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.
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 \( \sim 5 \) 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...].
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Electrostatic, linearised polarisation GK Vlasov-Maxwell system

TOOL: gyrokinetic field theory.
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TOOL: gyrokinetic field theory.

1) Establish a proper GK Lagrangian for particles and fields. 

2) Approximate the Lagrangian. 

3) Classical field theory: derive equations for particles and fields from variational principles.

The symmetry and conservation properties are preserved.
Particle Lagrangian with time dependence in Hamiltonian

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

\[
L_p \equiv \left( \frac{e}{c} A + p_\parallel b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H
\]

\(R\), gyrocenter positions; \(\mu \equiv \frac{mv^2}{2B}\), magnetic moment; \(p_\parallel \equiv mU - \frac{e}{c} J_0 A_\parallel\), canonical parallel momentum; \(\theta\), gyroangle; \(B = \nabla \times A\), 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 Hamiltonian \(H\).

[Hahm 1988, Brizard 2007, Miyato 2009,...].
GK total Lagrangian contains all the needed physics

Following [Sugama 2000], Lagrangian for particles AND fields is:

\[
L = \sum_{sp} \int dW_0 dV \ f(Z_0, t_0) L_p(Z(Z_0, t_0; t), \dot{Z}(Z_0, t_0; t), t) \\
+ \int dV \frac{E^2 - B^2_\perp}{8\pi}
\]

\[
Z \equiv (R, p_\parallel, \mu, \theta); \ dW \equiv \frac{2\pi}{m^2} B^* d\mu; \ B^2_\perp = |\nabla_\perp A_\parallel|^2
\]
GK total Lagrangian contains all the needed physics

Following [Sugama 2000], Lagrangian for particles AND fields is:

\[ L = \sum_{sp} \int dW_0 dV \ f(Z_0, t_0) L_p(Z(Z_0, t_0; t), \dot{Z}(Z_0, t_0; t), t) \]

\[ + \int dV \frac{E^2 - B^2}{8\pi} \]

The first term is the Lagrangian for charged particles.

\[ f(Z_0) \] is the distribution function for the species \( sp \) at an arbitrary initial time \( t_0 \).

\[ L_p \] is the Lie transformed particle Lagrangian written in terms of the gyro-center coordinates, *Lagrangian density*. 
GK total Lagrangian contains all the needed physics

Following [Sugama 2000], the GK total Lagrangian is:

\[ L = \sum_{sp} \int dW_0 dV \, f(Z_0, t_0) L_p(Z(Z_0, t_0; t), \dot{Z}(Z_0, t_0; t), t) \]

\[ + \int dV \frac{E^2 - B_{\perp}^2}{8\pi} \]

The second term is the Lagrangian for the electromagnetic fields.

Note: the particle Hamiltonian is not an invariant in GK theory. The conserved quantity is the total energy of the system.
Total Lagrangian contains the Vlasov equation

- Particle number conservation condition:
  \[ \text{d}W_0 \text{d}Vf(Z_0, t_0) = \text{d}W \text{d}Vf(Z, t) \]

- The time dependence in the distribution function \( f(Z, t) \) is:
  \[ \frac{2\pi}{m^2} B^* f(Z, t) = \int \text{d}W_0 \text{d}Vf(Z_0, t_0) \delta(Z - Z_0) \]

- Taking the time derivative of this equation, with some algebra, the **GK Vlasov equation** can be obtained:
  \[ \frac{\partial}{\partial t} f(Z, t) + \frac{dZ}{dt} \cdot \frac{\partial}{\partial Z} f(Z, t) = 0 \]

  Full derivation, for example: [Miyato 2009].
Total Lagrangian: summary

\[ L = \sum_{sp} \int dW dV \ f(Z, t) \int dV f(Z, t) \left( \frac{E^2 - B_\perp^2}{8\pi} \right) \]

\[ L_p = \left( \frac{e}{c} A + p_\parallel b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H \]

\[ H = H(\Phi, A_\parallel) \]

- Contains the Vlasov equation.
- Only one assumption on the Hamiltonian: it must contain the electrostatic potentials \( \Phi \) and the parallel component of the fluctuation magnetic potential \( A_\parallel \).
Total Lagrangian with simplest Hamiltonian [Hahm 1988]

\[
L = \sum_{sp} \int dW dV \ f(Z, t) L_p + \int dV \frac{E^2 - B^2}{8\pi} \\
L_p = \left( \frac{e}{c} A + p_{||} b \right) \cdot \dot{R} + \frac{mc}{e} \mu \theta - H \\
H = m\frac{U^2}{2} + \mu B + eJ_0 \Phi - \frac{mc^2}{2B^2} |\nabla \perp \Phi|^2
\]
Total Lagrangian with simplest Hamiltonian [Hahm 1988]

\[ L = \sum_{sp} \int dW dV \ f(\mathbf{Z}, t)L_p + \int dV \frac{E^2 - B_{\perp}^2}{8\pi} \]

\[ L_p = \left(\frac{e}{c} \mathbf{A} + p_{\parallel} \mathbf{b}\right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H \]

\[ H = m\frac{U^2}{2} + \mu B + eJ_0 \Phi - \frac{mc^2}{2B^2} \left| \nabla_{\perp} \Phi \right|^2 \]

- H is second order in the fields \( (p_{\parallel} \equiv mU - \frac{e}{c} J_0 A_{\parallel}) \)

\[ H = H_0 + H_1 + H_2 \]

\[ H_0 \equiv \frac{p_{\parallel}^2}{2m} + \mu B \]

\[ H_1 \equiv e(J_0 \Phi - \frac{p_{\parallel}}{mc} J_0 A_{\parallel}) \equiv eJ_0 \Psi \]

\[ H_2 \equiv \frac{e^2}{2mc^2} (J_0 A_{\parallel})^2 - \frac{mc^2}{2B^2} \left| \nabla_{\perp} \Phi \right|^2 \]
Total Lagrangian with simplest Hamiltonian [Hahm 1988]

\[ L = \sum_{sp} \int dW dV \ f(Z, t) L_p + \int dV \frac{E^2 - B_{\perp}^2}{8\pi} \]

\[ L_p = \left( \frac{e}{c} A + p_{\parallel} b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H \]

\[ H = \frac{p_{\parallel}^2}{2m} + \mu B + e(J_0 \Phi - \frac{p_{\parallel}}{mc} J_0 A_{\parallel}) + \frac{e^2}{2mc^2} (J_0 A_{\parallel})^2 - \frac{mc^2}{2B^2} |\nabla_{\perp} \Phi|^2 \]

- This is all we need from GK... from now on, field theory.

- In the context of field theory, this Lagrangian can be further approximated, without loosing self-consistency and energetic consistency of the final equations.

- Symmetry property of the Lagrangian will be automatically transferred to the equations.
Quasi-neutrality approximation

\[ L = \sum_{\text{sp}} \int dW dV \ f(Z, t) L_p + \int dV \left( \frac{E^2}{8\pi} - \frac{B^2}{8\pi} \right) \]

\[ L_p = \left( \frac{e}{c} A + p_{\parallel} b \right) \cdot \dot{R} + \frac{mc}{e} \dot{\mu} \dot{\theta} - H \]

\[ H = \frac{p_{\parallel}^2}{2m} + \mu B + e(J_0 \Phi - \frac{p_{\parallel}}{mc} J_0 A_{\parallel}) + \frac{e^2}{2mc^2} (J_0 A_{\parallel})^2 - \frac{mc^2}{2B^2} |\nabla_{\perp} \Phi|^2 \]
Quasi-neutrality approximation

\[ L = \sum_{sp} \int dW dV f(Z, t) L_p + \int dV \left( \frac{E^2}{8\pi} - \frac{B^2_\perp}{8\pi} \right) \]

\[ L_p = \left( \frac{e}{c} A + p_\parallel b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H \]

\[ H = \frac{p_\parallel^2}{2m} + \mu B + e(J_0 \Phi - \frac{p_\parallel}{mc} J_0 A_\parallel) + \frac{e^2}{2mc^2} (J_0 A_\parallel)^2 - \frac{mc^2}{2B^2} |\nabla_\perp \Phi|^2 \]

\[ \int dV \frac{E^2}{8\pi} + \int dW dV f \frac{m c^2}{2 B^2} |\nabla_\perp \Phi|^2 = \frac{1}{8\pi} \int dV \left( 1 + \frac{\rho_S^2}{\lambda_d^2} \right) |\nabla_\perp \Phi|^2 \]

\[ \lambda_d^2 \equiv \frac{k_B T_e}{4\pi n e^2} \text{ Debye length; } \rho_S^2 \equiv \frac{k_B T_e mc^2}{e^2 B^2} \text{ ion sound Larmor radius.} \]

Fusion plasmas: \[ \frac{\rho_S^2}{\lambda_d^2} = \frac{4\pi n mc^2}{B^2} = \frac{c^2}{v_a^2} \gg 1 \]

where \( v_a \) is the Alfvén velocity, \( c \) speed of light.
Quasi-neutrality approximation

\[ L = \sum_{sp} \int dW dV f(Z, t) L_p + \int dV \left( \frac{E^2}{8\pi} - \frac{B^2}{8\pi} \right) \]

\[ L_p = \left( \frac{e}{c} A + p_\parallel b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H \]

\[ H = \frac{p_\parallel^2}{2m} + \mu B + e(J_0\Phi - \frac{p_\parallel}{mc} J_0A_\parallel) + \frac{e^2}{2mc^2} (J_0A_\parallel)^2 - \frac{mc^2}{2B^2} |\nabla_\perp \Phi|^2 \]
Linearised polarisation approximation

\[
L = \sum_{sp} \int dV dW \left( \left( \frac{e}{c} A + p_{\parallel} b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H \right) f - \int dV \frac{B_{\perp}^2}{8\pi}
\]

- Start from \( H = H_0 + H_1 + H_2 \)
- In the Lagrangian \( H_0 + H_1 \) only multiplies \( f \): \((H_0 + H_1)f\)
- For \( H_2 \), \( f \) is replaced by an equilibrium distribution function \( f_M \) independent of time: \( H_2 f_M \)

\[
L = \sum_{sp} \int dV dW \left( \left( \frac{e}{c} A + p_{\parallel} b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H_0 - H_1 \right) f
\]

\[
+ \sum_{sp} \int dV dW H_2 f_M - \int dV \frac{B_{\perp}^2}{8\pi}
\]

This approximation will lead to linearised field equations.
Electrostatic model

- Although electromagnetic effects are important to correctly describe experimental plasmas, in the following we will neglect magnetic perturbations, $A_∥ = 0$ and $p_∥ = mU$.

$$L = \sum_{sp} \int dV dW \left( \left( \frac{e}{c} A + p_∥ b \right) \cdot \dot{R} + \frac{mc}{e} \mu \dot{\theta} - H_0 - H_1 \right) f$$

$$+ \sum_{sp} \int dV dW \frac{mc^2}{2B^2} |\nabla_⊥ \Phi|^2$$

- From now on, any additional approximation or ordering will break the symmetry and conservation properties of the underlying dynamical system.
Euler-Lagrange equations

- From the GK Lagrangian using variational principles for the action functional $I$, functional derivatives [Morrison 2005]:
  \[ \delta I = \int_{t_1}^{t_2} \delta L \, dt \]

- Euler-Lagrange equations, functional derivatives with respect to the particle phase space positions $Z = (R, p_\parallel, \mu)$:
  \[ \frac{\delta I}{\delta Z} = 0 \Rightarrow \frac{\delta L}{\delta Z} = 0 \]

as $t_1$ and $t_2$ are arbitrary.
Euler-Lagrange equations, electrostatic \( H \)

- With the simple Lagrangian:

\[
\dot{\mathbf{R}} = \dot{p}_\parallel \begin{pmatrix} B^* \frac{\partial (H_0 + H_1)}{\partial p_\parallel} \mathbf{B}^* - \frac{c}{eBB^*} \mathbf{F} \cdot \nabla (H_0 + H_1) \\
\frac{\partial (H_0 + H_1)}{\partial p_\parallel} \end{pmatrix}
\]

\[
\dot{p}_\parallel = -\frac{\mathbf{B}^*}{B^*_\parallel} \cdot \nabla (H_0 + H_1)
\]

where a drift tensor notation for the background magnetic field has been used, in which \( \epsilon \) it the rank-three Levi-Civita pseudotensor:

\[
\mathbf{F} = \nabla \mathbf{A} - (\nabla \mathbf{A})^T, \quad \mathbf{F} = \epsilon \cdot \mathbf{B}, \quad \nabla \times \mathbf{b} = -\nabla \cdot \frac{\mathbf{F}}{B}, \quad \mathbf{b} \times \mathbf{C} = -\frac{\mathbf{F}}{B} \cdot \mathbf{C} \quad \forall \mathbf{C}
\]

\[
\mathbf{A}^* = \mathbf{A} + p_\parallel \frac{c}{e} \mathbf{b}, \quad \mathbf{B}^* = \nabla \times \mathbf{A}^*
\]
Euler-Lagrange equations, no tensors

- Same equations in a more familiar form:

\[
\dot{R} = \frac{p_{\parallel}}{m} b - \left( \frac{p_{\parallel}}{m} \right)^2 \frac{mc}{eB^*_{\parallel}} b \times \frac{\nabla p}{B^2}
\]

\[
+ \left( \frac{\mu B}{m} + \left( \frac{p_{\parallel}}{m} \right)^2 \right) \frac{mc}{eB^*_{\parallel}} b \times \frac{\nabla B}{B} + \frac{c}{eB^*_{\parallel}} e b \times \nabla J_0 \Phi,
\]

\[
\dot{p}_{\parallel} = \mu B \nabla \cdot b + \frac{\mu c}{eB^*_{\parallel}} p_{\parallel} b \times \frac{\nabla p}{B^2} \cdot \nabla B
\]

\[
+ e \nabla J_0 \Phi \cdot \left( -b + \frac{c}{eB^*_{\parallel}} p_{\parallel} \left( b \times \frac{\nabla p}{B^2} - b \times \frac{\nabla B}{B} \right) \right)
\]

\[
\nabla p \equiv \frac{1}{4\pi} (\nabla \times \mathbf{B} \times \mathbf{B})
\]
Tensor formalism emphasizes symmetries

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

$$B^* \frac{\partial f}{\partial t} + \nabla H \cdot \frac{\partial G}{\partial p ||} \cdot \nabla f + (-\nabla \cdot G) \cdot \left( \frac{\partial H}{\partial p ||} \nabla f - \frac{\partial f}{\partial p ||} \nabla H \right) = 0$$

having defined $G \equiv \epsilon \cdot A^*$.
- This structure has the form of a triple bracket:

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

$ab$ are pairs of spatial indices, $z$ denotes the $p||$ coordinate.
- The two-bracket form is

$$[H, f]_{ab} = H, af, b - H, bf, a$$

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.
$\epsilon^{abcz}$ is the antisymmetric rank-four Levi-Civita pseudotensor.

- The antisymmetric bracket form of the GK Vlasov equations allows for \textit{straightforward conservation} of several quantities, including particle number and energy.
Field equation: Polarisation equation

- Functional derivative of $L$ with respect to $\Phi$:

$$\frac{\delta L}{\delta \Phi} = 0 \rightarrow \frac{\delta fH}{\delta \Phi} = 0$$

which implies, with some algebra,

$$\sum_{sp} \int dV \delta \Phi \int dW \left( eJ_0 f + \frac{1}{B^*_\parallel} \nabla (B^*_\parallel \frac{mc^2}{B^2} f_M \nabla \perp \Phi) \right) = 0$$

the $J_0$ operator must be Hermitian.

- The arbitrariness of $\delta \Phi$ implies:

$$\sum_{sp} \int dW \left( eJ_0 f + \frac{1}{B^*_\parallel} \nabla (\frac{mc^2}{B^2} B^*_\parallel f_M \nabla \perp \Phi) \right) = 0$$
Field equation: Polarisation equation

• $dp_{\parallel} d\mu$ commutes with $\nabla$:

$$\sum_{sp} \left( \int dW e J_0 f + \nabla n_0 mc^2 B^2 \nabla \perp mc^2 B^2 \Phi \right) = 0$$

$n_0$ 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 $\sum_{sp} en_{sp} = 0$, where $en_{sp}$ is the *particle* density, i.e. a quasi-neutrality condition.
Global energy conservation equation

\[ \frac{\partial f}{\partial t} + \frac{1}{\sqrt{gB^*_||}} \varepsilon^{abcz} H,_{af},bA^*_c,z = 0 \]

- Multiply by \( H \), use linearity of the derivatives in the brackets and symmetry:

\[ \frac{\partial fH}{\partial t} + \frac{1}{\sqrt{gB^*_||}} \varepsilon^{abcz} H,_{a(fH)},bA^*_c,z = f \frac{\partial H}{\partial t} \]

- Integrate over phase-space, sum over species:

\[ \sum_{sp} \int dWdV \frac{\partial fH}{\partial t} = \sum_{sp} \int dWdVf \frac{\partial H}{\partial t} \]

- Functional derivatives:

\[ \sum_{sp} \int dWdV \frac{\partial fH}{\partial t} = \int dV \sum_{sp} \frac{\delta fH}{\delta \Phi} \frac{\partial \Phi}{\partial t} = 0 \]
Global energy conservation equation

- Finally:

\[
\frac{\partial}{\partial t} \mathcal{E} \equiv \frac{\partial}{\partial t} \sum_{\text{sp}} \int dV dW f H = 0
\]

- The Hamiltonian is the global energy.

- Not true for electromagnetic (EM) Lagrangian:

\[
\frac{\partial}{\partial t} \mathcal{E} \equiv \frac{\partial}{\partial t} \left( \sum_{\text{sp}} \int dV dW f H + \int dV \frac{B^2}{8\pi} \right) = 0
\]

Note: the EM total energy is conserved only across-species.
Global energy conservation, electrostatic case

\[
\frac{\partial}{\partial t} \mathcal{E} = \frac{\partial}{\partial t} \left( \sum_{sp} \int dV dW f H \right) = 0
\]

\[
\frac{\partial}{\partial t} \left( \sum_{sp} \int dV dW f \left( \frac{m U^2}{2} + \mu B + e J_0 \Phi \right) \right) \equiv \dot{\mathcal{E}}_k + \dot{\mathcal{E}}_F = 0
\]

- It can be easily verified, using the Euler-Lagrange equations, that

\[
\dot{\mathcal{E}}_k = - \sum_{sp} \int dV dW f e \nabla (J_0 \Phi) \cdot \dot{\mathbf{R}}_0
\]

- Power balance equation:

\[
\frac{1}{2 \mathcal{E}_F} \dot{\mathcal{E}}_F = - \frac{1}{2 \mathcal{E}_F} \sum_{sp} \int dV dW f e \nabla (J_0 \Phi) \cdot \dot{\mathbf{R}}_0
\]
Power balance equation in CYCLONE, nonlinear PIC

- CYCLONE base case: DIII-D (circular) equilibrium.
Power balance is a powerful tool

- The power balance equation not only gives an indication of the quality of the simulation, but also provides, in linear simulations, a measure of the instantaneous growth rate:

\[
\mathcal{E}_F(R, t) = \bar{\mathcal{E}}_F(R) \exp(2\gamma t)
\]

\[
\gamma = \frac{1}{2\mathcal{E}_F} \sum_{sp} \int dV dWfe \nabla(J_0\Phi) \cdot \dot{R}_0
\]

\[
\dot{R}_0 = \frac{p_\parallel}{m} b - \left(\frac{p_\parallel}{m}\right)^2 \frac{mc}{eB^*_\parallel} b \times \frac{\nabla p}{B^2} + \left(\frac{\mu B}{m} + \left(\frac{p_\parallel}{m}\right)^2\right) \frac{mc}{eB^*_\parallel} b \times \frac{\nabla B}{B}
\]

\[
\gamma = \frac{1}{2\mathcal{E}_F} \sum_{sp} \int dV dWfe \nabla(J_0\Phi) \cdot (v_\parallel + v_{\nabla p} + v_{\nabla B})
\]
Instantaneous growth rate for ITG modes, linear

\[ \gamma = \frac{1}{2E_F} \sum_{sp} \int dV dWf e \nabla (J_0 \Phi) \cdot (v_\parallel + v \nabla p + v \nabla B) \]
Instantaneous growth rate for ITG modes, nonlinear
Summary: electrostatic, linear polarization GK equations

\[
\frac{\partial f}{\partial t} + \dot{\mathbf{R}} \cdot \nabla f + \dot{p}_\parallel \frac{\partial f}{\partial p_\parallel} = 0
\]

\[
\dot{\mathbf{R}} = \frac{p_\parallel B^*}{m B^*_\parallel} - \frac{c}{eBB^*} \mathbf{F} \cdot [\mu \nabla B + e \nabla J_0 \Phi]
\]

\[
p_\parallel = -\frac{B^*}{B^*_\parallel} \cdot [\mu \nabla B + e \nabla J_0 \Phi]
\]

\[
\sum_{sp} \left( \int dW e J_0 f + \nabla \cdot \left( \frac{n_0 mc^2}{B^2} \nabla \perp \Phi \right) \right) = 0
\]

- **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

\[
\frac{\partial f}{\partial t} + \mathbf{R} \cdot \nabla f + \dot{p}_\parallel \frac{\partial f}{\partial p_\parallel} = 0
\]

\[
\dot{\mathbf{R}} = \frac{p_\parallel B_\ast}{m B_\ast} - \frac{c}{eBB_\ast} \mathbf{F} \cdot [\mu \nabla B + e\nabla J_0 \Phi]
\]

\[
\dot{p}_\parallel = -\frac{B_\ast}{B_\ast} \cdot [\mu \nabla B + e\nabla J_0 \Phi]
\]

\[
\sum_{sp} \left( \int dW eJ_0 f + \nabla \cdot \left( \frac{n(t)mc^2}{B^2} \nabla_\bot \Phi \right) \right) = 0
\]

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.
Energetic consistency can be easily broken

\[
\frac{\partial f}{\partial t} + \dot{\bf R} \cdot \nabla f + \dot{\rho}_\parallel \frac{\partial f}{\partial \rho_\parallel} = 0
\]

\[
\dot{\bf R} = \frac{\rho_\parallel \bf B^*}{m B^*_\parallel} - \frac{c}{e BB^*_\parallel} \bf F \cdot [\mu \nabla B + e \nabla J_0 \Phi] + O(\Phi^2)
\]

\[
\dot{\rho}_\parallel = -\frac{\bf B^*}{B^*_\parallel} \cdot [\mu \nabla B + e \nabla J_0 \Phi] + O(\Phi^2)
\]

\[
\sum_{sp} \left( \int dW e J_0 f + \nabla \cdot \left( \frac{n(t)mc^2}{B^2} \nabla \perp \Phi \right) \right) = 0
\]

Energetic consistency is restored:

- nonlinear polarization implies using \((H_0 + H_1 + H_2)f\) in the Lagrangian for field equations;
- \(\rightarrow\) 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 $(\mathbf{R}(t), p_\parallel(t), \mu)$ and a weight $w$.

\[
f \simeq f_N(\mathbf{R}(t), p_\parallel(t), \mu) = \sum_{k=1}^{N} w_k \delta(\mathbf{R} - \mathbf{R}_k(t)) \delta(p_\parallel - p_\parallel_k(t)) \delta(\mu - \mu_k)
\]

- 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 time evolution is done by advancing the markers along the characteristics of the Vlasov equation:

\[
\dot{R}_k = \left( \frac{p_{\parallel k} B^*}{m} - \frac{c}{eB B^*} F \cdot [\mu_k \nabla B + e \nabla J_0 \Phi] \right)_{k} \\
\dot{p}_{\parallel k} = \left( -\frac{B^*}{B^*_{\parallel}} \cdot [\mu_k \nabla B + e \nabla J_0 \Phi] \right)_{k}
\]

given an initial condition \( R_k(0) = R_k^0, \mu_k, p_{\parallel k}(0) = p_{\parallel k}^0 \).

- \( J_0 \Phi \) at the marker position is needed.

- \( \Phi \) is computed by solving the polarisation equation on a grid of physical space, after having constructed the charge density \( \rho_N = \int dWeJ_0 f \) on the grid.
The gyroaverage operator $J_0$ has the form of Bessel-$J_0$

\[ J_0\Phi = \frac{1}{2\pi} \int_0^{2\pi} \Phi(R + \vec{\rho}_i) \, d\theta = \]

\[ = \frac{1}{2\pi} \int_0^{2\pi} \left( \int \frac{1}{(2\pi)^3} \hat{\Phi}(k) \, e^{ik \cdot (R + \vec{\rho}_i)} \, dk \right) \, d\theta = \]

\[ = \int \frac{1}{(2\pi)^3} \hat{\Phi}(k) \left( \frac{1}{2\pi} \int_0^{2\pi} e^{ik \cdot \rho_i \cos(\theta)} \, d\theta \right) \, e^{ik \cdot R} \, dk = \]

\[ = \frac{1}{(2\pi)^3} \int \hat{\Phi}(k) \, J_0(k \cdot \rho_i) \, e^{ik \cdot R} \, dk, \]

$\hat{\Phi}$ Fourier transformed $\Phi$, $\rho_i = \frac{k_B T m c^2}{e^2 B^2}$.

- $J_0$ has the form, in Fourier space, of a multiplication of Fourier coefficients by the zeroth Bessel functions $J_0(k \cdot \rho_i)$. 
The gyroaveraged electrostatic potential $J_0\Phi$

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

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

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

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

$\hat{\Phi}$ Fourier transformed $\Phi$, $\rho_i = \frac{k_B T m c^2}{e^2 B^2}$.

- $J_0$ has the form, in Fourier space, of a multiplication of Fourier coefficients by the zeroth Bessel functions $J_0(k_{\perp} \rho_i)$. 
Bessel $J_0$ smooths out small variations

- $J_0$ acts as a smoothing operator on $\Phi$. 
Bessel $J_0$ smooths out small variations

- $J_0$ acts as a smoothing operator on $\Phi$. 

$$J_0(k_{\perp \rho_1})$$

$$1 - 0.25(k_{\perp \rho_1})^2$$
A discretized gyroaverage operator

- Direct calculation of $J_0 \Phi$ for each individual marker has to account for its interaction with all the waves in the system, computationally prohibitive.

- Alternatively, the gyroaverage procedure can be approximated by an average over a number of points on the gyro-ring [Lee 1987].

$$J_0 \Phi = \frac{1}{2\pi} \int_0^{2\pi} \Phi(R + \vec{\rho}) \, d\theta \simeq \frac{1}{N_{\text{avg}}} \sum_{i=1}^{N_{\text{avg}}} \Phi(x_i)$$

When four quadrature points are used, this procedure is equivalent to replace $J_0$ with a Taylor expansion $J_0 (k_\perp \rho_i) \simeq 1 - \frac{1}{4} (k_\perp \rho_i)^2$ and to compute the transverse Laplacian using second order finite differences.
Simple proof

- Consider an equispaced 2D grid, with grid spacing $h = \rho_i$ in both directions.
- Each point of the grid is defined by a pair of indexes $(i, j)$:

$$J_0(R) \simeq \Phi - \frac{1}{4} \rho_i^2 \nabla^2 \Phi(R)$$

$$J_0 \Phi_{i,j} \simeq \Phi_{ij} + \frac{\rho_i^2}{4h^2}(\Phi_{i+1,j} + \Phi_{i-1,j} - 2\Phi_{i,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 2\Phi_{i,j})$$

$$= \frac{1}{4}(\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1})$$

where the standard second order centred finite difference scheme $\nabla^2 \Phi_j = (-\Phi_{j+1} + 2\Phi_j - \Phi_{j-1})/h^2$ was used in both directions.
Example: 4-point average in 2D, linear interpolation

\[ J_0 \Phi = \frac{1}{2\pi} \int_0^{2\pi} \Phi(R + \rho) \, d\theta \simeq \frac{1}{4} \sum_{i=1}^{4} \Phi(x_i) \]

- \( \Phi \) is defined on a grid (blue dots).
- Interpolation to get \( \Phi \) on some points (\( x_i \)) on the ring (red dots).
- Average to get \( J_0 \Phi \) at the tracer position.
Polarization (Poisson) equation, B-splines

The polarization equation is solved using finite elements:

$$
\Phi(x, t) = \sum_\mu \Phi_\mu(t) \Lambda_\mu(x)
$$

Where $\Phi_\mu(t)$ are real numbers, and $\Lambda_\mu(x) = \Lambda_j(x_1)\Lambda_k(x_2)\Lambda_l(x_3)$ is a 3D product of polynomial basis functions (cubic B-splines).
Polarization (Poisson) equation, B-splines

• The polarization equation becomes:

\[
\sum_{\text{sp}} \sum_{\mu} \Phi_{\mu} \left( -\nabla_{\perp} \cdot \frac{n_0 m c^2}{b^2} \nabla_{\perp} \Lambda_{\mu}(x) \right) = \sum_{\text{sp}} \int dW e J_0 f
\]

• Galerkin method:
  a) Multiply the equation by another test function \( g(x) = \Lambda_{\nu}(x) \).
  b) Integrate the resulting equation over configuration space.

\[
- \sum_{\mu} \Phi_{\mu} \int dV \sum_{\text{sp}} \Lambda_{\nu}(x) \nabla_{\perp} \cdot \frac{n_0 m c^2}{B^2} \nabla_{\perp} \Lambda_{\mu}(x) = \sum_{\text{sp}} \int dW dV e J_0 f \Lambda_{\nu}(x)
\]

having integrated the left hand side by parts.
• This equation is usually called the discretized weak form of the polarization equation.
Discretized polarization equation, set of linear equations

- The right hand side is now rewritten using the PIC approximation for \( J_0 f \) and by integrating the delta functions:

\[
- \sum_{\mu} \Phi_\mu \sum_{sp} \int dR \Lambda_\nu(R) \nabla_\perp \cdot \frac{n_0 mc^2}{B^2} \nabla_\perp \Lambda_\mu(R) = \\
\sum_{sp} \left( e \sum_{k=1}^{N} w_k \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} \Lambda_\nu(x_{k,\beta}) \right)
\]

- The previous equation is actually a set of linear equations:

\[
\sum_{\mu} A_{\mu \nu} \Phi_\mu = b_\nu
\]

- \( A_{\mu \nu} \) is a sparse, symmetric and positive definite matrix
Charge assignment, linear B-splines

\[ \sum_{sp} \left( e \sum_{k=1}^{N} \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} w_k \Lambda_\nu(x_k,\beta) \right) \]

- Scatter operation
- Each sample point (red dots) contributes to the charge of 4 grid points (blue dots).
- For 3D cubic B-Splines, 64 grid points.
Skeleton of a finite element PIC code

Initialization:

- Construct the matrix:

\[ A_{\mu\nu} = - \sum_{\mu} \Phi_{\mu} \sum_{sp} \int dR \Lambda_{\nu}(R) \nabla_{\perp} \cdot \frac{n_0 mc^2}{B^2} \nabla_{\perp} \Lambda_{\mu}(R) \]

- Initialize marker positions and weights:
\[ R_k(0) = R_k^0, \quad \mu_k, \quad p_{\parallel k}(0) = p_{\parallel k}^0, \quad w_k \]
Skeleton of a finite element PIC code

Main loop:

- Charge assignment:

\[ b_\nu = \sum_{sp} \left( e \sum_{k=1}^{N} w_k \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} \Lambda_\nu(x_{k,\beta}) \right) \]

- Solve \( \sum_\mu A_{\mu\nu} \Phi_\mu = b_\nu \) to get:

\[ \Phi(x, t) = \sum_\mu \Phi_\mu(t) \Lambda_\mu(x) \]

- Calculate \( J_0 \Phi \) at each marker position.
- Update marker position using Euler-Lagrange (ODEs):

\[ \dot{R}_k = \left( \frac{p_{\parallel k}}{m} \frac{B^*}{B^*_{\parallel}} - \frac{c}{eBB^*_{\parallel}} F \cdot [\mu_k \nabla B + e \nabla J_0 \Phi] \right)_k \]

\[ p_{\parallel k} = \left( -\frac{B^*}{B^*_{\parallel}} \cdot [\mu_k \nabla B + e \nabla J_0 \Phi] \right)_k \]
Control variate PIC ($\delta f$ method)

\[ f(R, v_||, \mu, t) = f_0(\psi_0, \epsilon, \mu, t) + \delta f(R, v_||, \mu, t) \]

- Particle kinetic energy $\epsilon = m_i (\mu B + U^2/2)$, the magnetic momentum $\mu$ and the toroidal canonical momentum $\psi_0 = \psi + (m_i/q_i)Rv_\phi$ are constant of motion on the unperturbed trajectories ($\Phi = 0$).
  $\rightarrow f_0$ is a stationary solution of the Vlasov equation with $\Phi = 0$.

- The PIC approximation of $f$ is now:
  \[
  f \approx f_0 + \delta f_N(R(t), p_||(t), \mu) \\
  = f_0 + \sum_{k=1}^{N} w_k \delta(R - R_k(t))\delta(p_|| - p_||_k(t))\delta(\mu - \mu_k)
  \]
Control variate PIC ($\delta f$ method)

- The Vlasov equation becomes a time evolution equation for $\delta f$:

$$\frac{d}{dt} f = \frac{d}{dt} \delta f + \frac{d}{dt} f_0 = 0$$

$$\frac{d}{dt} \delta f = -\frac{d}{dt} f_0 \equiv \tau (J_0 \Phi)$$

and consequently for the weights:

$$\dot{w}_k = \tau (J_0 \Phi)|_k$$
Skeleton of a finite element PIC code

Main loop:

• Charge assignment:

\[ b_\nu = \sum_{sp} \left( e \sum_{k=1}^{N} w_k \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} \Lambda_\nu(x_k, \beta) \right) \]

• Solve \( \sum_\mu A_{\mu \nu} \Phi_\mu = b_\nu \) to get:

\[ \Phi(x, t) = \sum_\mu \Phi_\mu(t) \Lambda_\mu(x) \]

• Calculate \( J_0 \Phi \) at each marker position.
• Update marker position using Euler-Lagrange (ODEs):

\[ \dot{R}_k = \ldots \\
\dot{p}_{\parallel k} = \ldots \\
\dot{w}_k = \tau(J_0 \Phi)|_k \]
Simple Monte-Carlo estimate for the noise

- **Statistical noise (Aydemir 1994):**
  Error $\epsilon$ introduced when the moment of the distribution function (density) is evaluated with a finite number $N$ of particles, $\epsilon \approx \sigma / \sqrt{N}$

$$
\rho^2_{\text{noise}} \simeq \frac{N_G}{N} \langle w^2 \rangle G ; \quad \langle w^2 \rangle \equiv \frac{1}{N} \sum_{i=1}^{N} w_i^2
$$

$N_G$, number of Fourier modes included in the simulation. $G$ accounts for FLR filtering and grid projection filtering.

- **Noise can be reduced by:**
  1. **Increasing** the number of tracers $N$.
  2. **Reducing** the number of modes $N_G \rightarrow$ Fourier filtering.
  3. **Reducing** $\langle w^2 \rangle$ (MC, reducing $\sigma$)
  4. Carefully choosing the projection algorithm, i.e. $G$. 
The statistical appears in the charge assignment

- In certain codes, the level of noise can be measured during the charge assignment:
  
  Direct measure of $|\rho|_{\text{noise}}^2$ by evaluating the average value of $|\rho_k|^2$ for the non-resonant (filtered) modes.

\[ <|\rho_k|^2>_{\text{noise}} / <n>^2 \]

Level of noise, $\rho_e^* = 1/80$
MC estimate validation: noise scaling with $N/N_G$

The scaling of the turbulence in number of particles per mode $N_G/N$ is satisfied

$$\frac{\rho_{\text{noise}}^2}{\langle w^2 \rangle} \approx \frac{N_G}{N} T$$

[a.u.]
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 simulation

- Time averaged spectrum: nonzonal electrostatic potential
Density fluctuation spectrum, slow converge in N

- Time averaged spectrum: density fluctuation


References (2)


- All the simulations were performed with the ORB5 (NEMORB) code:
  
  