Derivation of the particle-in-cell (PIC) method

As we have already seen, we use the Vlasov equation for the particle phase-space distribution function $f_s(\mathbf{x}, \mathbf{v}, t)$ for species s.

$$\partial_t f_s + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = \left(\frac{\partial f_s}{\partial t}\right)_{coll}$$

together with Maxwell's equations.

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \nabla \cdot \mathbf{B} = 0$$
$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \frac{\mathbf{j}}{\epsilon_0} \qquad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

Charge density and current density are obtained by integrating the distribution function over velocity space:

$$\rho = \sum_s q_s \int f(\mathbf{x}, \mathbf{v}, t)\, d^3v \qquad \mathbf{j} = \sum_s q_s \int \mathbf{v} f(\mathbf{x}, \mathbf{v}, t)\, d^3v$$

and satisfy the continuity equation

$$\partial_t \rho + \nabla \cdot \mathbf{j} = 0.$$

Numerical Approach

We now approximate the phase space distribution function as a sum of quasi-particles:

$$f_s(\mathbf{x}, \mathbf{v}, t) = \sum_p f_p(\mathbf{x}, \mathbf{v}, t)$$

Each quasi-particle represents a large number of particles that are close to each other in phase space. Instead of delta-functions which would represent a single particle, we now use shape function in configuration and velocity space to represent the distribution function belonging to the quasi-particle p:

$$f_p(\mathbf{x}, \mathbf{v}, t) = N_p S_{\mathbf{x}}(\mathbf{x} - \mathbf{x_p}(\mathbf{t})) S_{\mathbf{v}}(\mathbf{v} - \mathbf{v_p}(\mathbf{t}))$$

It makes sense to demand that the shape functions can be factorized as, e.g.,

$$S_{\mathbf{x}}(\mathbf{x} - \mathbf{x_p}(\mathbf{t})) = S_x(x - x_p(t)) S_y(y - y_p(t)) S_z(z - z_p(t))$$

We further demand certain properties of the shape functions:

- The support of the shape function is compact.
- The shape function is normalized. $\int_{-\infty}^{\infty} S_\xi(\xi - \xi_p)\, d\xi = 1$
- Symmetry. $S_\xi(\xi - \xi_p) = S_\xi(\xi_p - \xi)$

Particle shape functions

The standard PIC method chooses the velocity space shape functions to be delta-functions, so that the spatial shape function remains constant in time:

$$S_v(v - v_p) = \delta(v - v_p)$$

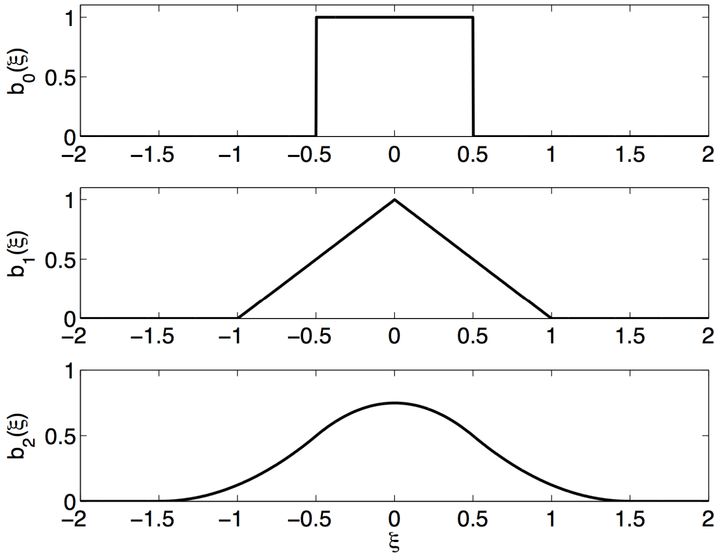
For the spatial shape function, *b-splines* are now commonly used. The first spline b_0 is defined as follows:

$$b_0(\xi) = \begin{cases} 1 & \text{if } |\xi| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$

The other b-splines are obtained by convoluting the previous spline with b_0:

$$b_l(\xi) = \int_{-\infty}^{\infty} b_0(\xi - \xi')b_{l-1}(\xi')\, d\xi'$$

The first 3 b-splines are shown here:



First three b-spline functions [Lapenta]

The actual spatial shape function is then chosen as

$$S_x(x - x_p) = \frac{1}{\Delta x} b_l\left(\frac{x - x_p}{\Delta x}\right)$$

where Δx is the scale length for the size of the computational particle.

Derivation of the equations of motion

So far, each particle has a position and velocity, $x_p and v_p$, whose evolution in time has not yet been specified. We obtain evolution equations by taking moments of the Vlasov equation. For simplicity, the following is written for the 1-d electrostatic case, but generalization to 3-d is straight-forward. The Vlasov equation for each quasi-particle distribution function looks like

$$\frac{\partial f_p}{\partial t} + v\frac{\partial f_p}{\partial x} + \frac{q_s E}{m_s}\frac{\partial f_p}{\partial v} = 0.$$

where the electric field is still determined by all particles together, though.

The Vlasov equation will not be satisfied for the prescribed particle shapes, however, we demand that the first moments are satisfied.

We obtain moments by integrating over configuration and velocity space:

$$\langle \ldots \rangle \equiv \int dx \int dv \ldots$$

Taking the 0th order moment of the Vlasov equation, it follows that

$$\frac{dN_p}{dt} = 0$$

That is, the number of physical particles represented by a quasi-particle remains constant in time.

Taking the moment of the Vlasov equation multiplied by x, we find

$$\frac{dx_p}{dt} = v_p$$

This is the same equation of motion that we had for a single real particle.

Finally, we take the moment of the Vlaosv equation multiplied by v and find

$$\frac{dv_p}{dt} = \frac{q_s}{m_s} E_p$$

where the electric field acting on the quasi particle is averaged over space according to the particle's shape function:

$$E_p = \int S_x(x - x_p) E_x$$

In conclusion, the particle in cell method actually solves the usual Newton's equations of motions for quasi-particles as we had for the actual particles, though the electric field is averaged due to the finite size of the quasi-particles.

The electric field is calculated on the grid and then assumed to be constant within each cell, so it is given as

$$E(x) = \sum_i E_i b_0 \left(\frac{x - x_i}{\Delta x} \right)$$

From the definition of E_p we get

$$E_p = \sum_i E_i \int b_0 \left(\frac{x - x_i}{\Delta x} \right) S_x(x - x_p) = \sum_i E_i W(x_i - x_p)$$

where the weight function W is essentially just the next higher order b-spline

$$W(x_i - x_p) = b_{l+1} \left(\frac{x_i - x_p}{\Delta x} \right)$$

where l is the order of the b-spline used in the particle shape function b-spline.

Time integration

The integration of the particle is staggered in time (leap-frog), too. We start with particle velocities at $\mathbf{v}_p^n$ and particle positions at $\mathbf{x}_p^{n+1/2}$. The positions $\mathbf{x}_p^{n+1/2}$ are used to interpolate the fields to the particle position at time $n + 1/2$ and calculate the Lorentz force $\mathbf{F}_p^{n+1/2}$. The Lorentz force is then used to update the particle velocity according to

$$m \frac{d\mathbf{v}_p}{dt} = F_p \Longrightarrow m \frac{\mathbf{v}_p^{n+1} - \mathbf{v}_p^n}{\Delta t} = F_p^{n+1/2}.$$

Then, the new particle positions can be found using $\mathbf{v}_p^{n+1}$:

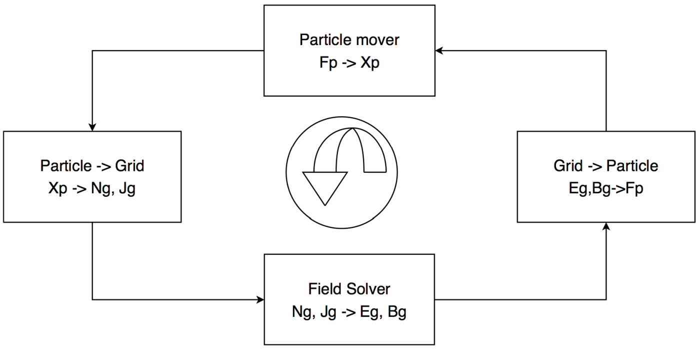
$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \Longrightarrow \frac{\mathbf{x}_p^{n+3/2} - \mathbf{x}_p^{n+1/2}}{\Delta t} = \mathbf{v}_p^{n+1}$$

The particle positions $\mathbf{x}^{n+1/2}$ and $\mathbf{x}^{n+3/2}$ are used to calculate the charge densities on the grid at those times. From the charge densities we then find the current densities $\mathbf{j}^{n+1}$ to satisfy discretely the charge continuity equation

$$\frac{d\rho}{dt} = \nabla \cdot \mathbf{j} \Longrightarrow \frac{\rho_{i,j,k}^{n+3/2} - \rho_{i,j,k}^{n+1/2}}{\Delta t} = (\nabla \cdot \mathbf{j})^{n+1}$$

The PIC cycle

The whole cycle showing the interaction between fields are particles is summarized in the following diagram.



PIC cylce [Lapenta]

Boris pusher

We skipped the details of numerically solving Newton’s 2nd Law with the Lorentz force, which contains the particle velocity, too. One common option is to used the pusher developed by Boris [1970]:

We split the Lorentz force into electric and magnetic parts:

$$\mathbf{F}_p = \mathbf{F}_{elec,p} + \mathbf{F}_{magn,p} = q_s \mathbf{E}_p + q_s \mathbf{v}_p \times \mathbf{B}_p$$

and then split the update as follows:

$$\begin{aligned} m_p \frac{\mathbf{v}^- - \mathbf{v}^n}{\Delta t} &= q_s \mathbf{E}_p^{n+1/2} \Longrightarrow \mathbf{v}^- = \mathbf{v}^n + \frac{q_p}{m_p} \mathbf{E}_p^{n+1/2} \\ m_p \frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} &= q_s \frac{\mathbf{v}^- + \mathbf{v}^-}{2} \times \mathbf{B}^{n+1/2} \Longrightarrow \mathbf{v}^+ = \text{rotation of } \mathbf{v}^- \text{ around } \mathbf{B}^{n+1/2} \\ m_p \frac{\mathbf{v}^{n+1} - \mathbf{v}^+}{\Delta t} &= q_s \mathbf{E}_p^{n+1/2} \Longrightarrow \mathbf{v}^{n+1} = \mathbf{v}^+ + \frac{q_p}{m_p} \mathbf{E}_p^{n+1/2} \end{aligned}$$