# Introduction to Particle-in-cell gyrokinetic simulations

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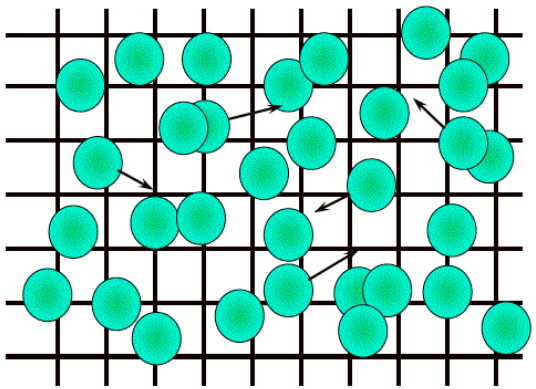
# The traditional PIC method in plasma physics

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 Lagrangian

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...].

# Self-consistent gyrokinetic equation from GK Lagrangian

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TOOL: gyrokinetic field theory.

# Self-consistent gyrokinetic equation from GK Lagrangian

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.

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.

IPP

# Particle Lagrangian with time dependence in Hamiltonian

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

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

$\mathbf{R}$, gyrocenter positions; $\mu \equiv \frac{mv_{\perp}^2}{2B}$, magnetic moment; $p_{\|} \equiv mU - \frac{e}{c}J_0 A_{\|}$, canonical parallel momentum; $\theta$, gyroangle; $\mathbf{B} = \nabla \times \mathbf{A}$, 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:

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}W_0 \mathrm{d}V \; f(\mathbf{Z}_0, t_0) L_p(\mathbf{Z}(\mathbf{Z}_0, t_0; t), \dot{\mathbf{Z}}(\mathbf{Z}_0, t_0; t), t) + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi}$$

$\mathbf{Z} \equiv (\mathbf{R}, p_\parallel, \mu, \theta)$; $\mathrm{d}W \equiv \frac{2\pi}{m^2} B_\parallel^* \mathrm{d}p_\parallel \mathrm{d}\mu$; $B_\perp^2 = |\nabla_\perp A_\parallel|^2$

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The first term is the Lagrangian for charged particles.

- $f(\mathbf{Z}_0)$ 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:

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}W_0 \mathrm{d}V \; f(\mathbf{Z}_0, t_0) L_p(\mathbf{Z}(\mathbf{Z}_0, t_0; t), \dot{\mathbf{Z}}(\mathbf{Z}_0, t_0; t), t) + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi}$$

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:

$$\mathrm{d}W_0\mathrm{d}Vf(\mathbf{Z}_0, t_0) = \mathrm{d}W\mathrm{d}Vf(\mathbf{Z}, t)$$

- The time dependence in the distribution function $f(\mathbf{Z}, t)$ is:

$$\frac{2\pi}{m^2} B_{\|}^* f(\mathbf{Z}, t) = \int \mathrm{d}W_0\mathrm{d}Vf(\mathbf{Z}_0, t_0)\delta(\mathbf{Z} - \mathbf{Z_0})$$

- Taking the time derivative of this equation, with some algebra, the GK Vlasov equation can be obtained:

$$\frac{\partial}{\partial t} f(\mathbf{Z}, t) + \frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} \cdot \frac{\partial}{\partial \mathbf{Z}} f(\mathbf{Z}, t) = 0$$

Full derivation, for example: [Miyato 2009].

# Total Lagrangian: summary

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z}, t) L_p + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi} \\
L_p &= \left( \frac{e}{c} \mathbf{A} + p_\parallel \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H \\
H &= H(\Phi, A_\parallel)
\end{aligned}
$$

- 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]

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z}, t) L_p + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi} \\
L_p &= \left( \frac{e}{c} \mathbf{A} + p_\parallel \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H \\
H &= m \frac{U^2}{2} + \mu B + e J_0 \Phi - \frac{mc^2}{2B^2} |\nabla_\perp \Phi|^2
\end{aligned}
$$

# Total Lagrangian with simplest Hamiltonian [Hahm 1988]

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z},t) L_p + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi} \\
L_p &= \left( \frac{e}{c}\mathbf{A} + p_\parallel \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e}\mu\dot{\theta} - H \\
H &= m\frac{U^2}{2} + \mu B + eJ_0\Phi - \frac{mc^2}{2B^2}|\nabla_\perp \Phi|^2
\end{aligned}
$$

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

$$
\begin{aligned}
H &= H_0 + H_1 + H_2 \\
H_0 &\equiv \frac{p_\parallel^2}{2m} + \mu B \\
H_1 &\equiv e(J_0\Phi - \frac{p_\parallel}{mc} J_0 A_\parallel) \equiv eJ_0\Psi \\
H_2 &\equiv \frac{e^2}{2mc^2}(J_0 A_\parallel)^2 - \frac{mc^2}{2B^2}|\nabla_\perp \Phi|^2
\end{aligned}
$$

# Total Lagrangian with simplest Hamiltonian [Hahm 1988]

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z}, t) L_p + \int \mathrm{d}V \frac{E^2 - B_\perp^2}{8\pi} \\
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H &= \frac{p_\parallel^2}{2m} + \mu B + e(J_0\Phi - \frac{p_\parallel}{mc} J_0 A_\parallel) + \frac{e^2}{2mc^2}(J_0 A_\parallel)^2 - \frac{mc^2}{2B^2}|\nabla_\perp \Phi|^2
\end{aligned}
$$

- 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.

- Simmetry property of the Lagrangian will be automatically transferred to the equations.

# Quasi-neutrality approximation

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z}, t) L_p + \int \mathrm{d}V \left( \frac{E^2}{8\pi} - \frac{B_\perp^2}{8\pi} \right) \\
L_p &= \left( \frac{e}{c} \mathbf{A} + p_\parallel \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H \\
H &= \frac{p_\parallel^2}{2m} + \mu B + e(J_0 \Phi - \frac{p_\parallel}{mc} J_0 A_\parallel) + \frac{e^2}{2mc^2} (J_0 A_\parallel)^2 - \frac{mc^2}{2B^2} |\nabla_\perp \Phi|^2
\end{aligned}
$$

# Quasi-neutrality approximation

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}W\mathrm{d}V\ f(\mathbf{Z},t)L_p + \int \mathrm{d}V \left( \frac{E^2}{8\pi} - \frac{B_\perp^2}{8\pi} \right)$$

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

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

$$\int \mathrm{d}V \frac{E^2}{8\pi} + \int \mathrm{d}W\mathrm{d}V\ f \frac{m}{2}\frac{c^2}{B^2}|\nabla_\perp\Phi|^2 = \frac{1}{8\pi}\int \mathrm{d}V \left(1 + \frac{\rho_S^2}{\lambda_d^2}\right)|\nabla_\perp\Phi|^2$$

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

$$\text{Fusion plasmas}: \quad \frac{\rho_S^2}{\lambda_d^2} = \frac{4\pi n m c^2}{B^2} = \frac{c^2}{v_a^2} \gg 1$$

where $v_a$ is the Alfvén velocity, $c$ speed of light.

# Quasi-neutrality approximation

$$
\begin{aligned}
L &= \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \; f(\mathbf{Z}, t) L_p + \int \mathrm{d}V \left( \frac{E^2}{8\pi} - \frac{B_\perp^2}{8\pi} \right) \\
L_p &= \left( \frac{e}{c} \mathbf{A} + p_\parallel \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H \\
H &= \frac{p_\parallel^2}{2m} + \mu B + e(J_0 \Phi - \frac{p_\parallel}{mc} J_0 A_\parallel) + \frac{e^2}{2mc^2} (J_0 A_\parallel)^2 - \frac{mc^2}{2B^2} |\nabla_\perp \Phi|^2
\end{aligned}
$$

# Linearised polarisation approximation

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W \left( \left( \frac{e}{c}\mathbf{A} + p_{\parallel}\mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e}\mu\dot{\theta} - H \right) f - \int \mathrm{d}V \frac{B_{\perp}^2}{8\pi}$$

- 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: $H_2 f_M$

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W \left( \left( \frac{e}{c}\mathbf{A} + p_{\parallel}\mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e}\mu\dot{\theta} - H_0 - H_1 \right) f$$
$$+ \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W H_2 f_M - \int \mathrm{d}V \frac{B_{\perp}^2}{8\pi}$$

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, $A_{\parallel} = 0$ and $p_{\parallel} = mU$.

$$L = \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W \left( \left( \frac{e}{c} \mathbf{A} + p_{\parallel} \mathbf{b} \right) \cdot \dot{\mathbf{R}} + \frac{mc}{e} \mu \dot{\theta} - H_0 - H_1 \right) f$$
$$+ \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W \frac{mc^2}{2B^2} |\nabla_{\perp} \Phi|^2$$

• From now on, any additional approximation or odering 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]:

$$\delta I = \int_{t1}^{t2} \delta L \mathrm{d}t$$

• Euler-Lagrange equations, functional derivatives with respect to the particle phase space positions $\mathbf{Z} = (\mathbf{R}, p_{\|}, \mu)$:

$$\frac{\delta I}{\delta \mathbf{Z}} = 0 \Rightarrow \frac{\delta L}{\delta \mathbf{Z}} = 0$$

as $t_1$ and $t_2$ are arbitrary.

# Euler-Lagrange equations, electrostatic H

- With the simple Lagrangian:

$$\dot{\mathbf{R}} = \frac{\partial(H_0 + H_1)}{\partial p_\parallel}\frac{\mathbf{B}^*}{B_\parallel^*} - \frac{c}{eBB_\parallel^*}\mathbf{F}\cdot\nabla(H_0 + H_1)$$

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

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:

$$
\begin{aligned}
\dot{\mathbf{R}} &= \frac{p_\parallel}{m}\mathbf{b} - \left(\frac{p_\parallel}{m}\right)^2 \frac{mc}{eB^*_\parallel}\mathbf{b}\times\frac{\nabla p}{B^2} \\
&\quad + \left(\frac{\mu B}{m} + \left(\frac{p_\parallel}{m}\right)^2\right)\frac{mc}{eB^*_\parallel}\mathbf{b}\times\frac{\nabla B}{B} + \frac{c}{eB^*_\parallel}e\mathbf{b}\times\nabla J_0\Phi, \\
\dot{p_\parallel} &= \mu B\nabla\cdot\mathbf{b} + \frac{\mu c}{eB^*_\parallel}p_\parallel\mathbf{b}\times\frac{\nabla p}{B^2}\cdot\nabla B \\
&\quad + e\nabla J_0\Phi\cdot\left(-\mathbf{b} + \frac{c}{eB^*_\parallel}p_\parallel\left(\mathbf{b}\times\frac{\nabla p}{B^2} - \frac{\mathbf{b}\times\nabla B}{B}\right)\right) \\
\nabla p &\equiv \frac{1}{4\pi}(\nabla\times\mathbf{B}\times\mathbf{B})
\end{aligned}
$$

# Tensor formalism emphasizes symmetries

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

$$B_{\parallel}^{*}\frac{\partial f}{\partial t}+\nabla H\cdot\frac{\partial \mathbf{G}}{\partial p_{\parallel}}\cdot\nabla f+(-\nabla\cdot\mathbf{G})\cdot\left(\frac{\partial H}{\partial p_{\parallel}}\nabla f-\frac{\partial f}{\partial p_{\parallel}}\nabla H\right)=0$$

having defined $\mathbf{G}\equiv\epsilon\cdot\mathbf{A}^{*}$.

- This structure has the form of a triple bracket:

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

$ab$ are pairs of spatial indices, $z$ denotes the $p_{\parallel}$ coordinate.

- The two-bracket form is

$$[H,f]_{ab}=H_{,a}f_{,b}-H_{,b}f_{,a}$$

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

# Vlasov equation has a symmetric form

• $\mathbf{A}^*$ 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 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,

$$\sum_{\mathrm{sp}} \int \mathrm{d}V \delta\Phi \int \mathrm{d}W \left( eJ_0 f + \frac{1}{B_{\parallel}^*} \nabla \left( B_{\parallel}^* \frac{mc^2}{B^2} f_M \nabla_{\perp} \Phi \right) \right) = 0$$

the $J_0$ operator must be Hermitian.

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

$$\sum_{\mathrm{sp}} \int \mathrm{d}W \left( eJ_0 f + \frac{1}{B_{\parallel}^*} \nabla \left( \frac{mc^2}{B^2} B_{\parallel}^* f_M \nabla_{\perp} \Phi \right) \right) = 0$$

# Field equation: Polarisation equation

- $\mathrm{d}p_{\parallel}\mathrm{d}\mu$ commutes with $\nabla$:

$$\sum_{\mathrm{sp}}\left(\int \mathrm{d}WeJ_0 f + \nabla\frac{n_0 mc^2}{B^2}\nabla_{\perp}\frac{mc^2}{B^2}\Phi\right) = 0$$

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

# Global energy conservation equation

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

- Multiply by $H$, use linearity of the derivatives in the brackets and symmetry:

$$\frac{\partial fH}{\partial t} + \frac{1}{\sqrt{g} B_{\parallel}^{*}} \epsilon^{abcz} H_{,a} (fH)_{,b} A_{c,z}^{*} = f \frac{\partial H}{\partial t}$$

- Integrate over phase-space, sum over species:

$$\sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \frac{\partial fH}{\partial t} = \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V f \frac{\partial H}{\partial t}$$

- functional derivatives:

$$\sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V \frac{\partial fH}{\partial t} = \int \mathrm{d}V \sum_{\mathrm{sp}} \frac{\delta fH}{\delta \Phi} \frac{\partial \Phi}{\partial t} = 0$$

# Global energy conservation equation

- Finally:

$$\frac{\partial}{\partial t}\mathcal{E} \equiv \frac{\partial}{\partial t}\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W f H = 0$$

- The Hamiltonian is the global energy.

- Not true for electromagnetic (EM) Lagrangian:

$$\frac{\partial}{\partial t}\mathcal{E} \equiv \frac{\partial}{\partial t}\left(\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W f H + \int \mathrm{d}V\frac{B_{\perp}^2}{8\pi}\right) = 0$$

Note: the EM total energy is conserved only across-species.

# Global energy conservation, electrostatic case

$$\frac{\partial}{\partial t}\mathcal{E} = \frac{\partial}{\partial t}\left(\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W f H\right) = 0$$

$$\frac{\partial}{\partial t}\left(\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W f\left(m\frac{U^2}{2} + \mu B + eJ_0\Phi\right)\right) \equiv \dot{\mathcal{E}}_k + \dot{\mathcal{E}}_F = 0$$

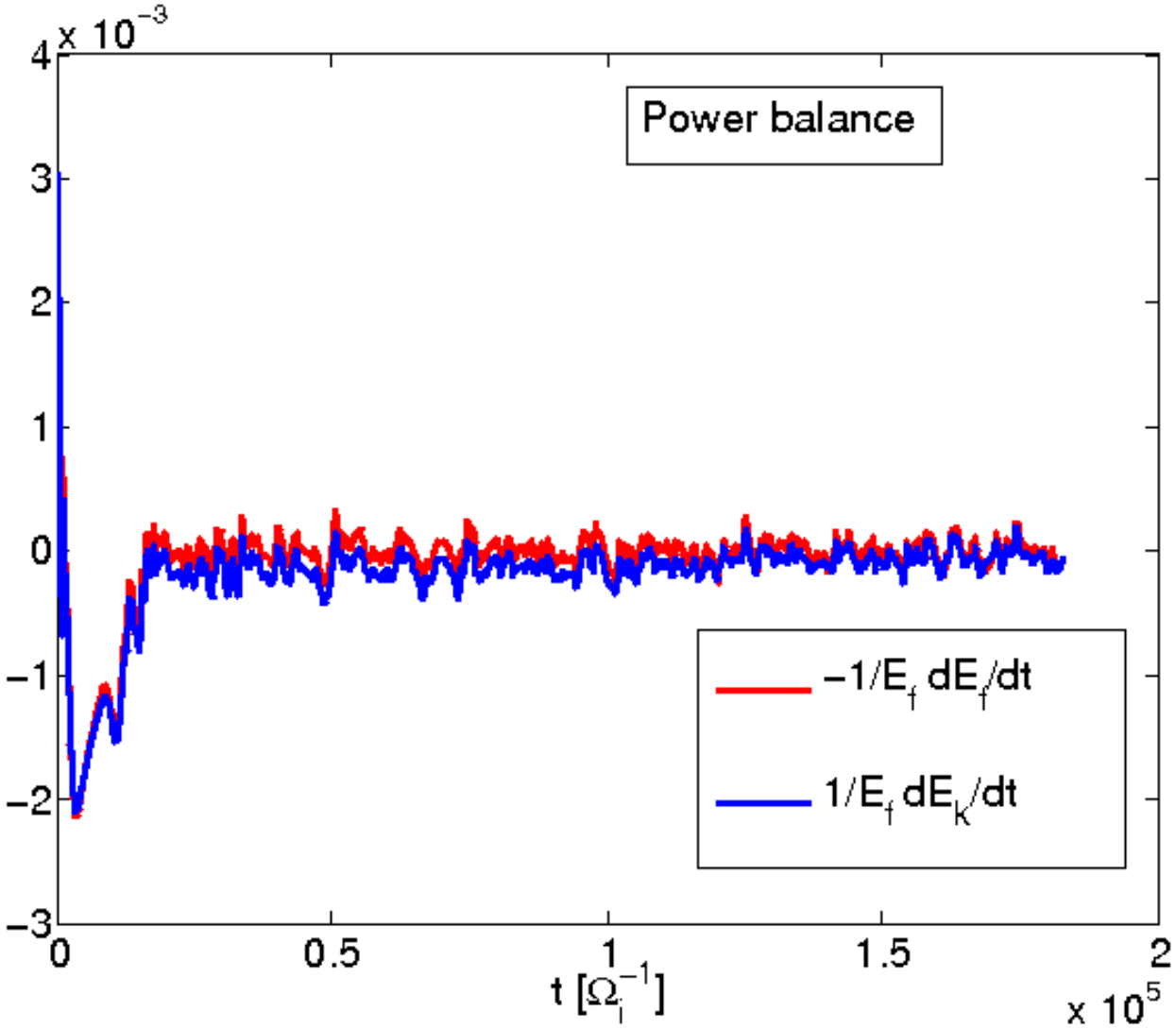
- It can be easily verified, using the Euler-Lagrange equations, that

$$\dot{\mathcal{E}}_k = -\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W fe\nabla(J_0\Phi)\cdot\dot{\mathbf{R}}_0$$

- Power balance equation:

$$\frac{1}{2\mathcal{E}_F}\dot{\mathcal{E}}_F = -\frac{1}{2\mathcal{E}_F}\sum_{\mathrm{sp}}\int \mathrm{d}V\mathrm{d}W fe\nabla(J_0\Phi)\cdot\dot{\mathbf{R}}_0$$

# 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:

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

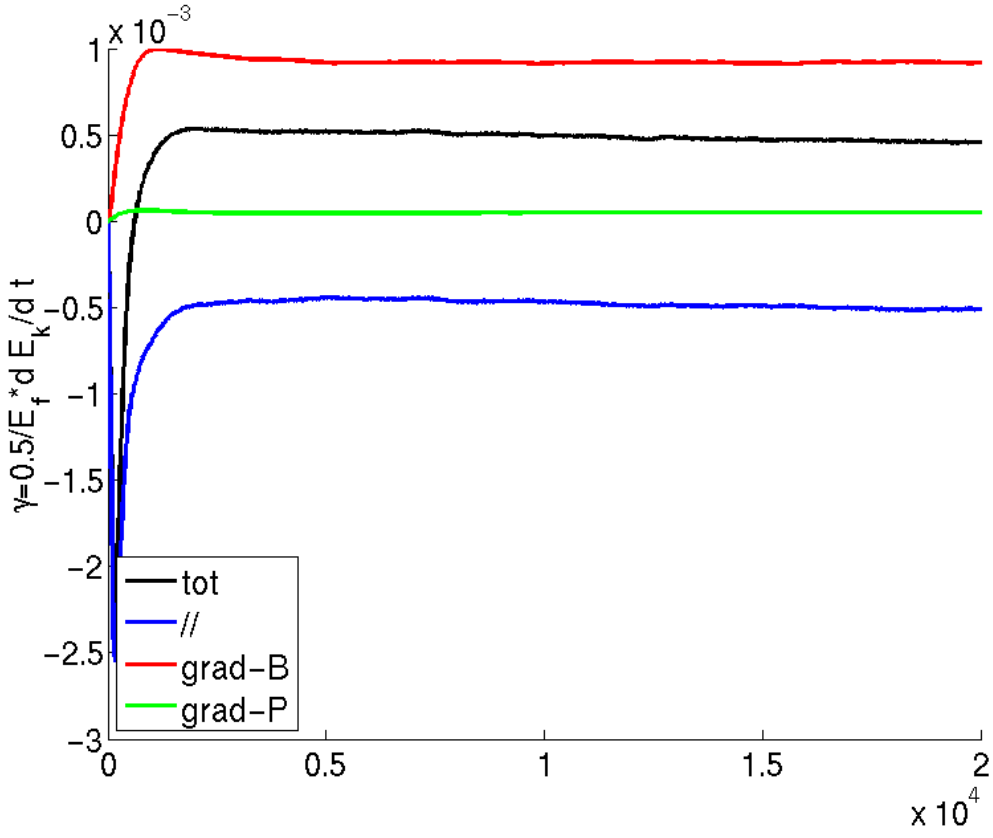
$$\gamma = \frac{1}{2\mathcal{E}_F} \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W f e \nabla (J_0 \Phi) \cdot \dot{\mathbf{R}}_0$$

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

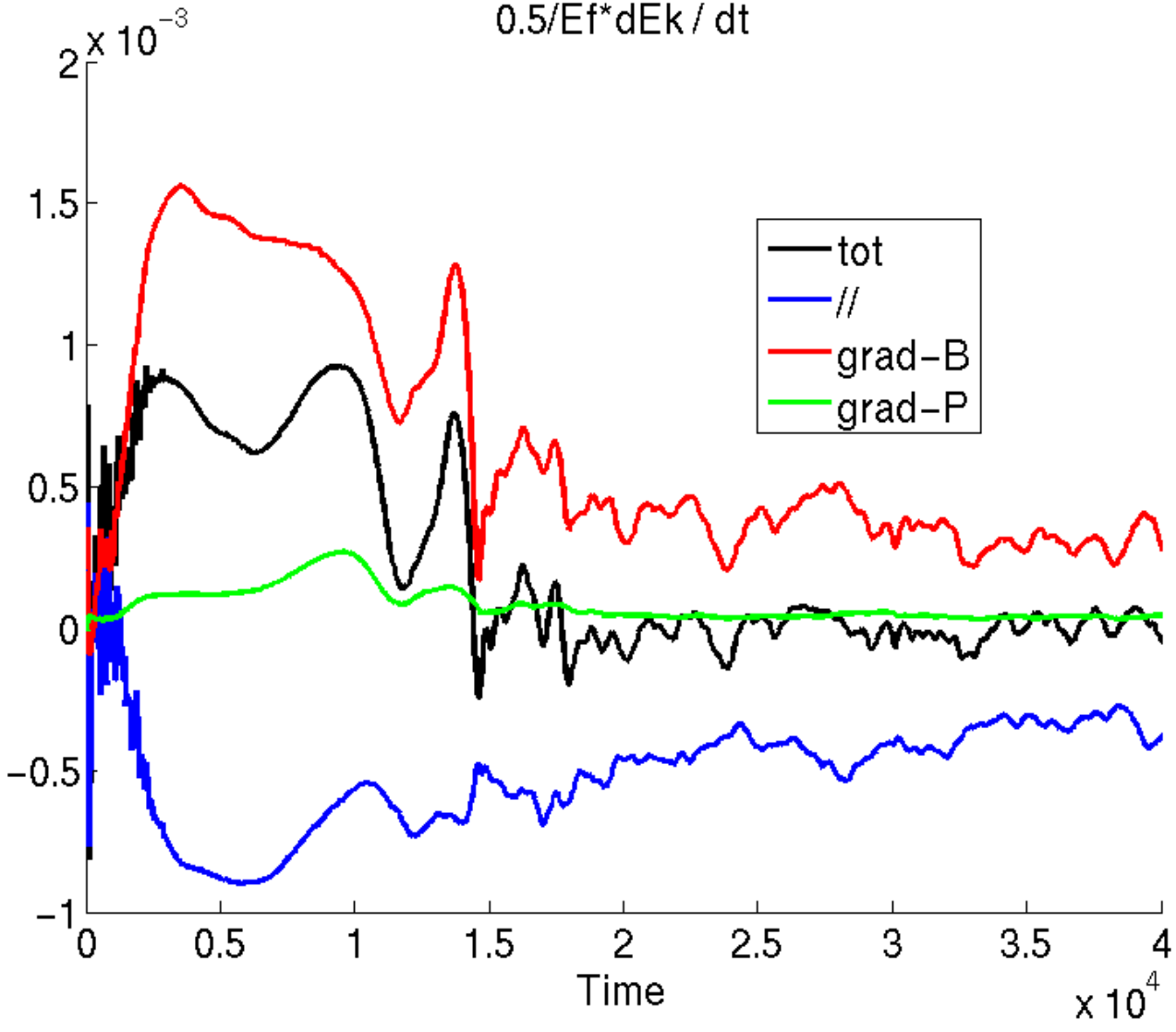
$$\gamma = \frac{1}{2\mathcal{E}_F} \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W f e \nabla (J_0 \Phi) \cdot (\mathbf{v}_\parallel + \mathbf{v}_{\nabla p} + \mathbf{v}_{\nabla B})$$

# Instantenous growth rate for ITG modes, linear

$$\gamma = \frac{1}{2\mathcal{E}_F} \sum_{\mathrm{sp}} \int \mathrm{d}V \mathrm{d}W f e \nabla (J_0 \Phi) \cdot (\mathbf{v}_{\parallel} + \mathbf{v}_{\nabla p} + \mathbf{v}_{\nabla B})$$



# Instantenous growth rate for ITG modes, nonlinear



# Summary: electrostatic, linear polarization GK equations

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

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

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

$$\sum_{\mathrm{sp}} \left( \int \mathrm{d}W e J_0 f + \nabla \cdot \left( \frac{n_0 m c^2}{B^2} \nabla_\perp \Phi \right) \right) = 0$$

• 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

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

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

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

$$\sum_{\mathrm{sp}} \left( \int \mathrm{d}W e J_0 f + \nabla \cdot \left( \frac{n(t) m c^2}{B^2} \nabla_{\perp} \Phi \right) \right) = 0$$

Energetic consistency is broken:

• nonlinear polarization implies using $(H_0 + H_1 + H_2)f$ in the Lagrangian for field equations;

$\rightarrow$ second order terms must be included in the Euler-Lagrange equations.

# Energetic consistency can be easily broken

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

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

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

$$\sum_{\mathrm{sp}} \left( \int \mathrm{d}W e J_0 f + \nabla \cdot \left( \frac{n(t) m c^2}{B^2} \nabla_{\perp} \Phi \right) \right) = 0$$

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:

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

$$\dot{p_{\|k}} = \left( -\frac{\mathbf{B}^*}{B^*_\|} \cdot [\mu_k \nabla B + e \nabla J_0 \Phi] \right)_k$$

given an initial condition $\mathbf{R_k}(0) = \mathbf{R_k}^0$, $\mu_k$,$p_{\|k}(0) = p^0_{\|k}$.

• $J_0\Phi$ 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 $\rho_N = \int \mathrm{d} W e J_0 f$ on the grid.

# The gyroaverage operator $J_0$ has the form of Bessel-$J_0$

$$
\begin{aligned}
J_0\Phi &= \frac{1}{2\pi}\int_0^{2\pi} \Phi(\mathbf{R}+\vec{\rho}_i)\,\mathrm{d}\theta = \\
&= \frac{1}{2\pi}\int_0^{2\pi}\left(\int \frac{1}{(2\pi)^3}\,\hat{\Phi}(\mathbf{k})\,e^{i\mathbf{k}\cdot(\mathbf{R}+\vec{\rho}_i)}\,\mathrm{d}\mathbf{k}\right)\,\mathrm{d}\theta = \\
&= \int \frac{1}{(2\pi)^3}\,\hat{\Phi}(\mathbf{k})\left(\frac{1}{2\pi}\int_0^{2\pi} e^{ik_\perp\rho_i\cos(\theta)}\,\mathrm{d}\theta\right)e^{i\mathbf{k}\cdot\mathbf{R}}\,\mathrm{d}\mathbf{k} = \\
&= \frac{1}{(2\pi)^3}\int \hat{\Phi}(\mathbf{k})\,J_0\left(k_\perp\rho_i\right)\,e^{i\mathbf{k}\cdot\mathbf{R}}\,\mathrm{d}\mathbf{k}\quad ,
\end{aligned}
$$

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

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

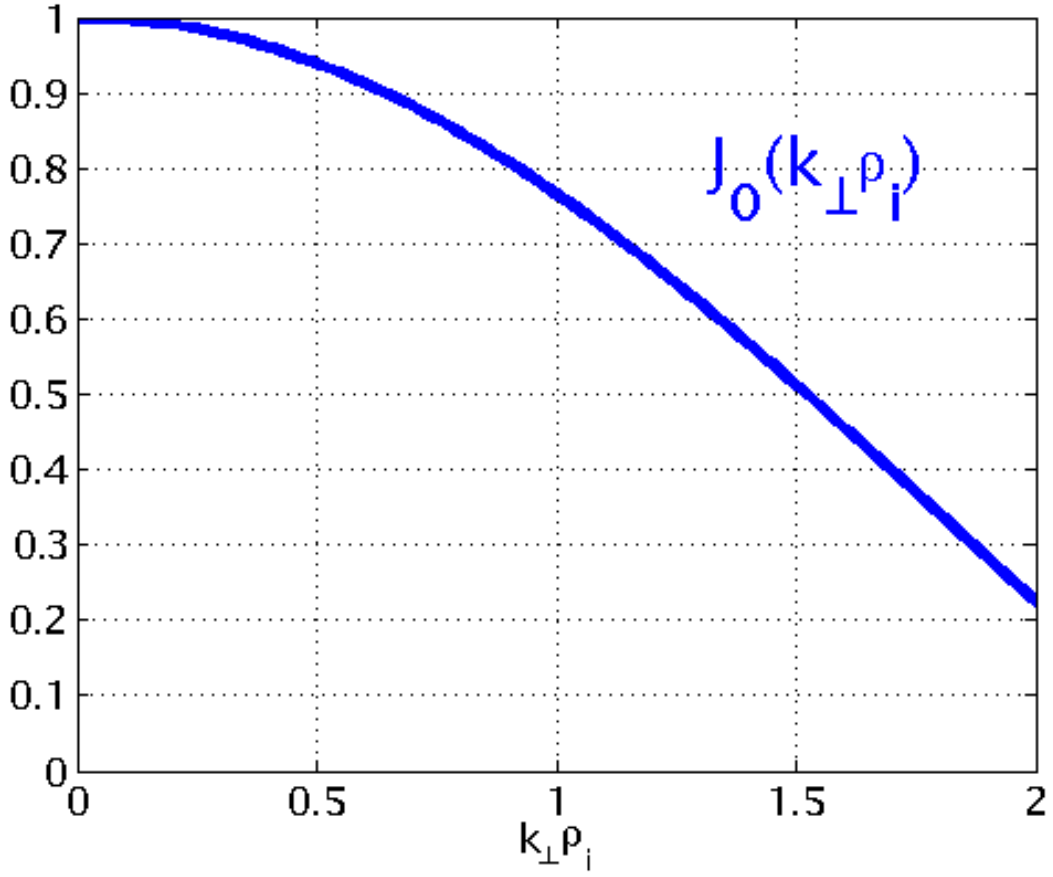
# The gyroaveraged electrostatic potential $J_0\Phi$

$$
\begin{aligned}
J_0\Phi &= \frac{1}{2\pi}\int_0^{2\pi} \Phi(\mathbf{R}+\vec{\rho}_i)\,\mathrm{d}\theta = \\
&= \frac{1}{2\pi}\int_0^{2\pi}\left(\int \frac{1}{(2\pi)^3}\,\hat{\Phi}(\mathbf{k})\,e^{i\mathbf{k}\cdot(\mathbf{R}+\vec{\rho}_i)}\,\mathrm{d}\mathbf{k}\right)\,\mathrm{d}\theta = \\
&= \int \frac{1}{(2\pi)^3}\,\hat{\Phi}(\mathbf{k})\left(\frac{1}{2\pi}\int_0^{2\pi} e^{ik_\perp\rho_i\cos(\theta)}\,\mathrm{d}\theta\right)e^{i\mathbf{k}\cdot\mathbf{R}}\,\mathrm{d}\mathbf{k} = \\
&= \frac{1}{(2\pi)^3}\int \hat{\Phi}(\mathbf{k})\,J_0\left(k_\perp\rho_i\right)\,e^{i\mathbf{k}\cdot\mathbf{R}}\,\mathrm{d}\mathbf{k}\quad ,
\end{aligned}
$$

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

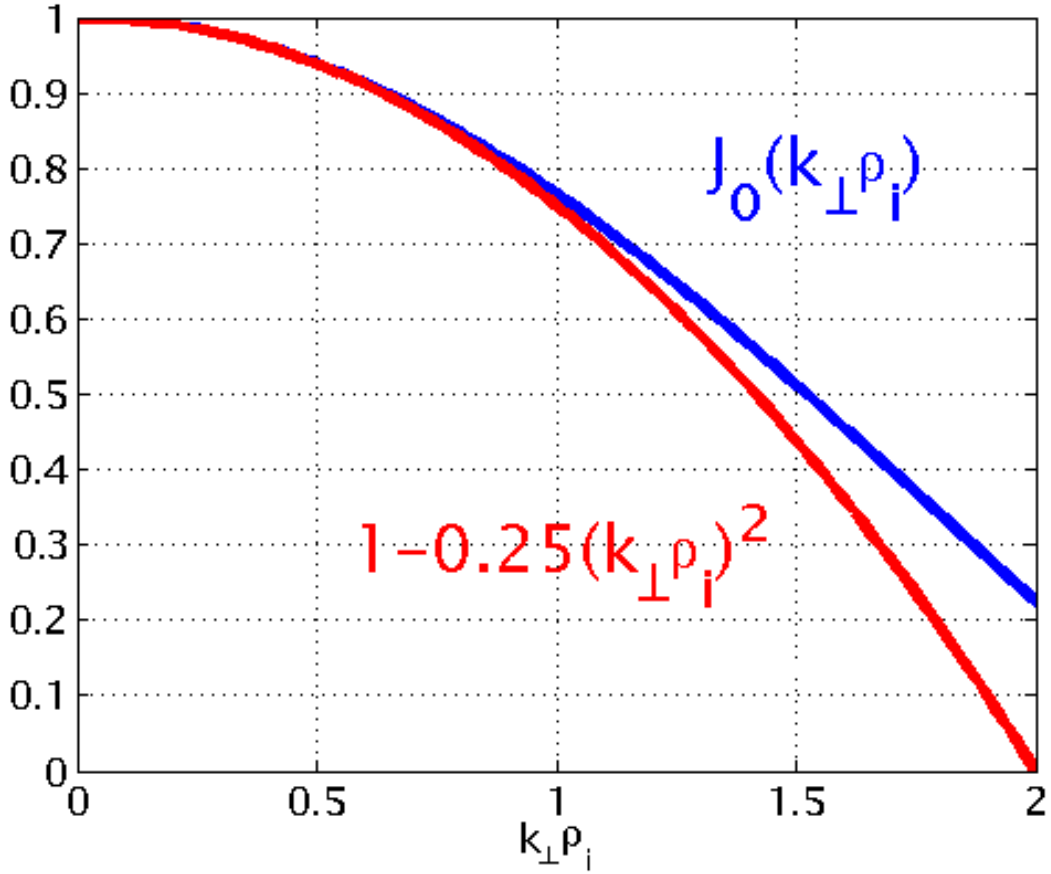
- $J_0$ has the form, in Fourier space, of a multiplication of Fourier coefficients by the zeroth Bessel functions $J_0(k_\perp\rho_i)$.

# 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 $\Phi$.

# 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].

$$J_0\Phi = \frac{1}{2\pi}\int_0^{2\pi} \Phi(\mathbf{R}+\vec{\rho})\ \mathrm{d}\theta \simeq \frac{1}{N_{avg}}\sum_{i=1}^{N_{avg}} \Phi(\mathbf{x}_i)$$

When four quadrature points are used, this procedure is equivalent to replace $J_0$ with a Taylor expansion $J_0\left(k_\perp\rho_i\right) \simeq 1 - \frac{1}{4}\left(k_\perp\rho_i\right)^2$ 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 $(i, j)$:

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

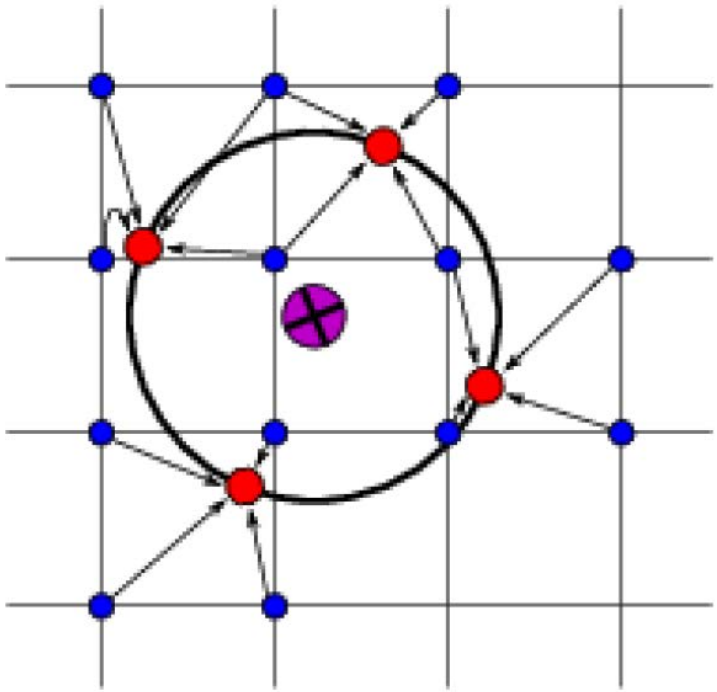
$$J_0\Phi_{i,j} \simeq \Phi_{ij} + \frac{\rho_i^2}{4h^2}(\Phi_{i+1,j} + \Phi_{i-1,j} - 2\Phi_{i,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 2\Phi_{i,j})$$

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

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

$$J_0\Phi = \frac{1}{2\pi}\int_0^{2\pi} \Phi(\mathbf{R}+\rho)\,\mathrm{d}\theta \simeq \frac{1}{4}\sum_{i=1}^{4}\Phi(\mathbf{x}_i)$$



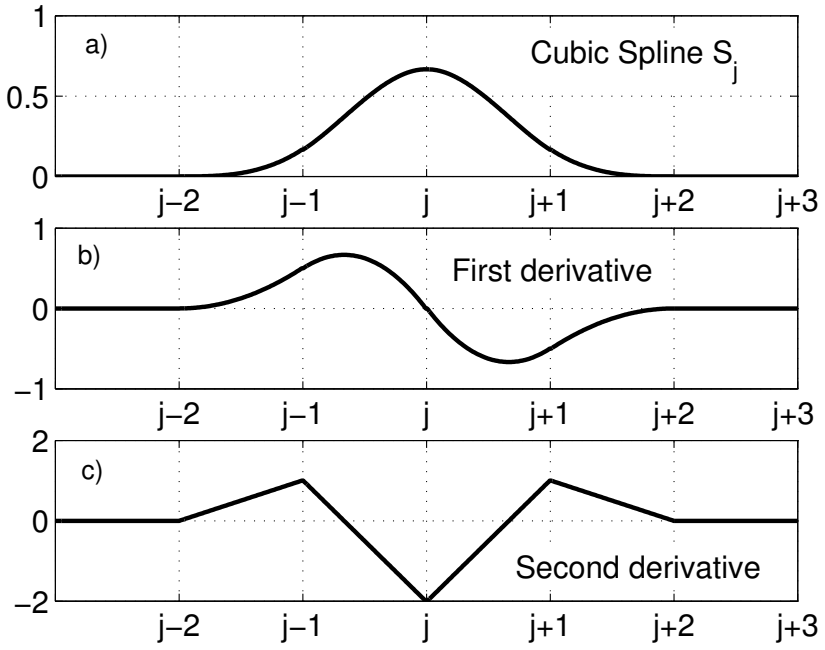
- $\Phi$ is defined on a grid (blue dots).
- interpolation to get $\Phi$ on some points ($\mathbf{x}_i$) on the ring (red dots).
- Average to get $J_0\Phi$ at the tracer position.

# Polarization (Poisson) equation, B-splines

The polarisation equation is solved using finite elements:

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

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



# Polarization (Poisson) equation, B-splines

- The polarization equation becomes:

$$\sum_{\mathrm{sp}} \sum_{\mu} \Phi_{\mu} \left( -\nabla_{\perp} \cdot \frac{n_0 m c^2}{b^2} \nabla_{\perp} \Lambda_{\mu}(\mathbf{x}) \right) = \sum_{\mathrm{sp}} \int \mathrm{d}W e J_0 f$$

- Galerkin method:

a) Multiply the equation by another test function $g(\mathbf{x}) = \Lambda_{\nu}(\mathbf{x})$.

b) Integrate the resulting equation over configuration space.

$$-\sum_{\mu} \Phi_{\mu} \int \mathrm{d}V \sum_{\mathrm{sp}} \Lambda_{\nu}(\mathbf{x}) \nabla_{\perp} \cdot \frac{n_0 m c^2}{B^2} \nabla_{\perp} \Lambda_{\mu}(\mathbf{x}) = \sum_{\mathrm{sp}} \int \mathrm{d}W \mathrm{d}V e J_0 f \Lambda_{\nu}(\mathbf{x})$$

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:

$$-\sum_{\mu}\Phi_{\mu}\sum_{\mathrm{sp}}\int \mathrm{d}\mathbf{R}\Lambda_{\nu}(\mathbf{R})\nabla_{\perp}\cdot\frac{n_0 mc^2}{B^2}\nabla_{\perp}\Lambda_{\mu}(\mathbf{R}) =$$

$$\sum_{\mathrm{sp}}\left(e\sum_{k=1}^{N}w_k\frac{1}{N_{gr,k}}\sum_{\beta=1}^{N_{gr,k}}\Lambda_{\nu}(\mathbf{x}_{k,\beta})\right)$$

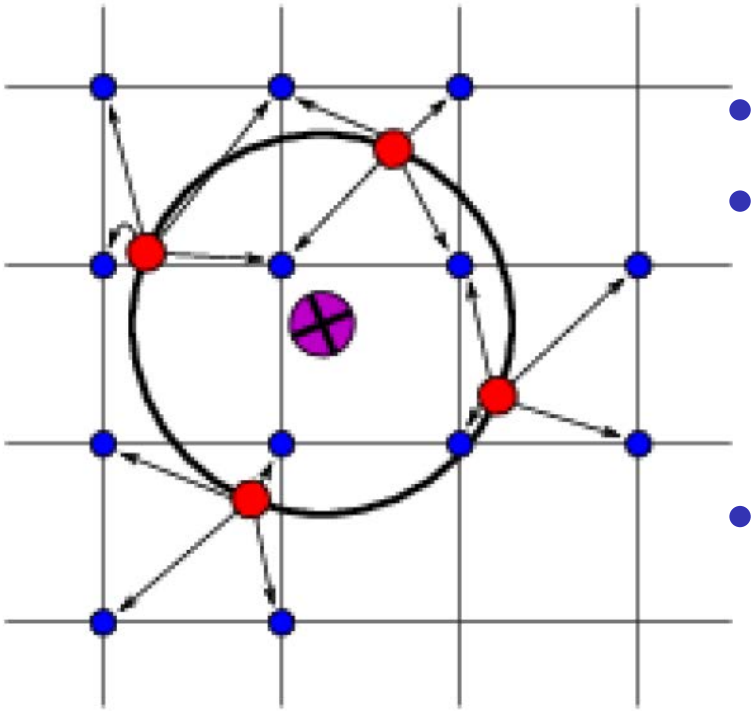
- The previous equation is actually a set of linear equations:

$$\sum_{\mu}A_{\mu\nu}\Phi_{\mu} = b_{\nu}$$

- $A_{\mu\nu}$ is a sparse, symmetric and positive definite matrix

# Charge assignment, linear B-splines

$$\sum_{\mathrm{sp}} \left( e \sum_{k=1}^{N} \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} w_k \Lambda_\nu(\mathbf{x}_{k,\beta}) \right)$$



- Scatter operation
- each smaple 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:

$$A_{\mu\nu} = -\sum_{\mu} \Phi_{\mu} \sum_{\mathrm{sp}} \int \mathrm{d}\mathbf{R} \Lambda_{\nu}(\mathbf{R}) \nabla_{\perp} \cdot \frac{n_0 m c^2}{B^2} \nabla_{\perp} \Lambda_{\mu}(\mathbf{R})$$

- Initialize marker positions and weights:

$\mathbf{R_k}(0) = \mathbf{R_k}^0, \;\; \mu_k, \;\; p_{\|k}(0) = p^0_{\|k}, \;\; w_k$

# Skeleton of a finite element PIC code

Main loop:

- Charge assignment:

$$b_\nu = \sum_{\mathrm{sp}} \left( e \sum_{k=1}^{N} w_k \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} \Lambda_\nu(\mathbf{x}_{k,\beta}) \right)$$

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

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

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

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

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

# Control variate PIC ($\delta f$ method)

$$f(\mathbf{R}, v_{\|}, \mu, t) = f_0(\psi_0, \epsilon, \mu, t) + \delta f(\mathbf{R}, v_{\|}, \mu, t)$$

• Particle kinetic energy $\epsilon = m_i\ (\mu B + U^2/2)$, the magnetic momentum $\mu$ and the toroidal canonical momentum $\psi_0 = \psi + (m_i/q_i) R v_\varphi$ 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:

$$\begin{aligned} f &\simeq f_0 + \delta f_N(\mathbf{R}(t), p_{\|}(t), \mu) \\ &= f_0 + \sum_{k=1}^{N} w_k \delta(\mathbf{R} - \mathbf{R}_k(t)) \delta(p_{\|} - p_{\|k}(t)) \delta(\mu - \mu_k) \end{aligned}$$

# Control variate PIC ($\delta f$ method)

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

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

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

and consequently for the weights:

$$\dot{w}_k = \tau(J_0 \Phi)|_k$$

# Skeleton of a finite element PIC code

Main loop:

- Charge assignment:

$$b_\nu = \sum_{\mathrm{sp}} \left( e \sum_{k=1}^{N} w_k \frac{1}{N_{gr,k}} \sum_{\beta=1}^{N_{gr,k}} \Lambda_\nu(\mathbf{x}_{k,\beta}) \right)$$

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

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

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

$$\begin{aligned} \dot{\mathbf{R}}_k &= \ldots \\ \dot{p_{\|}}_k &= \ldots \\ \dot{w}_k &= \tau(J_0\Phi)|_k \end{aligned}$$

# 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, $\epsilon \simeq \sigma/\sqrt{N}$

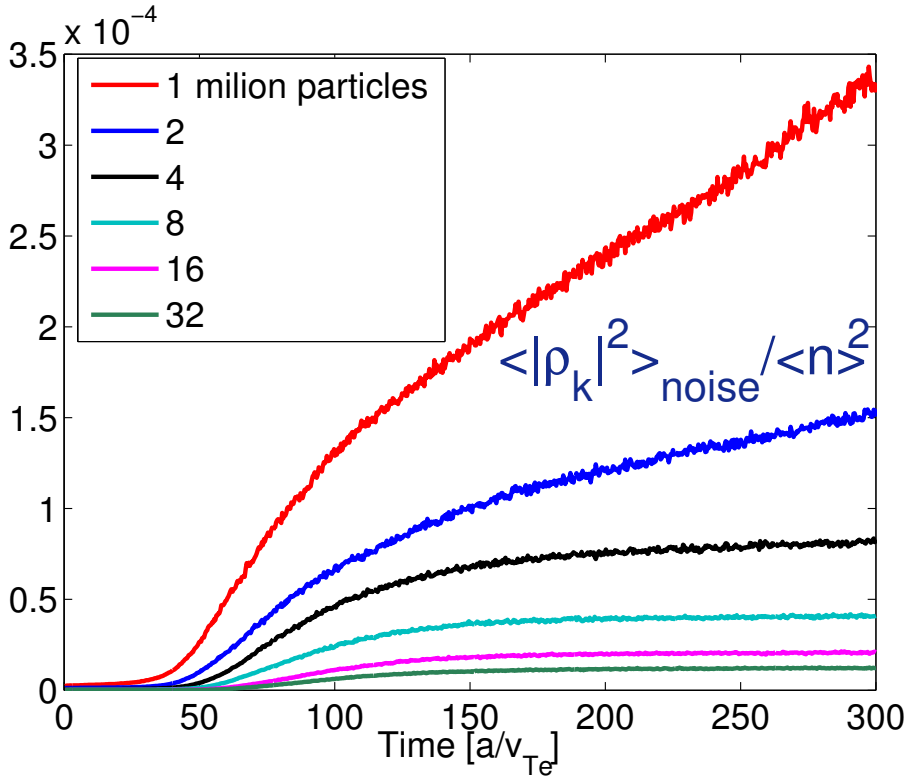
$$\rho^2_{noise} \simeq \frac{N_G}{N}\langle w^2\rangle G \quad ; \qquad \langle w^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} w_i^2$$

  $N_G$, 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. $G$.

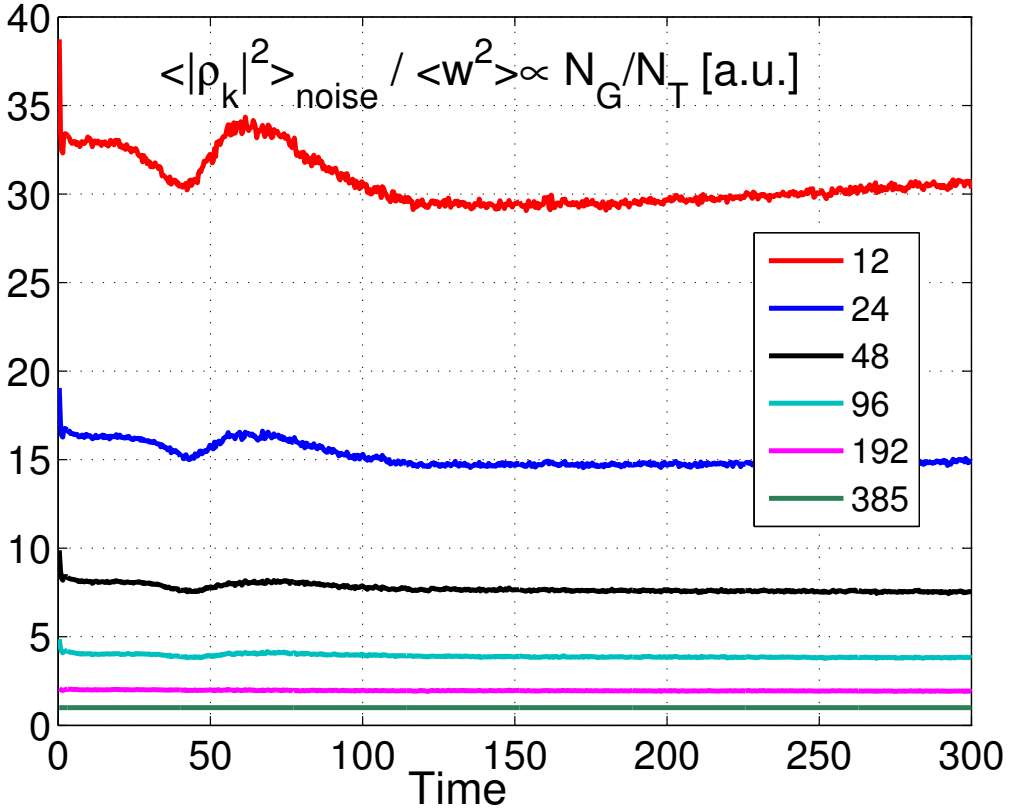
# The statistical appears in the charge assignment

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




*Level of noise*, $\rho_e^* = 1/80$

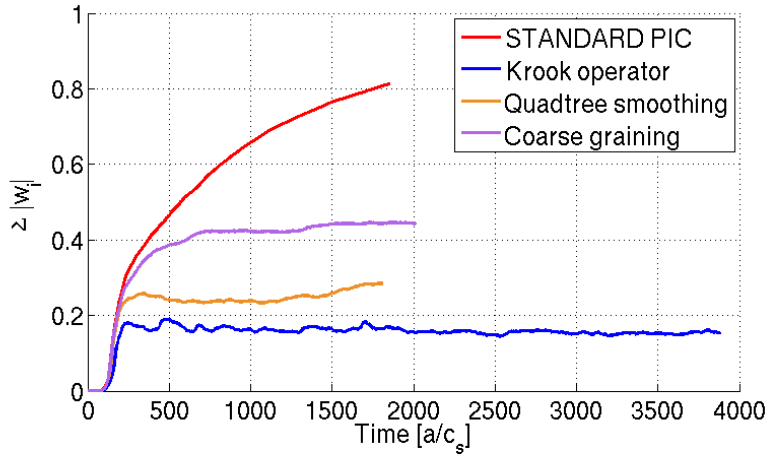
# MC estimate validation: noise scaling with $N/N_G$

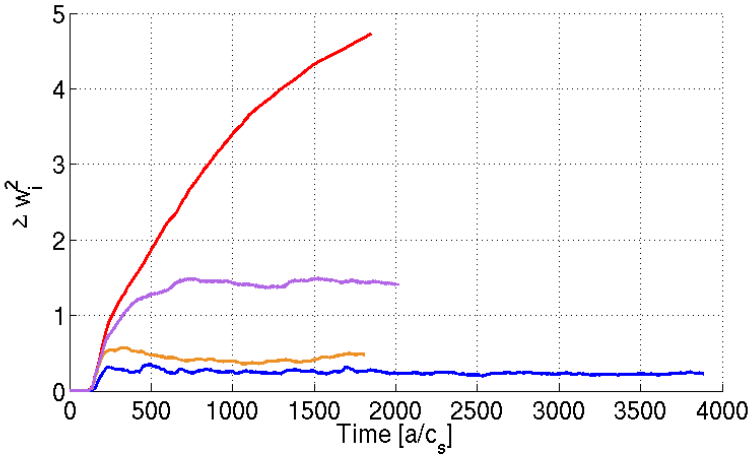


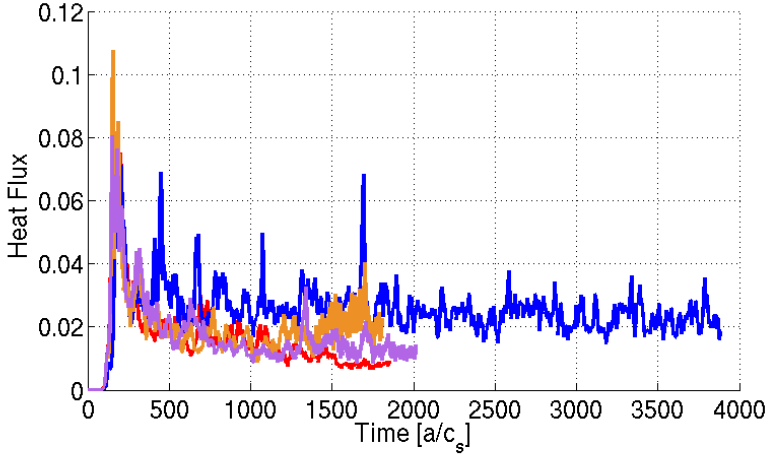

The scaling of the turbulence in number of particles per mode $N_G/N$ is satisfied

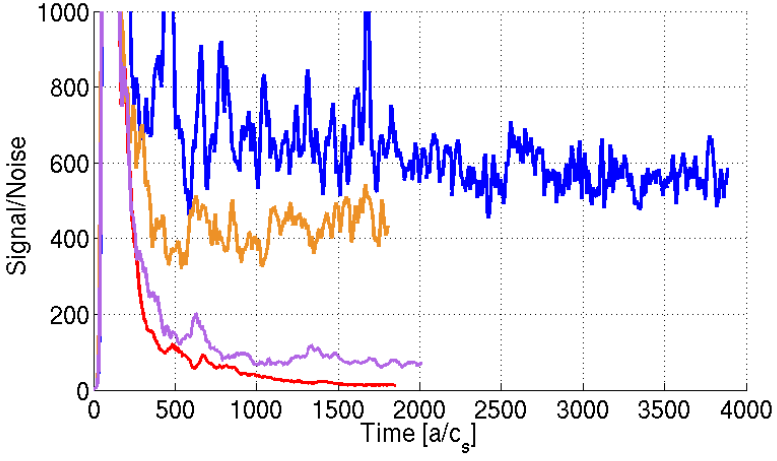
$$\frac{\rho^2_{noise}}{\langle w^2 \rangle} \simeq \frac{N_G}{N} G$$

# Variance reduction techniques (Monte-Carlo)



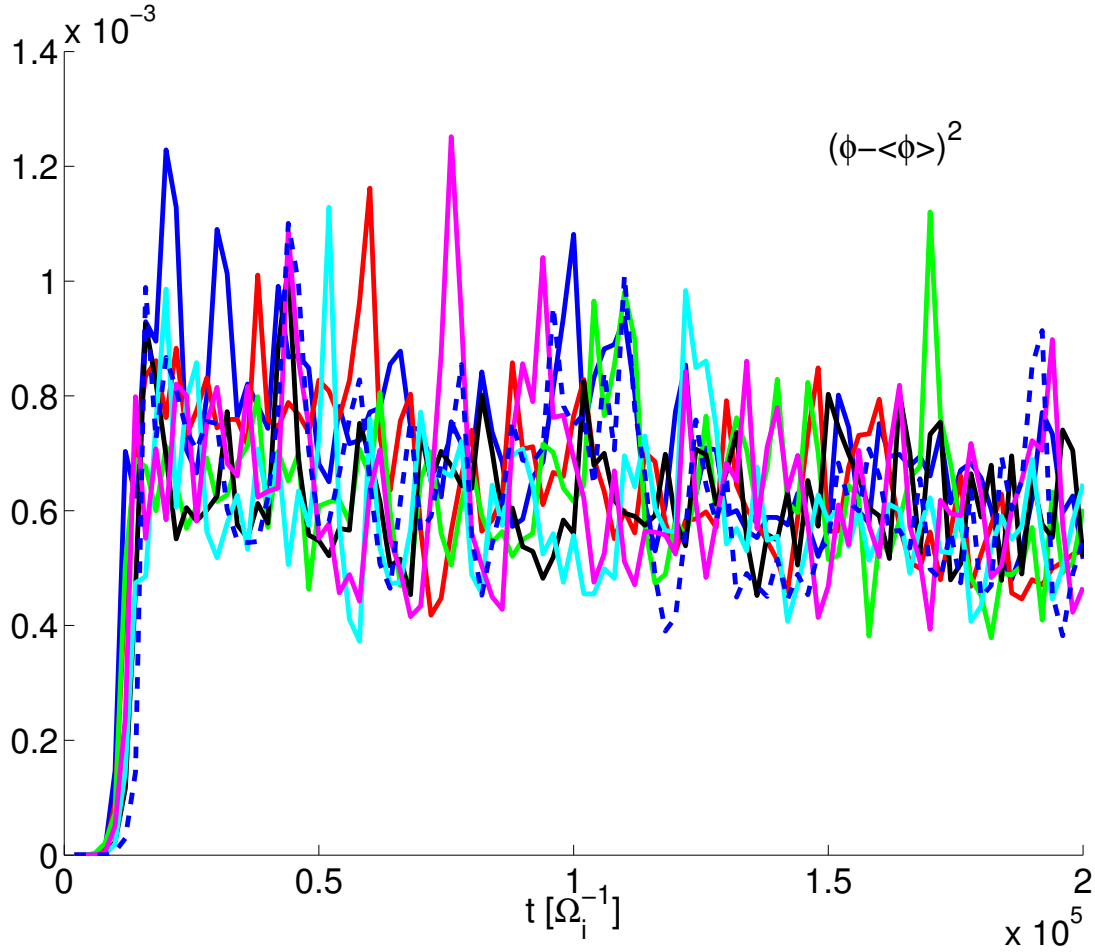




- Very long simulations; Different heat sources $\rightarrow$ different fluxes.

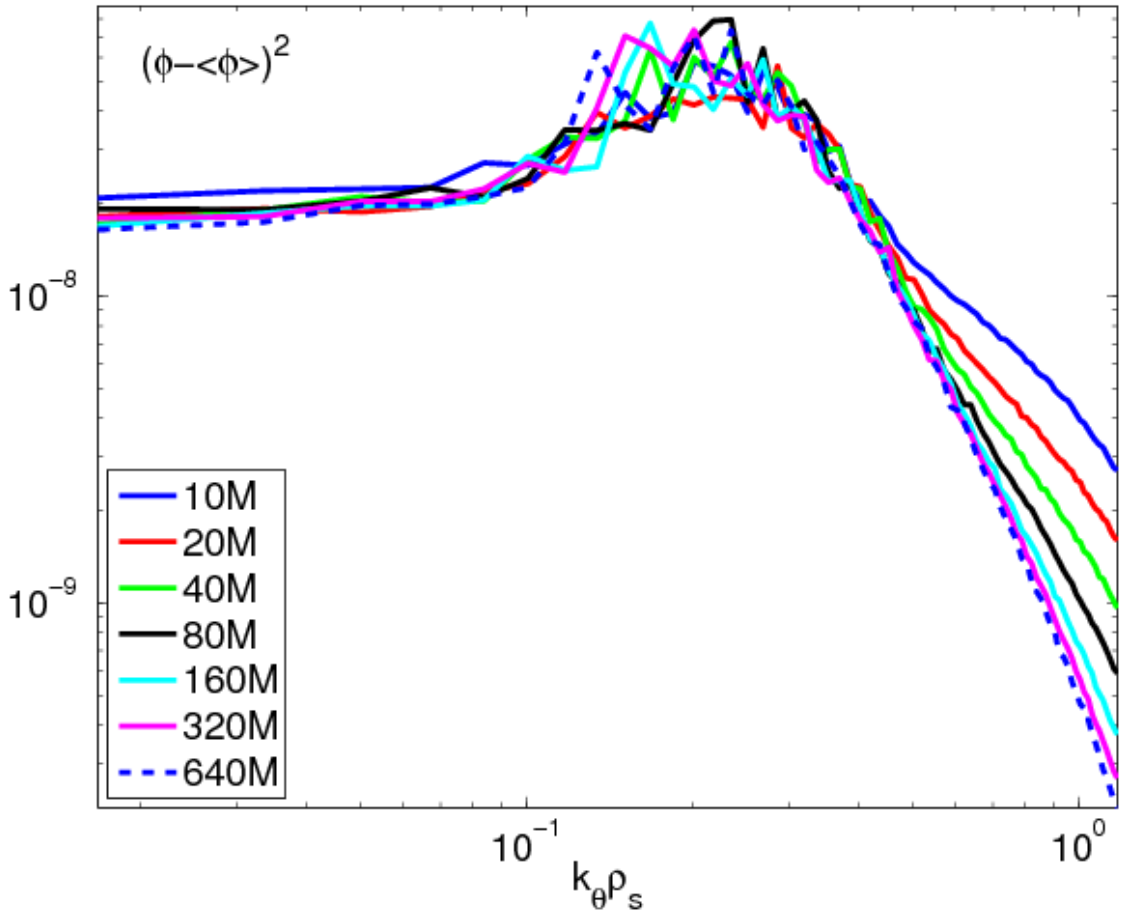
# Convergence in number of markers N

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



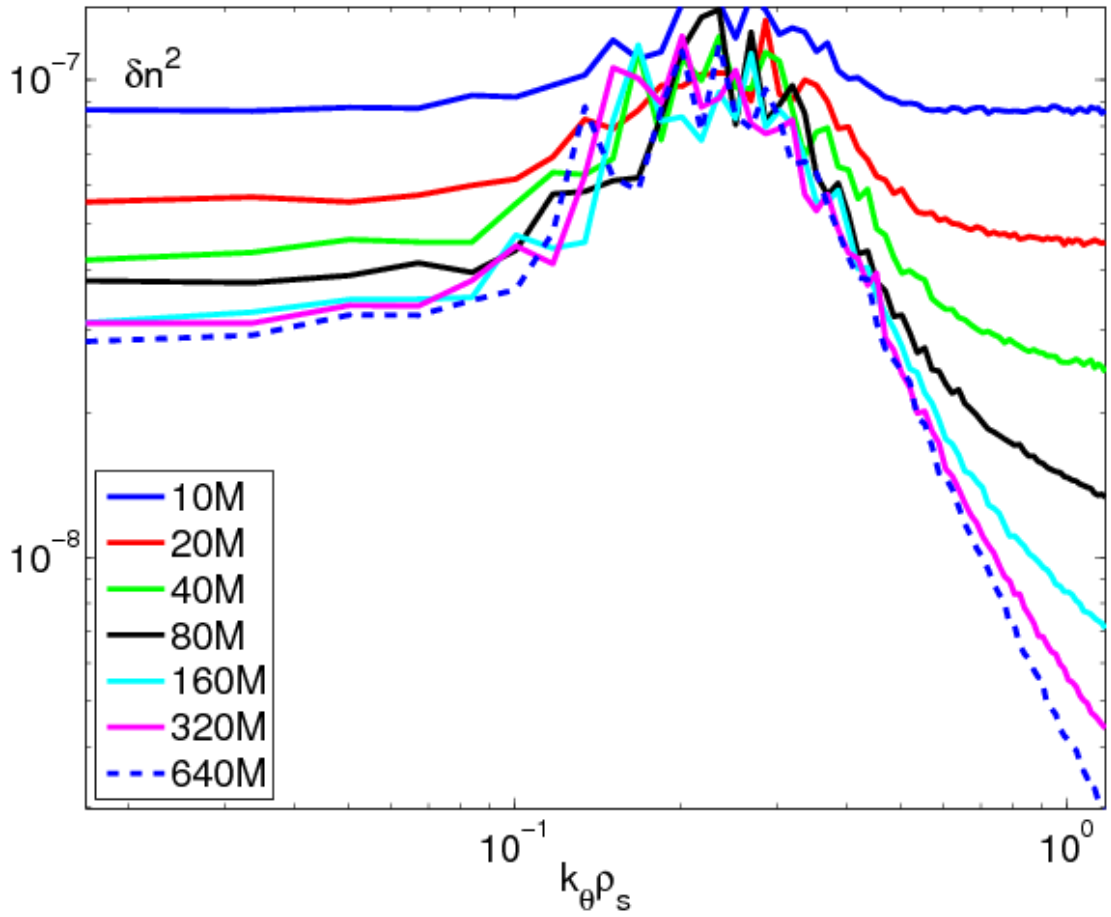
# Spectra give good insights on the quality of the simulation

- Time averaged spectrum: nonzonal electrostatic potential



# Density fluctuation spectrum, slow converge in N

- Time averaged spectrum: density fluctuation



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

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