Particle in Cell method

Birdsall and Langdon: *Plasma Physics via Computer Simulation*
Dawson: Particle simulation of plasmas
Hockney and Eastwood: Computer Simulations using Particles

we start with an electrostatic 1d-1v collisionless plasma: Lecture by G. Lapenta

Vlasov equation for distribution function $f_s$:

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

$q_s, m_s$: charge and mass of the species

Poisson equation:

$$\frac{\partial^2 \phi}{\partial x^2} = -\rho$$

charge density $\rho$ follows from distribution function

$$\rho(x, t) = \sum_s \int f_s(x, v, t) dv$$
moving finite elements or \textit{superparticles}: \( f_p \)

\[
f_s(x, v, t) = \sum_{p} f_p(x, v, t)
\]

\textbf{Ansatz:} tensor product of shape functions:

\[
f_p(x, v, t) = N_p S_x(x - x_p(t)) S_v(v - v_p(t))
\]

\( S_x, S_v \): shape functions
\( N_p \): number of real particles in the \textit{superparticle}

\textbf{Assumptions:}

1. compact support
2. normalisation:

\[
\int_{-\infty}^{\infty} S_\zeta(\zeta - \zeta_p) d\zeta = 1
\]

\( \zeta = x \) or \( v \)
3. symmetric shapes:

\[
S_\zeta(\zeta - \zeta_p) = S_\zeta(\zeta_p - \zeta)
\]
Selection of particle shape

\[ S_v(v - v_p) = \delta(v - v_p) \]

b-splines

first b-spline: flat-top function \( b_0(\xi) \)

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

subsequent b-splines:

\[ b_l(\xi) = \int_{-\infty}^{\infty} d\xi' \, b_0(\xi - \xi') b_{l-1}(\xi') \]
Mathematical Derivation of the PIC method

Fig. 1.1. First three b-spline functions. The length scale is indicated by $H$.

The majority uses b-splines of order 0, a choice referred to as cloud in cell because the particle is a uniform square cloud in phase space with infinitesimal span in the velocity direction and a finite size in space.

1.3 Derivation of the equations of motion

To derive the evolution equations for the free parameters $x_p$ and $v_p$, we require that the first moments of the Vlasov equation to be exactly satisfied by the functional forms chosen for the elements. This procedure requires some explanations:

(i) The Vlasov equation is formally linear in $f_s$ and the equation satisfied by each element is still the same Vlasov equation. The
spatial shape function

\[ S_x(x - x_p) = b_l \left( \frac{x - x_p}{\Delta_p} \right) \]

\( \Delta_p \): size of superparticle

Remarks:
few PIC codes use splines of order 1 but most use order 0
Vlasov equation looks linear, \textbf{but} is nonlinear due to E-field.

Equation for superparticle:

\[
\frac{\partial f_p}{\partial t} + v \frac{\partial f_p}{\partial x} + \frac{qE}{m} \frac{\partial f_p}{\partial v} = 0
\]

The arbitrary functional form chosen for the elements does not satisfy exactly the Vlasov equation. The usual procedure of the finite element method is to require that the moments of the equations be satisfied.

Notation: \( \langle \ldots \rangle := \int dx \int dv \)
Moment 0

\[ \frac{\partial \langle f_p \rangle}{\partial t} + \langle v \frac{\partial f_p}{\partial x} \rangle + \langle \frac{qE}{m} \frac{\partial f_p}{\partial v} \rangle = 0 \]

second and third term = 0 \implies N_p = \text{const}

Moment 1_x

\[ \frac{\partial \langle xf_p \rangle}{\partial t} + \langle xv \frac{\partial f_p}{\partial x} \rangle + \langle \frac{qx E}{m} \frac{\partial f_p}{\partial v} \rangle = 0 \]

last term = 0
consider first term:

$$
\langle xf_p \rangle = N_p \left( \int S_v(v-v_p)dv \right) \left( \int xS_x(x-x_p)dx \right)
= N_p \int (x' + x_p)S_x(x')dx'
= N_p x_p \quad \text{using symmetry of } S_x
$$

consider second term:

$$
\int vdv \int x \frac{\partial f_p}{\partial x} dx = - \int v f_p dx dv = - \langle vf_p \rangle
$$

$$
\langle vf_p \rangle = N_p \left( \int vS_v(v-v_p)dv \right) \left( \int S_x(x-x_p)dx \right)
= N_p \int (v' + v_p)S_v(v')dv'
= N_p v_p \quad \text{using symmetry of } S_v
$$

thus

$$
\frac{dx_p}{dt} = v_p
$$
Moment $1_v$

$$\frac{\partial \langle vf_p \rangle}{\partial t} + \left \langle v^2 \frac{\partial f_p}{\partial x} \right \rangle + \left \langle \frac{qE_v}{m} \frac{\partial f_p}{\partial v} \right \rangle = 0$$

second term = 0
first term has already been computed: $\langle vf_p \rangle = N_p v_p$

remaining term:

$$\int \frac{q_s E}{m} dx \int v \frac{\partial f_p}{\partial v} dv = - \int \frac{q_s E}{m} dx \int f_p dv = - \left \langle \frac{q_s E}{m} f_s \right \rangle$$

This defines average electric field $E_p$ acting on computational particle:

$$\left \langle \frac{q_s E}{m} f_s \right \rangle = N_p \frac{q_s}{m} E_p$$

thus

$$\frac{dv_p}{dt} = \frac{q_s}{m} E_p$$
Equations of motion

\[ \frac{dN_p}{dt} = 0 \]
\[ \frac{dx_p}{dt} = v_p \]
\[ \frac{dv_p}{dt} = \frac{q_s}{m_s} E_p \]

Field equations: finite volume approach

cell centres: \( x_i \)  

cell faces: \( x_{i+1/2} \)

cell-averaged values \( \phi_i \) of potential

Poisson equation:

\[ \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2} = q \rho_i \]

with cell-averaged density:

\[ \rho_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x) \, dx \]
recall definition of b-spline of order 0

\[
\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x) \, dx = \int_{-\infty}^{\infty} b_0 \left( \frac{x - x_i}{\Delta x} \right) \rho(x) \, dx
\]

recall definition of the density

\[
\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x) \, dx = \sum_p \int_{-\infty}^{\infty} b_0 \left( \frac{x - x_i}{\Delta x} \right) S_x(x - x_p) \, dx
\]

define interpolation function

\[
W(x_i - x_p) = \int S_x(x - x_p) b_0 \left( \frac{x - x_i}{\Delta x} \right) \, dx
\]

and get:

\[
\rho_i = \sum_p \frac{q_p}{\Delta x} W(x_i - x_p) \quad \text{with } q_p = q_s N_p
\]
very simple expression, when we choose: $\Delta p = \Delta x \implies$

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

Electric field from central differences

$$E_i = -\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

E field is constant in each cell:

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

recall definition of $E_p$:

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

and recall definition of interpolation function

$$E_p = \sum_i E_i W(x - x_i)$$
Simplest symplectic integrator: leap-frog

\[ x_p^{n+1} = x_p^n + \Delta t v_p^{n+1/2} \]
\[ v_p^{n+3/2} = v_p^{n+1/2} + \Delta t E_p(x_p^n) \]

initial step: Euler forward

\[ v^{1/2} = v_p^0 + \Delta t E_p(x_p^0) \]

Stability

\[ c \Delta t < \Delta x \]
\[ \omega_{pe} < 2 \]
\[ \Delta x < \lambda_{De} \]