jersey, 1976.

Press, W. H., B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes (in C or in FORTRAN and Pascal), Cambridg*e University Press, Cambridge, 1988.

Richtmyer, R. D., and K. W. Morton, *Difference Methods for Initial-Value Problems,* 2nd edition, John Wiley & Sons, Inc., 1967.

Shampine, L. F., and M. K. Gordon, *Computer Solution of Ordinary Differential Equation: the Initial Value Problem,* W. H. Freeman and Company, San Francisco, 1975.

Snell, J. L., *Introduction to Probability Theory With Computing,* Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1975.

*System/360 Scientific Subroutine Package Version III, Programmer's Manual,* 5th edition, IBM, New York, 1970.

*Computer Simulation of Space Plasmas*, edited by H. Mstsumoto and T. Sato, D. Reidel Publishing Co., Boston, 1985.