The numerics behind electromagnetic gyrokinetic particle-in-cell simulation — the cancellation problem resolved

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Outline

- The Vlasov-Maxwell equations
- The PIC method
- Discretization of the PIC method
- The cancellation problem
- Control variates as variance reduction method
- The adjustable control variate (ACV)
- Numerical results
- Summary

The Vlasov equation

The usual basis for kinetic treatments of a collisionless plasma is the Vlasov equation:

$$\frac{\partial \hat{f}_s}{\partial t} + \mathbf{v} \cdot \frac{\partial \hat{f}_s}{\partial \mathbf{x}} + \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial \hat{f}_s}{\partial \mathbf{v}} = 0$$

Here, $\hat{f}_s(\mathbf{x}, \mathbf{v}, t)$ is the distribution function of the sth species in six-dimensional phase space with the spatial coordinate $\mathbf{x}$ and the velocity coordinate $\mathbf{v}$.

The Vlasov equation can be written in the following form:

$$\frac{\mathrm{D}\hat{f}_s}{\mathrm{D}t} \overset{\text{def}}{=} \frac{\partial \hat{f}_s}{\partial t} + \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \cdot \frac{\partial \hat{f}_s}{\partial \mathbf{x}} + \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \cdot \frac{\partial \hat{f}_s}{\partial \mathbf{v}} = 0$$

where

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \quad , \quad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \qquad \textbf{equations of motion} \qquad (1)$$

Its short form $\mathrm{D}\hat{f}_s/\mathrm{D}t = 0$ means that the total derivative vanishes along the characteristics given by the integration of Eqs. (1).

In physical terms:
If we follow the particles along their trajectories by integrating the equations of motion, Eqs. (1), in six-dimensional phase space, the initial value of $\hat{f}_s(\mathbf{x}(t_0), \mathbf{v}(t_0))$ will not change.

This method is well known by the name "method of characteristics" and can be used to evolve $\hat{f}_s$ in time (initial value problem).

The Vlasov-Maxwell equations

The self-consistent electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ which appear in the force law are calculated from Poisson's equation and Ampère's law, two of the Maxwell equations:

$$\epsilon_0 \nabla \cdot \mathbf{E} = \varrho \qquad \nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

Here, the charge density ϱ and current density $\mathbf{j}$ are to be obtained at each point in space from the appropriate moments of the distribution function itself:

$$\varrho(\mathbf{x}, t) = \sum_s q_s \int \hat{f}_s \, \mathrm{d}^3 v \qquad \mathbf{j}(\mathbf{x}, t) = \sum_s q_s \int \mathbf{v} \hat{f}_s \, \mathrm{d}^3 v$$

where the summation is over the species of particles present in the plasma.

The PIC method

The Particle-In-Cell method (PIC) is a numerical technique used to solve a certain class of partial differential equations:

- Individual (macro) particles in a Lagrangian frame are traced in continuous phase space
- Moments of the distribution function are computed simultaneously on a Eulerian (stationary) mesh to solve the self-consistent field equations

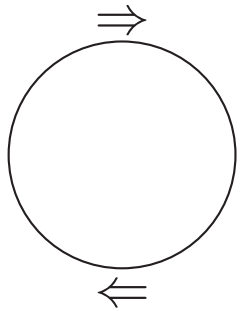
The PIC method is a so-called Particle-Mesh (PM) method which includes interactions of particles only through the average fields.

Area of application in plasma physics:
laser-plasma interactions, electron acceleration and ion heating in the auroral ionosphere, magnetic reconnection, . . ., gyrokinetics

Schematic diagram of the PIC method

Integration of the equations of motion

Interpolation of the fields from the mesh to the particle locations



Interpolation of charge and current source terms onto the potential mesh

Computation of the potentials on the mesh

Monte Carlo evaluation of integrals

Of special interest is the evaluation of moments of the distribution function f over the phase space volume V, i.e. general integrals of the form

$$I(\Lambda) \stackrel{\text{def}}{=} \int_V \Lambda(\mathbf{z}) f(\mathbf{z}) \, \mathrm{d}\mathbf{z}$$

where $\Lambda(\mathbf{z})$ is a general function of the phase-space coordinates $\mathbf{z}$.
For example, $I(\Lambda)$ would be the number density in configuration space if $\Lambda = 1$, and the integral is evaluated over the velocity space.

The sampling distribution of our Monte-Carlo sampling points (marker) is done by a continuous probability density function $g(\mathbf{z})$ such that

$$\int_V g(\mathbf{z}) \, \mathrm{d}\mathbf{z} = 1$$

Now, the integral for $I(\Lambda)$ can be written in the following form

$$\mathcal{E}[\lambda(\mathbf{z})] \stackrel{\text{def}}{=} \int_V \lambda(\mathbf{z}) g(\mathbf{z})\,\mathrm{d}\mathbf{z} \qquad \textbf{where} \qquad \lambda(\mathbf{z}) \stackrel{\text{def}}{=} \frac{\Lambda(\mathbf{z}) f(\mathbf{z})}{g(\mathbf{z})}$$

and $\mathcal{E}[\lambda]$ is the expected value of the random variable λ. In addition, we define the variance of λ by

$$\sigma^2 \equiv \mathcal{V}[\lambda(\mathbf{z})] \stackrel{\text{def}}{=} \int_V \{\lambda(\mathbf{z}) - \mathcal{E}[\lambda(\mathbf{z})]\}^2 g(\mathbf{z})\,\mathrm{d}\mathbf{z}$$

The crude Monte-Carlo estimator for the integral $I(\Lambda)$ is given by the sum over the marker weights w_n

$$I(\Lambda) = \frac{1}{N}\sum_{n=1}^{N} \Lambda(\mathbf{z}_n) w_n \pm \epsilon \qquad \textbf{where} \qquad \epsilon \stackrel{\text{def}}{=} \frac{\sigma}{\sqrt{N}}, \qquad w_n \stackrel{\text{def}}{=} \frac{f(\mathbf{z}_n)}{g(\mathbf{z}_n)}$$

Liouville's theorem

A phase space volume $\Omega_p \overset{\text{def}}{=} \Omega(\mathbf{z}_p)$ moving in phase space according to the equations of motion does not change its volume, although in general it can change its shape (Liouville's theorem):

$$\int_{\Omega_p} \mathrm{d}\mathbf{z} = \textbf{const.}$$

As the marker distribution and phase space volumes Ω_p are related by

$$g_p = \frac{V}{\Omega_p} = \textbf{const.}$$

it follows for the marker weights from $f_p = \textbf{const.}$ that

$$w_p = \frac{f_p}{g_p} = \textbf{const.}$$

The gyrokinetic Vlasov equation (W.W. Lee, 1983)

The average of the Vlasov equation over the fast gyro-motion leaves just the guiding center motion and thus reduces the dimensionality of the problem:

$$\frac{\partial f_s}{\partial t} + \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t} \cdot \frac{\partial f_s}{\partial \mathbf{R}} + \frac{\mathrm{d}v_\parallel}{\mathrm{d}t} \cdot \frac{\partial f_s}{\partial v_\parallel} = 0 \quad ; \quad \frac{\mathrm{d}\mu}{\mathrm{d}t} = 0 \quad , \quad \mu \stackrel{\mathrm{def}}{=} \frac{v_\perp^2}{2B}$$

Here, $f_s(\mathbf{R}, v_\parallel, \mu, t)$ is the guiding center distribution function of the sth species in the reduced five-dimensional phase space with the guiding center coordinate $\mathbf{R}$ and the parallel velocity coordinate $v_\parallel$ and the magnetic moment μ.

$$v_{\mathrm{gc}}(\langle\phi\rangle, \langle\mathbf{A}\rangle) \stackrel{\mathrm{def}}{=} \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}, \quad a_{\mathrm{gc}}(\langle\phi\rangle, \langle\mathbf{A}\rangle) \stackrel{\mathrm{def}}{=} \frac{\mathrm{d}v_\parallel}{\mathrm{d}t}$$ **guiding center velocity/acceleration**

with the gyro-averaged electrostatic and magnetic potentials $\langle\phi\rangle$ and $\langle\mathbf{A}\rangle$.

The discretized f

The full-f PIC approximation is given by a sum of δ functions:

$$f(\mathbf{R}, v_\parallel, \mu, t) = \sum_{p=1}^{N} \frac{w_p}{\mathcal{J}_{\mathrm{red}}} \delta(\mathbf{R} - \mathbf{R}_p(t))\, \delta(v_\parallel - v_{\parallel p}(t))\, \delta(\mu - \mu_p(t_0))$$

with the Jacobian in the reduced phase space $\mathcal{J}_{\mathrm{red}} = 2\pi B^\star_\parallel$.

Each marker (macro particle, tracer, ...) p is defined by:

- **its position in the 5-dim phase space $(\mathrm{R}_p, v_{\parallel p}, \mu_p)$**
- **its phase-space volume Ω_p assigned by the initial marker distribution $g(t_0)$**
- **its constant weight w_p**
- **its averaged value of $f_p = w_p/\Omega_p$ over the phase-space volume Ω_p**

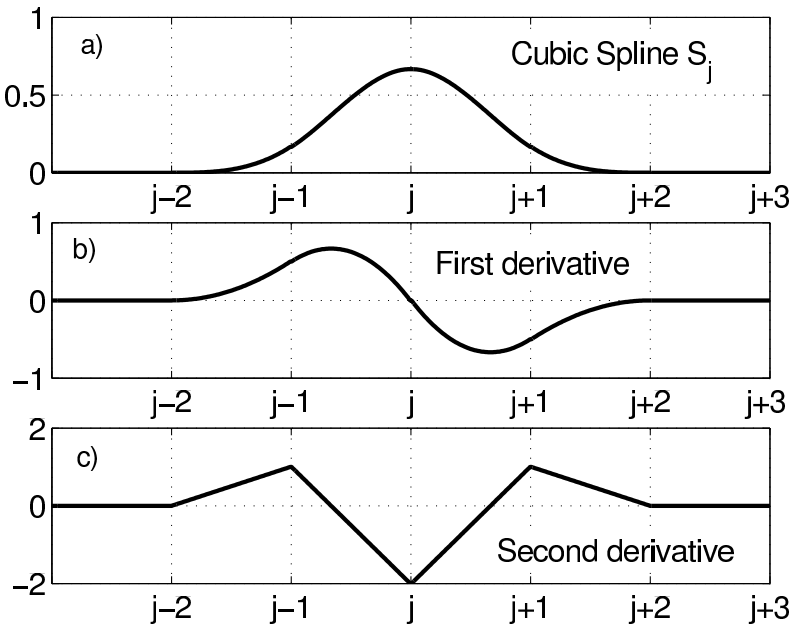
Discretization of parallel Ampère's law

The Helmholtz type Ampère's law equation is discretized with a finite element method:

$$A_{\parallel}(\mathbf{x},t) = \sum_{\nu} A_{\parallel\nu}(t)\Lambda_{\nu}(\mathbf{x})$$

where $\Lambda_{\mu}(\mathbf{x})$ is a product of unidimensional B-splines S of order k:

$$\Lambda_{\mu}(\mathbf{x}) = B_l^k(r)B_m^k(\chi)B_n^k(\varphi)$$



Tensor product of B-splines:

B-splines can be extended to higher dimensions, e.g. three dimensions:

$$B_{lmn}(\mathbf{x}) \stackrel{\text{def}}{=} B_l(x)\, B_m(y)\, B_n(z)$$

Monograph: Carl de Boor, A practical guide to splines, Revised edition, Springer-Verlag 2001.

Advantages of finite elements (B-splines):

- **Conservation laws, e.g. particle number and energy conservation for PIC are consistently preserved**
- **Complicated geometries and non-equidistant meshes are easy to implement**

Discretization of Ampère's law using Galerkin's method

$$-\nabla_\perp \cdot \left[(1-\beta_\mathrm{i})\nabla_\perp A_\parallel\right] + \left(\frac{\beta_\mathrm{i}}{\rho_\mathrm{i}^2} + \frac{\beta_\mathrm{e}}{\rho_\mathrm{e}^2}\right) A_\parallel = \mu_0 \left(\langle j_{\parallel\mathrm{i}}\rangle + j_{\parallel\mathrm{e}}\right)$$

1. Insert the discretized form of $A_\parallel(\mathbf{x},t) = \sum_{\nu'} A_{\parallel\nu'}(t)\Lambda_{\nu'}(\mathbf{x})$
2. Multiply the equation by a test function $\Lambda_\nu(\mathbf{x})$
3. Integrate the whole equation over the entire plasma volume

LHS:

$$\sum_{\nu'} \int \left[(1-\beta_\mathrm{i})\nabla_\perp\Lambda_\nu \cdot \nabla_\perp\Lambda_{\nu'} + \left(\frac{\beta_\mathrm{i}}{\rho_\mathrm{i}^2} + \frac{\beta_\mathrm{e}}{\rho_\mathrm{e}^2}\right)\Lambda_\nu\Lambda_{\nu'}\right] \mathrm{d}\mathbf{x}\; A_{\parallel\nu'}(t) \stackrel{\mathrm{def}}{=} \sum_{\nu'} \left[L_{\nu\nu'} + S_{\nu\nu'}\right] A_{\parallel\nu'}$$

Polarization density (Laplacian operator): integrated by parts (weak form)
$\Rightarrow$ Discretization consists of B-splines and B-spline first derivatives only

Discretization of $\langle j_{\|\mathrm{i}} \rangle$ at RHS:

$$\sum_{p=1}^{N} v_{\|\mathrm{i}p} w_{\mathrm{i}p} \frac{1}{2\pi} \int_0^{2\pi} \int \Lambda_\nu(\mathbf{x})\, \delta(\mathbf{R}_{\mathrm{i}p} + \boldsymbol{\rho}_{\mathrm{i}p} - \mathbf{x})\, \mathrm{d}\mathbf{x}\, \mathrm{d}\alpha = \sum_{p=1}^{N} v_{\|\mathrm{i}p} w_{\mathrm{i}p} \frac{1}{2\pi} \int_0^{2\pi} \Lambda_\nu(\mathbf{R}_{\mathrm{i}p} + \boldsymbol{\rho}_{\mathrm{i}p})\, \mathrm{d}\alpha$$

using

1. **The definition of the gyro-averaged ion current which smears out the density along the gyro-ring of radius ρ_i:**

$$\langle j_{\|\mathrm{i}} \rangle \overset{\mathrm{def}}{=} \int v_{\|\mathrm{i}} f_\mathrm{i}\, \delta(\mathbf{R} + \boldsymbol{\rho}_\mathbf{i} - \mathbf{x})\, \mathrm{d}^6\mathbf{Z} = \int v_{\|\mathrm{i}} f_\mathrm{i}\, \delta(\mathbf{R} + \boldsymbol{\rho}_\mathbf{i} - \mathbf{x})\, B_\|^\star\, \mathrm{d}\mathbf{R}\, \mathrm{d}v_\|\, \mathrm{d}\mu\, \mathrm{d}\alpha$$

2. **The discretized f_i:**

$$f_\mathrm{i} = \sum_{p=1}^{N} \frac{1}{2\pi B_\|^\star} w_{\mathrm{i}p}(t)\, \delta(\mathbf{R} - \mathbf{R}_{\mathrm{i}p}(t))\, \delta(v_\| - v_{\|\mathrm{i}p}(t))\, \delta(\mu - \mu_{\mathrm{i}p}(t_0))$$

The interpolation of the current onto the grid

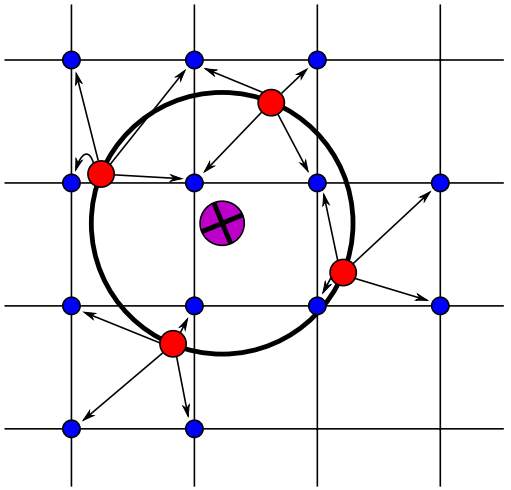
The construction of the RHS is the so-called current assignment:

$$j_{\parallel \mathrm{i}\nu}(t) \stackrel{\mathrm{def}}{=} \sum_{p=1}^{N} v_{\parallel \mathrm{i}p} w_{\mathrm{i}p} \frac{1}{2\pi} \int_0^{2\pi} \Lambda_\nu(\mathbf{R}_{\mathrm{i}p} + \boldsymbol{\rho}_{\mathrm{i}p}) \, \mathrm{d}\alpha$$

Projection of the weights $w_{\mathrm{i}p}$ in the form of gyro-rings onto the B-spline basis.

The charge assignment is a scatter operation, e.g. each sample point contributes to 64 grid points for cubic B-splines in 3-dim.

The figure shows linear interpolation for linear B-splines in 2-dim.



The interpolation of $\nabla\langle A_\parallel \rangle$ from the grid

The gyro-averaged magnetic potential $\langle A_\parallel \rangle$ is defined by:

$$\langle A_\parallel \rangle \overset{\text{def}}{=} \frac{1}{2\pi} \int_0^{2\pi} \int A_\parallel(\mathbf{x})\, \delta(\mathbf{R} + \boldsymbol{\rho}_\text{i} - \mathbf{x})\, \mathrm{d}\mathbf{x}\, \mathrm{d}\alpha = \frac{1}{2\pi} \int_0^{2\pi} A_\parallel(\mathbf{R} + \boldsymbol{\rho}_\text{i})\, \mathrm{d}\alpha$$

The gyro-averaged $\nabla\langle \mathbf{A}_\parallel \rangle$ is defined by:

$$\nabla\langle \mathbf{A}_\parallel \rangle \overset{\text{def}}{=} \nabla_\mathbf{R} \langle A_\parallel \rangle = \frac{1}{2\pi} \int_0^{2\pi} \nabla_\mathbf{R} A_\parallel(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{R}+\boldsymbol{\rho}_\text{i}} \mathrm{d}\alpha + \mathcal{O}(\epsilon_\text{B})$$

Inserting the discretized form of $A_\parallel(\mathbf{x}, t) = \sum_\nu A_{\parallel\nu}(t) \Lambda_\nu(\mathbf{x})$ gives:

$$\nabla\langle \mathbf{A}_\parallel \rangle = \sum_\nu \frac{A_{\parallel\nu}}{2\pi} \int_0^{2\pi} \nabla\Lambda(\mathbf{R} + \boldsymbol{\rho}_\text{i})\, \mathrm{d}\alpha + \mathcal{O}(\epsilon_\text{B})$$

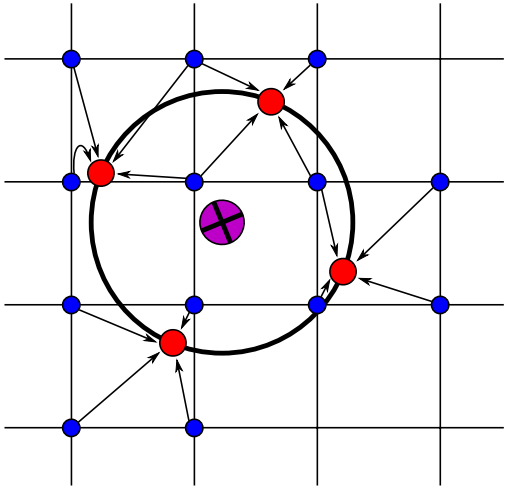
The gyro-averaged $\nabla\langle \mathbf{A}_\parallel \rangle$ is an analytic differential of the potential represented by the B-splines, i.e., the gradient is computed exactly using:

$$\nabla\Lambda_\nu(s,\vartheta,\varphi) = \frac{\partial\Lambda_\nu}{\partial s}\nabla s + \frac{\partial\Lambda_\nu}{\partial\vartheta}\nabla\vartheta + \frac{\partial\Lambda_\nu}{\partial\varphi}\nabla\varphi$$

The N_{av} field vectors $\nabla\mathbf{A}_{\parallel n}$ on the gyro-ring are calculated from the B-spline representation of the potential and then averaged.

The $\nabla\mathbf{A}_{\parallel n}$ calculation is a gather operation, e.g. each sample point is assembled from 64 grid points for cubic B-splines in 3-dim.

The figure shows linear interpolation for linear B-splines in 2-dim.



The cancellation problem

The electron distribution function f_e includes an adiabatic (Boltzmann) part responding to $A_\parallel$:

$$\delta f_\mathrm{e} = \delta f_\mathrm{e}^\mathrm{ad} + \delta f_\mathrm{e}^\mathrm{nonad} \qquad \textbf{where} \qquad \delta f_\mathrm{e}^\mathrm{ad} = -\frac{e v_\parallel f_{0\mathrm{e}}}{k_\mathrm{B} T_\mathrm{e}} A_\parallel$$

The electron skin term in Ampère's law coincides with the adiabatic current term:

$$\frac{\beta_\mathrm{e}}{\rho_\mathrm{e}^2} A_\parallel = \frac{\mu_0 n_0 e^2}{m_\mathrm{e}} A_\parallel = -\mu_0 e \int \mathrm{d}^6 Z \, \delta f_\mathrm{e}^\mathrm{ad} \, v_\parallel \, \delta(\mathbf{R} - \mathbf{x}) = \mu_0 j_{\parallel\mathrm{e}}^\mathrm{ad}$$

$$\Downarrow$$

In theory the skin terms cancel the adiabatic current terms.

$$-\nabla_\perp \cdot \left[(1 - \beta_\mathrm{i}) \nabla_\perp A_\parallel \right] = \mu_0 \left(\langle j_{\parallel\mathrm{i}} \rangle^\mathrm{nonad} + j_{\parallel\mathrm{e}}^\mathrm{nonad} \right)$$

The PIC method expresses inseparably the adiabatic and nonadiabatic current.

$$\Downarrow$$

Signal-to-noise problem when adiabatic current dominates.

$$\frac{j_{\|\mathrm{e}}^{\mathrm{ad}}}{\langle j_{\|\mathrm{i}}\rangle^{\mathrm{nonad}} + j_{\|\mathrm{e}}^{\mathrm{nonad}}} \approx \frac{\beta_{\mathrm{e}}/\rho_{\mathrm{e}}^2 A_{\|}}{\nabla_{\perp}^2 A_{\|}} \propto \frac{n_0 A_{\|}}{\nabla_{\perp}^2 A_{\|}}$$

Due to the signal-to-noise problem the numerical cancellation of the skin terms is inaccurate which is called the "cancellation problem".

The nonadiabatic part is the minor part of the total electron distribution for

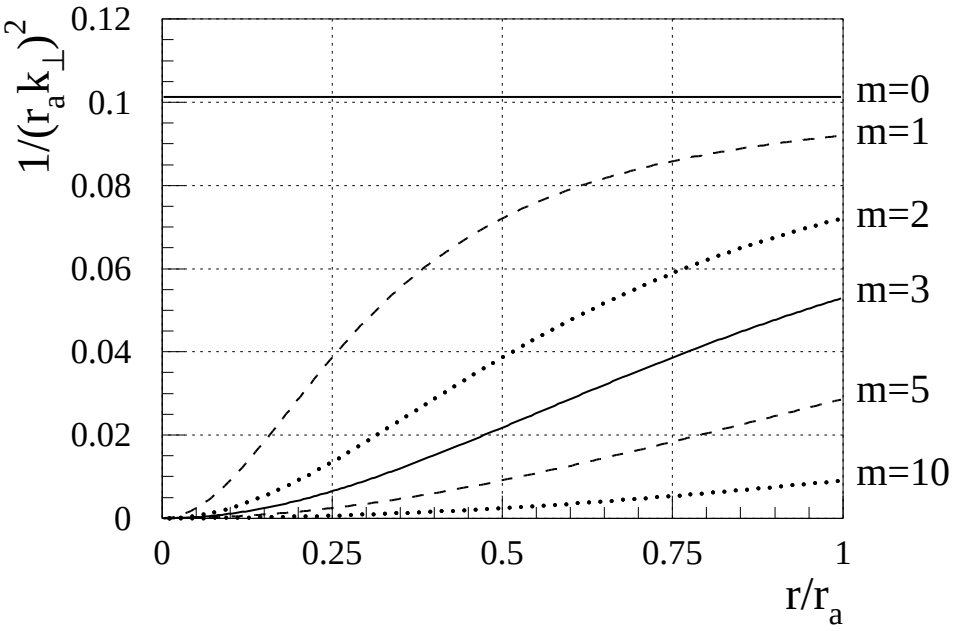
- **high beta cases,** $\beta \gtrsim 1\ \%$
- **the MHD limit** $k_{\perp} \to 0$

The cancellation problem scales with n_0 **and** $1/k_{\perp}^2(s)$**.**

$1/k_\perp^2$ dependency of the cancellation problem for a cylindrical configuration

$$\frac{1}{k_\perp^2} = \frac{r_\mathrm{a}^2}{\left(\frac{m}{r/r_\mathrm{a}}\right)^2 + \pi^2}$$

where m is the poloidal mode number and the minimal k_r is assumed.



- **The cancellation problem is most pronounced for the $m = 0$ mode**
  $\Rightarrow$ negative effect on the accuracy of the zonal flows
- **For $m \neq 0$ the cancellation problem is most pronounced at the edge**
- **The cancellation problem scales with r_a^2**

The cancellation problem in the quasineutrality equation

The contribution of the total adiabatic part to the electron number density n_e is:

$$\int \mathrm{d}^6 Z\, \delta(\mathbf{R}-\mathbf{x})\, \frac{e f_{0\mathrm{e}}}{k_\mathrm{B} T_e}\phi - \underbrace{\int \mathrm{d}^6 Z\, \delta(\mathbf{R}-\mathbf{x})\, \frac{e v_\parallel \mathrm{e} f_{0\mathrm{e}}}{k_\mathrm{B} T_\mathrm{e}} A_\parallel}_{=0}$$

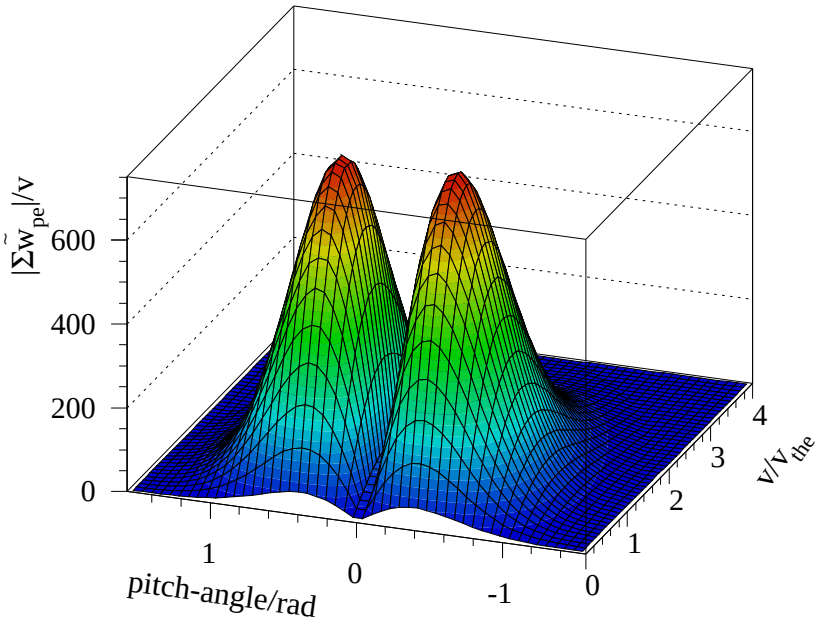
The last term has to "cancel with a zero" and is a source of a potentially large statistical error in each spatial bin Λ_ν:

$$e \sum_{p=1}^{N_\mathrm{e}^\nu} \Lambda_\nu \Omega_{p\mathrm{e}}\, \frac{v_{\parallel p\mathrm{e}} f_{0\mathrm{e}}}{k_\mathrm{B} T_\mathrm{e}} A_\parallel \Big|_{R_p, v_{\parallel p}, \mu_p} \neq 0$$

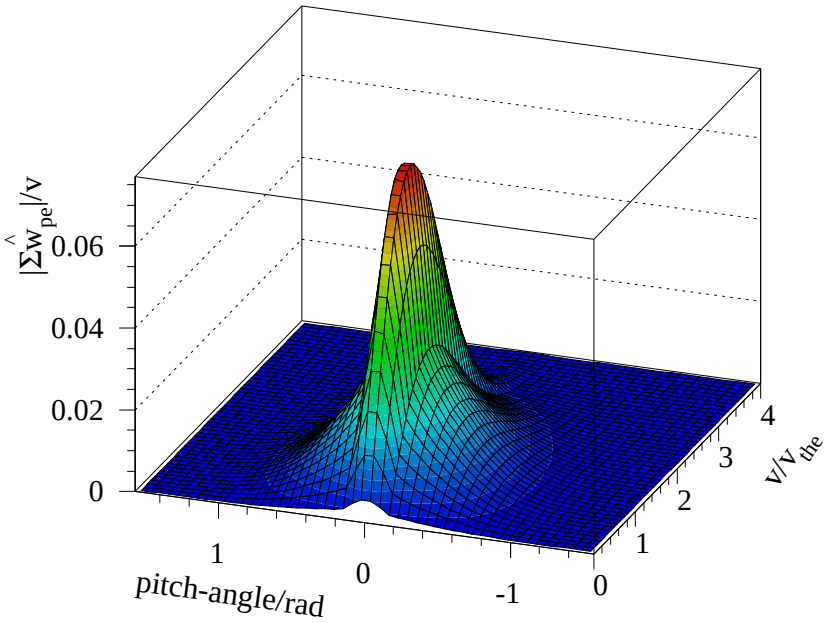
$\Rightarrow$ The cancellation problem has its counterpart in the quasineutrality equation.

The electron distribution function in velocity space at the MHD-limit

adiabatic and nonadiabatic part



nonadiabatic part



⇒ **The nonadiabatic part can be drastically smaller than the adiabatic part.**

Control variates as variance reduction method

One tries to utilize (strong) correlation between the observed variable X and some auxiliary variable Y, the so called control variable whose expected value $\mathcal{E}[Y] = \nu$ has to be known analytically.

The task is to estimate the expected value $\mathcal{E}[X] = \mu$ with a preferably smaller standard deviation than $\mathcal{V}[X]$.

Hence, we define the variable Z which has the same expected value as $\mathcal{E}[X]$ by

$$Z \stackrel{\text{def}}{=} X - \alpha(Y - \nu) = \tilde{Z} + \alpha\nu \qquad \text{where} \qquad \tilde{Z} \stackrel{\text{def}}{=} X - \alpha Y$$

The parameter α can be used to further optimize the variance reduction property of the control variate. Here we omit this opportunity by setting $\alpha = 1$.

The expected value of Z is as predicted

$$\mathcal{E}[Z] = \mathcal{E}[\tilde{Z}] + \nu = \mathcal{E}[X] - (\mathcal{E}[Y] - \nu) = \mathcal{E}[X].$$

Only the variable $\tilde{Z}$ will be discretized by our control variate schemes as the expected value ν is known analytically and can be added at any time.

The variance of Z is

$$\mathcal{V}[Z] = \mathcal{V}[\tilde{Z}] = \mathcal{V}[X - Y] = \mathcal{V}[X] - 2\mathrm{Cov}[X, Y] + \mathcal{V}[Y]$$

where the covariance is defined by

$$\mathrm{Cov}[X, Y] \stackrel{\mathrm{def}}{=} \mathcal{E}[(X - \mu)(Y - \nu)].$$

We seek for the case $\mathcal{V}[Z] < \mathcal{V}[X]$ to reduce the statistical error.

Effective control variates

The auxiliary variable Y is an effective control variate if the correlation is strong enough, i.e.

$$\frac{\mathrm{Cov}[X,Y]}{\mathcal{V}[Y]} > \frac{1}{2} \qquad \Rightarrow \qquad \mathcal{V}[\tilde{Z}] < \mathcal{V}[X].$$

For PIC simulations one can use the knowledge about the initial state $f(t_0)$ of the system to construct an effective control variate as long as the system does not evolve too far from its initial state.

For such situations the usage of a control variate is a valuable enhancement of the full-f PIC method which has naturally problems to resolve relatively small changes of the system.

The standard error ϵ (statistical noise) can be reduced in some cases drastically.

Ordinary charge assignment with a control variate

$$b(t) = \frac{1}{N}\sum_{p=1}^{N} w_p\,\Lambda(\mathbf{R}_p) \simeq \frac{1}{N}\sum_{p=1}^{N} \Omega_p \underbrace{\left[f_p - f_0(\mathbf{R}_p(t),\mathbf{v}_p(t))\right]}_{\tilde{Z}=X-Y}\Lambda(\mathbf{R}_p) + \underbrace{\int f_0\,\Lambda\,\mathrm{d}\mathbf{R}\,\mathrm{d}\mathbf{v}}_{\mathcal{E}[Y]=\nu}$$

$$= \frac{1}{N}\sum_{p=1}^{N} \underbrace{\left[w_p - \Omega_p f_{0,p}(t)\right]}_{\tilde{w}_p(t)}\Lambda(\mathbf{R}_p) + \hat{b} \qquad \textbf{where} \qquad \hat{b} \stackrel{\mathrm{def}}{=} \int f_0\,\Lambda\,\mathrm{d}\mathbf{R}\,\mathrm{d}\mathbf{v}$$

- The B-spline coefficient vector $\hat{\mathbf{b}}$ is the result of the analytic projection of the control variate f_0 onto the B-spline basis.
- As long as the control variate is time independent the B-spline coefficient vector $\hat{\mathbf{b}}$ has to be calculated only once at the initialization.

The δf method

The popular δf method chooses the following ansatz:

$$\delta f = f - f_0$$

For PIC simulations it is only used as an efficient noise reduction method if

$$\delta f \ll f_0$$

It can be interpreted as a control variate method which has set $\alpha = 1$:

$$b = \frac{1}{N}\sum_{p=1}^{N} \Omega_p [f_p - f_{\mathrm{M},p}]\, \Lambda(\mathbf{R}_p) + \hat{b} = \frac{1}{N}\sum_{p=1}^{N} \Omega_p \delta f_p\, \Lambda(\mathbf{R}_p) + \hat{b} = \frac{1}{N}\sum_{p=1}^{N} \tilde{w}_p(t)\, \Lambda(\mathbf{R}_p) + \hat{b}$$

It usually integrates an unnecessary evolution equation to derive $\delta f_p(t)$.

The adjustable control variate

An effective control variate can be constructed under the assumption of the presence of a dominant part responding adiabatically to the magnetic potential in the perturbation of the distribution function of the electrons:

$$\delta f_\mathrm{e} \approx \delta f_\mathrm{e}^\mathrm{ad} = -\frac{e v_\parallel f_{0\mathrm{e}}}{k_\mathrm{B} T_\mathrm{e}} A_\parallel$$

We define the stochastic variable $\tilde{Z}$ by introducing a "noise reduced" species of electron marker weights:

$$\bar{w}_{p\mathrm{e}} \stackrel{\mathrm{def}}{=} \Omega_{p\mathrm{e}} (\delta f_\mathrm{e} - \delta f_\mathrm{e}^\mathrm{ad}) = \tilde{w}_{p\mathrm{e}} + \Omega_{p\mathrm{e}} \frac{e v_\parallel f_{0\mathrm{e}}}{k_\mathrm{B} T_\mathrm{e}} A_\parallel \Big|_{R_p, v_{\parallel p}, \mu_p}$$

Problem: We don't know $A_\parallel$ in advance!

Ampère's law discretized in a B-spline finite element basis

$$(L + S_\mathrm{i} + S_\mathrm{e})\,\mathbf{c} = \mu_0 \langle \mathbf{j}_{\parallel \mathrm{i}} \rangle + \underbrace{\mu_0 \mathbf{j}_{\parallel \mathrm{e}} - J^{\mathrm{ad}}_{\parallel \mathrm{e}}\,\mathbf{c}}_{\tilde{Z}=X-Y} + \underbrace{S_\mathrm{e}\mathbf{c}}_{\mathcal{E}[Y]=\nu}$$

Capital letters depict matrices, $\mathbf{c}$ is the B-spline coefficient vector to be solved for and $\mathbf{j}_\parallel$'s are the coefficient vectors after current assignment of the weights.

$$\Downarrow$$

The cancellation problem can be resolved analytically by eliminating the electron skin term $S_\mathrm{e}\mathbf{c}$ on both sides:

$$(L + S_\mathrm{i} + J^{\mathrm{ad}}_{\parallel \mathrm{e}})\,\mathbf{c} = \mu_0 (\langle \mathbf{j}_{\parallel \mathrm{i}} \rangle + \mathbf{j}_{\parallel \mathrm{e}})$$

$$\Downarrow$$

This "noise reduced" matrix equation can be solved for $\mathbf{c}$ to achieve $A_\parallel(x)$.

The iterative scheme

$$\mathbf{c} = (L+S)^{-1}[I-M]^{-1}\mathbf{b} = (L+S)^{-1}\left(\mathbf{b} + \sum_{i=1}^{\infty}\mathbf{b}^{(i)}\right)$$

where

$$S \stackrel{\text{def}}{=} (S_\text{i} + S_\text{e}), \quad M \stackrel{\text{def}}{=} (S_\text{e} - J^{\text{ad}}_{\|\text{e}})(L+S)^{-1}, \quad \mathbf{b} \stackrel{\text{def}}{=} \mu_0(\langle \mathbf{j}_{\|\text{i}}\rangle + \mathbf{j}_{\|\text{e}}), \quad \mathbf{b}^{(i)} \stackrel{\text{def}}{=} M^i\,\mathbf{b}$$

We use the Neumann series with the sufficient convergence condition $\|M\| < 1$.

The solution vector $\mathbf{c} = \lim_{i\to\infty} c^{(i)}$ can be calculated iteratively by:

$$\mathbf{c}^{(0)} = (L+S)^{-1}\,\mathbf{b}, \qquad \mathbf{c}^{(n+1)} = (L+S)^{-1}[\mathbf{b} + (S_\text{e} - J^{\text{ad}}_{\|\text{e}})\mathbf{c}^{(n)}]$$

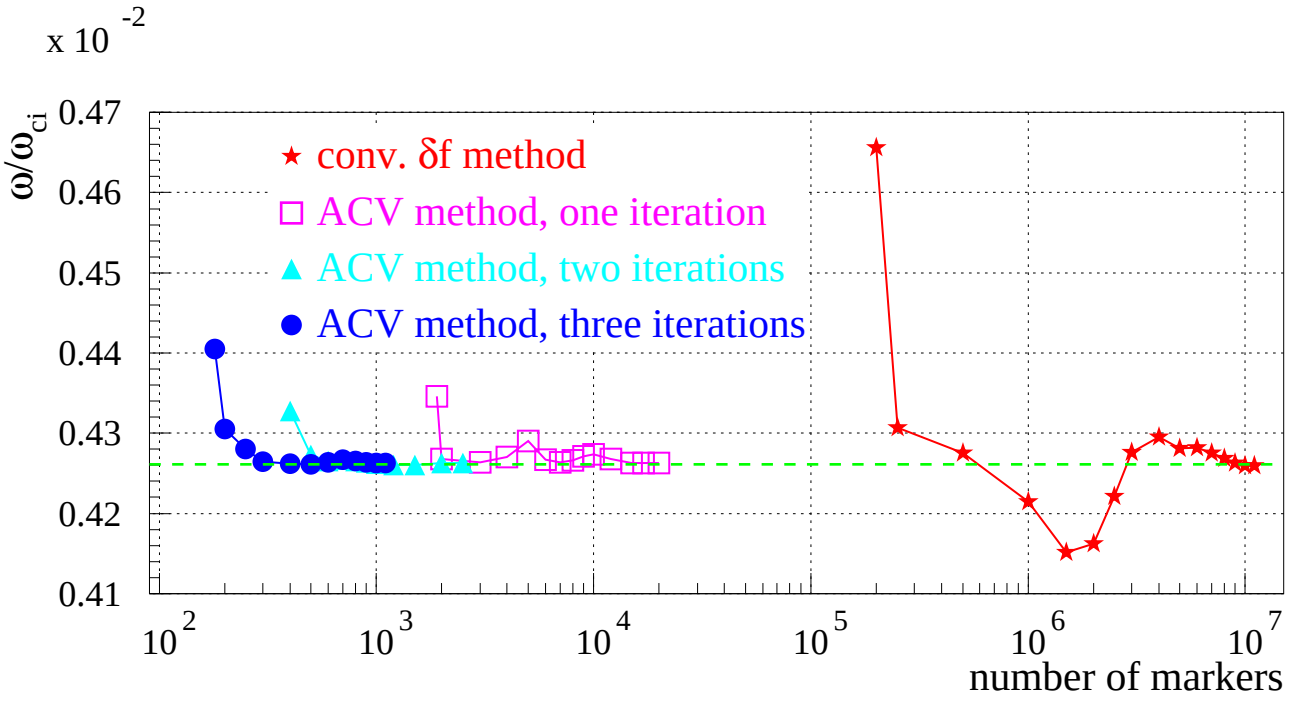
- **Usually just one or two iterations are sufficient**
- **A Cholesky decomposition is only necessary at the initialization**

Numerical results

Shear Alfvén wave in the MHD limit $k_\perp \to 0$

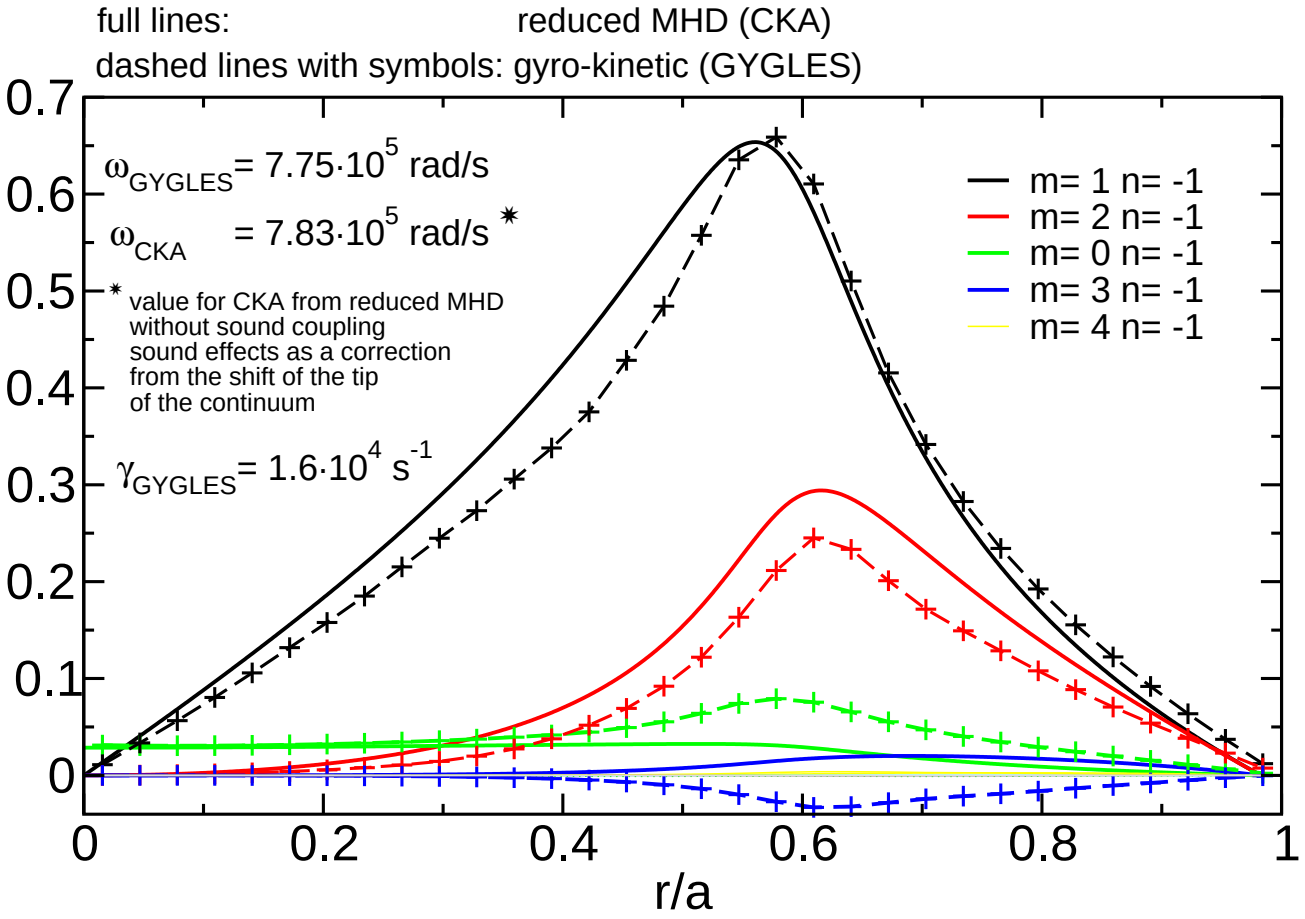
Slab model:

$k_x \rho_i = 0.023$
$k_y \rho_i = 0.015$
$k_z \rho_i = 7.43 \times 10^{-4}$
$\beta = 3.04\ \%$



Reduction of the number of markers by more than four orders of magnitude!

Global linear tokamak simulation of a low n TAE with the GYGLES code

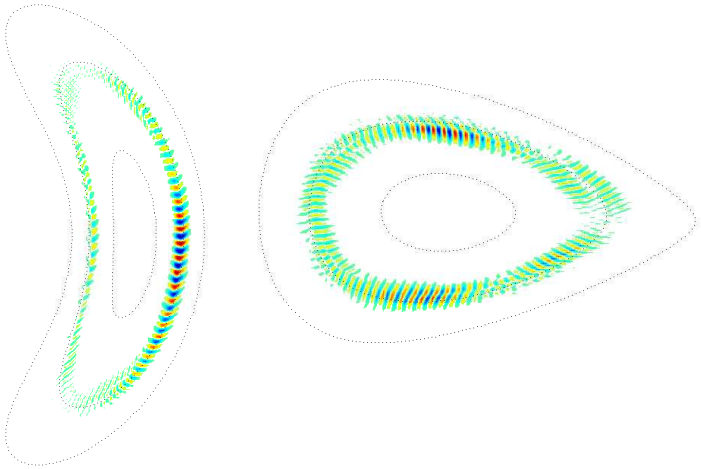


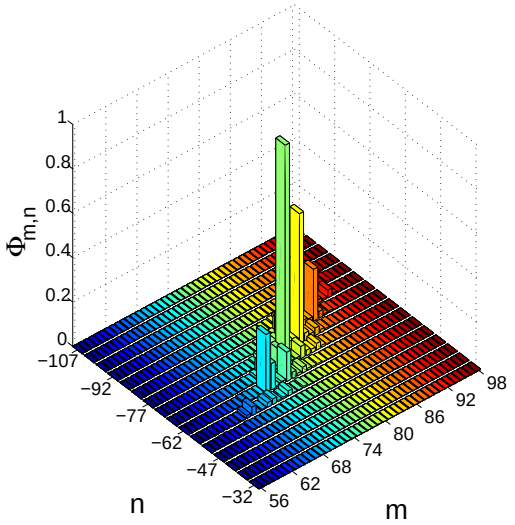
More at this conference!

Global stellarator simulation with the EUTERPE code

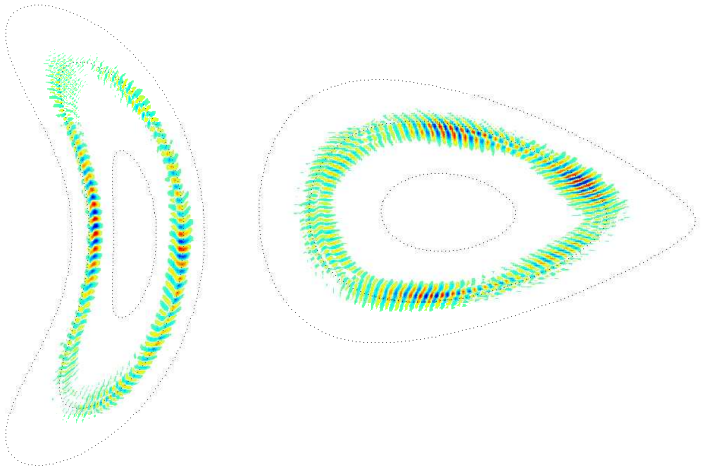
- **Equilibrium: Wendelstein 7-X**
- **Linear simulation of electromagnetic ITG with** $\beta = 1\%$
- **Fully kinetic electrons** $\Rightarrow$ **small time step**
- **Marker numbers:** $N_\mathrm{i} = 32 \cdot 10^6$**,** $N_\mathrm{e} = 128 \cdot 10^6$
- **Grid size** $(s, \vartheta, \varphi) : 100 \times 128 \times 128$
- **Computing time:** $\approx 100\,000$ **CPU hours on 128 cores**

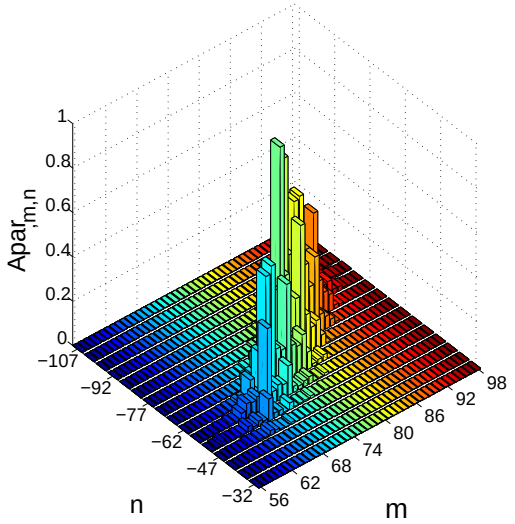
Φ





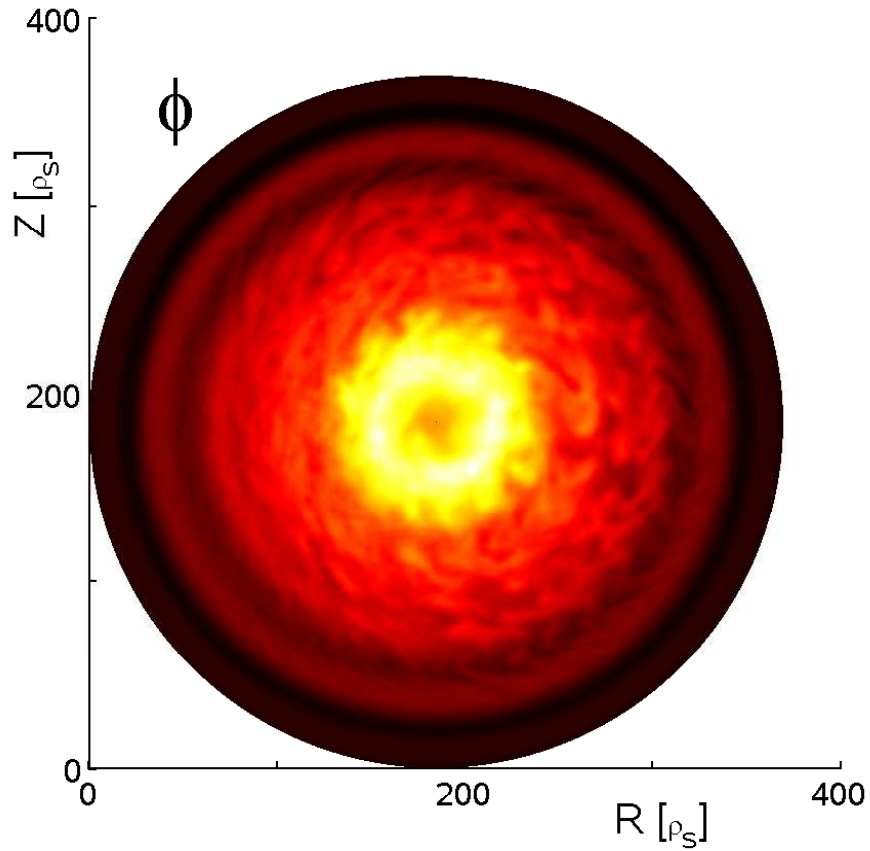
$A_{||}$

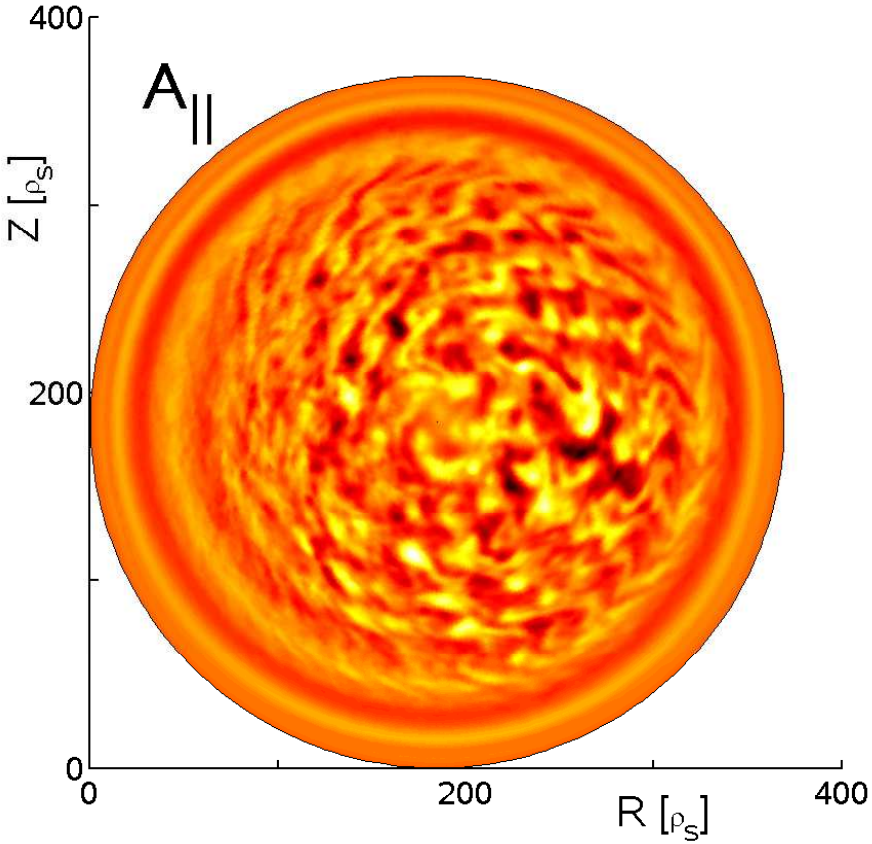




More at this conference!

Global nonlinear simulation in a tokamak with the NEMORB code





A. Bottino et al., *IEEE Transactions on Plasma Science*, **38, p. 2129–2135 (2010)**

Summary

- **The established δf scheme for PIC is a control variate method belonging to a group of Monte Carlo methods used for variance reduction.**
- **An iterative implementation of an adaptive control variate can be used to solve the "cancellation" problem very efficiently.**
- **There are no limitations concerning the geometry of the configuration.**
- **The method works for linear and nonlinear simulations.**
- **Fully kinetic electromagnetic PIC simulations become more and more the standard.**

References

- **C.K. Birdsall and A.B. Langdon:** *Plasma physics via computer simulation*, **in Plasma Physics Series edited by E. W. Laing (Institute of Physics Publishing, Bristol, 1995).**
- **R.W. Hockney and J.W. Eastwood:** *Computer simulation using particles* **(Adam Hilger, Bristol, 1989).**
- **A.Y. Aydemir,** *A unified Monte Carlo interpretation of particle simulations and applications to non-neutral plasmas*, **Physics of Plasmas 1, p. 822–831 (1994).**
- **R. Hatzky, A. Könies, and A. Mishchenko,** *Electromagnetic gyrokinetic PIC simulation with an adjustable control variates method*, **Journal of Computational Physics, 225: p. 568–590 (2007).**
- **R. Kleiber, R. Hatzky, A. Könies, K. Kauffmann, and P. Helander,** *An improved control-variate scheme for particle-in-cell simulations with collisions*, **Computer Physics Communications, 182: p. 1005–1012 (2011).**
- **URL: www.efda-hlst.eu**