Max-Planck-Insititut
für Plasmaphysik

Entropy evolution and dissipation in collisionless particle-in-cell gyrokinetic simulations

A. Bottino

Objectives

- Develop a **numerical tool** able to reproduce and predict **turbulence** and **transport** in tokamaks.

- **Physics:** **Gyrokinetics, nonlinear**
- **Numerics:** **Particle-in-cell**
- **Geometry:** **Global, Tokamak**

- **Gyrokinetics**: suitable theory, good compromise between physics needs and numerical constraint.
- **Nonlinear**: turbulence is a nonlinear process.
- **Particle-in-cell**: well suited for high dimensional system, high resolution in velocity space, high performances on parallel supercomputing.
- **Global**: allow profile variation, simulation box from magnetic axis to plasma boundary.

Outline

- A brief introduction to Gyrokinetics
- Particle-in-cell for Gyrokinetics
- From linear to nonlinear PIC simulations: statistical noise and entropy evolution
- The tool: the NEMORB code
- Conclusions and outlook

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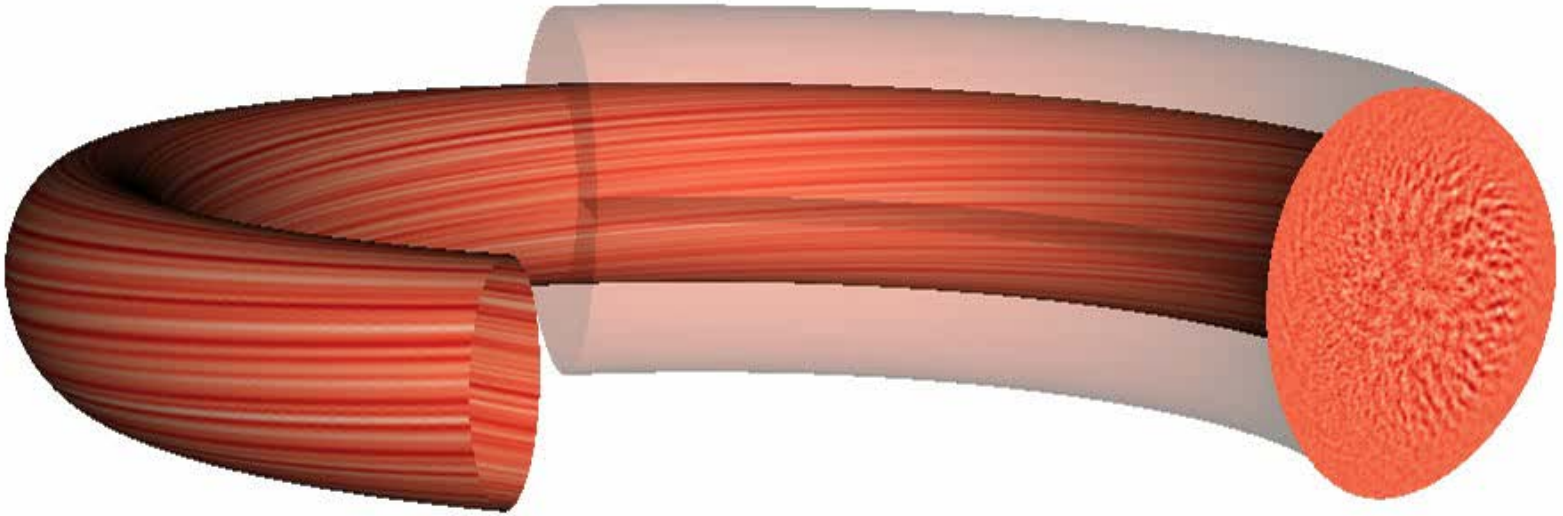
GK approximation of the Vlasov-Maxwell problem

Gyrokinetic is a system of equations for treating **low frequency fluctuations** in magnetized plasmas.

- Traditional basic assumption, **Gyrokinetic Ordering:**
  - dynamics **slower** than **gyrofrequency**
  - Scale of **background larger** than gyroradius
  - **energy** of field perturbation **smaller** than thermal
  - but **perturbation scale** can be **small**

$$\frac{\omega}{\Omega_{ci}} = O(\epsilon); \frac{\rho_i}{L} = O(\epsilon); \quad \frac{e\phi}{T} = O(\epsilon); \quad k_\perp \rho_i = O(1); \quad k_\parallel \rho_i = O(\epsilon)$$

Turbulence, perpendicular vs. parallel



Modern gyrokinetic field theory

- **Lagrangian formulation**: Equations derived by applying the Principle of Least Action for both particles and fields [Brizard, Scott, Sugama,..].
- **Coordinate transforms** are used to **eliminate** the **gyroangle** dependence in the Lagrangian at every desired order.
- Reduced dimensionality: **5D** (3D space + 2D velocity).
- Variational principle on Lagrangian gives **Euler-Lagrange** equations.
- Variational principle on Lagrangian density gives equations for the fields, **Polarization** and (parallel) **Ampére's equations**.
- Degree of freedom for the choice of the velocity coordinates.

Vlasov equation for f(R,μ, $p_{||}$)

Vlasov equation:

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \dot{\mathbf{R}} \cdot \frac{\partial f}{\partial \mathbf{R}} + \dot{p}_{||} \cdot \frac{\partial f}{\partial p_{||}} = 0 \quad ; \quad \dot{\mu} = 0$$

$$p_{||} \equiv mU + \frac{e}{c} J_0 A_{||} \qquad \text{canonical parallel momentum}$$

$$\mu \equiv v_{\perp}^2 / 2B \qquad \text{magnetic moment}$$

Euler-Lagrange equations:

$$\begin{aligned}
\dot{\mathbf{R}} &= \left(p_{||} - \frac{e}{c} J_0 A_{||}\right) \frac{\mathbf{B}^*}{m B_{||}^*} - \frac{c}{eBB_{||}^*} \mathbf{F} \cdot \left[\mu \nabla B + e \nabla \left(J_0 \Phi - \frac{p_{||}}{mc} J_0 A_{||}\right)\right] \\
&\simeq U\mathbf{b} + \mathbf{v}_D + \mathbf{v}_{ExB} + \mathbf{v}_{A||} \\
\dot{p}_{||} &= -\frac{\mathbf{B}^*}{B_{||}^*} \cdot \left[\mu \nabla B + e \nabla \left(J_0 \Phi - \frac{p_{||}}{mc} J_0 A_{||}\right)\right] \\
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J_0 gyroaverage operator

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Polarization equation

- Long wavelength limit ($k_\perp \rho_s < 1$) :

$$\sum_{\text{species}} e\langle \delta n \rangle + \nabla_\perp \left(\sum_{\text{species}} \frac{m n_0}{B^2} \right) \nabla_\perp \Phi = 0$$

- Equation of motion does not contain polarization drifts. In GK **polarization** enters in the **polarization equation** only.

- The GK+Polarization system contains the FLR generalization of the well-known physics of the fluid equations (like R-MHD), but it packages that physics differently **formally proven by [Scott 2010]**.

- **GK** equations: **ExB** drifts and **magnetic** drifts**.**

- **Polarization** equation: **Polarization** and **diamagnetic** drifts**.**

Ampére's law in $p_{||}$ formulation

- Different from the "usual" formulation, (skin terms):

$$\left(\sum_{\text{species}} \frac{n_0 e^2}{m} A_{\parallel}\right) - \frac{1}{\beta}\nabla_{\perp}^2 A_{\parallel} = \sum_{\text{species}} \langle \delta j_{\parallel} \rangle$$

- The fact that all the equations have been derived from a **Lagrangian** assure **consistency**. Even if approximations are made in the Lagrangian, all the **symmetry** properties will be preserved.

- This entire system of equation: GK Vlasov + Polarization + Ampére, has been proven be energy and momentum conserving via gyrokinetic field theory [Scott 2010].

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Particle-in-cell method in physics

The Particle-in-cell method (**PIC**) is a **numerical technique** used to solve a certain class of partial differential equations. Two steps:

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

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

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

Particle-in-cell method in GK

- The Vlasov equation is recast in the following form (control variate method):

$$\frac{\mathrm{D}f}{\mathrm{D}t} = \frac{\mathrm{D}(f_0 + \delta f)}{\mathrm{D}t} = 0 \rightarrow \frac{\mathrm{D}\delta f}{\mathrm{D}t} = -\frac{\mathrm{D}f_0}{\mathrm{D}t}$$

- **f_0** is an **analytically known** function, possibly (but not necessary) an equilibrium distribution function.

- **No changes** in the **equations** (only adding and subtracting the same term in the moment equation):

$$\int M(\mathbf{v}) f \,\mathrm{d}\mathbf{v} = \int M(\mathbf{v})(f - f_0)\mathrm{d}\mathbf{v} + \int M(\mathbf{v}) f_0 \mathrm{d}\mathbf{v}$$

- **δf** is discretized with numerical particles (**markers**):

$$\delta f \equiv \sum_{p=1}^{N} w_p(t)\ \delta(\mathbf{R} - \mathbf{R}_p(t))\ \delta(p_{\|} - p_{\|p}(t))\ \delta(\mu - \mu_p(t_0))$$

Particle-in-cell method in GK

- The **Vlasov** equation becomes a set of **N equations** for the particles weights, integrated using the method of the characteristics:

$$\frac{\mathrm{d}w_p}{\mathrm{d}t} = -\frac{\partial f_0}{\partial \mathbf{R}}\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\Big|_p - \frac{\partial f_0}{\partial p_\parallel}\frac{\mathrm{d}p_\parallel}{\mathrm{d}t}\Big|_p$$

- The RHS contains **gyroaveraged** potentials **$J_0(A_\parallel)$** and **$J_0(\phi)$**

- The gyroaverage operator in real space looks like:

$$\langle \phi \rangle_{\mathbf{R}} = \sum_{\mathbf{k}} \phi_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{R}}\, J_0(k_\perp \rho_L)$$

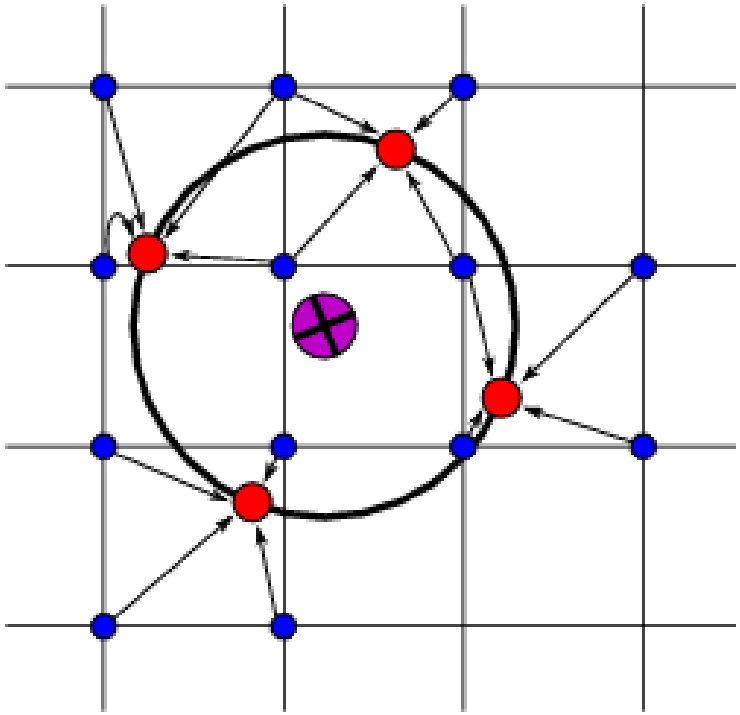
- This should be calculated N times at every time step.

Computationally prohibitive!!!

Gyroaverage in PIC simulations

- **Gyroaveraged** potential at the particle position is **approximated** by an **average** of the potential on some points on the **gyroring**:

$$\langle \phi \rangle = \frac{1}{2\pi} \int_0^{2\pi} \phi(\vec{R} + \vec{\rho}) \, \mathrm{d}\theta \simeq \frac{1}{N_{avg}} \sum_{i=1}^{N_{avg}} \phi(\vec{x}_i)$$



- **Start from ϕ on the grid and a particle p.**
- **Choose some points on the gyroring.**
- **Calculate via interpolation the values of ϕ on points of the gyroring.**
- **Calculate the average value.**
- **[Lee 1983]**

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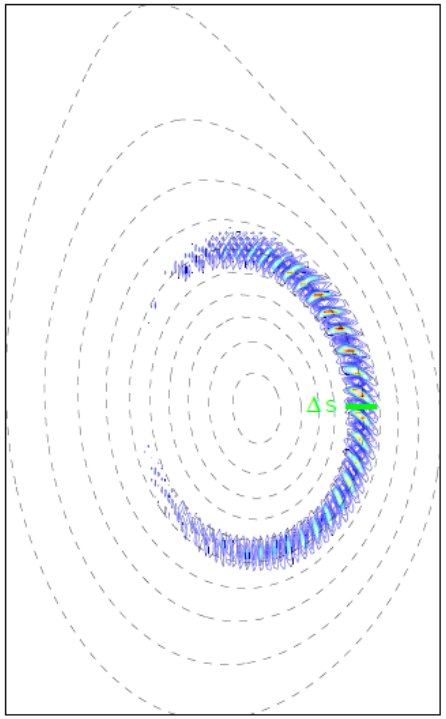
Linear simulations in tokamaks

- **Linearize** the equations, markers will move on **unperturbed trajectories**.
- Choose an **MHD equilibrium**, **temperature** and **density** profiles.
- Select one toroidal mode n.
- Put an initial perturbation on an equilibrium distribution function.
- Run the code.

ITG in AUG 13149 [Bottino et al. 2004]



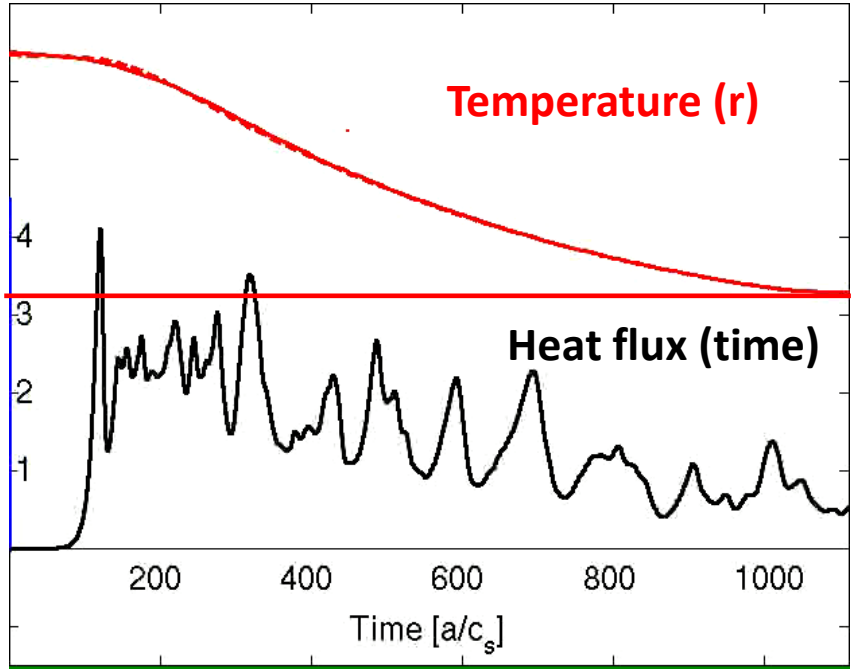
Non linear global simulations in tokamaks

Issues when moving from linear to nonlinear global simulations:

- Heat and particle fluxes: **profile evolution**.
- **Statistical noise.**
- **Collisionless**: lack of **dissipation** or the "**entropy paradox**".
- Massively parallel simulations required.
- Deal with a lot (TB of) data.
- Inclusion of collision becomes problematic.

Profile evolution is very rapid

- In nonlinear global simulations with **adiabatic electrons** only **temperature evolves** in time (no net particle transport).
- Temperature gradient decays until critical gradient is reached.
- A real steady state is never reached: the heat flux continuously decays.
- In reality, the heat flux reaches a finite value determined by the discretization (in PIC mostly number of particles).
- **Heat source** terms must be added on the right hand side of the Vlasov equation.



Example: ITM cyclone case (circular DIII-D)

Origin of the noise in GK PIC

- **δf** is discretized with N markers.

- Besides diagnostics purposes, **δf** itself **does not enter in the PIC algorithm, the moments of δf do**, e.g.:

$$\sum_{\text{species}} e\langle \delta n \rangle + \nabla_\perp \left(\sum_{\text{species}} \frac{m n_0}{B^2} \right) \nabla_\perp \Phi = 0$$

- Calculating the moments is equivalent to a Monte-Carlo integration, i.e. solving [Aydemir 94]:

$$\int_V f(\mathbf{Z}) \mathrm{d}\mathbf{Z}$$

using only a **discrete random sample** for f :

$$(\mathbf{Z_1}, \mathbf{Z_2}, .., \mathbf{Z_N}) \rightarrow (f(\mathbf{Z_1}), f(\mathbf{Z_2}), .., f(\mathbf{Z_N})).$$

The noise is the statistical error in MC integration

- The **error** in Monte-Carlo integral evaluation is well known:

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

N, number of sampling points.
σ^2 variance of the distribution of the test function.

- The **error ε** in the density integration is the **statistical noise**.

- The charge density calculated with particles will be:

$$\rho(\mathbf{Z}) = \rho(\mathbf{Z})_{\text{signal}} + \epsilon = \rho(\mathbf{Z})_{\text{signal}} + \rho(\mathbf{Z})_{\text{noise}}$$

- The **Polarization equation transfers** the statistical **noise** (error) from the charge density to the **electrostatic potential**.

Noise in GK PIC can be estimated

- Error introduced when the moment of the GK distribution function (density) can be analytically evaluated, a crude but useful approximation is:

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

NG , number of Fourier modes included in the simulation.

G accounts for FLR filtering and grid projection filtering.

Derivation: DFT on discretized Polarization Equation, velocity dependence is removed by averaging the contribution of the Bessel functions with a Maxwellian distribution.

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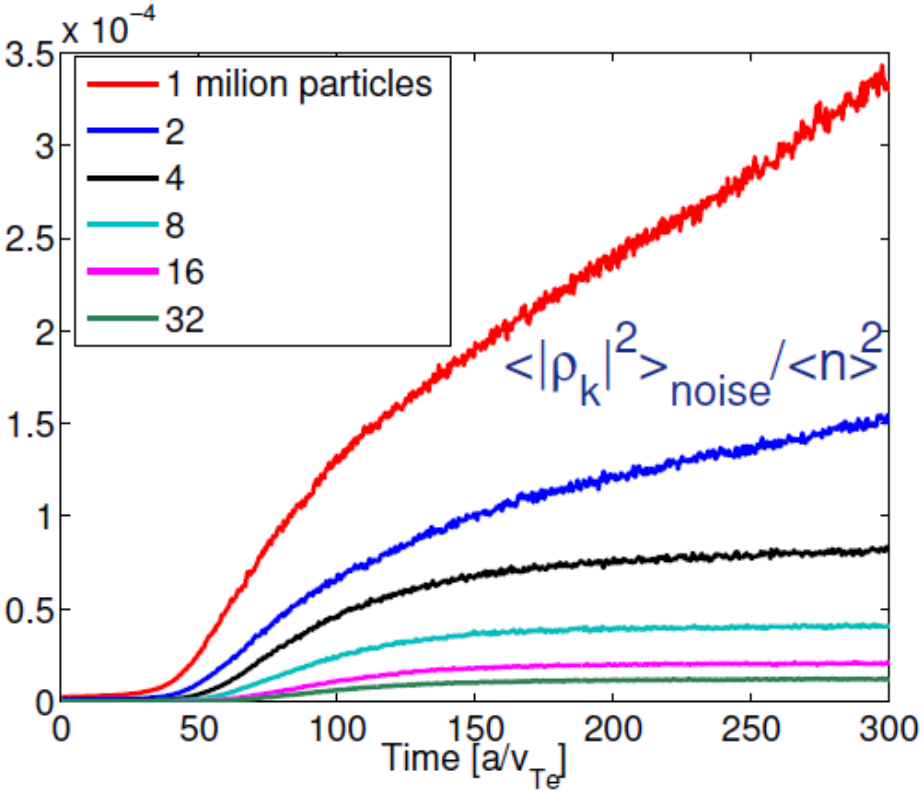

- PIC is different from MC: **noise constantly grows in time**. Why?

The dissipation in PIC

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- **Without dissipation a true steady state cannot be reached in δf PIC simulations.** Without dissipation fluctuation entropy always increases in time in PIC [Krommes et al. 1994, 1999].

Entropy in PIC delta-f

- Entropy fluctuation:

$$\delta S = \int (f \ln f - f_0 \ln f_0)\, \mathrm{d}\mathbf{Z} \simeq \int \frac{\delta f^2}{f_0} \mathrm{d}\mathbf{Z} \rightarrow \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \frac{w_i^2}{f_{0i}} = \langle \frac{w^2}{f_0} \rangle$$

- Time evolution (multiply Vlasov eq. times $\delta f/f_0$, integrate over phase space):

$$\frac{\mathrm{d}\delta S}{\mathrm{d}t} = \mathrm{D}_{\mathrm{flux}} + \mathrm{D}_{\mathrm{field}}$$

$$\mathrm{D}_{\mathrm{flux}} \simeq \frac{a}{V} \left(\frac{a}{L_{Ti}} \right)^2 \chi_i \; n_0$$

$$\mathrm{D}_{\mathrm{field}} \simeq \frac{1}{T} \frac{\mathrm{d}E_f}{\mathrm{d}t}$$

*- **D_{flux}**, proportional to the heat diffusivity (contains **heat flux** and **T gradient**)*

*- **D_{field}**, entropy variation by the **transfer** of energy **from particles** to the **fields**.*

[Jolliet et al. 2009]

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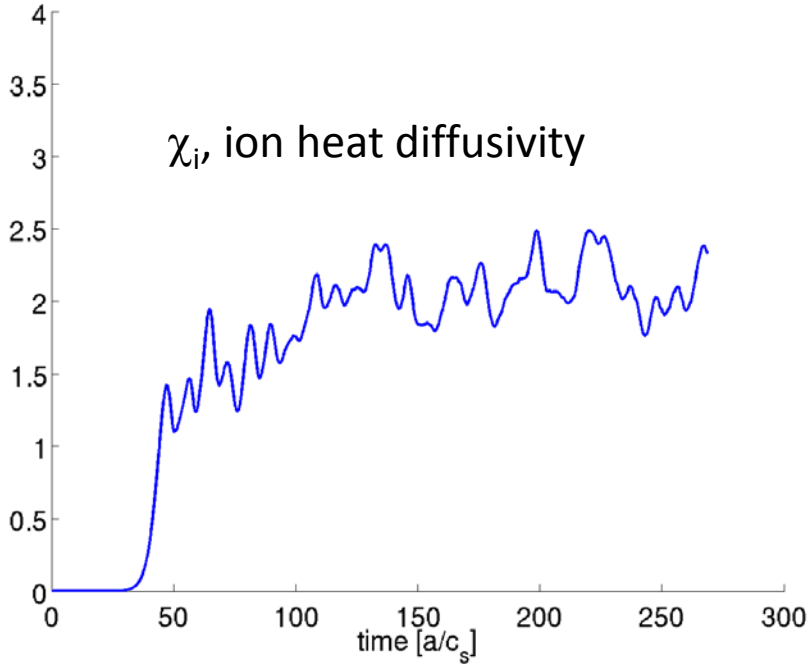

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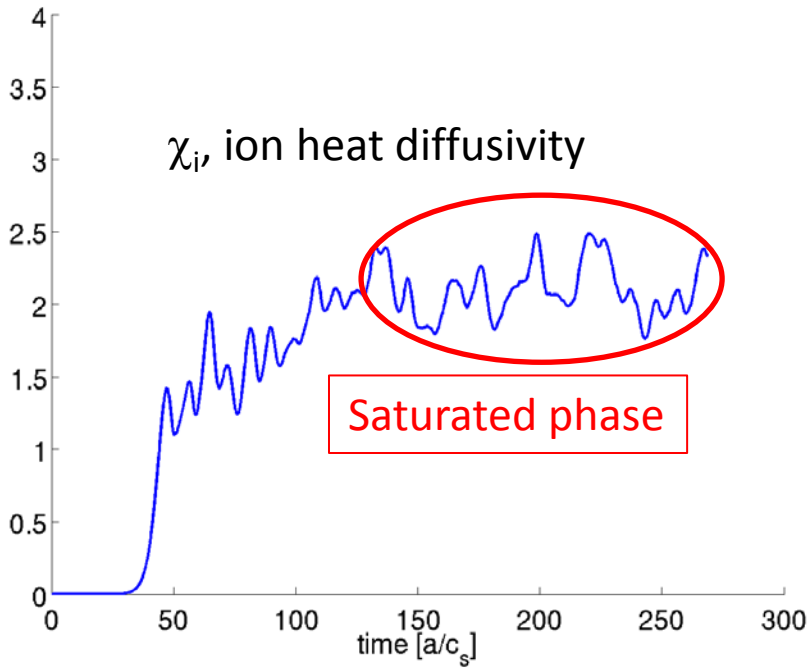

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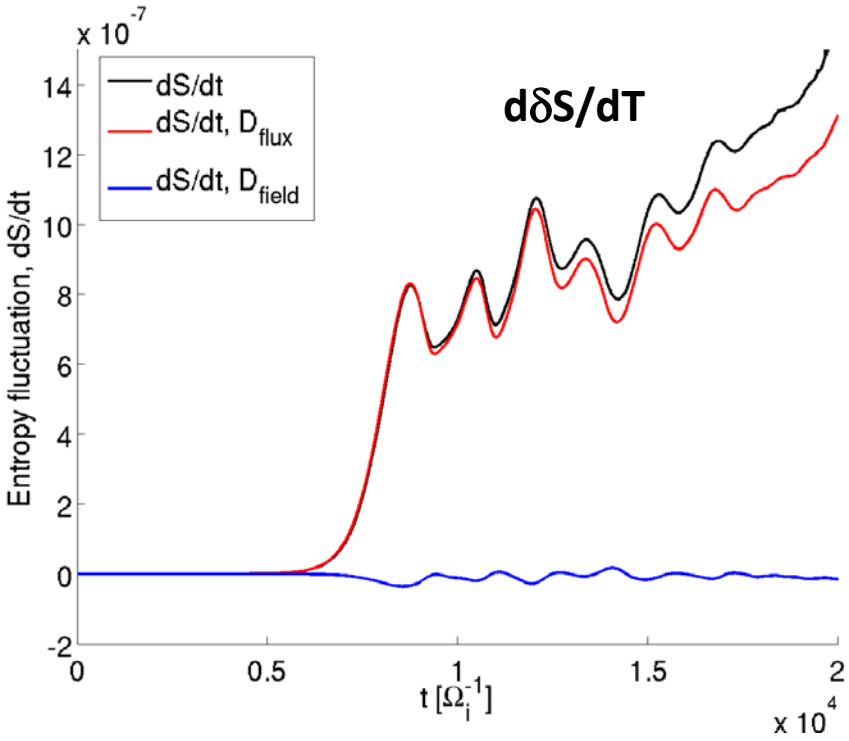


*- D_{flux}, proportional to the heat diffusivity (contains **heat flux** and **T gradient**)*

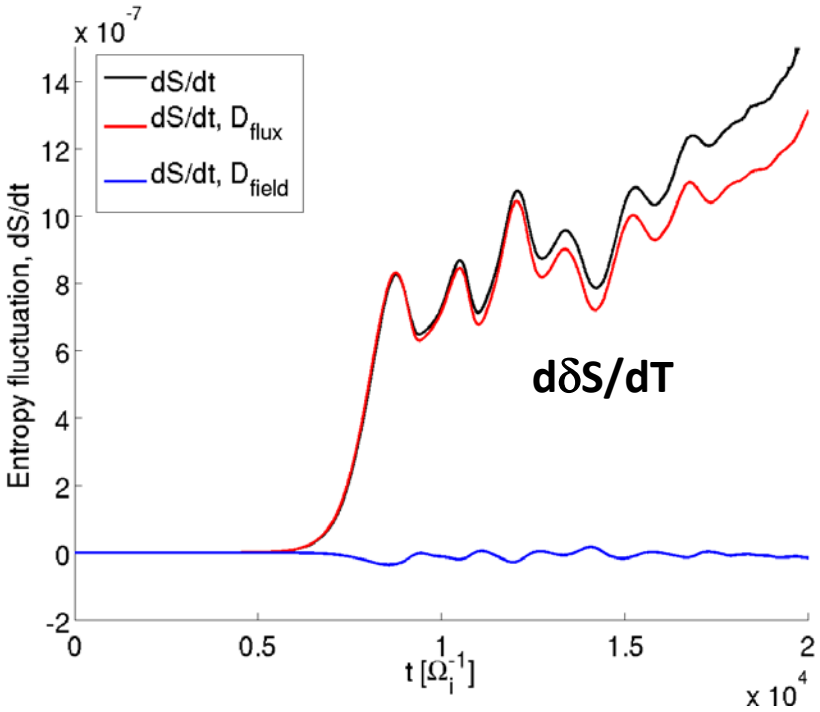
*- D_{field}, entropy variation by the **transfer** of energy **from particles** to the **fields**.*

Entropy in PIC delta-f

- Entropy fluctuation:

$$\delta S = \int (f \ln f - f_0 \ln f_0)\, \mathrm{d}\mathbf{Z} \simeq \int \frac{\delta f^2}{f_0} \mathrm{d}\mathbf{Z} \rightarrow \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} \frac{w_i^2}{f_{0i}} = \langle \frac{w^2}{f_0} \rangle$$

This is the "**entropy paradox**": In a state which appears to be steady (finite and **stationary heat flux**) the entropy (sum of the weight square) **increases in time**.



A physics picture of the entropy growth

- Without **dissipation** the system will develop structures at smaller and **smaller scales in velocity** space.

- The **low moments** of **δf saturate**, but the growth of fine-scale velocity structures contributes to the monotonical increase of the **entropy** (δf^2).

The "entropy paradox" is real physics, and it is what the PIC simulations show!

A physics picture of the entropy growth

- Without **dissipation** the system will develop structure at **smaller and smaller scale in velocity** space.
- The **low moments** of **δf saturate** but the growth of fine-scale velocity structures contributes to the monotonical increase of the **entropy** (**δf^2**):
- **This is real physics, and it is what the PIC simulations get!**
- **What about the noise?**
- **The noise is also a δf^2 term:** $$\rho^2_{noise} \simeq \frac{N_G}{N} \langle w^2 \rangle G$$
- The **markers try to resolve the new small scales**, i.e. the **weights** will unavoidably **grow** in absolute value: **noise will increase**!

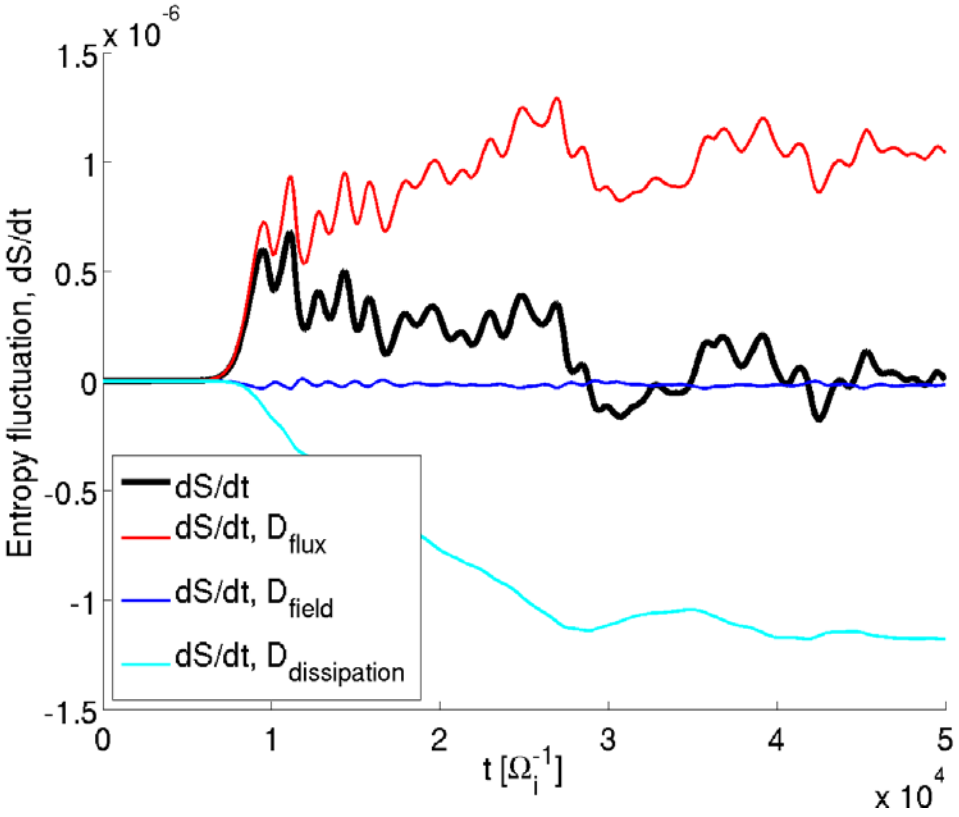
The cure: add dissipation

- **Dissipation can be introduced in different ways, e.g. Particle-Continuum methods** [Parker et al 2008] **or Krook–like operators** [McMillan et al. 2009]**.**

$$\frac{\mathrm{d}\delta S}{\mathrm{d}t} = \mathrm{D}_{\mathrm{flux}} + \mathrm{D}_{\mathrm{field}} + \mathrm{D}_{\mathrm{dissipation}}$$

The cure: add dissipation

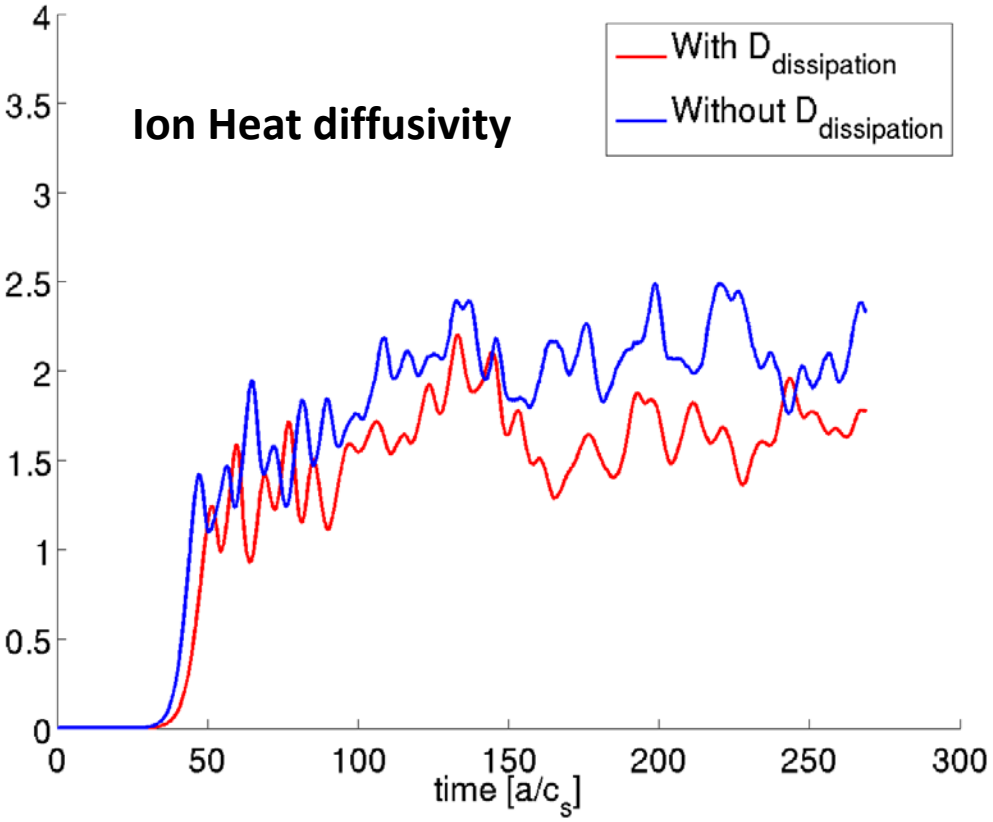
$$\frac{d\delta S}{dt} = D_{flux} + D_{field} + D_{dissipation}$$



A. Bottino, NumKin 2013, 5/09/2013

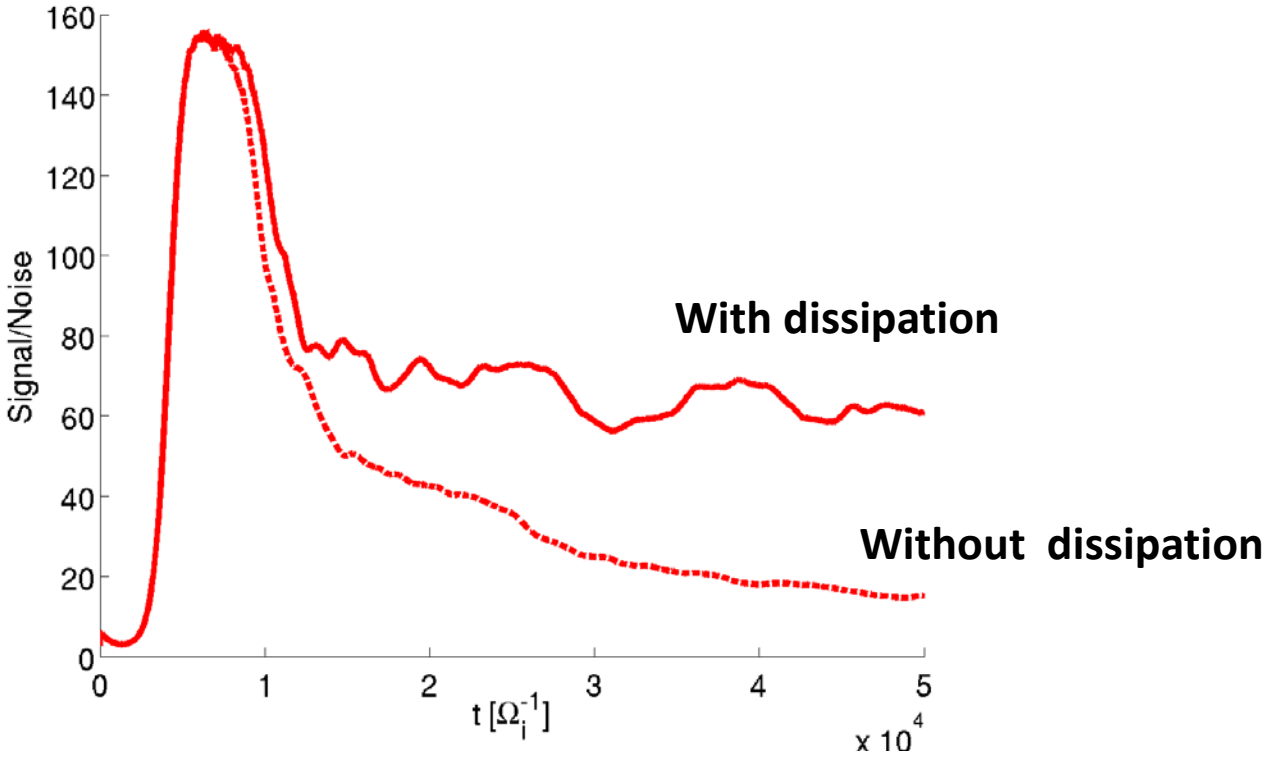
Transport is unaffected on short time scale

- Although entropy behaves so differently, ITG fluxes appear to be robust:



Noise growth is a show stopper

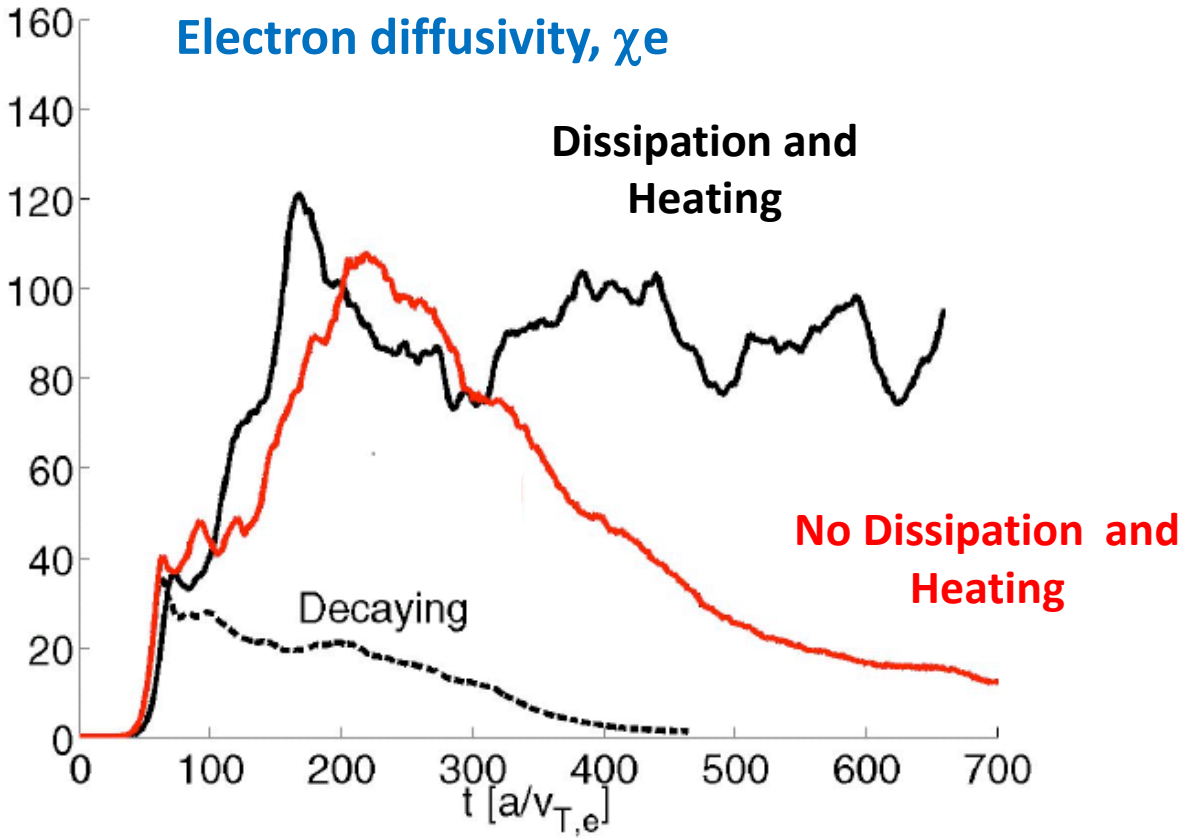
- **But**, simulations **without dissipation cannot be run forever**, the **signal to noise** will drop and finally crash the simulation.



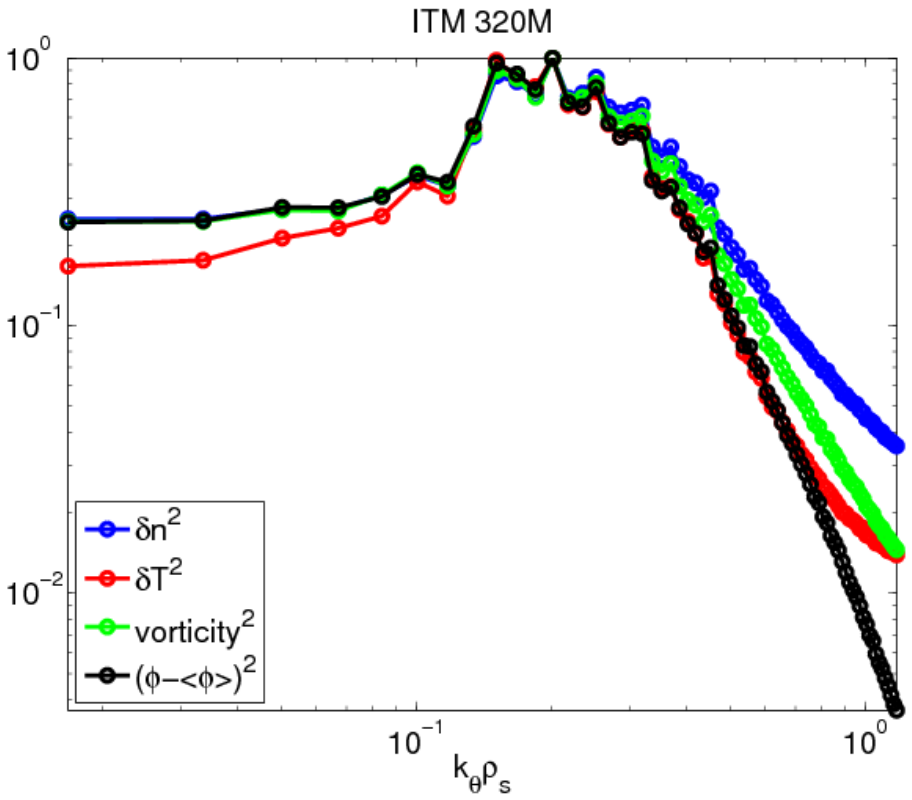
ETG: noise growth leads to wrong fluxes

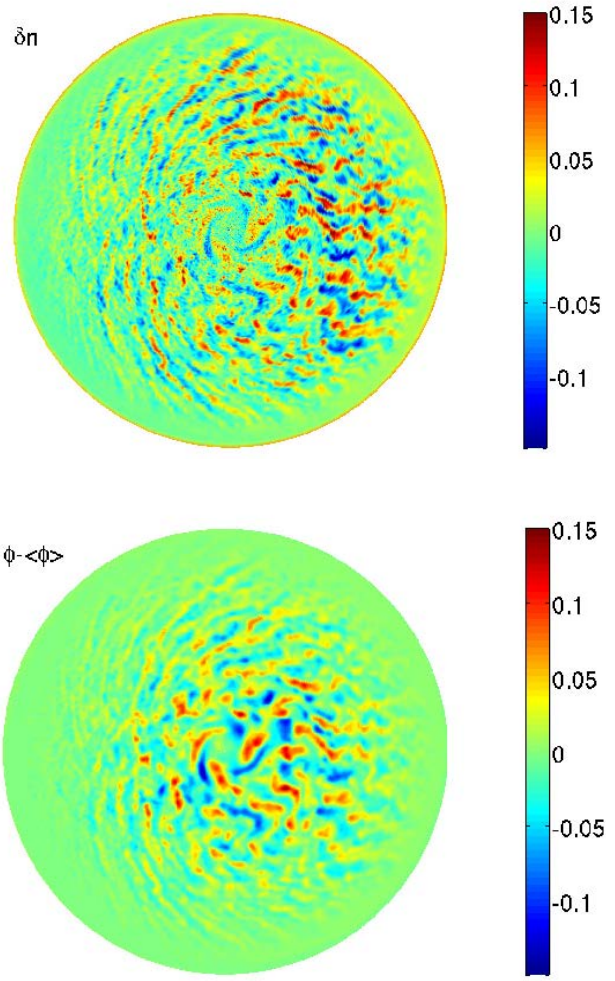
- For **ETG turbulence**, the growth of the **noise** and the consequent spurious density charge strongly **reduces** the **transport**

  [Nevins et al. 2005, Bottino et al. 2006].



Convergence: the Cyclone base case





DIII-D like plasma (ρ^*=1/186), circular, electrostatic, R/L_T=6.9, adiabatic electrons , collisionless, 320M markers.

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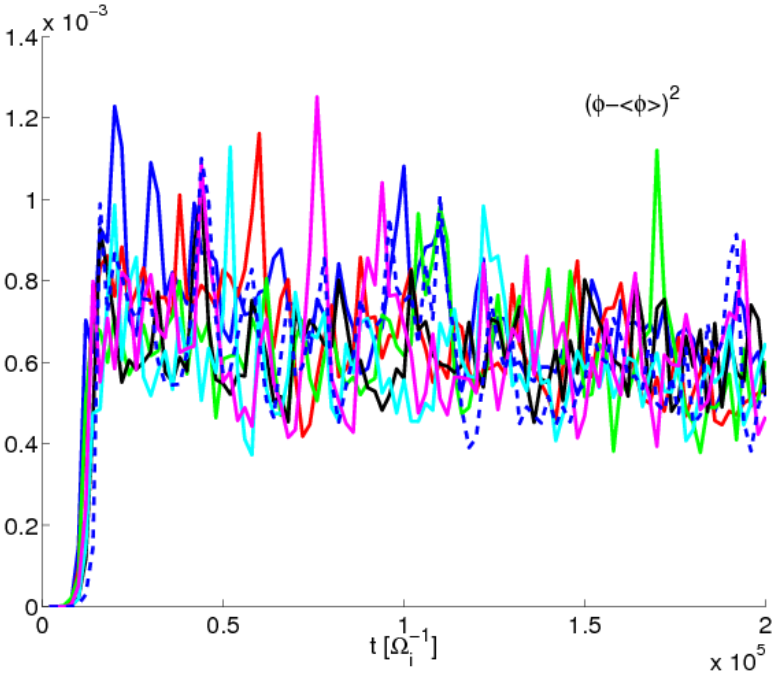
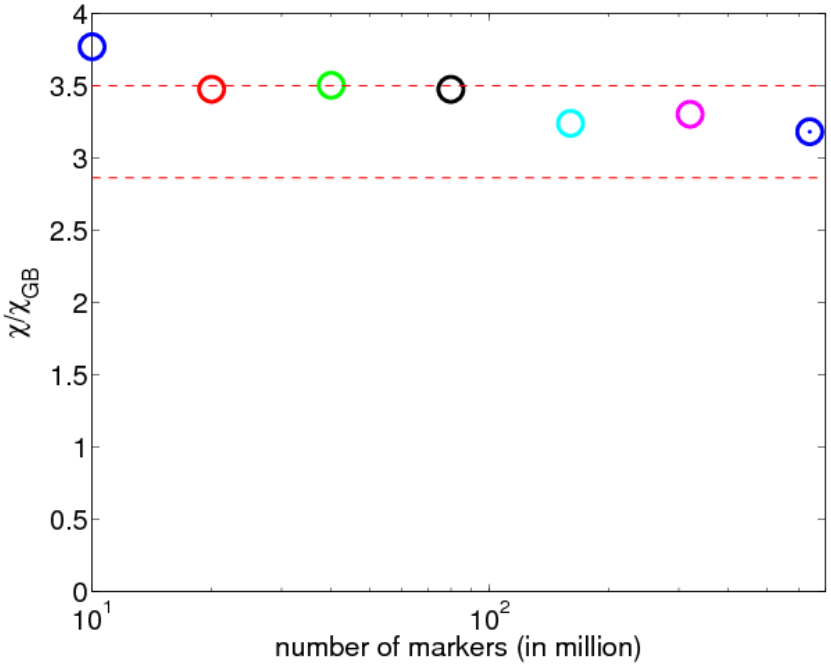
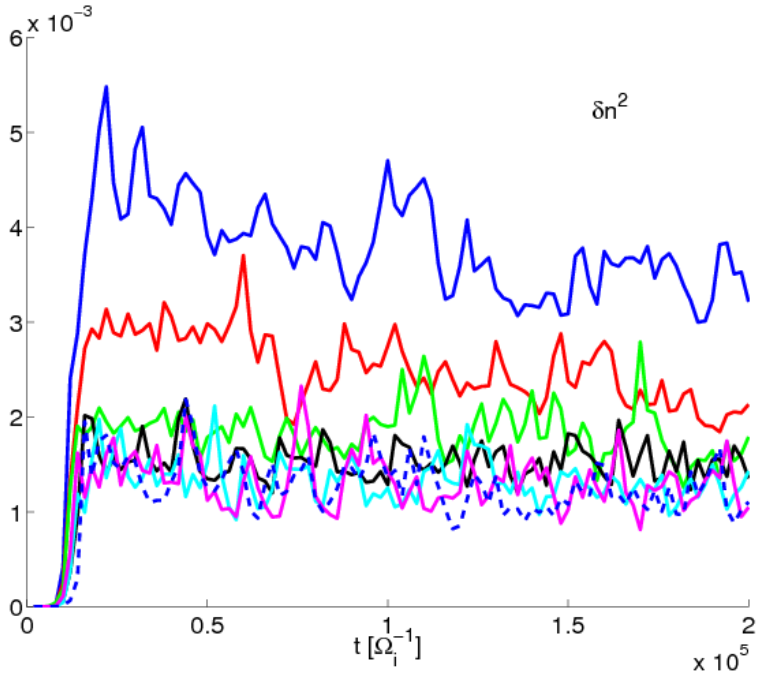
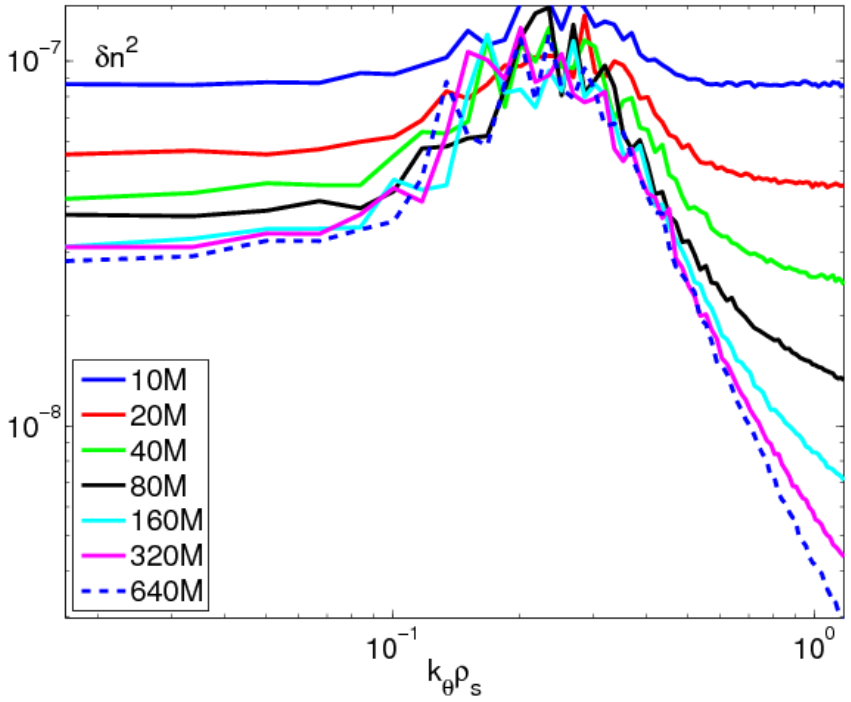
Noise convergence ($R/L_T=10$)

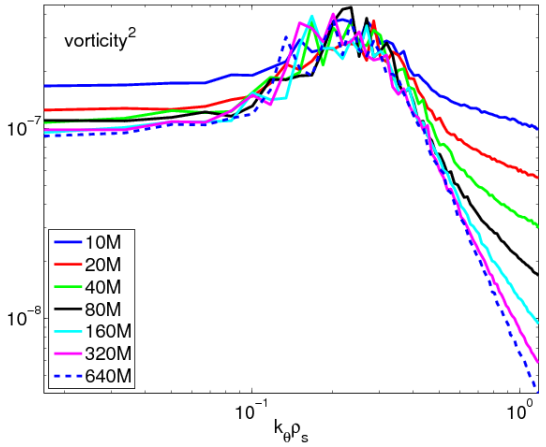




Noise convergence ($R/L_T=10$)







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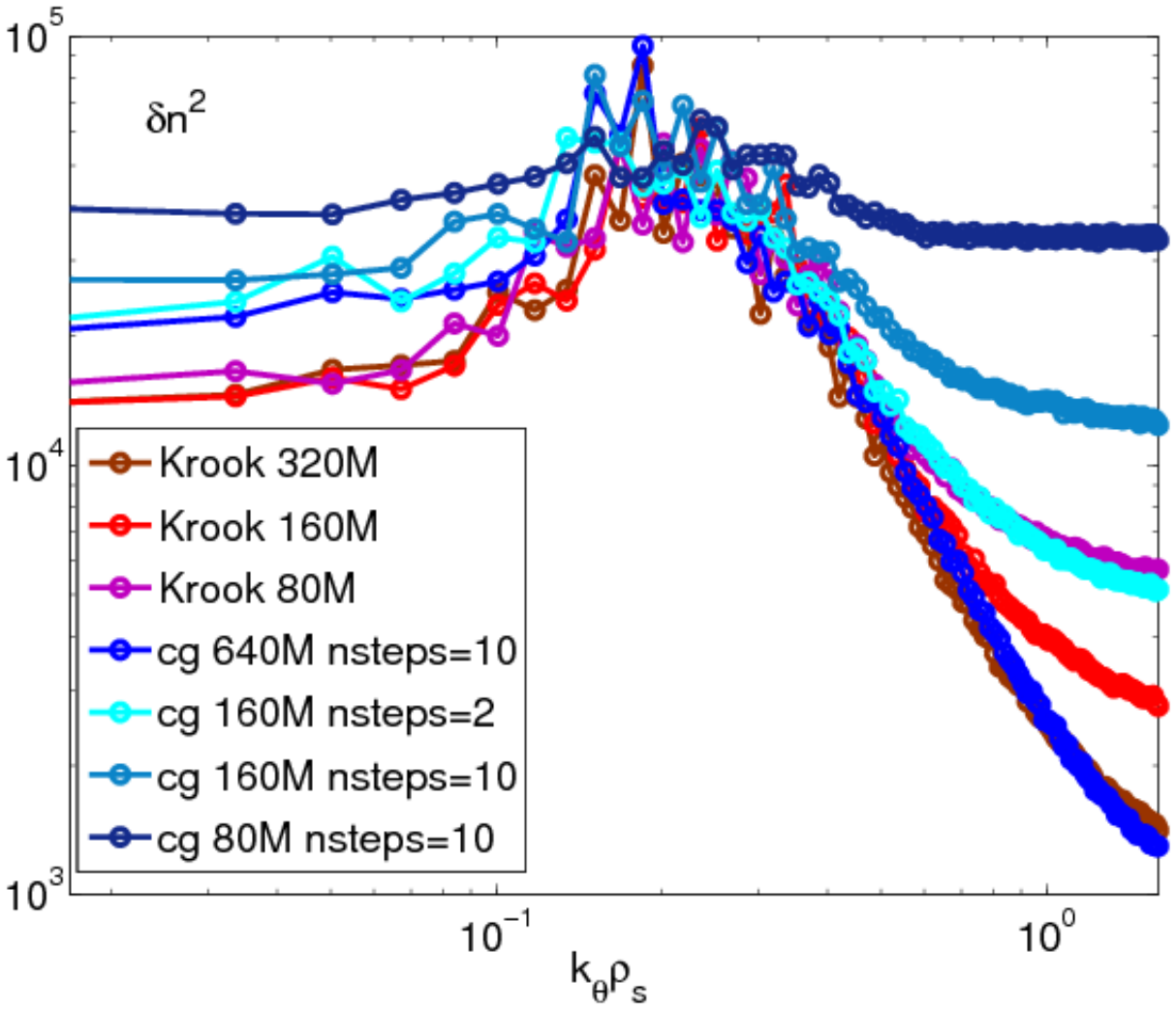
Krook op. vs coarse graining



Outline

- **The tool: the NEMORB code**

Timeline of ORB5

- **1998**: *T.M. Tran*, adiabatic electrons, no ZF response, cylindrical coordinates, MHD equilibria, long wavelength approximation in Polarization.

- **2001-2003:** *A. Bottino*, electron model (linear), improved Polarization, simple ZF response; *P. Angelino*, ZF response;
- **2002: first nonlinear physics studies.**

- **2004-2008:** *S. Jolliet*, magnetic coordinates, field aligned solver, electron model, field aligned Fourier filtering (with *P. Angelino*), *A.Bottino*, domain cloning, *B.F. McMillan*, dissipation, Solver in Fourier space;
- **2006 first massively parallel simulations**.

- **2009-now:** *B.F. McMillan*, equilibrium flows; *T. Vernay*, collisions.
- **2009**: *A.Bottino*, parallel Ampére's law, multispecies*: **NEMORB***.

Now: three groups, CRPP (L. Villard), Warwick U. (B.F.Mcmillan), IPP (Bottino)

The NEMORB code

- Upgrade of the **ORB5** [Jolliet et al. 2007] code.
- **Global tokamak** geometry (including magnetic axis).
- **Gyrokinetic Vlasov** equation for **multiple ion species** (DK for electrons).
- Linearized Polarization equation and **parallel Ampére's law**.
- Electron-ion **collisions**, self-collisions (pitch angle scattering).
- Ideal **MHD** equilibria (CHEASE code).
- **Equilibrium flows**.
- Dissipation in collisionless simulations

Heat transport predictions with NEMORB

- Follow the ORB5 timeline and see **how the heat transport predictions would have changed over the years**.

- **Equilibrium**: AUG 26754.

- **Profiles**: stronger gradients than experiment and localized around mid-radius ($R/L_T \sim 7.5$).

- Definitions:

  Q, heat flux: kinetic energy flux due to the V_{EXB} velocity.

$$\chi_i = \frac{Q}{n_i |\nabla T_i|} \qquad \chi_{GB} = \frac{\rho_s^2 c_s}{a}$$

ORB5 in the year 1998

- Electrostatic, adiabatic electrons

$$\langle \delta n_D \rangle + \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_D} \nabla_\perp \phi \right) = \frac{e n_0}{k_B T_e} (\phi - \bar{\phi})$$

- $\bar{\phi}$ is the “zonal” (flux surface averaged) component of the electrostatic potential.

- Calculating $\bar{\phi}$ beyond the numerical possibilities at that time.

- Toroidal mode number **n=0 was filtered out** of the simulations.

ORB5 in the year 1998

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$$\langle \delta n_D \rangle + \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_D} \nabla_\perp \phi \right) = \frac{e n_0}{k_B T_e} \left(\phi - \cancel{\bar{\phi}} \right)$$

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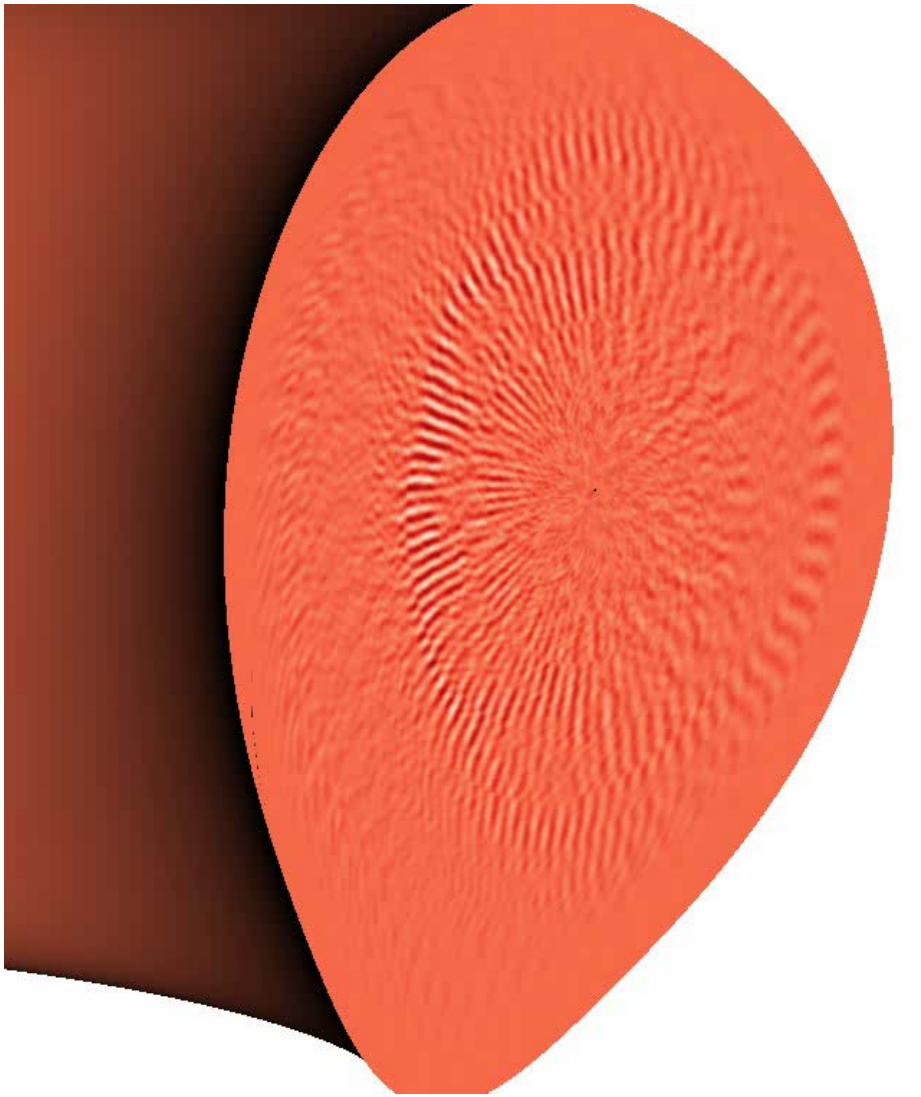
- Calculating $\bar{\phi}$ beyond the numerical possibilities at that time.

- Toroidal mode number **n=0 was filtered out** of the simulations.

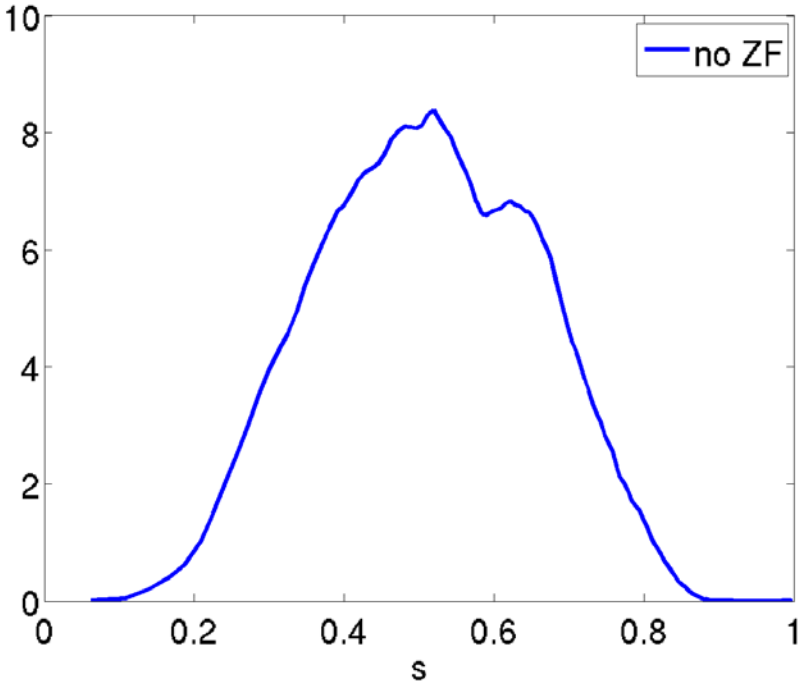
Electrostatic potential, no n=0



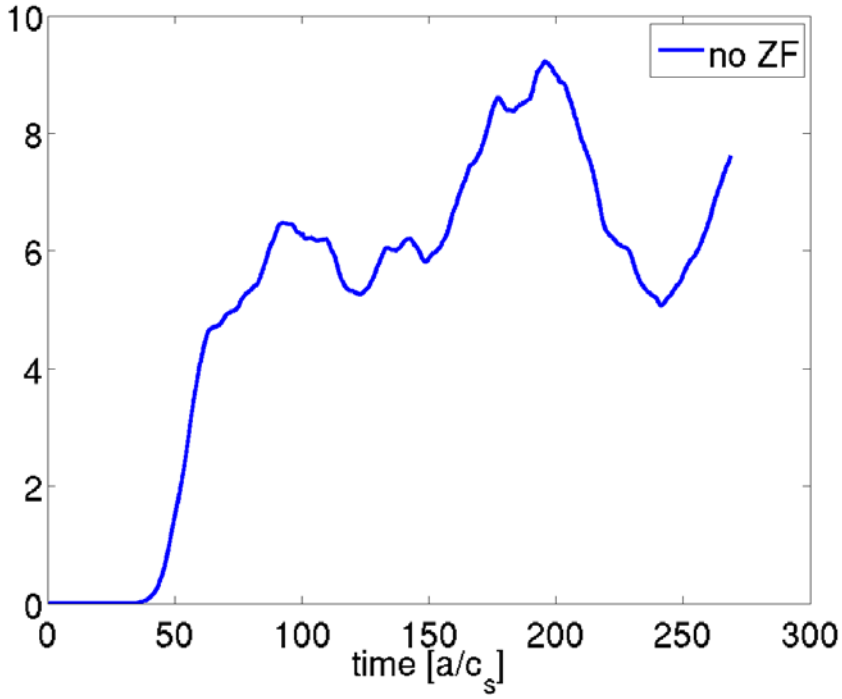
Without ZF, very high heat transport

➢ **Ion heat conductivity is very large**

Time average, χ/χ_{GB}



Radial average , χ/χ_{GB}



ORB5 in the year 2001

- Electrostatic, adiabatic electrons, **zonal flow correctly treated**

- Polarization equation:

$$\langle \delta n_D \rangle + \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_D} \nabla_\perp \phi \right) = \frac{e n_0}{k_B T_e} (\phi - \bar{\phi})$$

- $\bar{\phi}$ is the "zonal" (flux surface averaged) component of the electrostatic potential

- Simulation similar to the first work that made particle-in-cell global simulations popular:

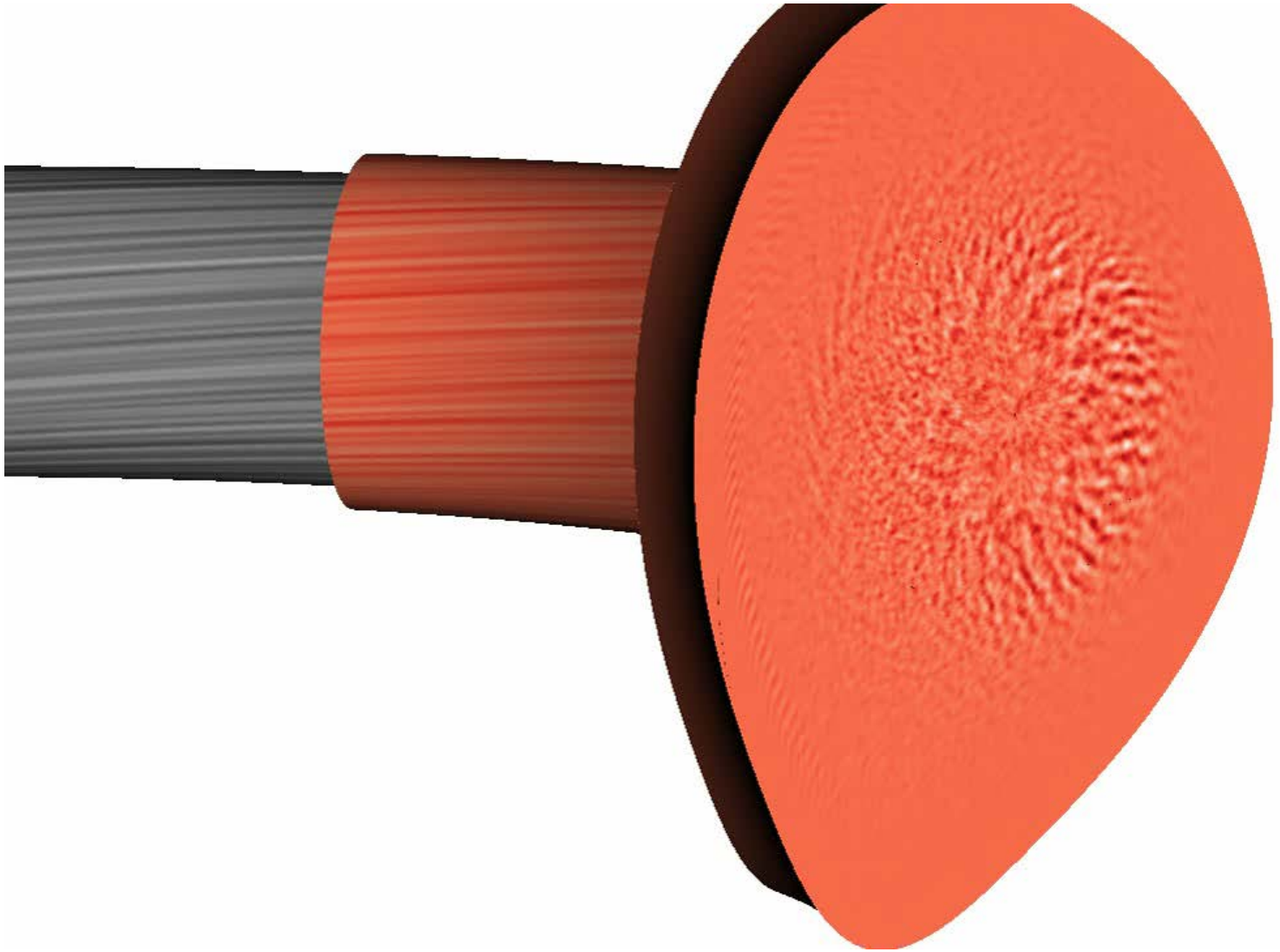
  Z.Lin,

  "Turbulent transport reduction by zonal flows: massively parallel simulations"

  [Science 1998],

  i.e., CYCLONE base case with ZF, using the GTC code.

Non zonal electrostatic potential



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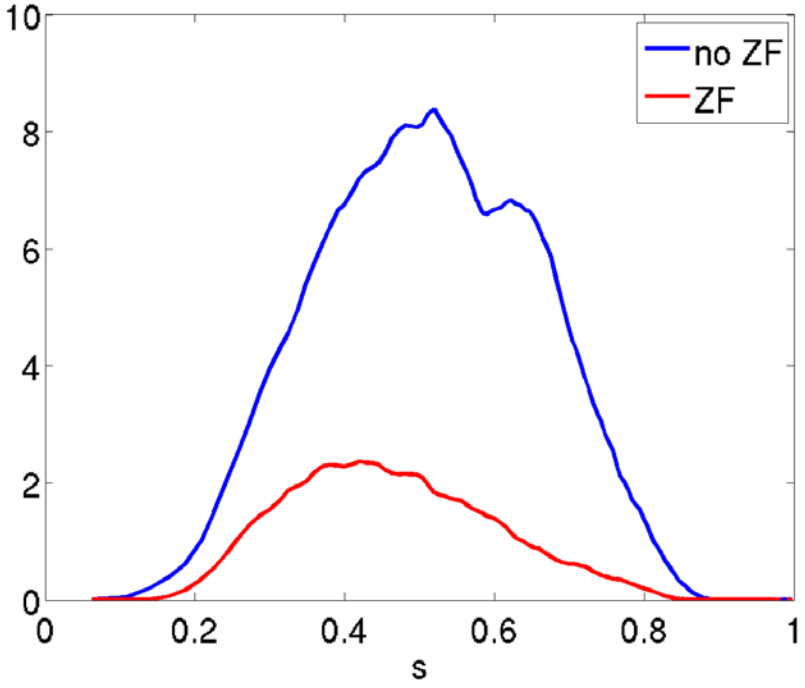
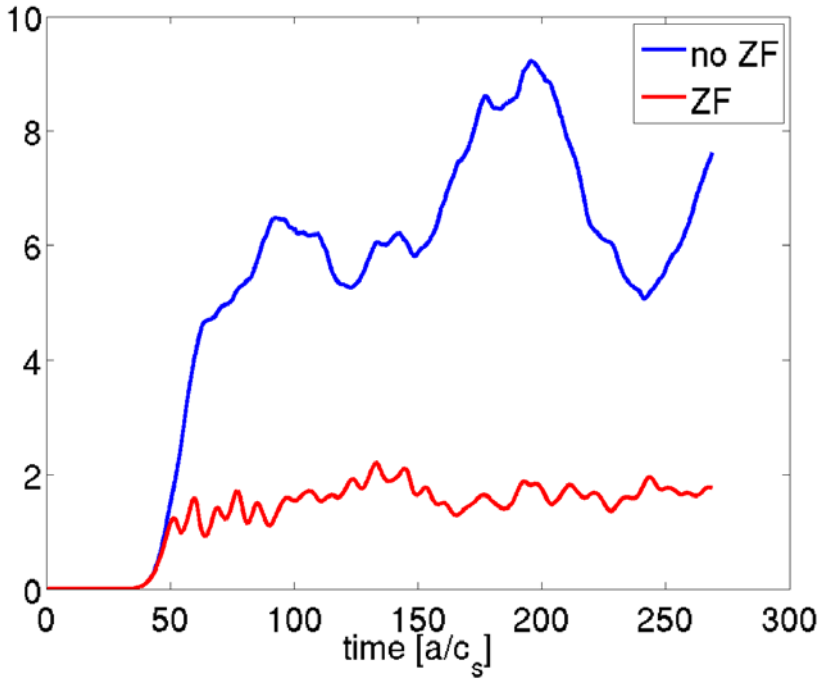
ZFs strongly reduce heat transport

➢ **Ion heat conductivity is strongly reduced**

Time average, χ/χ_{GB}



Radial average , χ/χ_{GB}



ORB5 in the year 2005

- Electrostatic, **adiabatic passing electrons**, zonal flow correctly treated and **kinetic trapped electrons.**

- Polarization equation:

$$\langle \delta n_D \rangle + \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_D} \nabla_\perp \phi \right) = (1-\alpha) \frac{e n_0}{k_B T_e} (\phi - \bar{\phi}) + \delta n_{e,trapped}$$

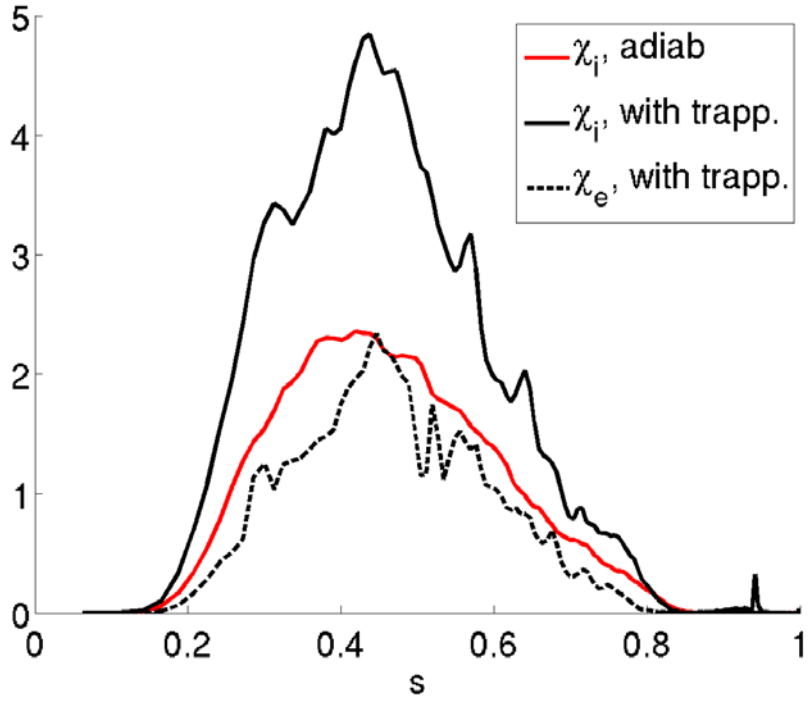
  α, fraction of trapped particles.

- No need to follow the fast parallel electron dynamics:
  time step is still comparable with adiabatic electron simulations.

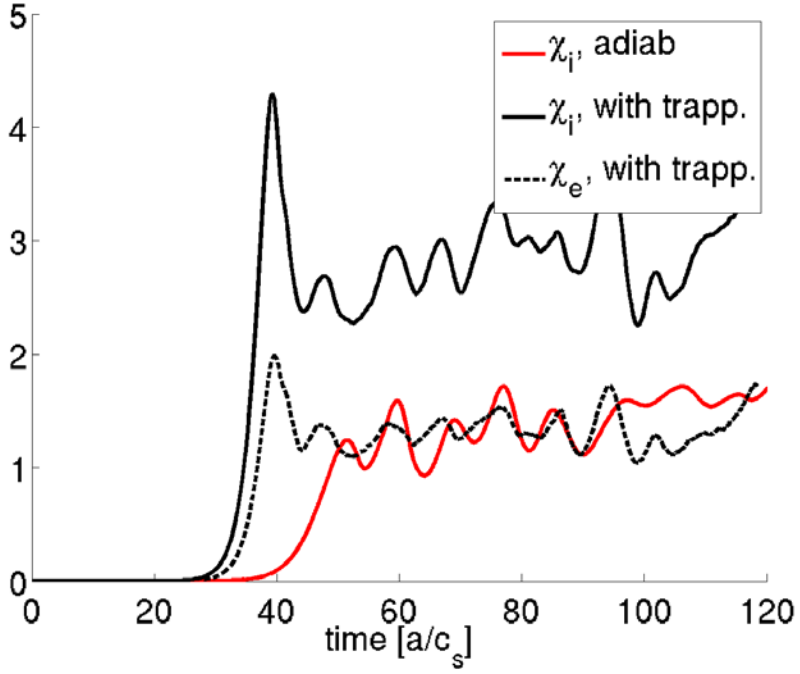
Trapped particles increase heat transport

➢ **Mode is still ITG, further destabilized by trapped particles**

Time average, χ/χ_{GB}



Radial average , χ/χ_{GB}



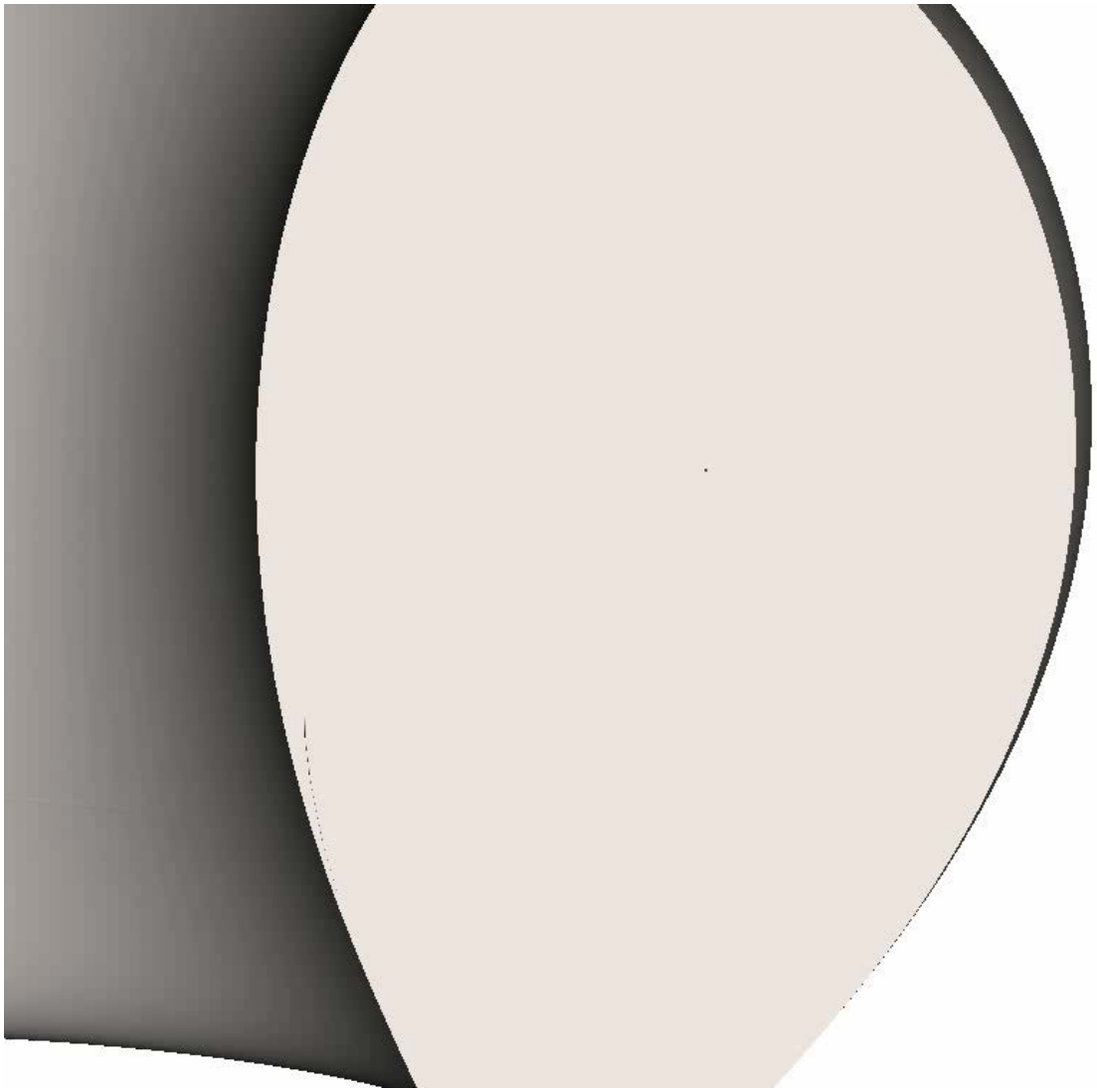
ORB5 in the year 2013

- **Electromagnetic**, passing and trapped kinetic electrons,
- Polarization equation:

$$\langle \delta n_D \rangle + \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_D} \nabla_\perp \phi \right) = \delta n_e$$

- Need to follow the fast parallel electron dynamics, time step must be $(m_i/m_e)^{1/2}$ smaller then adiabatic electron simulations.
- **Wall-clock time: 10^6 cpu/hours**.
- Rescaled density profile to have β_e**=0.1 %** at mid-radius.

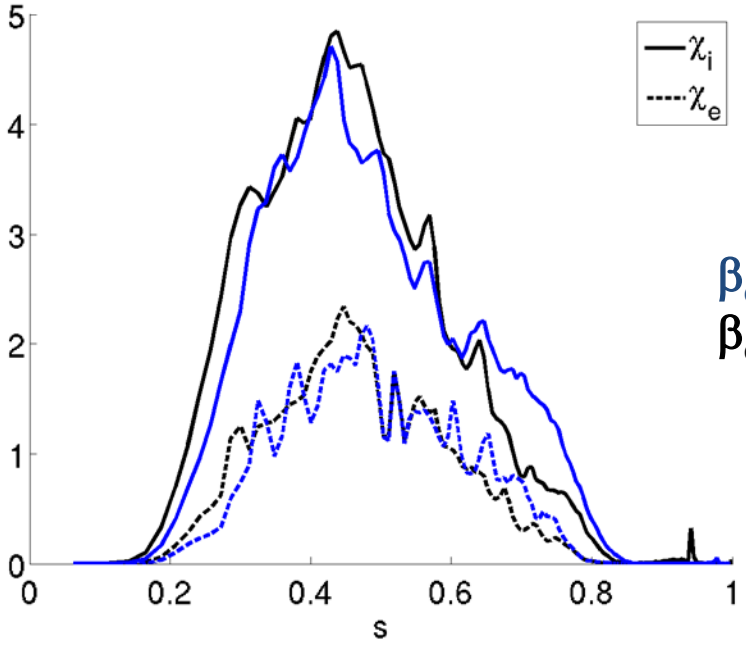
Parallel magnetic potential, $A_{||}$



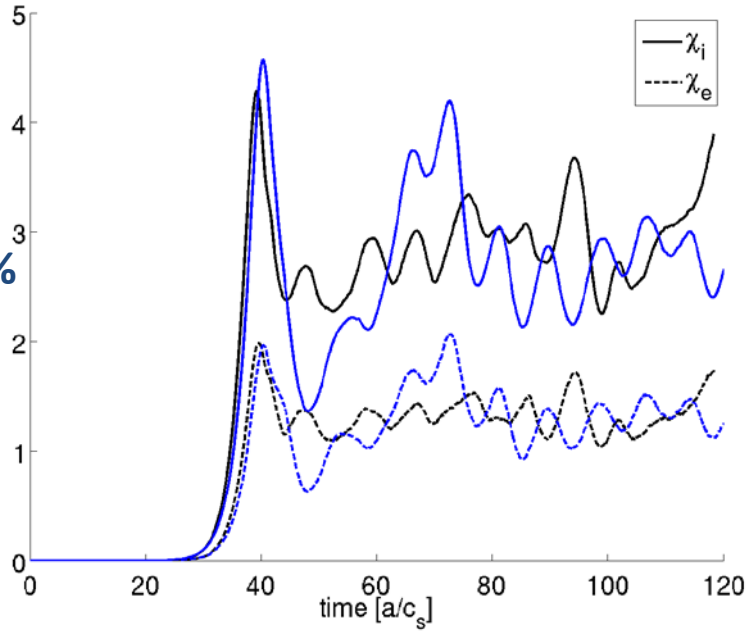
Finite β effect on transport

➢ β_e=0.1 %, no effect on transport

Time average, χ/χ_{GB}



Radial average , χ/χ_{GB}



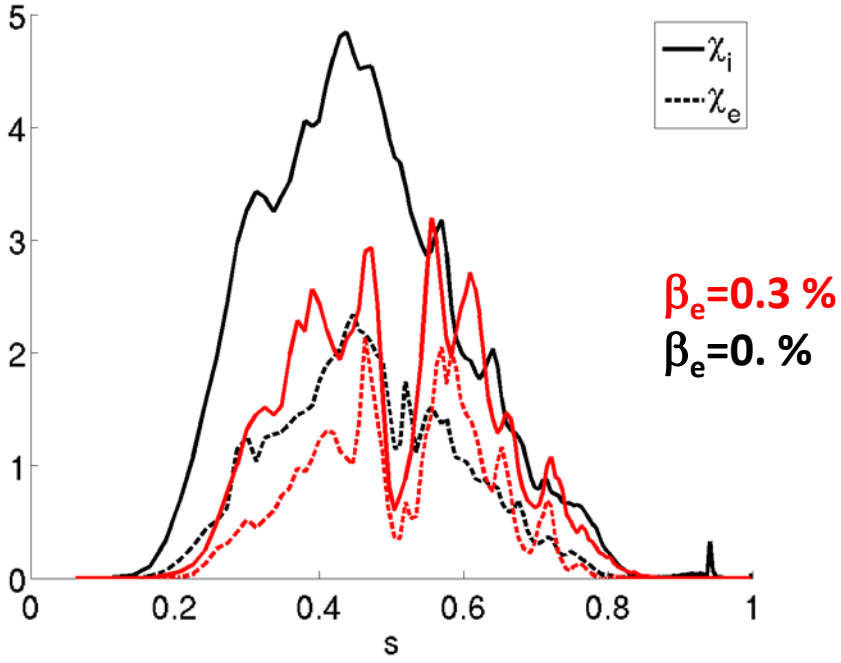
β_e=0.1 %

β_e=0. %

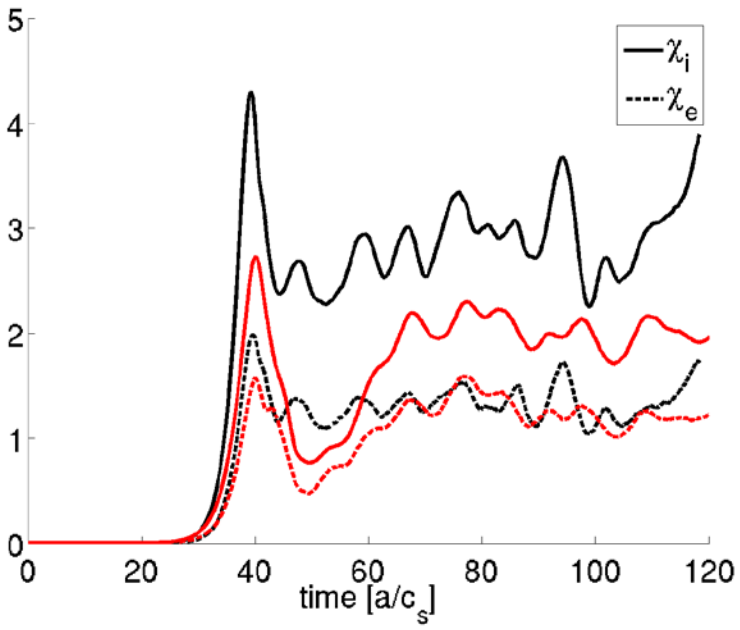
Finite β effect on transport

➢ β_e=0.3 %, transport reduction, ITG "almost TEM"

Time average, χ/χ_{GB}



Radial average , χ/χ_{GB}



Outline

- A brief introduction to Gyrokinetics
- Particle-in-cell for Gyrokinetics
- From linear to nonlinear PIC simulations: statistical noise and entropy evolution.
- The tool: the NEMORB code
- **Conclusions and outlook**

Conclusions

- **Nonlinear electrostatic GK PIC simulations are mature**: comparisons with existent experiments are now possible, when trapped electron dynamics is included.

- **Noise is understood** and kept under control.

- Cancellation problem in electromagnetic simulations is cured using control variate method: **EM simulations are challenging but feasible**. It is still a work in progress… the model is not complete and some results are questionable.

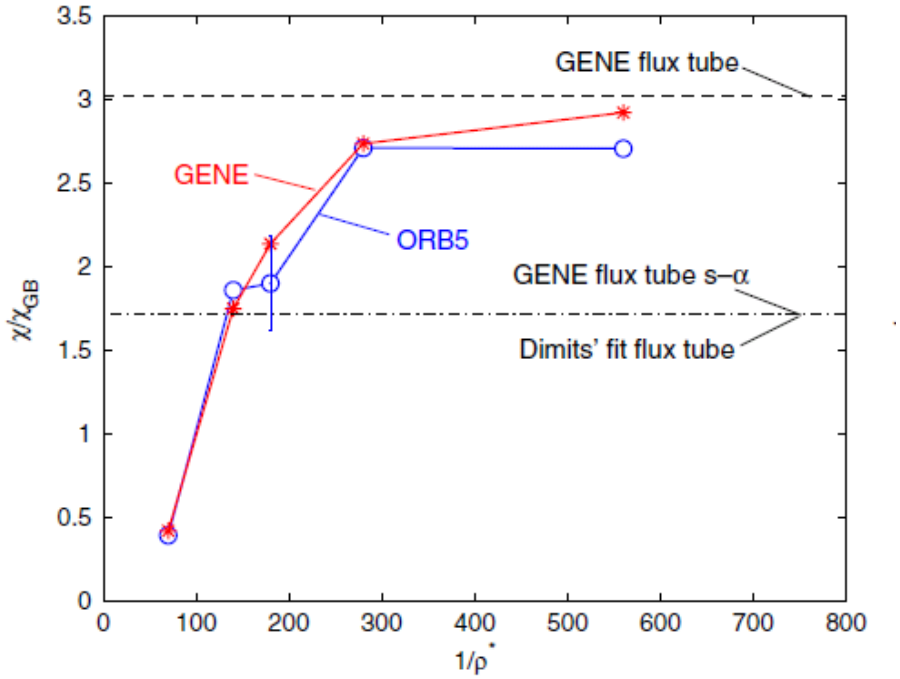
- Open problems in NEMORB:
  - **conciliate collisions and EM**
  - **push the scaling of the code (accelerators?)**

- **Outlook**: **fast particles** and their **self consistent** interplay with **Alfvénic modes.**

- Backup slides

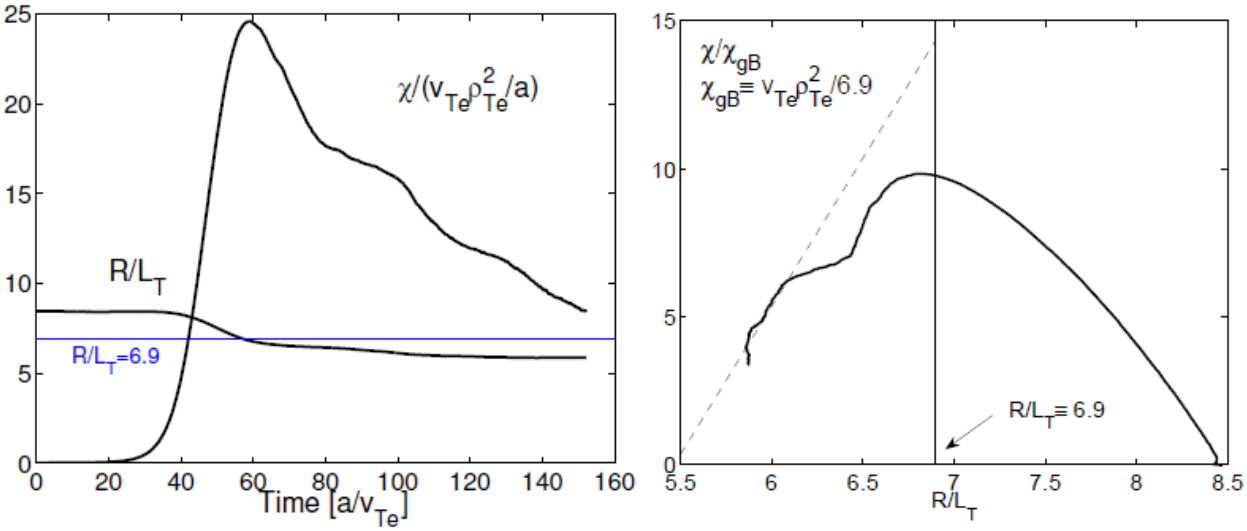
System size effects

- Controversy between GYRO and GTC results concerning the scaling of the turbulence with the machine size and the transition to the Gyro-Bohm regime.
- Controversy was solved when the same MHD equilibria (and not s-alpha) were used in ORB5 and GENE simulations [McMillan 2007].



ETG turbulence, relevance for transport

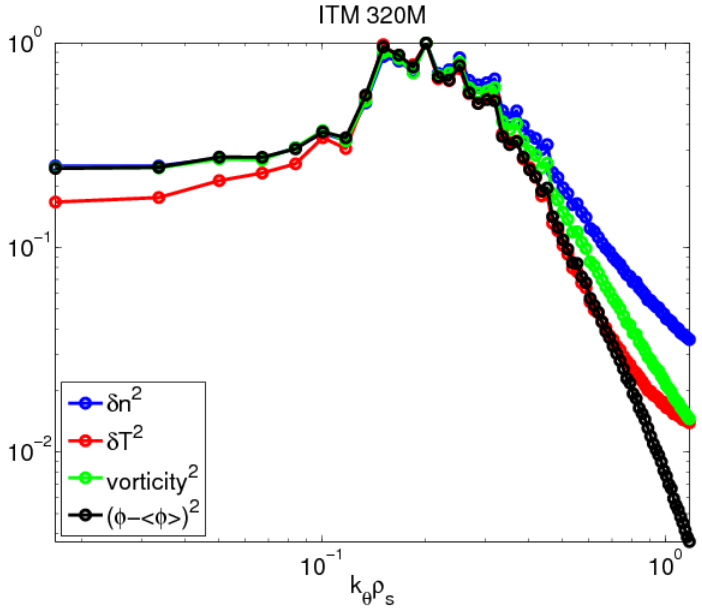
- Main motivation for my “noise” studies.
- In 2005 global PIC simulations [Lin 2005] showed that ETG modes lead to lower transport level than flux tube simulations [Jenko 2002].
- Physics or an artifact of the numerical scheme? [Nevins 2005].
- ORB5 simulations proved that when the noise was kept under control, the original flux-tube results were retrieved.

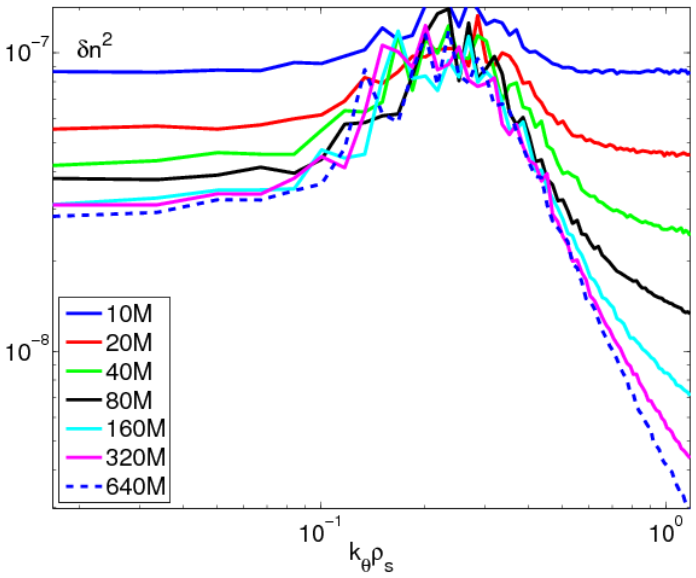


Standard diagnostics in NEMORB

- Radial profiles

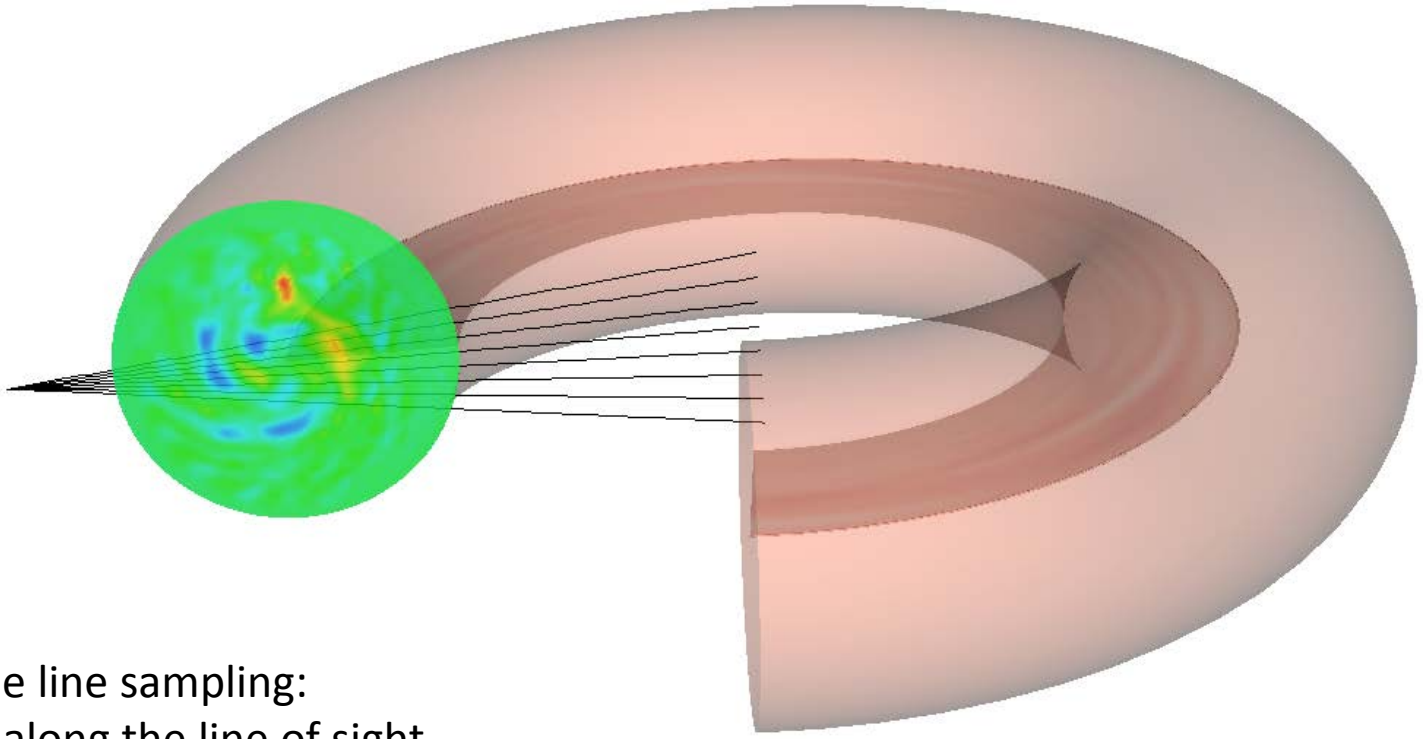
- Spectra:





- Converged spectra are difficult to get, convergence slower than fluxes.
- Spectra are reconstructed from 3D data, local spectra are possible.

Synthetic diagnostics: line sampler



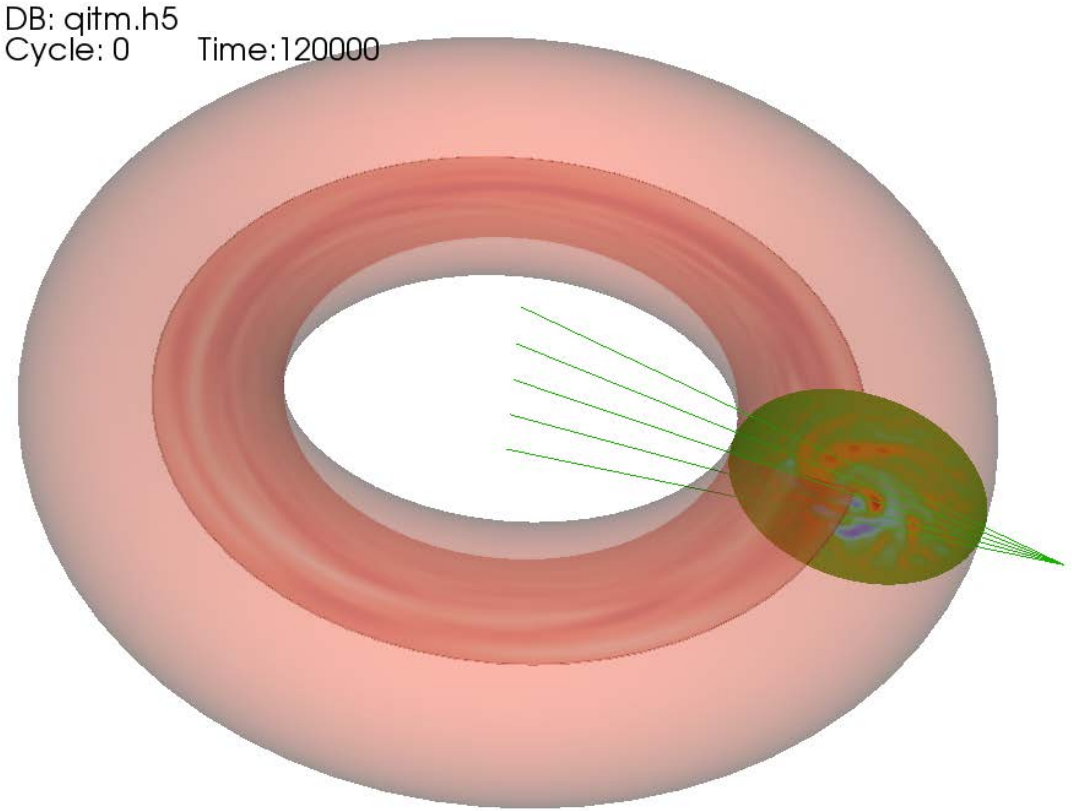
Very flexible line sampling:

- Profiles along the line of sight
- Integrated values

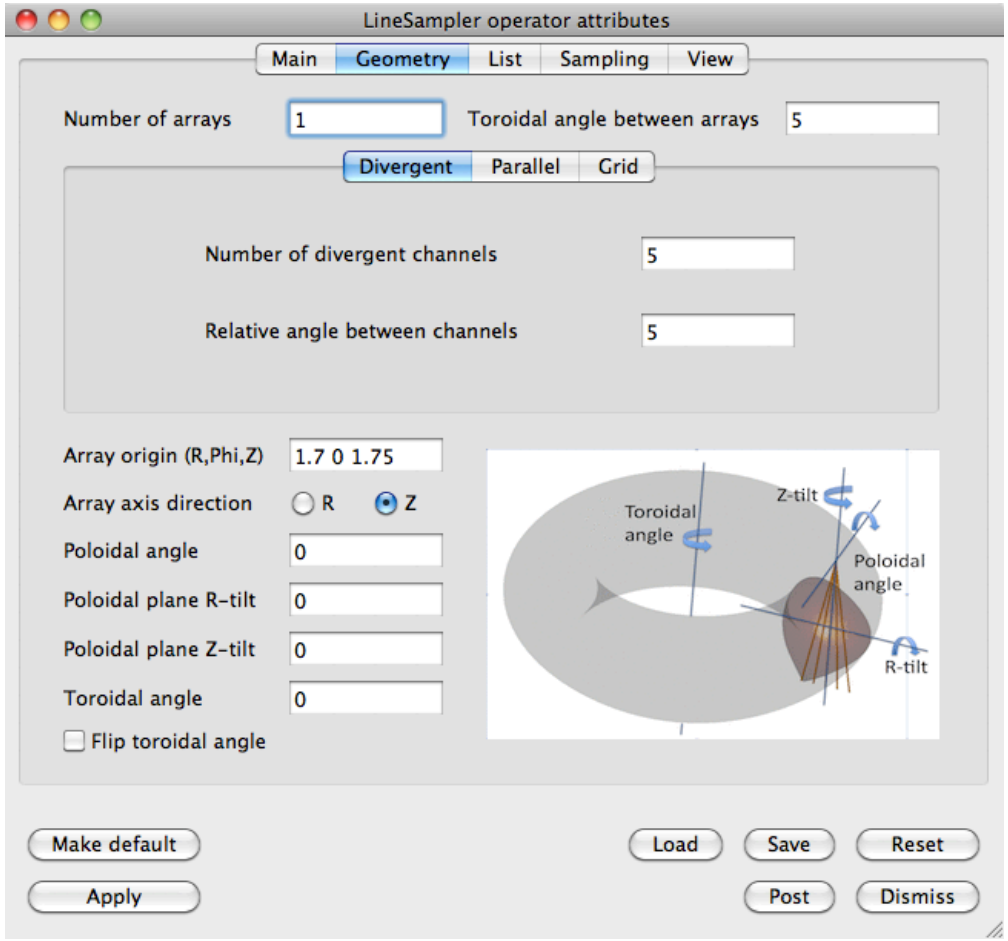
Computationally costly (for AUG, visualization cluster required)

3D diagnostics

- Sampling 3D data along 1D chords (or points)



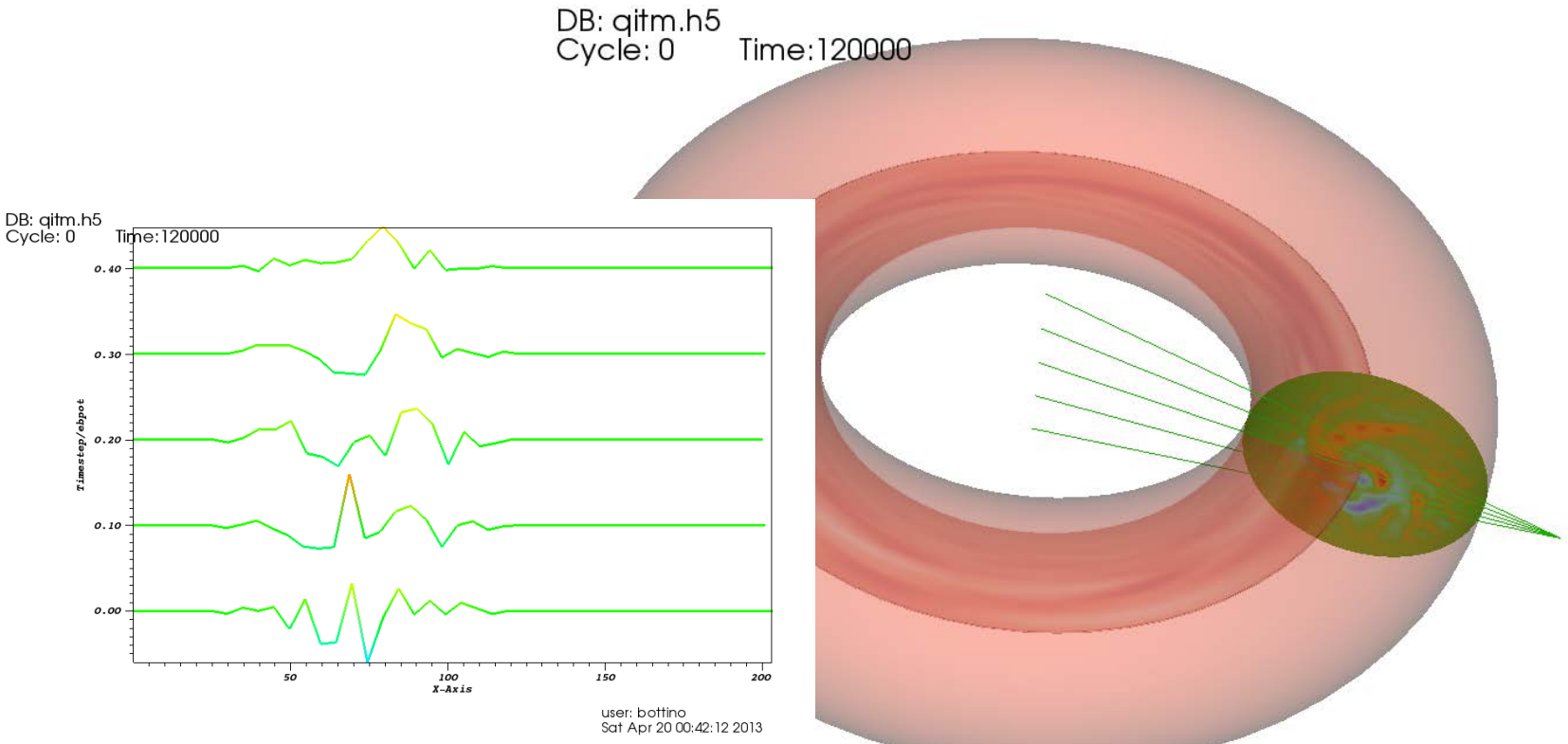
Visit: LineSampler tool



- Very flexible, easy to use BUT extremly computationally intensive.

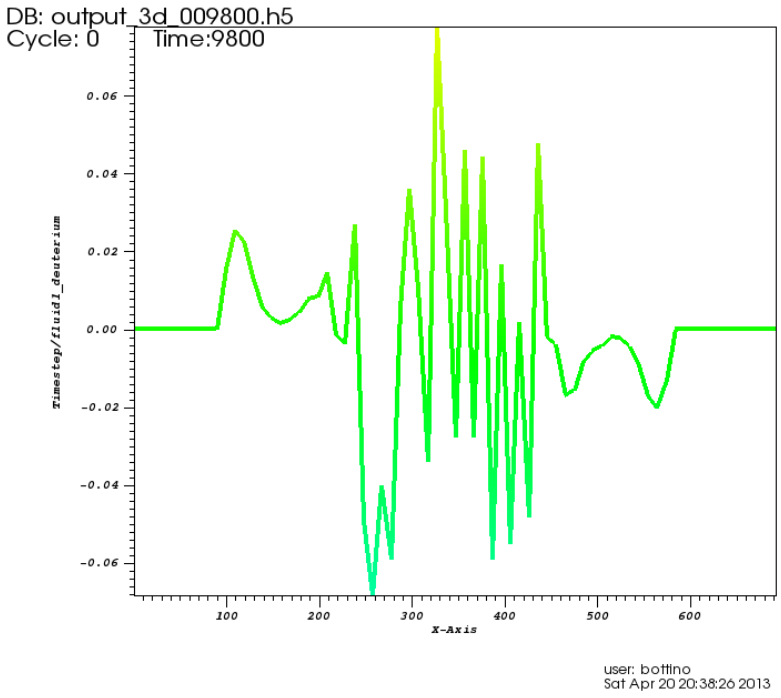
3D diagnostics

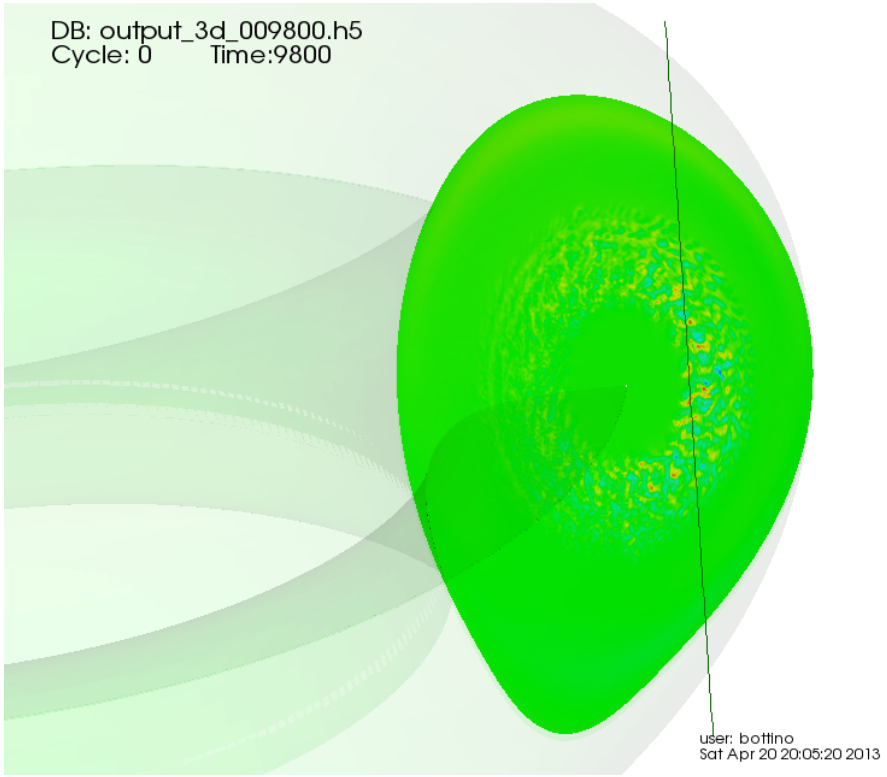
- Sampling 3D data along 1D chords (or points)



user: bottino
Fri Apr 19 23:52:04 2013

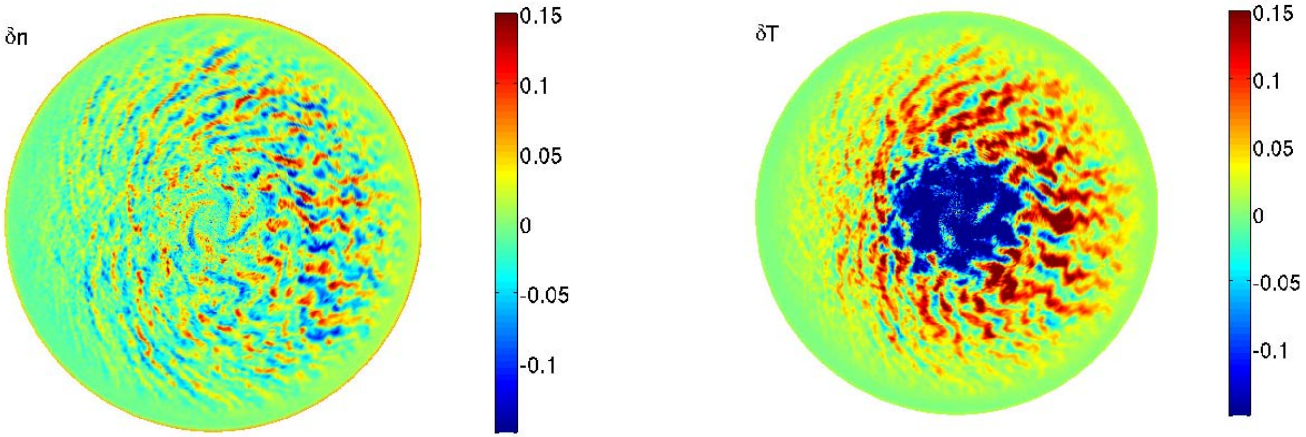
AUG application: density fluctuations





3D diagnostics

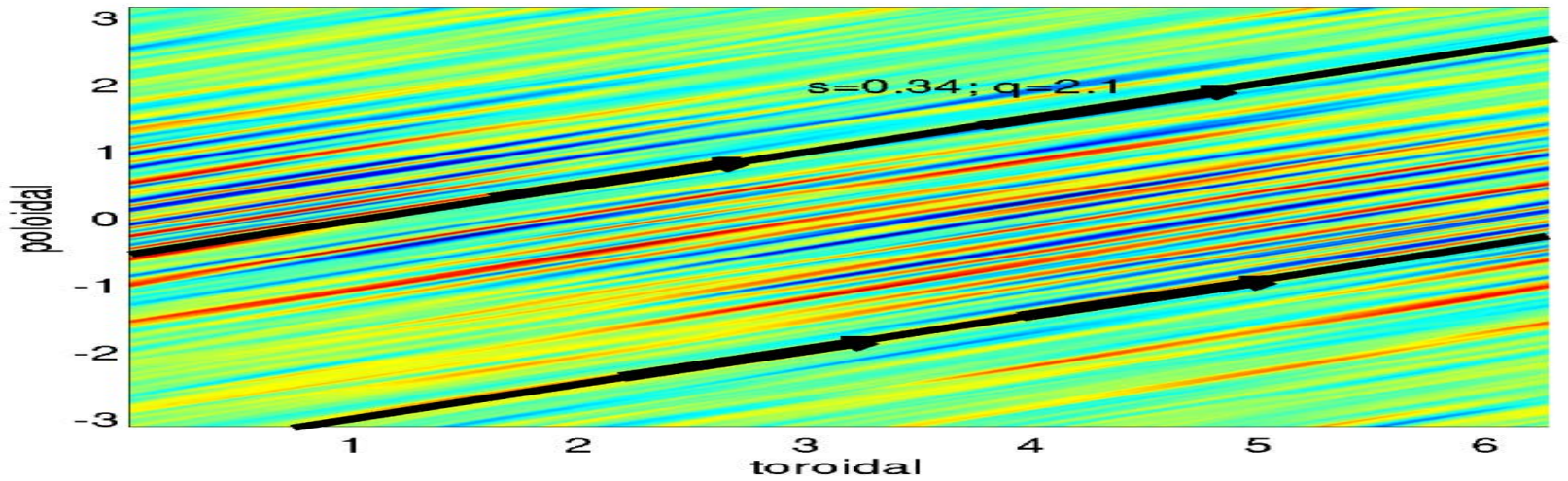
- Poloidal plots from 3D data:



- Track passive particle in turbulent or stationary fields.

- Use full 3D data (several hundreds of GB) for analysis using VisIt.

Turbulence on a flux-surface



$$\nabla_\perp^2 A_\parallel = \mu_0 \sum_{\text{species}} j_\parallel \tag{10}$$

where $j_\parallel$ is the current density linearized on the background Maxwellian f_0:

$$j_\parallel = e \int \mathrm{d}W \delta(\mathbf{R}+\boldsymbol{\rho}-\mathbf{x}) p_z \left[f - \frac{e p_z}{T} f_0 J_0 A_\parallel \right] \quad . \tag{11}$$

Eq. (10) can be rewritten as:

$$\left(\sum_{\text{species}} \frac{\mu_0 n_0 e^2}{m} \langle A_\parallel \rangle \right) - \nabla_\perp^2 A_\parallel = \mu_0 \sum_{\text{species}} \delta j_\parallel \tag{12}$$

where $\delta j_\parallel = e \int \mathrm{d}W (p_z/m) \delta f \delta(\mathbf{R}+\boldsymbol{\rho}-\mathbf{x})$ and $\langle A_\parallel \rangle \equiv (n_0)^{-1} \int \mathrm{d}W f_0 J_0 A_\parallel \delta(\mathbf{R}+\boldsymbol{\rho}-\mathbf{x})$. For $C(f) = 0$ and $S = 0$, the set of gyrokinetic equations given by (7,8,9,12) is energy and momentum conserving. An elegant proof is given in Ref. [15].
Defining for a species s the thermal gyroradius, $\rho_s \equiv \sqrt{m_s T_s}/(eB_0)$, and the plasma β, $\beta_s = \mu_0 n_0 T / B_0^2$, eq. (12) becomes, for a single ion species:

$$\frac{\beta_s}{\rho_s^2} \langle A_\parallel \rangle_s + \frac{\beta_e}{\rho_e^2} \langle A_\parallel \rangle_e - \nabla_\perp^2 A_\parallel = \mu_0 \sum_{\text{species}} \delta j_\parallel \quad . \tag{13}$$

$$H = m\frac{U^2}{2} + m\mu B + eJ_0\Phi + \mathcal{O}(\Phi^2) \simeq \frac{p_z^2}{2m} + m\mu B + e\left(J_0\Phi - \frac{p_z}{m}J_0A_\parallel\right) \quad .(3)$$

The p_z formulation implies the appearance of large unphysical terms in the parallel Ampère's law (13). Considering the Hamiltonian (3), one can define the adiabatic part of the distribution function as

$$F^{\mathrm{ad}} \equiv -\frac{ef_0}{T}(J_0\Phi - p_z J_0 A_\parallel) \tag{14}$$

and an adiabatic current $j_\parallel^{\mathrm{ad}}$:

$$\begin{aligned}\mu_0 j_\parallel^{\mathrm{ad}} &\equiv \mu_0 e \int \mathrm{d}W \delta(\mathbf{R} + \boldsymbol{\rho} - \mathbf{x}) F^{\mathrm{ad}} p_z \\ &= \mu_0 e \int \mathrm{d}W \delta(\mathbf{R} + \boldsymbol{\rho} - \mathbf{x}) \frac{ef_0 p_z^2}{T} J_0 A_\parallel = \frac{\beta_s}{\rho_s^2}\langle A_\parallel \rangle \quad .\end{aligned} \tag{15}$$

$$A_{\parallel}(\mathbf{x},t) = \sum_{\mu} \phi_{\mu}(t)\Lambda_{\mu}(\mathbf{x}) \tag{17}$$

where $\Lambda_{\mu}(\mathbf{x})$ is a tensor product of 1D B-splines. Using the Galerkin's method, equation (16) can be written in matrix form as:

$$(\hat{\mathbf{L}} + \hat{\mathbf{S}}_{\mathbf{i}} + \hat{\mathbf{S}}_{\mathbf{e}})\phi = \mu_0(\mathbf{j}_{\parallel \mathbf{i}} + \mathbf{j}_{\parallel \mathbf{e}}) \quad . \tag{18}$$

In the following, the "hat" quantities are matrices, ϕ is the B-spline coefficient vector to be solved for and the $\mathbf{j}_{\parallel}$'s are the coefficient vectors after current-assignment of the weights. The matrix elements of Eq. (18) are defined by

$$\hat{L}_{kj} \equiv \int (1-\beta_{\mathrm{i}})\nabla_{\perp}\Lambda_j \cdot \nabla_{\perp}\Lambda_k \, \mathrm{dx} \tag{19}$$

$$\hat{S}_{i,kj} \equiv \int \frac{\beta_{\mathrm{i}}}{\rho_{\mathrm{i}}^2}\Lambda_j\Lambda_k \, \mathrm{dx} \tag{20}$$

$$\hat{S}_{e,kj} \equiv \int \frac{\beta_e}{\rho_e^2}\Lambda_j\Lambda_k \, \mathrm{dx} \tag{21}$$

and the current-assignment vectors are:

$$j_{\|\mathrm{e},k} = \sum_{p=1}^{N_\mathrm{e}} p_{z,\mathrm{p}} w_{\mathrm{e,p}} \Lambda_k \tag{22}$$

$$j_{\|\mathrm{i},k} = \sum_{p=1}^{N_\mathrm{i}} p_{z,\mathrm{p}} w_{\mathrm{i,p}} J_0 \Lambda_k \quad ; \tag{23}$$

$w_{e,p}$ and $w_{i,p}$ are the marker weights, for which $\delta f_s = \sum_{p=1}^{N_s} w_s \delta(W - W_\mathrm{p})$ where $W_\mathrm{p} \equiv (\mathbf{R}_\mathrm{p}, p_{z,\mathrm{p}}, \mu_\mathrm{p})$ represents a point in the 5D phase space. N_s is the total number of markers. In order to solve the cancellation problem, we define a "noise reduced" marker weight:

$$\tilde{w}_\mathrm{p} = w_\mathrm{p} - \Omega_\mathrm{p} \frac{e f_0}{T} J_0 A_\| \tag{24}$$

Ω_p is the phase space volume, initially centered around W_p, associated with the marker p (see Ref.[10]). The current-assignment vector, for the new weight $\tilde{w}_\mathrm{p}$ becomes:

$$\mu_0 \tilde{\mathbf{j}}_\| = \mu_0 (\mathbf{j}_\| - \hat{\mathbf{j}}_\|^{\mathrm{ad}} \phi) \tag{25}$$

$$\mu_0 \hat{\mathbf{j}}_\|^{\mathrm{ad}} \phi \equiv \sum_{p=1}^{N_\mathrm{s}} \mu_0 p_{z,p} \Omega_p \frac{e p_z f_0}{T} J_0 A_\| \Lambda_k \tag{26}$$

$$\simeq \mu_0 e \int \mathrm{d}W \delta(\mathbf{R} + \boldsymbol{\rho} - \mathbf{x}) \frac{e f_0 p_z^2}{T} J_0 A_\| \Lambda_k = \hat{\mathbf{S}} \phi \tag{27}$$

having used the definition of adiabatic current of Eq. (15). Since the cancellation problem affects mainly the electrons, noise-reduced weights are used for the electrons only. Therefore, the discretized parallel Ampère's law is:

$$(\hat{\mathbf{L}} + \hat{\mathbf{S}}_\mathrm{i} + \hat{\mathbf{S}}_\mathrm{e})\phi = \mu_0(\mathbf{j}_{\parallel \mathrm{i}} + \mathbf{j}_{\parallel \mathrm{e}} - \hat{\mathbf{j}}^{\mathrm{ad}}_{\parallel \mathrm{e}}\,\phi) + \hat{\mathbf{S}}_\mathrm{e}\phi \quad . \tag{28}$$

A formal proof of the equivalence of this algorithm with a control variate method is given in [6] (scheme two). This equation can be solved by an iterative procedure (see Appendix B of Ref. [6]). The cancellation problem can be solved analytically by eliminating the term $\hat{\mathbf{S}}_\mathrm{e}\phi$ on both sides of eq. (28).