A particle-in-cell method with adaptive phase-space remapping for kinetic plasmas

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Outline

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  Vlasov equation
  Numerical methods for the Vlasov equation

Particle Methods
  The particle in cell method
  What is particle noise?

Noise Reduction: Phase-space Remapping
  Conservative, high order and positive remapping
  Mesh refinement

Numerical results
We consider a collisionless electrostatic plasma with two species, electron and ion, described by the Vlasov-Poisson equation.

**Vlasov equation**

\[
\frac{\partial f_e}{\partial t} + \mathbf{v} \cdot \nabla_x f_e + \mathbf{F} \cdot \nabla_v f_e = 0
\]

\[
\mathbf{F} = -\frac{q_e}{m_e} \mathbf{E}
\]

**Poisson equation**

\[
\rho = 1 - q_e \int_{\mathbb{R}^n} f_e d\mathbf{v}
\]

\[
\Delta \phi = -\rho \quad \mathbf{E} = -\nabla \phi
\]

\(f_e(\mathbf{x}, \mathbf{v}, t)\): the electron distribution function in phase space

\(\mathbf{F}(\mathbf{x}, t)\): Lorentz force (electrostatic case)

\(\mathbf{E}(\mathbf{x}, t)\): the self-consistent electrostatic field
Lagrangian description of the system

The distribution function $f$ is conserved along the characteristics. At time $s$ and $t$

$$f(X(t), V(t), t) = f(X(t_0), V(t_0), t_0)$$

where $(X(t), V(t))$ is the characteristics of the Vlasov equation:

$$\frac{dX}{dt} = V(t)$$
$$\frac{dV}{dt} = F(t)$$

where $X(t_0) = x_0$ and $V(t_0) = v_0$
Review of numerical methods: grid methods

1. Grid-based methods include spectral methods (Knorr 63, Armstrong 69, Flimas-Farrell 94), semi-Lagrangian methods (Cheng-Knorr 76, Sonnendrucker 99, Nakamura-Yabe 99), finite volume methods (Fijalkow 99, Filbet 01, Colella 11) and finite element methods (Zaki 88, Kilimas-Farrell 94).

2. They have drawn much attention in the past decade thanks to increasing processing power.
   - Advantage: Smooth representation of $f$
   - Disadvantage: High dimensions (up to 6) $\rightarrow$ high computational cost (specifically memory)
Particle methods, e.g., the PIC method, are widely used and are preferred for high dimensions.

**Advantages:**
- Naturally adaptive, since particles only occupy spaces where the distribution function is not zero
- Simpler to implement, in particular in high dimensions

**Disadvantages:**
- particle noise → difficulties to get precise results in some cases, for example, in simulating the problems with large dynamic ranges
Particle methods

- In particle methods, we approximate the distribution function by a collection of finite-size particles

\[ f(x, v, t) \approx \sum_k q_k \delta_{\epsilon_x}(x - \tilde{X}_k(t)) \delta_{\epsilon_v}(v - \tilde{V}_k(t)) \]

where \( q_k = f(x_i, v_i, 0) h_x h_v \)

\( \delta_{\epsilon_x}(y) = \frac{1}{\epsilon_x} u\left(\frac{y}{\epsilon_x}\right) \)

- At each time step, particles are transported along trajectories described by the equation of motion

\[ \frac{dq_k}{dt} = 0 \]
\[ \frac{d\tilde{X}_k}{dt} = \tilde{V}_k(t) \]
\[ \frac{d\tilde{V}_k}{dt} = \tilde{F}_k(t) \]

where \( \tilde{X}_k(0) = x_k \) and \( \tilde{V}_k(0) = v_k \).
The PIC method

- Charge assignment:
  \[ \tilde{\rho}(x_j, t^n) = \sum_k q_k \frac{u_1}{\varepsilon_x}(\frac{x_j - \tilde{X}_k(t^n)}{\varepsilon_x}) \]

  where \( j \) is the grid index.

- Field solver: i.e., FFTs or multigrid methods
  \[ \frac{\phi_{j-1} - 2\phi_j + \phi_{j+1}}{\varepsilon_x^2} = \tilde{\rho}_j \]

  \[ E_j = \frac{\phi_{j-1} - \phi_{j+1}}{2\varepsilon_x} \]

- Force interpolation:
  \[ \tilde{E}(\tilde{X}_k, t^n) = \sum_j E_j u_1(\frac{x_j - \tilde{X}_k(t^n)}{\varepsilon_x}) \]
What is particle noise?

Particle noise: the numerical error introduced when evaluating the moments of the distribution function using particles in phase space and **the particle disorder induced by the numerical error**

Error analysis:

- Monte Carlo estimate (Aydemir 93)

\[
\text{error} \propto \frac{\sigma}{\sqrt{N}}
\]

where \( \sigma \) is the standard deviation depends on the particle sampling and the distribution function.

- The approach in vortex methods: consistency error + stability error (Cottet-Raviart 84):

\[
\text{error} \propto \text{consistency error} \times (\exp(at) - 1)
\]

where \( a \) is a physical parameter.
Error Analysis of the PIC method for the VP system

The charge density error is

\[
|\rho(x, t) - \bar{\rho}(x, t)| = |\rho(x, t) - \sum_k q_k \delta_{\varepsilon_x}(x - \tilde{X}_k(t))|
\]

\[
\leq \left| \rho(x, t) - \int_{\mathbb{R}} \rho(y, t) \delta_{\varepsilon_x}(x - y) dy \right|
\]

moment error: \(e_m(x, t) \propto \varepsilon_x^2\)

\[
+ \left| \int_{\mathbb{R}} \rho(y, t) \delta_{\varepsilon_x}(x - y) dy - \sum_k q_k \delta_{\varepsilon_x}(x - X_k(t)) \right|
\]

discretization error: \(e_d(x, t) \propto \varepsilon_x^2 \left( \frac{h_x}{\varepsilon_x} \right)^2\)

\[
+ \left| \sum_k q_k \delta_{\varepsilon_x}(x - X_k(t)) - \sum_k q_k \delta_{\varepsilon_x}(x - \tilde{X}_k(t)) \right|
\]

stability error: \(e_s(x, t) \propto \frac{1}{\varepsilon_x} \max_k |X_k - \tilde{X}_k|\)

\[
|E(x, t) - \bar{E}(x, t)| \propto \left( \varepsilon_x^2 + \varepsilon_x^2 \left( \frac{h_x}{\varepsilon_x} \right)^2 + \max_k |\tilde{X}_k(t) - X_k(t)| \right)
\]
By following Cottet and Raviart (84):

\[(\tilde{X}_k - X_k)(t) = \int_0^t (\tilde{V}_k - V_k)(t') dt'\]

and

\[(\tilde{V}_k - V_k)(t) = -\int_0^t \left( (\tilde{E} - E)(\tilde{X}_k, t') + \frac{\partial E}{\partial x}(\tilde{X}_k - X_k)(t') \right) dt'\]
By using a variation on Gronwall’s inequality, we get

\[
\max_k (|X_k(t) - \tilde{X}_k(t)| + |V_k(t) - \tilde{V}_k(t)| + \|E - \tilde{E}(:, t)\|_{L^\infty})
\leq C_1 \left[ \varepsilon_x^2 + \varepsilon_x^2 \left( \frac{h_x}{\varepsilon_x} \right)^2 \right]
\leq C_1 \left[ \underbrace{\varepsilon_x^2 + \varepsilon_x^2 \left( \frac{h_x}{\varepsilon_x} \right)^2}_{e_c(x,t)} + \underbrace{e_s(x,t) \left( \exp(at) - 1 \right)}_{e_s(x,t)} \right]
\]

where \(a\) is \(\max(1, \| \frac{\partial E}{\partial x}(:, t) \|_{L^\infty})\), but not \(\varepsilon_x\) and \(h_x\).

**Requirements for Convergence**

- Particle overlapping: \(\frac{h_x}{\varepsilon_x} \leq 1\)
- Particle regularization: control the exponential-like term

ref: Cottet-Raviart 84 and Wang, Miller, Colella 11
Options if we want to reduce particle noise

- **Perturbative methods, such as the $\delta f$ method** (Kotschenreuther 88, Dimits-Lee 93, Parker-Lee 93): discretize the perturbation with respect to a (local) Maxwellian in velocity space using particles

  $\Rightarrow$ reduce $\sigma$ (error $\propto \frac{\sigma}{\sqrt{N}}$)

- **Our approach: remapping**: remap the distorted charge distribution on regularized grid(s) in phase space and then create a new set of particle charges from the grids with regularized distribution

  $\Rightarrow$ reduce exponential term
Conservative remapping on phase space \((x, v)\)

Particle charges are remapped (interpolated) to a grid in phase space

\[ q_i = q_k u\left(\frac{x_k - x_{i_x}}{h_x}\right) u\left(\frac{v_k - v_{i_v}}{h_v}\right) \]

Total charge and momentum are conserved if the interpolation function \(u\) satisfies

\[
\sum_{i \in \mathbb{Z}} u\left(\frac{x-x_i}{h}\right) = 1 \\
\sum_{i \in \mathbb{Z}} x_i u\left(\frac{x-x_i}{h}\right) = x
\]
High order interpolation

A modified B-spline by Monaghan (85)

\[ u_2(y) = \begin{cases} 
1 - \frac{5|y|^2}{2} + \frac{3|y|^3}{2} & 0 \leq |y| \leq 1 \\
\frac{1}{2}(2 - |y|)^2(1 - |y|) & 1 < |y| \leq 2 \\
0 & \text{otherwise}
\end{cases} \]

\( u_2 \) can approximate a quadratic function exactly (error is \( O(h^3) \)). Moreover, its first and second order derivatives are continuous.
Positivity for high order interpolation functions

**Algorithm**: Global mass redistribution based on flux corrected transport (Zalesak 78)

Treat interpolation as advection

\[ f_{i}^{n+1} = f_{i}^{n} + \nabla \cdot F \]

\[ f_{i}^{n+1} = \sum_{k} q_{k} \frac{1}{h x h v} u_{1 |2}(\frac{x_{i} - x_{k}}{h}) \]

\[ f_{i}^{n} = \sum_{k} q_{k} \frac{1}{h x h v} u_{0}(\frac{x_{i} - x_{k}}{h}) \]

Obtain the flux by solving a Poisson equation \( \nabla \cdot F = f_{i}^{n+1} - f_{i}^{n} \)

Define a low order flux \( F^{lo} \) and a high order flux \( F^{hi} \) as being using a low order \( u_{1} \) and a high order \( u_{2} \) interpolation.

Correct the low interpolation value by using the idea of FCT.
Algorithm: Local mass redistribution by Chern-Colella (87)

We redistribute the undershoot of cell $i$

$$
\delta f_i = \min(0, f_i^n)
$$

to neighboring cells in proportion to their capacity $\xi$

$$
\xi_{i+\ell} = \max(0, f_{i+\ell}^n)
$$

The distribution function is conserved, which fixes the constant of proportionality

$$
f_{i+\ell}^{n+1} = f_{i+\ell}^n + \frac{\xi_{i+\ell}}{\sum_{\ell' \neq 0} \xi_{i+\ell'}} \delta f_i
$$
Mesh refinement

**Motivation:** Remapping creates too many small strength particles at the edge of the distribution function.

**Algorithm:** Interpolate as in uniform grid first, then transfer the charge from invalid cells to valid cells.

The valid deposit cells: filled circles  The invalid cell: open circles
Introduction collision term

1. Remapping provides an opportunity to integrate collision models with a grid-based solver.
2. Example: simplified Fokker-Planck equation suggested by Rathmann and Denavit (75)

\[
\left( \frac{\partial f}{\partial t} \right)_c = \nabla_v \cdot [\nu vf + D\nabla_v (\nu f)]
\]

where \((\nu, D)\) are constants.

- Discretize it using a finite volume discretization and a second order \(L_0\) stable, implicit scheme
- Solve the matrix system using multigrid method
- Couple it with the Vlasov equation with operator splitting

\[
\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} - E \cdot \frac{\partial f}{\partial v} = \left( \frac{\partial f}{\partial t} \right)_c
\]
1D Vlasov-Poisson: linear Landau damping

The initial distribution of linear Landau damping is

\[ f_0(x, v) = \frac{1}{\sqrt{2\pi}} \exp(-v^2/2)(1 + \alpha \cos(kx)) \]

where \( \alpha = 0.01 \), \( k = 0.5 \), \( L = 2\pi/k \).

The evolution of the amplitude of the electric field: exponential decay with rate \( \gamma = -0.1533 \)

![Graph](image1)

\[ \text{w/o remapping} \]

particle number: 960

CPU times: 3.99 seconds

![Graph](image2)

\[ \text{w/ remapping} \]

particle number: 960-1,539

CPU times: 5.21 seconds
1D Vlasov-Poisson: linear Landau damping

\[ \gamma = -0.1533 \]

- **w/o remapping**
  - Particle number: 60,416
  - CPU times: 141.60 seconds

- **w/ remapping**
  - Particle number: 1,539
  - CPU times: 5.21 seconds
1D Vlasov-Poisson: the two stream instability

The initial distribution of the two stream instability is

\[ f_0(x, v) = \frac{1}{\sqrt{2\pi}} v^2 \exp(-v^2/2)(1 + \alpha \cos(kx)) \]

where \( \alpha = 0.05, k = 0.5, L = 2\pi/k \).

The evolution of \( f(x,v,t) \)

\[\text{w/o remapping, particle number: 18,360} \quad \text{w/ remapping, particle number: 18,360-24,242}\]
1D Vlasov-Poisson: the two stream instability

Comparison of $f(x, v, t)$ at the same instant of time $t = 20$

w/o remapping $\max_c = 1.740$ vs. $\max_e = 0.3$

w/ remapping $\max_c = 0.3082$ vs. $\max_e = 0.3$
1D Vlasov-Poisson: the two stream instability

E field Errors and convergence rates

w/o remapping

w/ remapping
1D Vlasov-Poisson-Fokker-Planck: the two stream instability

The evolution of $f(x,v,t)$

Simulation w/o (left) and w/ (right) collision at $t=30$
The initial distribution of linear Landau damping in 2D is

\[ f_0(x, y, v_x, v_y) = \frac{1}{2\pi} \exp\left(-\frac{(v_x^2 + v_y^2)}{2}\right)(1 + \alpha \cos(kx) \cos(ky)) \]

where \( \alpha = 0.05, k = 0.5, L = \frac{2\pi}{k}. \)

The evolution of the electric energy \( \xi_e \): exponential decay with constant rate \( \gamma \)

Without remapping, particle number: 1,228,800

With remapping, particle number: 1,228,800-1,835,008
2D Vlasov-Poisson: the two stream instability

The initial distribution for the two stream instability in 2D is

\[ f_0(x, y, v_x, v_y) = \frac{1}{12\pi} \exp\left(-\frac{v_x^2 + v_y^2}{2}\right)(1 + \alpha \cos(k_x x))(1 + 5v_x^2) \]

where \( \alpha = 0.05 \), \( k_x = 0.5 \), \( L = 2\pi/k \).

Comparison of projected distribution function in \((x, v_x)\) at time \( t = 20 \)

\[ \begin{array}{c}
\text{w/o remapping, particle number: 14,408,192} \\
\text{w/ remapping particle number: 14,408,192-22,184,217}
\end{array} \]
The parallel and multidimensional Vlasov-Poisson solver is implemented using Chombo framework, a C/C++ and FORTRAN library for the solutions of partial differential equations on a hierarchy of block-structured grid with finite difference methods developed in the ANAG group of LBNL.

- The physical domain is decomposed into patches
- Each patch is assigned to a processor
- Particles are assigned to a processor according to their physical position
- Particles are transferred between patches using MPI

Continuous work in ANAG: scalable multidimensional particle in cell code with remapping
Future Work

- Adaptivity on creating a hierarchy of grids for remapping
- Apply the method to magnetic fusion plasmas, e.g., gyrokinetic particle in cell method
- Parallel scalability
- GPU acceleration of remapping
Thank you!

Questions?