Basic Equations

of

Particle Code Simulations

Part 1: The Klimontovich-Maxwell Equations

Let us define a microscopic distribution function of the αth species in the six-dimensional phase space

$$N_\alpha(\mathbf{x},\mathbf{v},t)=\sum_{k=1}^{N_0}\delta[\mathbf{x}-\mathbf{x}_k(t)]\delta[\mathbf{v}-\mathbf{v}_k(t)] \tag{1}$$

where $\alpha = i$ or e; $\delta(a-b)=0$ if $a \neq b$, and $\delta(a-b)=1$ if $a=b$. The $\mathbf{x}_k(t)$ and $\mathbf{v}_k(t)$ in Eq. (1) satisfy the following equations of motion

$$\frac{d\mathbf{x}_k(t)}{dt}=\mathbf{v}_k(t) \tag{2}$$

$$\frac{d\mathbf{v}_k(t)}{dt}=\frac{e_\alpha}{m_\alpha}\{\mathbf{E}^m[\mathbf{x}_k(t),t]+\mathbf{v}_k(t)\times\mathbf{B}^m[\mathbf{x}_k(t),t]\} \tag{3}$$

where $\mathbf{E}^m(\mathbf{x},t)$ and $\mathbf{B}^m(\mathbf{x},t)$ are the microscopic electric field and magnetic field, respectively. The Klimontovich equation can be obtained by evaluating the time derivative of $N_\alpha(\mathbf{x},\mathbf{v},t)$. It yields (e.g., Nicholson, 1983; Lyu, 2010)

$$\frac{\partial N_\alpha(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v} \cdot \frac{\partial N_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{x}} + \frac{e_\alpha}{m_\alpha}[\mathbf{E}^m(\mathbf{x},t) + \mathbf{v} \times \mathbf{B}^m(\mathbf{x},t)] \cdot \frac{\partial N_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}} = 0 \quad (4)$$

Eq. (4) is the Klimontovich equation of the microscopic distribution function $N_\alpha(\mathbf{x},\mathbf{v},t)$.

The microscopic electric field and magnetic field satisfy the following Maxwell equations

$$\nabla \cdot \mathbf{E}^m(\mathbf{x},t) = \frac{1}{\varepsilon_0}\sum_\alpha e_\alpha[\iiint N_\alpha(\mathbf{x},\mathbf{v},t)d^3v] \tag{5}$$

$$\nabla \times \mathbf{E}^m(\mathbf{x},t) = -\frac{\partial \mathbf{B}^m(\mathbf{x},t)}{\partial t} \tag{6}$$

$$\nabla \cdot \mathbf{B}^m(\mathbf{x},t) = 0 \tag{7}$$

$$\nabla \times \mathbf{B}^m(\mathbf{x},t) = \mu_0\sum_\alpha e_\alpha[\iiint N_\alpha(\mathbf{x},\mathbf{v},t)\mathbf{v}d^3v] + \frac{1}{c^2}\frac{\partial \mathbf{E}^m(\mathbf{x},t)}{\partial t} \tag{8}$$

Application of the Klimontovich-Maxwell Equations to the Particle Simulation

In the particle code simulations, we evaluate the microscopic electric field, magnetic field, and the microscopic distribution functions at each grid point. The Eq. (3) can be rewritten as

$$\frac{d\mathbf{v}_k(t)}{dt} = \frac{e_\alpha}{m_\alpha}[\mathbf{E}^m(\mathbf{x},t) + \mathbf{v}_k(t) \times \mathbf{B}^m(\mathbf{x},t)]\delta[\mathbf{x} - \mathbf{x}_k(t)] \quad (9)$$

The $\delta[\mathbf{x} - \mathbf{x}_k(t)]$ in Eqs. (1) and (9) is replaced by a Taylor expansion of the delta function with respect to the nearest grid point in the UCLA simulation scheme, but the nearest half grid point in the PIC simulation scheme and in the higher-order interpolation scheme proposed in this study.

Part 2: The Vlasov-Maxwell Equations

Let $f_\alpha(\mathbf{x},\mathbf{v},t)$, $\mathbf{E}(\mathbf{x},t)$, and $\mathbf{B}(\mathbf{x},t)$ be the ensemble average of $N_\alpha(\mathbf{x},\mathbf{v},t)$, $\mathbf{E}^m(\mathbf{x},t)$, and $\mathbf{B}^m(\mathbf{x},t)$, respectively and let

$$N_\alpha(\mathbf{x},\mathbf{v},t) = f_\alpha(\mathbf{x},\mathbf{v},t) + \delta N_\alpha(\mathbf{x},\mathbf{v},t)$$

$$\mathbf{E}^m(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t) + \delta\mathbf{E}^m(\mathbf{x},t)$$

$$\mathbf{B}^m(\mathbf{x},t) = \mathbf{B}(\mathbf{x},t) + \delta\mathbf{B}^m(\mathbf{x},t)$$

If we use $\langle A \rangle$ to denote the ensemble average of A, then taking the ensemble average of Eq. (4), it yields

$$\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{x}} + \frac{e_\alpha}{m_\alpha}[\mathbf{E}(\mathbf{x},t) + \mathbf{v}\times\mathbf{B}(\mathbf{x},t)]\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}}$$
$$+\frac{e_\alpha}{m_\alpha}\left\langle[\delta\mathbf{E}^m(\mathbf{x},t) + \mathbf{v}\times\delta\mathbf{B}^m(\mathbf{x},t)]\cdot\frac{\partial \delta N_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}}\right\rangle = 0 \tag{10}$$

The last term in Eq. (10) is a result of the interactions among the microscopic fields, $\delta\mathbf{E}^m(\mathbf{x},t)$, and $\delta\mathbf{B}^m(\mathbf{x},t)$, and the microscopic distribution functions, $\delta N_i(\mathbf{x},\mathbf{v},t)$ and $\delta N_e(\mathbf{x},\mathbf{v},t)$. For convenience, we define the last term in Eq. (10) to be an effective collision in the collision-free plasma, i.e.,

$$-\frac{e_\alpha}{m_\alpha}\left\langle[\delta\mathbf{E}^m(\mathbf{x},t) + \mathbf{v}\times\delta\mathbf{B}^m(\mathbf{x},t)]\cdot\frac{\partial \delta N_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}}\right\rangle = \left.\frac{\delta f_\alpha(\mathbf{x},\mathbf{v},t)}{\delta t}\right|_{collision}$$

Then, Eq. (10) can be rewritten as

$$\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{x}} + \frac{e_\alpha}{m_\alpha}[\mathbf{E}(\mathbf{x},t)+\mathbf{v}\times\mathbf{B}(\mathbf{x},t)]\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}} = \left.\frac{\delta f_\alpha(\mathbf{x},\mathbf{v},t)}{\delta t}\right|_{collision} \tag{11}$$

Eq. (11) is the Boltzmann equation. For $\delta f_\alpha(\mathbf{x},\mathbf{v},t)/\delta t\big|_{collision}=0$, the Boltzmann equation is reduced to the Vlasov equation (Vlasov, 1945):

$$\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{x}} + \frac{e_\alpha}{m_\alpha}[\mathbf{E}(\mathbf{x},t)+\mathbf{v}\times\mathbf{B}(\mathbf{x},t)]\cdot\frac{\partial f_\alpha(\mathbf{x},\mathbf{v},t)}{\partial \mathbf{v}} = 0 \tag{12}$$

The electric field and magnetic field satisfy the following Maxwell equations

$$\nabla \cdot \mathbf{E}(\mathbf{x},t) = \frac{1}{\varepsilon_0} \sum_{\alpha} e_{\alpha} [\iiint f_{\alpha}(\mathbf{x},\mathbf{v},t) d^3 v] \tag{13}$$

$$\nabla \times \mathbf{E}(\mathbf{x},t) = -\frac{\partial \mathbf{B}(\mathbf{x},t)}{\partial t} \tag{14}$$

$$\nabla \cdot \mathbf{B}(\mathbf{x},t) = 0 \tag{15}$$

$$\nabla \times \mathbf{B}(\mathbf{x},t) = \mu_0 \sum_{\alpha} e_{\alpha} [\iiint f_{\alpha}(\mathbf{x},\mathbf{v},t) \mathbf{v} d^3 v] + \frac{1}{c^2} \frac{\partial \mathbf{E}(\mathbf{x},t)}{\partial t} \tag{16}$$

Eqs. (13) ~ (16) can be obtained by the ensemble average of the equations (5) ~ (8) respectively.

Application of the Vlasov-Maxwell Equations to the Particle Simulation

In the particle code simulations, due to insufficient number of simulation particles, we mimic the ensemble average by a finite-size shape function $S(\mathbf{x})$ to reduce the inter particle collision. Namely,

$$f_\alpha(\mathbf{x},\mathbf{v},t) = \int N_\alpha(\mathbf{x}',\mathbf{v},t) S(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'$$

The electric field and magnetic field can be divided into two parts, the external fields and the internal fields. The sources of the external fields are located outside the simulation domain. The internal fields are produced by the plasma in the simulation system. Thus, we have

$$\mathbf{E}(\mathbf{x},t) = \mathbf{E}^e(\mathbf{x},t) + \int \mathbf{E}^{i,m}(\mathbf{x}',t) S(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'$$

$$\mathbf{B}(\mathbf{x},t) = \mathbf{B}^e(\mathbf{x},t) + \int \mathbf{B}^{i,m}(\mathbf{x}',t) S(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'$$

The electric field and magnetic field in our simulation can be determined by the following Maxwell equations

$$\nabla \cdot \mathbf{E}^{e}(\mathbf{x},t) = 0 \tag{17a}$$

$$\nabla \cdot \mathbf{E}^{i}(\mathbf{x},t) = \frac{1}{\varepsilon_0}\sum_{\alpha} e_{\alpha}\{\iiint [\int N_{\alpha}(\mathbf{x}',\mathbf{v},t)S(\mathbf{x}-\mathbf{x}')d\mathbf{x}']d^3v\} \tag{17b}$$

$$\nabla \times \mathbf{E}^{e}(\mathbf{x},t) = -\frac{\partial \mathbf{B}^{e}(\mathbf{x},t)}{\partial t} \tag{18a}$$

$$\nabla \times \mathbf{E}^{i}(\mathbf{x},t) = -\frac{\partial \mathbf{B}^{i}(\mathbf{x},t)}{\partial t} \tag{18b}$$

$$\nabla \cdot \mathbf{B}^{e}(\mathbf{x},t) = 0 \tag{19a}$$

$$\nabla \cdot \mathbf{B}^{i}(\mathbf{x},t) = 0 \tag{19b}$$

$$\nabla \times \mathbf{B}^e(\mathbf{x},t) = \frac{1}{c^2}\frac{\partial \mathbf{E}^e(\mathbf{x},t)}{\partial t} \tag{20a}$$

$$\nabla \times \mathbf{B}^i(\mathbf{x},t) = \mu_0 \sum_\alpha e_\alpha \{\iiint [\int N_\alpha(\mathbf{x}',\mathbf{v},t) S(\mathbf{x}-\mathbf{x}') d\mathbf{x}'] \mathbf{v} d^3v\} + \frac{1}{c^2}\frac{\partial \mathbf{E}^i(\mathbf{x},t)}{\partial t} \tag{20b}$$

where $\mathbf{E}^e(\mathbf{x},t)$ and $\mathbf{B}^e(\mathbf{x},t)$ are the external fields and $\mathbf{E}^i(\mathbf{x},t)$ and $\mathbf{B}^i(\mathbf{x},t)$ are the internal fields

The force acting on the finite-size particle is also affected by the shape function. The momentum equation of the *k*th particle can be rewritten as

$$\begin{aligned}\frac{d\mathbf{v}_k(t)}{dt} &= \frac{e_\alpha}{m_\alpha}[\mathbf{E}^e(\mathbf{x},t)+\mathbf{v}_k(t)\times\mathbf{B}^e(\mathbf{x},t)]\delta[\mathbf{x}-\mathbf{x}_k(t)] \\ &\quad + \frac{e_\alpha}{m_\alpha}\int[\mathbf{E}^i(\mathbf{x}',t)+\mathbf{v}_k(t)\times\mathbf{B}^i(\mathbf{x}',t)]S(\mathbf{x}-\mathbf{x}')d\mathbf{x}'\}\delta[\mathbf{x}-\mathbf{x}_k(t)]\end{aligned} \tag{21}$$

The shape function $S(\mathbf{x})$ is a probability density function, which satisfies $\int S(\mathbf{x})d\mathbf{x}=1$ and $S(\mathbf{x})\geq 0$ for all $\mathbf{x}$. A Gaussian-shaped distribution function is used in the UCLA finite-size particle simulation code. A uniform distribution function with size equal to the grid size is used in the classical PIC simulation. A higher-order shape function is proposed in this study.

Basic Equations of Particle Code Simulation With Relativistic Plasma

$$\frac{d\mathbf{x}_{\alpha,k}(t)}{dt} = \mathbf{u}_{\alpha,k}(t) / \sqrt{1 + \frac{u_{\alpha,k}^2}{c^2}}$$

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

$$+ \frac{e_\alpha}{m_\alpha}\{\int [\mathbf{E}^i(\mathbf{x}',t) + \frac{\mathbf{u}_{\alpha,k}(t)}{\sqrt{1 + \frac{u_{\alpha,k}^2}{c^2}}} \times \mathbf{B}^i(\mathbf{x}',t)]S(\mathbf{x} - \mathbf{x}')d\mathbf{x}'\}\delta[\mathbf{x} - \mathbf{x}_k(t)]$$

where the external fields $\mathbf{E}^e(\mathbf{x},t)$, $\mathbf{B}^e(\mathbf{x},t)$; and the internal fields $\mathbf{E}^i(\mathbf{x},t)$, $\mathbf{B}^i(\mathbf{x},t)$ satisfy the following Maxwell's equations:

$$\frac{\partial \mathbf{B}^e(\mathbf{x},t)}{\partial t} = -\nabla \times \mathbf{E}^e(\mathbf{x},t)$$

$$\frac{\partial \mathbf{B}^i(\mathbf{x},t)}{\partial t} = -\nabla \times \mathbf{E}^i(\mathbf{x},t)$$

$$\frac{\partial \mathbf{E}^e(\mathbf{x},t)}{\partial t} = c^2 \nabla \times \mathbf{B}^e(\mathbf{x},t)$$

$$\frac{\partial \mathbf{E}^i(\mathbf{x},t)}{\partial t} = c^2 \nabla \times \mathbf{B}^i(\mathbf{x},t)$$

$$-\frac{1}{\varepsilon_0}\sum_\alpha e_\alpha \{\iiint [\int \sum_{k=1}^{N_0} \delta[\mathbf{x}' - \mathbf{x}_{\alpha,k}(t)]\delta[\mathbf{u} - \mathbf{u}_{\alpha,k}(t)]\, S(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}'] \frac{\mathbf{u}}{\sqrt{1+\frac{u^2}{c^2}}} d^3u\}$$

and the following initial conditions:

$\nabla \cdot \mathbf{B}^e(\mathbf{x}, t=0) = 0$, $\nabla \cdot \mathbf{B}^i(\mathbf{x}, t=0) = 0$, $\nabla \cdot \mathbf{E}^e(\mathbf{x}, t=0) = 0$, and

$$\nabla \cdot \mathbf{E}^i(\mathbf{x}, t=0)$$

$$= \frac{1}{\varepsilon_0} \sum_\alpha e_\alpha \{ \iiint [\int \sum_{k=1}^{N_0} \delta[\mathbf{x}' - \mathbf{x}_{\alpha,k}(t=0)] \delta[\mathbf{u} - \mathbf{u}_{\alpha,k}(t=0)] \, S(\mathbf{x} - \mathbf{x}') d\mathbf{x}'] d^3u \}$$

where $S(\mathbf{x})$ is a finite-size shape function which satisfies $\int S(\mathbf{x}) d\mathbf{x} = 1$ and $S(\mathbf{x}) \geq 0$ for all $\mathbf{x}$.

The $\delta[\mathbf{x} - \mathbf{x}_{\alpha,k}(t)]$ is replaced by a Taylor expansion of the delta function with respect to the nearest grid point of $\mathbf{x}_{\alpha,k}(t)$ in the UCLA simulation scheme, but the nearest half grid point of $\mathbf{x}_{\alpha,k}(t)$ in the PIC simulation scheme and in the higher-order interpolation scheme proposed in this study.