Introduction to Particle-in-cell gyrokinetic simulations

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The traditional PIC method in plasma physics

Method to simulate collective phenomena in plasmas:

Plasma is described by a small number of super-particles (SP),
each SP represents many ions or electrons,
each SP describes a piece of the distribution function f.

The motion of the SPs is straightforwardly described by the Newton-Maxwell equations.

The self-consistent fields are calculated by projecting on a spatial grid charge and current associated with each SP.

The PIC method in general..

The PIC method is a numerical technique used to solve a certain class of partial differential equations:

- individual particles (or fluid elements) in a Lagrangian frame are tracked in continuous phase space
- moments of the distribution function are computed simultaneously on Eulerian (stationary) mesh points.

Solid and fluid mechanics, cosmology,...
Plasma physics:
laser-plasma interactions, electron acceleration and ion heating in the auroral ionosphere, magnetic reconnection...Gyrokinetics

Outline

Construct a set of gyrokinetic (GK) equations, suited for simulations:

1) Must preserve symmetries: conserved quantities (energy).
2) Must contain (only) relevant physics: approximation are needed, but must not break self-consistency.

General procedure: GK field theory.
Example: Electrostatic, linearised polarisation GK Vlasov-Maxwell.

PIC discretization for particle and field eqs. (finite elements).

Properties of the discretised equations (conservation, errors, convergences,..).

Examples, simulations of experimental plasmas.

Self-consistent gyrokinetic equation from GK Lagrangi

GOAL: construct a simple self-consistent, energy conserving set of gyrokinetic equations, suited for PIC discretisation: Electrostatic, linearised polarisation GK Vlasov-Maxwell system.

Not only an academic problem: state of the art up 5 years ago, still useful for many physics problems.

Traditionally, iterative method [Friemann & Chen 1979...] or Hamiltonian representation to get Vlasov equation from particle Lagrangian; a back transformation (Lie) was used to obtain the field equations [Hahm 1988...].

Self-consistent gyrokinetic equation from GK Lagrangi

GOAL: construct a simple self-consistent, energy conserving set of gyrokinetic equations, suited for PIC discretisation:
Electrostatic, linearised polarisation GK Vlasov-Maxwell system

TOOL: gyrokinetic field theory.

Particle Lagrangian with time dependence in Hamiltoni

STARTING POINT: Lie transformed low-frequency particle Lagrangian in gyrocenter coordinates

$$L_p \qquad \frac{e}{c}A + p_k b \qquad R + \frac{mc}{e} \quad - \quad H$$

R, gyrocenter positions; $\frac{mv_?^2}{2B}$, magnetic moment;
$p_k \quad mU \quad \frac{e}{c}J_0 A_k$, canonical parallel momentum;, gyroangle;
$B = r \quad A$, background (static) magnetic field; J_0 gyroaverage operator, U parallel velocity.

Lie transform method is rather general: choices can be made to arrange L_p so that the symplectic part depends only on the background, while all the time varying fields are contained in the

Euler-Lagrange equations, electrostatic H

With the simple Lagrangian:

$$\underline{R} = \frac{\partial(H_0 + H_1)}{\partial p_\parallel}\frac{B}{B_\parallel} \quad \frac{c}{eBB_\parallel}F \quad \nabla \; (H_0 + H_1)$$

$$\underline{p_\parallel} = \frac{B}{B_\parallel} \quad \nabla \; (H_0 + H_1)$$

where a drift tensor notation for the background magnetic field has

Euler-Lagrange equations, no tensors

Tensor formalism emphasizes symmetries

The previous equation can be cast in the form of an antisymmetric generalised bracket [Scott 2010]:

$$B_k \frac{\partial f}{\partial t} + \nabla H \quad \frac{\partial G}{\partial p_k} \quad \nabla f + (\nabla \qquad G) \qquad \frac{\partial H}{\partial p_k} \nabla f \qquad \frac{\partial f}{\partial p_k} \nabla H \quad = 0$$

having defined $G \qquad A$.

This structure has the form of a triple bracket:

$$[H; G^{ab}; f]_{azb} = \frac{\partial G^{ab}}{\partial p_k} [H; f]_{ab} + (\nabla_a G^{ab})[H; f]_{bz} + (\nabla_b G^{ab})[H; f]_{za}$$

ab are pairs of spatial indices, z denotes the p_k coordinate.

The two-bracket form is

$$[H; f]_{ab} = H_{;a} f_{;b} \qquad H_{;b} f_{;a}$$

$g_{;a}$ denotes differentiation with respect to variable with index a.

Vlasov equation has a symmetric form

A has no $p_\parallel$ component:
additional fictitious 3-brackets can be added, leading to a remarkably symmetric expression for the gyrokinetic Vlasov equation.

$$\frac{\partial f}{\partial t} + \frac{1}{\sqrt{g} B_\parallel} \epsilon^{abcz} H_{;a} f_{;b} A_{c;z} = 0$$

where Einstein summation convention is assumed.
ϵ^{abcz} is the antisymmetric rank-four Levi-Civita pseudotensor.

The antisymmetric bracket form of the GK Vlasov equations allows for straightforward conservation of several quantities,

Field equation: Polarisation equation

Functional derivative of L with respect to :

$$\frac{L}{} = 0 \; ! \quad \frac{fH}{} = 0$$

which implies, with some algebra,

$$\overset{}{\underset{sp}{X}} Z \, dV \; Z \, dW \quad eJ_0 f + \frac{1}{B_k} r \; \left(B_k \frac{mc^2}{B^2} f_M \, r \; _{?} \right)^{!} = 0$$

the J_0 operator must be Hermitian.

The arbitrariness of implies:

$$\underset{sp}{X} Z \, dW \quad eJ_0 f + \frac{1}{B_k} r \; \left(\frac{mc^2}{B^2} B_k f_M \, r \; _{?} \right)^{!} = 0$$

Field equation: Polarisation equation

$dp_k d$ commutes with r :

$$\underset{sp}{X} \; Z \; dW e J_0 f + r \, \frac{n_0 mc^2}{B^2} r_{?} \frac{mc^2}{B^2} = 0$$

n_0 is the density associated with the equilibrium Maxwellian f_M.

The polarization equation clarifies the approximations made:

1) It is a linear equation.

2) It has the form of $\underset{sp}{P} en_{sp} = 0$, where en_{sp} is the particle density, i.e. a quasi-neutrality condition.

Global energy conservation equation

Finally:

$$\frac{\partial}{\partial t}E \quad \frac{\partial}{\partial t}\sum_{sp}\int dV\,dW fH = 0$$

The Hamiltonian is the global energy.

Global energy conservation, electrostatic case

X

@

E =

@t @t Z sp !

X dV dWfH !

@t Z sp + B eJ0)

U2 2

dV dWf (m

X

2EF 2EF Z sp

@

dV dWfer (@)E

Power balance equation in CYCLONE, nonlinear PIC

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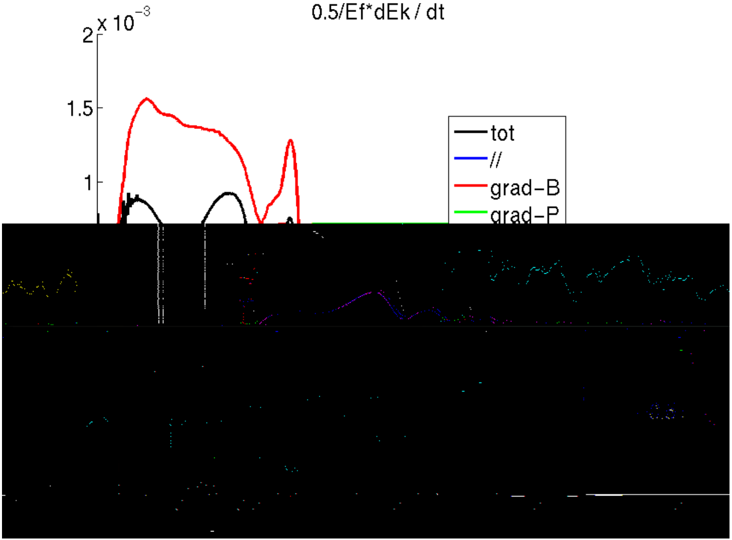
CYCLONE base case: DIII-D (circular) equilibrium.

Power balance is a powerful tool

Instantenous growth rate for ITG modes, nonlinear



Summary: electrostatic, linear polarization GK equatio

$$\frac{@f}{@t} + \underline{R} \ r \ f + \underline{p}_k \frac{@f}{@p_k} = 0$$

$$\underline{R} = \frac{p_k}{m}\frac{B}{B_k} \qquad \frac{c}{eBB_k} F \ [\ r \ B + er \ J_0 \,]$$

$$\underline{p}_k = \qquad \frac{B}{B_k} \ [\ r \ B + er \ J_0 \,]$$

$$X_{sp} \ Z \ dWeJ_0 f + r \qquad \frac{n_0 mc^2}{B^2} r_{?} \qquad = 0$$

Energetic consistency: the same Hamiltonian must be used to construct the polarization equation and the gyrokinetic Vlasov equations.

This also implies that the approximations made cannot be relaxed once the equations have been derived.

Energetic consistency can be easily broken

$$\frac{\partial f}{\partial t} + \dot{R}\,\nabla f + \dot{p}_\| \frac{\partial f}{\partial p_\|} = 0$$

$$\dot{R} = \frac{p_\|}{m}\frac{B}{B_\|} \quad \frac{c}{eBB_\|}F\ [\ \nabla B + e\nabla J_0\ ]$$

$$\dot{p}_\| = \quad \frac{B}{B_\|}\ [\ \nabla B + e\nabla J_0\ ]$$

$$\sum_{sp}\int dW eJ_0 f + \nabla \quad \frac{n(t)mc^2}{B^2}\nabla_\perp \quad = 0$$

Energetic consistency is broken:
nonlinear polarization implies using $(H_0 + H_1 + H_2)f$ in the Lagrangian for field equations;
→ second order terms must be included in the Euler-Lagrange equations.

PIC discretization

f is approximated by a sum of N markers, each defined by a position in phase-space $(R(t); p_k(t);\ )$ and a weight w.

$$f \ ' \ f_N(R(t); p_k(t);\ ) = \sum_{k=1}^{N} w_k \ (R \ \ R_k(t)) \ (p_k \ \ p_{kk}(t)) \ (\ \ _k)$$

The weights w_k are time independent (replace f in Vlasov eq...).

The weights are distributed accordingly to a certain probability density function g (importance sampling).

Euler-Lagrange equations, time evolution

The gyroaverage operator J_0 has the form of Bessel J_0

$$J_0 \quad = \frac{1}{2}\int_0^{2} (\ R + \tilde{}_i)\, d \quad =$$

$$= \frac{1}{2}\int_0^{2}\int \frac{1}{(2\ )^3}\hat{(}\ k)\, e^{ik(R+\tilde{}_i)}\, dk \quad d \quad =$$

$$= \int \frac{1}{(2\ )^3}\hat{(}\ k)\ \frac{1}{2}\int_0^{2} e^{ik_{?}\ _i\cos(\ )}\, d \quad e^{ikR}\, dk =$$

$$= \frac{1}{(2\ )^3}\int \hat{(}\ k)\ J_0(k_{?}\ _i)\ e^{ikR}\, dk \quad ;$$

$\hat{}$Fourier trasformed , $\ _i = \frac{k_B T m c^2}{e^2 B^2}$.

J_0 has the form, in Fourier space, of a multiplication of Fourier coefficients by the zeroth Bessel functions $J_0(k_{?}\ _i)$.

The gyroaveraged electrostatic potential $J_0\phi$

$$J_0\phi = \frac{1}{2\pi}\int_0^{2\pi}\phi(\mathbf{R}+\vec{\rho}_i)\,d\theta =$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\int \frac{1}{(2\pi)^3}\hat{\phi}(\mathbf{k})\,e^{i\mathbf{k}\cdot(\mathbf{R}+\vec{\rho}_i)}\,d\mathbf{k}\,d\theta =$$

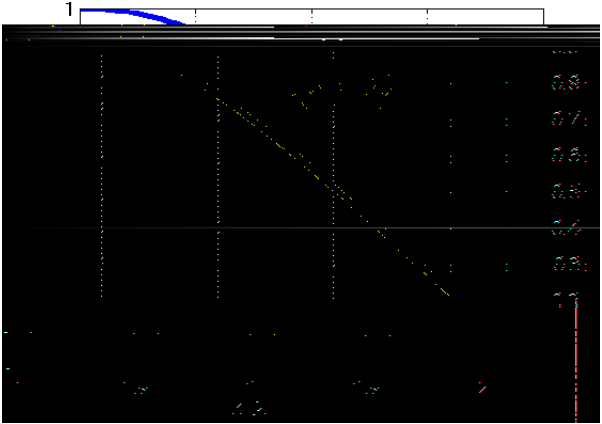
$$= \int \frac{1}{(2\pi)^3}\hat{\phi}(\mathbf{k})\,\frac{1}{2\pi}\int_0^{2\pi} e^{ik_\perp\rho_i\cos(\theta)}\,d\theta\,e^{i\mathbf{k}\cdot\mathbf{R}}\,d\mathbf{k} =$$

$$= \frac{1}{(2\pi)^3}\int \hat{\phi}(\mathbf{k})\,J_0(k_\perp\rho_i)\,e^{i\mathbf{k}\cdot\mathbf{R}}\,d\mathbf{k}\;;$$

$\hat{\phi}$ Fourier trasformed ϕ, $\rho_i = \frac{k_B T m c^2}{e^2 B^2}$.

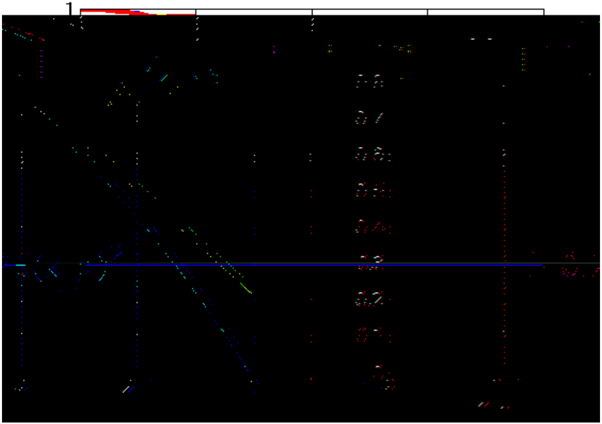
$J_0\phi$ has the form, in Fourier space, of a multiplication of Fourier coefficients by the zeroth Bessel functions $J_0(k_\perp\rho_i)$.

Bessel J_0 smooths out small variations



J_0 acts as a smoothing operator on .

Bessel J_0 smooths out small variations



J_0 acts as a smoothing operator on .

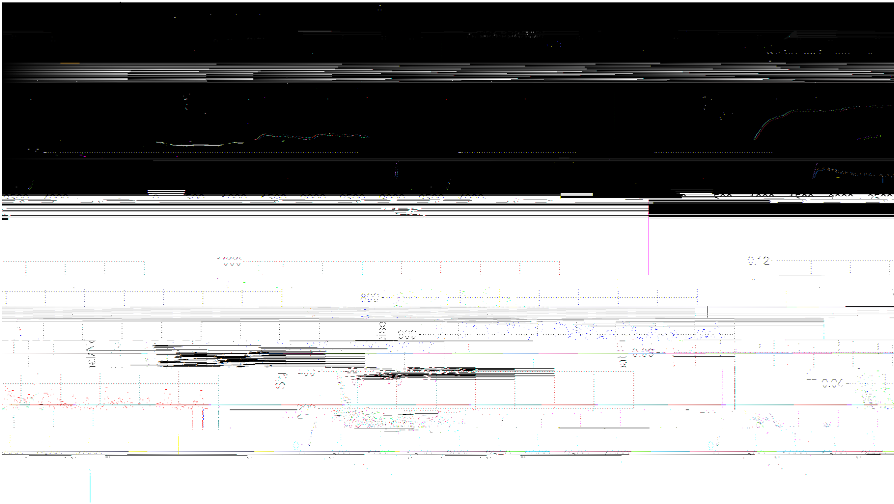
Polarization (Poisson) equation, B-splines

The polarisation equation is solved using finite elements:

$$(x;t) = \sum (t)\quad (x)$$

Where (t) are real numbers, and $(x) = {}_j(x_1)\ {}_k(x_2)\ {}_l(x_3)$ is a 3D product of polynomial basis functions (cubic B-splines).

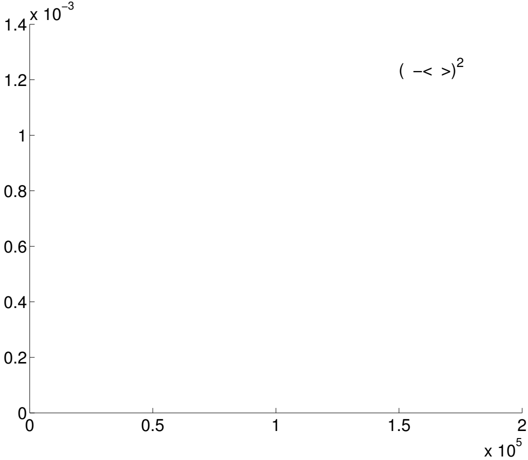
Variance reduction techniques (Monte-Carlo)



Very long simulations; Different heat sources different fluxes.

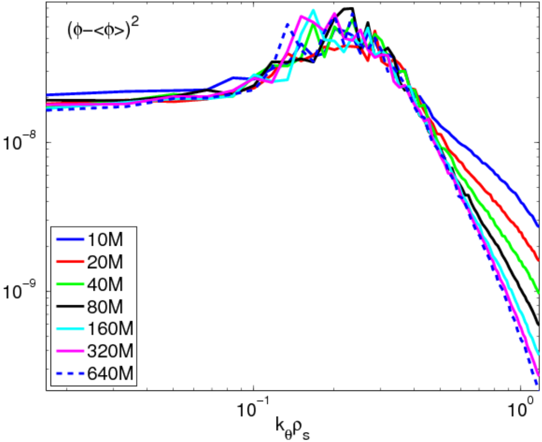
Convergence in number of markers N

Radial averaged heat fluxes or electrostatic potentials are very robust... not a good choice.



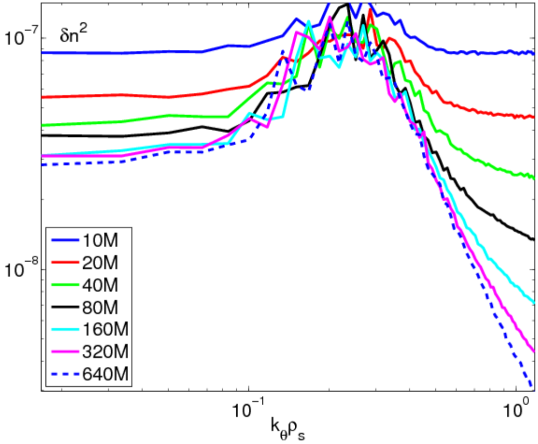
Spectra give good insights on the quality of the simulat

Time averaged spectrum: nonzonal electrostatic potential



Density fluctuation spectrum, slow converge in N

Time averaged spectrum: density fluctuation



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