DE LA RECHERCHE À L'INDUSTRIE

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GYROKINETIC SIMULATIONS OF MAGNETIC FUSION PLASMAS: GYSELA CODE

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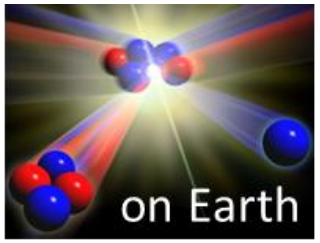
Main challenges for Magnetic Fusion

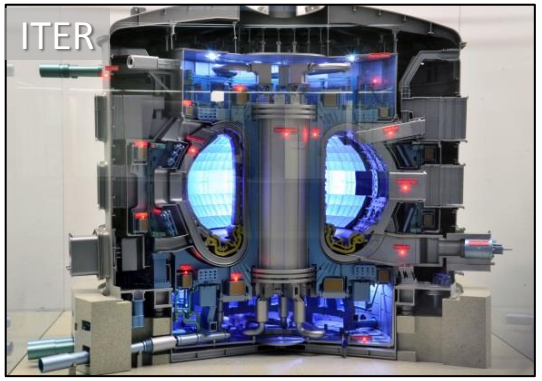
- **Goals of fusion researches**: To control fusion reactions on earth that occur naturally in sun for instance
  - Fusion reactions only at high temperatures (~150 Million °C)
  - How to confine turbulent plasmas ?
  - Most advanced concept = Tokamak



$D+T \rightarrow {}^4He+n$

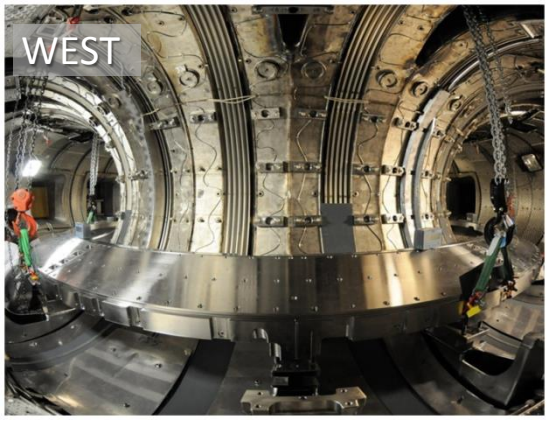
p+p

- Main **goals of ITER** (Cadarache) ~2025
  - International project under construction
  - To demonstrate the scientific and technological feasibility of fusion energy on earth, thus leading to a reliable source of energy with low environmental impacts.



Plasma volume: 840 m^3

- Main **goals of WEST** (IRFM) ~2017
  - Upgrade of Tore Supra french tokamak exploits at IRFM CEA for almost 30 years
  - Tests of ITER like actively cooled divertor elements

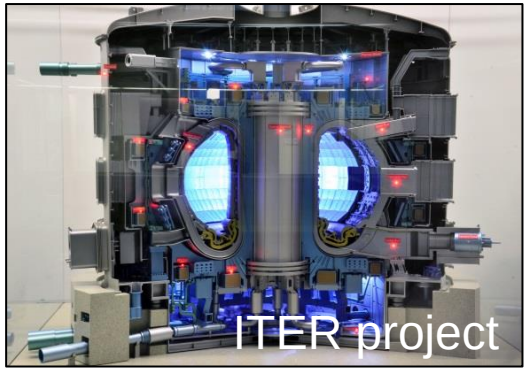


Plasma volume ~ 20 m^3

ITER building site at Cadarache

Plasma turbulence simulations → Kinetic approach mandatory

- Turbulence generates loss of heat and particles
  - ↘ Confinement properties of the magnetic configuration
  - Understanding, predicting and controlling turbulence is a subject of utmost importance
- Tokamak plasmas weakly collisional → Kinetic approach is mandatory



Outline

1. Gyrokinetic codes for plasma turbulence

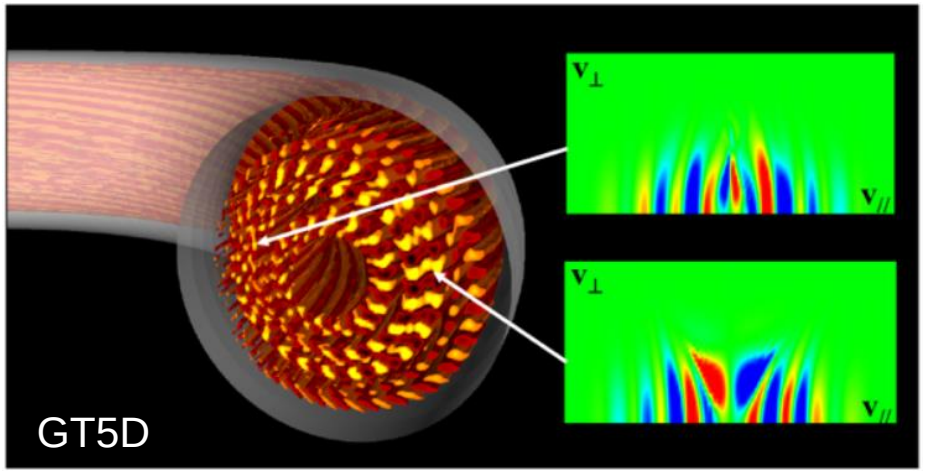
2. GYSELA code: How to treat kinetic electrons ?

   → How to prepare to exascale needs

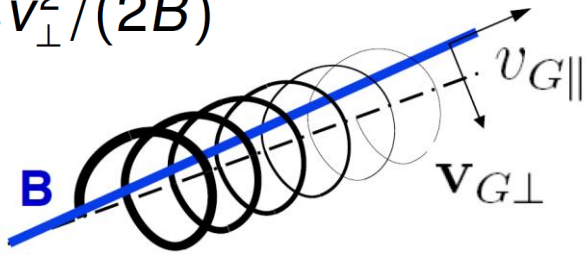
Gyrokinetic plasma turbulence simulations

- Kinetic theory: 6D distribution function of particles (3D in space + 3D in velocity) $F_s(r, \theta, \varphi, v_{\parallel}, v_{\perp}, \alpha)$
- Fusion plasma turbulence is low frequency:

$$\omega_{\text{turb}} \sim 10^5 s^{-1} \ll \omega_{ci} \sim 10^8 s^{-1}$$



- Phase space reduction 6D to 5D: fast gyro-motion is averaged out
  - Adiabatic invariant: magnetic momentum $\mu = m_s v_\perp^2/(2B)$
  - Velocity drifts of guiding-centers



☺ Large reduction memory / CPU time

☹ Complexity of the system

- Gyrokinetic theory: 5D distribution function of guiding-centers $\bar{F}_s(r, \theta, \varphi, v_{G\parallel}, \mu)$ where μ parameter

References for modern GK derivation

- For an overview and a modern formulation of the gyrokinetic derivation, see the review paper by A.J. Brizard and T.S. Hahm, *Foundations of nonlinear gyrokinetic theory*, Rev. Mod. Phys (2007).

- This new approach is based on Lagrangian formalism and Lie perturbation theory (see *e.g.* J.R Cary *[Physics Reports (1981)]*, J.R Cary and Littlejohn *[Annals of Physics (1983)]*

- The advantage of this approach is to preserve the first principles by construction, such as the symmetry and conservation properties of the Vlasov equation – particle number, momentum, energy and entropy.

[See N. Tronko talk for more recent works, Thursday morning]

GK codes require state-of-the-art HPC (1/2)

- Gyrokinetic codes require state-of-the-art HPC techniques and must run efficiently on several thousand processors
  - Non-linear 5D simulations + multi-scale problem in space and time

$\rho_i \rightarrow$ machine size a : $\rho_* \equiv \rho_i / a \ll 1$ $(\rho_*^{\mathrm{ITER}} \approx 10^{-3})$; $\Delta t \approx \gamma^{-1} \sim 10^{-6} s \rightarrow t_{\mathrm{simul}} \approx$ few $\tau_E \sim 10 s$

GK codes already use Petascale capabilities

- Various simplifications in terms of physics:

			complex →	
- δf: scale separation between equilibrium and perturbation		$\neq$		Full-f
- Flux-tube: domain considered = a vicinity of a magnetic field line		$\neq$		Global
- Fixed gradient: no sources		$\neq$		Flux-driven
- Collisionless: no neoclassical transport		$\neq$		Collisions
- Adiabatic electrons: no particle transport		$\neq$		Kinetic electrons
- Electrostatic: $\mathbf{B} = \mathrm{const}$		$\neq$		Electromagnetic

→ None of the codes cover all physical aspects

New generation of codes: Global full-f flux-driven code with collisions

GK codes require state-of-the-art HPC (2/2)

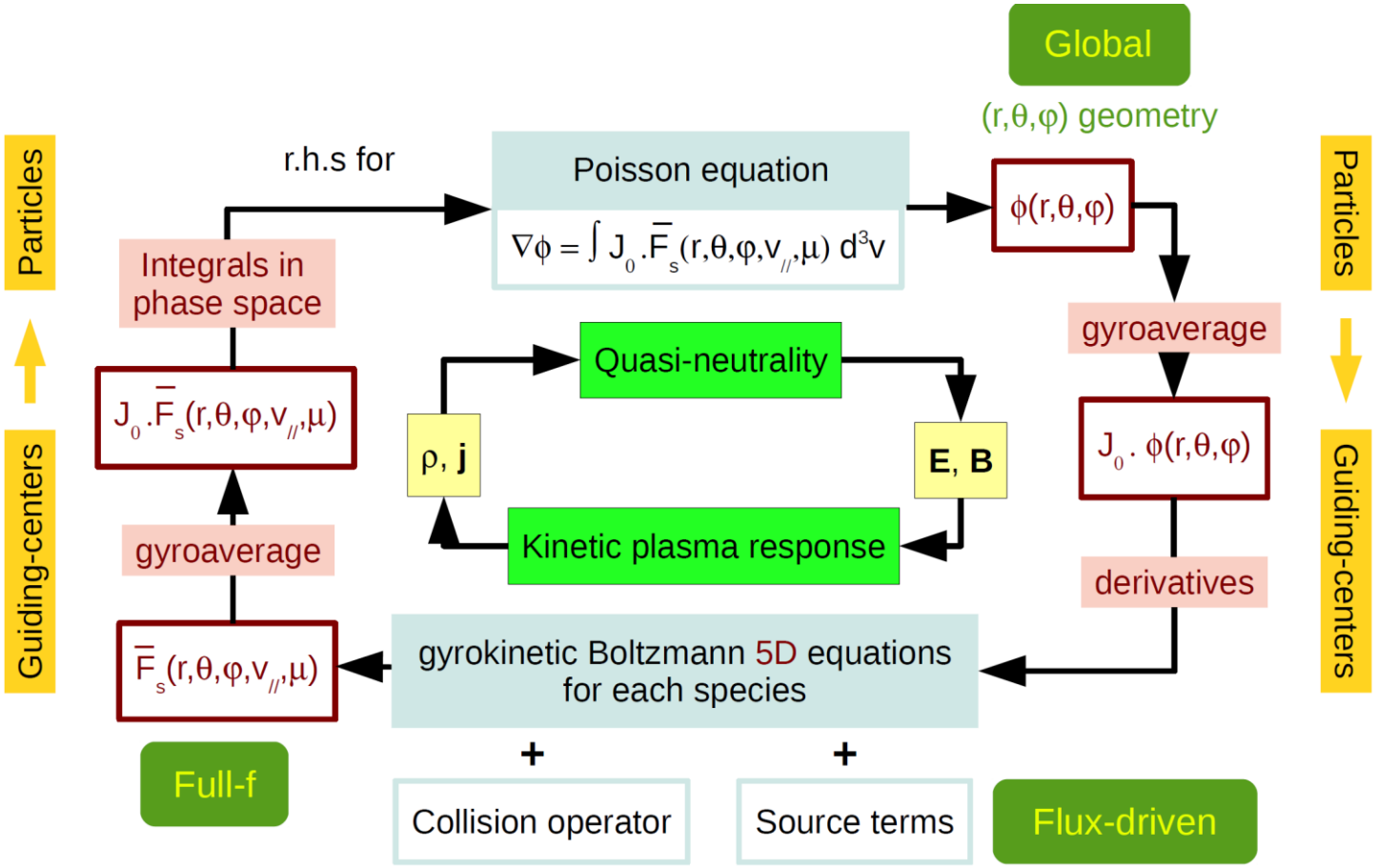
- Various numerical schemes: [Grandgirard, Panorama & Synthèse 2012]
  - Lagrangian (PIC), Eulerian or Semi-Lagrangian
- GK code development is a highly international competitive activity
  - US: ~ 8 codes - EU: 5 codes - Japan: 2 codes
- EuroFusion project “GK code benchmark” (2015-2017)
  - Linear benchmarks between 3 EU codes successfully achieved

[Goerler, PoP 2016 ; Biancalani, PoP 2017]

→ITER simulations without any assumptions are unreacheable

GK code – schematic view

- Gyrokinetic complexity: Poisson is solved with the charge density of particles and the Vlasov equation describe the guiding-center evolution
  - Gyrokinetic operator is more complex for global codes



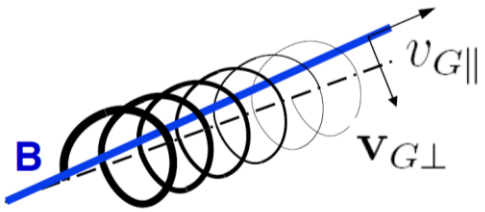
5D Boltzmann eq. + 3D quasi-neutrality eq.

- Time evolution of the gyrocenter distribution function for s species $\bar{F}_s(r, \theta, \varphi, v_\parallel, \mu)$ governed by 5D gyrokinetic Fokker-Planck equation with an additional realistic heating source:

$$B^*_{\parallel s}\frac{\partial \bar{F}_s}{\partial t} + \nabla \cdot \left(\frac{d\mathbf{x_G}}{dt} B^*_{\parallel s} \bar{F}_s\right) + \frac{\partial}{\partial v_{G\parallel}}\left(\frac{dv_{G\parallel}}{dt} B^*_{\parallel s} \bar{F}_s\right) = \underbrace{C(\bar{F}_s)}_{\text{collision operator}} + \underbrace{S}_{\text{heating source}}$$

where $\frac{d\mathbf{x_G}}{dt} = \mathbf{v}_G = v_{G\parallel}\mathbf{b} + v_{G\perp}$

with $v_{G\perp} \approx \frac{\mathbf{E}\times\mathbf{B}}{B^2} + v_{d0} R \frac{\mathbf{B}\times\nabla B}{B^2}$



$\mathbf{E} = \nabla\left(J_0 \cdot \phi\right)$ with $\phi(\mathbf{x})$ electrostatic potential and J_0 the gyroaverage operator.

5D Boltzmann eq. + 3D quasi-neutrality eq.

- Time evolution of the gyrocenter distribution function for s species $\bar{F}_s(r, \theta, \varphi, v_\parallel, \mu)$ governed by 5D gyrokinetic Fokker-Planck equation with an additional realistic heating source:

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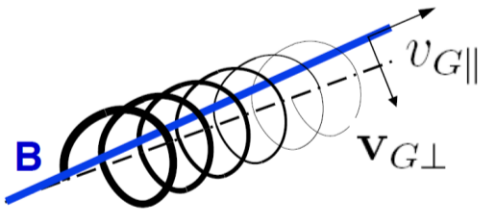
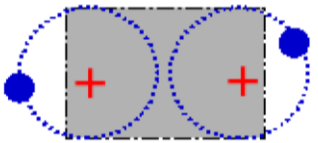


$\mathbf{E} = \nabla\left(J_0 \cdot \phi\right)$ with $\phi(\mathbf{x})$ electrostatic potential and J_0 the gyroaverage operator.

- Self-consistency ensured by a 3D quasi-neutrality equation:



$$\underbrace{\frac{e}{T_{e,\mathrm{eq}}}(\phi - \langle\phi\rangle_{\mathrm{FS}})}_{\delta n_e \text{ for adiabatic electrons}} = \underbrace{\frac{1}{n_{e_0}}\sum_s Z_s \int J_0 \cdot \left(\bar{F}_s - \bar{F}_{s,\mathrm{eq}}\right) d^3v}_{\sum_s \delta n_{GCs}} + \underbrace{\frac{1}{n_{e_0}}\sum_s Z_s \nabla_\perp \cdot \left(\frac{n_{s,\mathrm{eq}}}{B\Omega_s}\nabla_\perp \phi\right)}_{\delta n_{\text{polarization}} \text{ particles} \neq \text{guiding-centers}}$$

Outline

1. Gyrokinetic codes for plasma turbulence

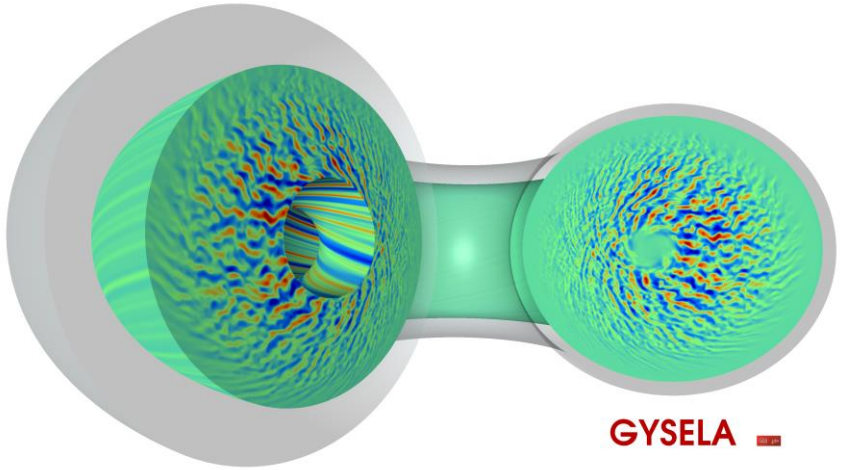
2. GYSELA code: How to treat kinetic electrons ?

- Increase code Parallelization
  → Prepare GYSELA to Exascale machine
- Separation of dynamics (//, ⊥)
  → Weak discretization in // direction
- Heavy electrons
  → spatial / temporal discretization x $(m_i/m_e)^2$
- Linear benchmarks
  - Damping of GAM due to kinetic electrons
  - Linear growth of ITG-TEM instability

GYSELA = GYrokinetic SEmi LAgrangian code

- GYSELA developed at CEA-IRFM since 2001: Unique code based on a Semi-Lagrangian method (mix between PIC and Eulerian schemes) [Grandgirard, CPC 2016]

- GYSELA strength:
  - Global: simulate entire tokamak
    → boundary conditions
  - Full-f: multi-scale physics
  - Flux-Driven (heat, momentum, … sources)
    → steady state on τ_E
  - Multi-ion species → impurity transp.
  - Collision operator → synergy between neoclassical & turbulent transports



- Present GYSELA limitations:
  - Adiabatic electrons
  - Circular magnetic configuration
  - Electrostatic

→ Kinetic electrons mandatory: particle transport + trapped electron modes

Time-splitting for Boltzmann equation

- A time-splitting of Strang is applied to the 5D non-linear Boltzmann equation:

$$B^*_{\|s}\frac{\partial \bar{F}_s}{\partial t} + \nabla\cdot\left(\frac{d\mathbf{x_G}}{dt}B^*_{\|s}\bar{F}_s\right) + \frac{\partial}{\partial v_{G\|}}\left(\frac{dv_{G\|}}{dt}B^*_{\|s}\bar{F}_s\right) = C(\bar{F}_s) + S$$

- Let us define three advection operators (with $\mathcal{X}_G = (r,\theta)$)

$$B^*_{\|s}\frac{\partial \bar{F}_s}{\partial t} + \nabla\cdot\left(B^*_{\|s}\frac{\mathrm{d}\mathcal{X}_G}{\mathrm{d}t}\bar{F}_s\right) = 0 \qquad : (\tilde{\mathcal{X}}_G)$$

$$B^*_{\|s}\frac{\partial \bar{F}_s}{\partial t} + \frac{\partial}{\partial \varphi}\left(B^*_{\|s}\frac{\mathrm{d}\varphi}{\mathrm{d}t}\bar{F}_s\right) = 0 \qquad : (\tilde{\varphi})$$

$$B^*_{\|s}\frac{\partial \bar{F}_s}{\partial t} + \frac{\partial}{\partial v_{G\|}}\left(B^*_{\|s}\frac{\mathrm{d}v_{G\|}}{\mathrm{d}t}\bar{F}_s\right) = 0 \qquad : (\tilde{v_{G\|}})$$

➠ Semi-Lagrangian scheme

- And the collision operator $(\tilde{C})$ on a Δt : $\partial_t \bar{F}_s = C(\bar{F}_s)$ ➠ Crank-Nicolson
- And the source operator $(\tilde{S})$ on a Δt : $\partial_t \bar{F}_s = S$ ➠ Crank-Nicolson
- Then, a Boltzmann solving sequence $(\tilde{\mathcal{B}})$ is performed:

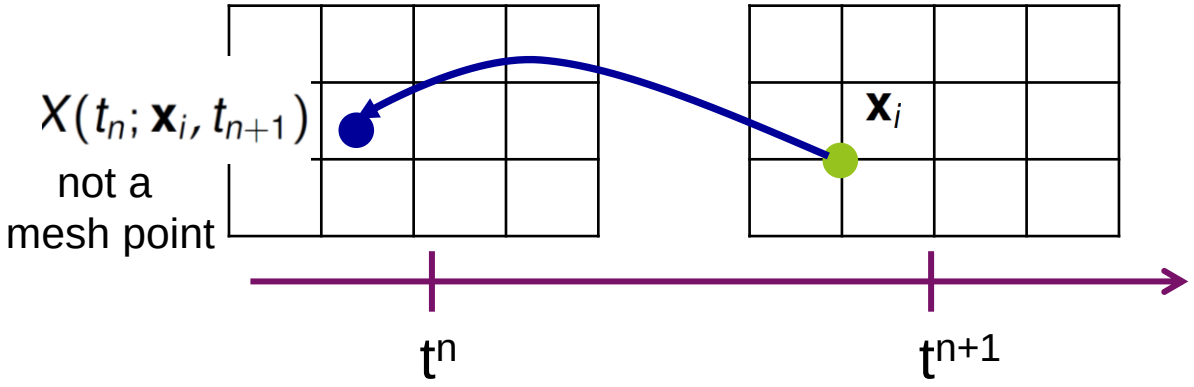
$$(\tilde{\mathcal{B}}) \equiv \left(\frac{\tilde{S}}{2},\frac{\tilde{C}}{2}\right)\left(\frac{\tilde{v_{G\|}}}{2},\frac{\tilde{\varphi}}{2},\tilde{\mathcal{X}}_G,\frac{\tilde{\varphi}}{2},\frac{\tilde{v_{G\|}}}{2}\right)\left(\frac{\tilde{C}}{2},\frac{\tilde{S}}{2}\right)$$

Example of Backward Semi-Lagrangian (BSL) approach for 2D advection operator

We consider the advection equation: $B^*_{\|s}\frac{\partial \bar{F}_s}{\partial t} + \nabla \cdot \left(B^*_{\|s}\frac{\mathrm{d}X_G}{\mathrm{d}t}\bar{F}_s \right) = 0$ (with $X_G = (r, \theta)$)

The Backward Semi-Lagrangian scheme: *(mix between PIC and Eulerian approach)*

- Fixed grid on phase-space *(Eulerian character)*
- Method of characteristics : ODE $\longrightarrow$ origin of characteristics *(PIC character)*



- f is conserved along the characteristics, i.e $f^{n+1}(\mathbf{x}_i) = f^n(X(t_n; \mathbf{x}_i, t_{n+1}))$
- Interpolate on the origin using known values of previous step at mesh points (initial distribution f^0 known).
  - Cubic spline interpolation: good compromise between accuracy and complexity.

Several Semi-Lagrangian schemes tested

$$(\tilde{\mathcal{V}}) \equiv \left(\frac{\tilde{v_{G\|}}}{2}, \frac{\tilde{\varphi}}{2}, \tilde{\mathcal{X}}_G, \frac{\tilde{\varphi}}{2}, \frac{\tilde{v_{G\|}}}{2} \right)$$

- Each Vlasov sequence $\tilde{\mathcal{V}}$ is solved by using Semi-Lagrangian techniques
- Several new Semi-Lagrangian have been tested in collaboration with Strasbourg university.
  - Conservative Semi-Lagrangian (CSL) *[Braeunig, INRIA-report 2010]*
  - Forward Semi-Lagrangian (FSL) *[Latu, INRIA-report 2012]*
- GYSELA is still based on the classical semi-lagrangian scheme
  - Backward Semi-lagrangian (BSL) *[Grandgirard, JoCP 2006]*
    ↪ Good properties of energy conservation shown for 4D simplified models

➠ SELALIB INRIA platform for testing numerical schemes for 4D Vlasov equations: born out the observation that efficient schemes in 2D can be irrelevant for our 5D plasma turbulence problem.

Kinetic electrons: A modeling bottleneck

- Long simulation ($\rightarrow$ self-organisation on τ_E) with adiabatic electrons on huge meshes (e.g. 272 10^9) run ~ 1 month on several thousands cores

[Dif-Pradalier, PRL 2015]

- GYSELA is already using currently Petascale machines (~ 100 million hours/year)

- GYSELA runs efficiently on the totality of the biggest EU machine (~ 450 kcores)

- Numerical issues for kinetic electrons:

$v_{the} \sim (m_i/m_e)^{1/2} \times v_{thi} \sim 10^8 m.s^{-1}$ → time step / $(m_i/m_e)^{1/2} \sim 60$

$\rho_e \sim \rho_i/(m_i/m_e)^{1/2} \sim \rho_i/60 \sim 50\mu m$ → nb grid points $\times (m_i/m_e)^{3/2} \sim 60^3$

→ (ρ_e , v_{the}) and (ρ_i, v_{thi}) in same simulation more than exascale ?

Parallelisation optimisation
→ Lagrange instead of cubic splines

- Trend: computations cheaper and cheaper in comparison to mem. access
  → FLOPs achieved by high-order methods tends to increase
- Idea: Replace cubic splines used for interpolation in semi-Lagrangian scheme by high-order Lagrange polynomials
  - Lagrange are more local than cubic splines
  - Lagrange polynomials degree 5 → best compromise (accuracy)
- **But** Lagrange involves extra operations

Kind of interpolation	Mem. load	Mem. store	Multiply	Add	Divide
1D spline	1	1	26	16	1
1D Lagrange 6-pts	1	1	30	25	0
2D spline	1	1	60	40	2
2D Lagrange 6-pts	1	1	90	74	0

- **However**:
  - Compiler vectorises well Lagrange formula
  - Division is costly on KNL

Parallelisation optimisation
→ Improvement of the vectorisation

- GYSELA is now ported on KNL machine

[EoCoE european Project + CVT GENCI + HLST IPP Garching + Atos-France]

Benchmark on one node Broadwell / KNL / Skylake (Marconi machine)

Adding of vectorisation + Lagrange

Steps \ Hardware	Broadwell	KNL	Skylake
advec1D in vpar	12.7 (-78%)	12.2 (-85%)	6.4 (-86%)
advec2D (r,theta)	16.3 (-60%)	24.7 (-43%)	8.9 (-70%)
comm. transpose	31.2 (-25%)	12.9 (-48%)	15.5 (-53%)
heat source	5.6 (-50%)	7.9 (-64%)	3.2 (-60%)
...			
Total	139 (-45%)	124 (-55%)	86 (-58%)

Table: Breakdown of timing (in s) for a small run. In parentheses, improvement compared to **initial version**.

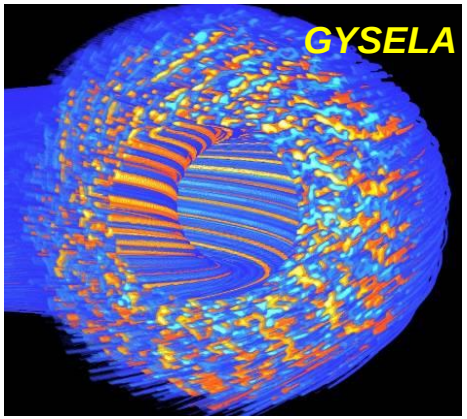
[G. Latu, 2017]

- CPU time on one KNL node comparable with one Broadwell node
- Improvement of vectorisation essential for KNL

  → positive impact on Broadwell and Skylake machine

Taking benefit of the strong anisotropy

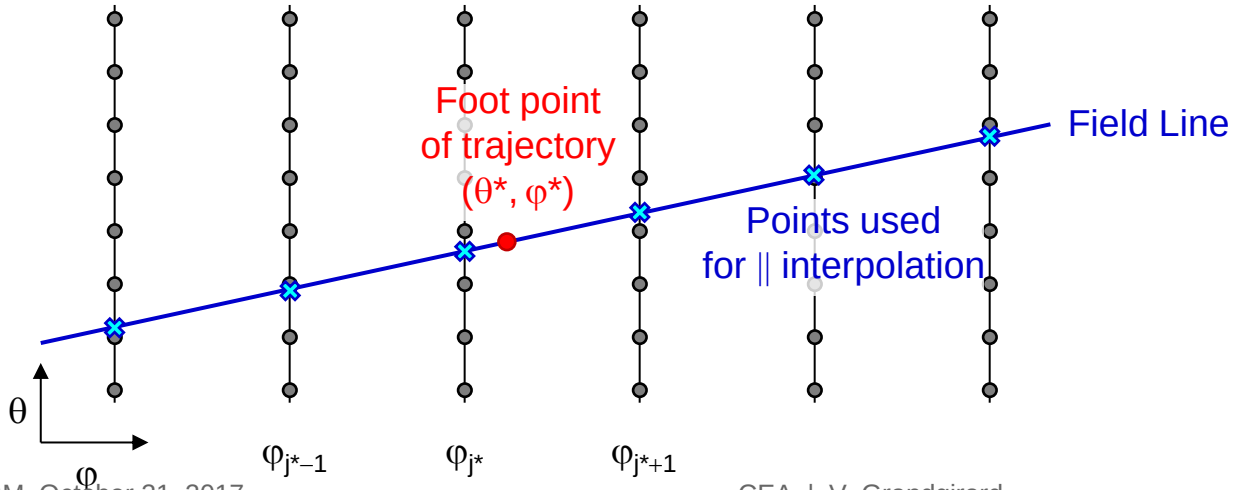
Objective: take benefit of strong anisotropy (// vs. ⊥) to reduce nb. of grid points in 1direction



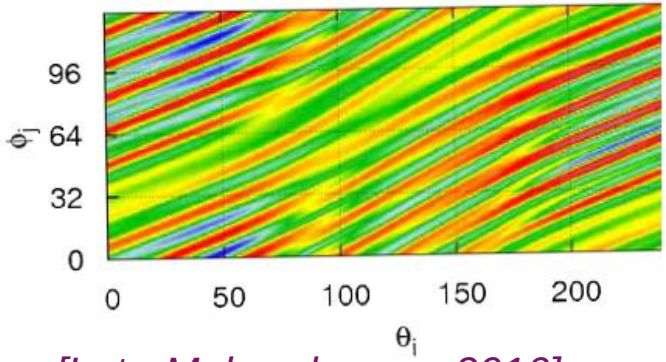
- Drawbacks of using aligned coordinates:
  - GYSELA uses (r,θ,φ) coord. system
    → would require complete rewritting
  - Not periodic → loss of natural double periodicity of torus

- Development of a "field-aligned coordinate" method inspired from Flux-Coordinate Independent approach

[Ottaviani 2011, Stegmeir 2014, Hariri 2015,]



Structures aligned along field lines



[Latu-Mehrenberger, 2016]

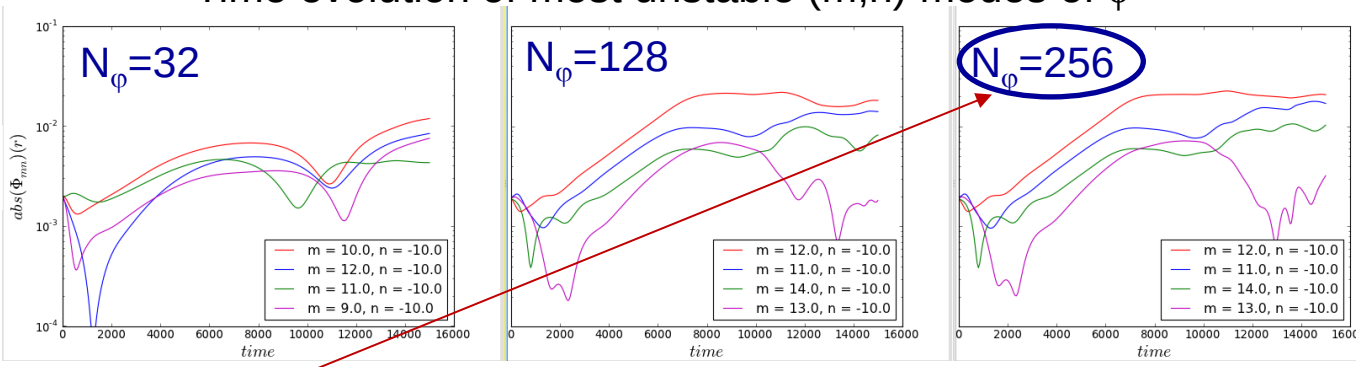
"Field aligned coordinates" method

- Standard method → Nb of grid points ~ ρ_*^{-3}
- New "aligned-coordinates" method = take advantage of weak $\nabla_{//}$
  - Decouples // & ⊥ dynamics → Nb of grid points ~ ρ_*^{-2} → crucial for kinetic e-

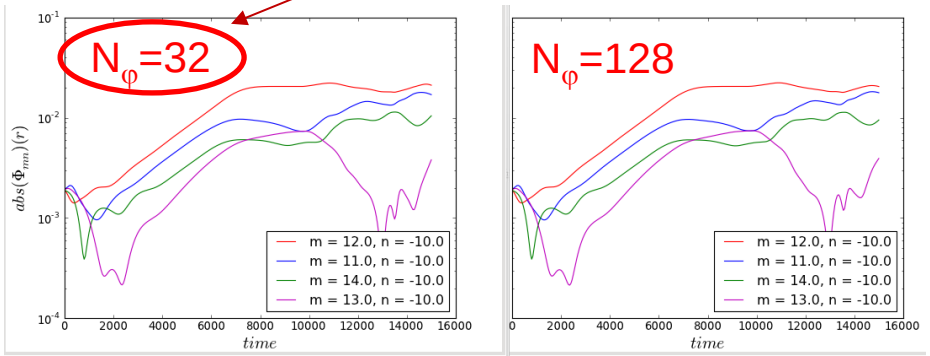
Comparison for adiabatic electrons

Time evolution of most unstable (m,n) modes of ϕ

Standard



Aligned



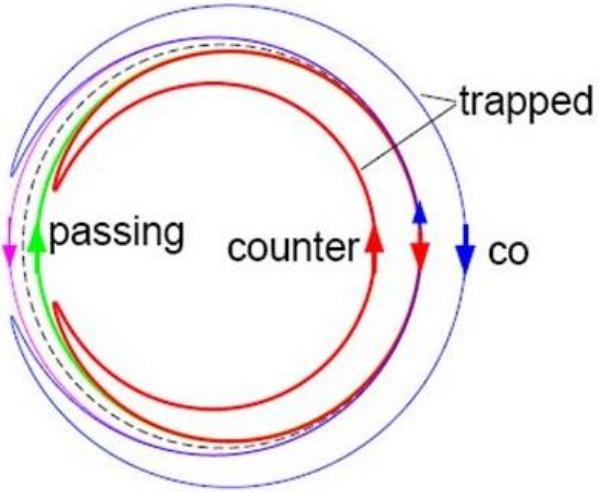
→ Less toroidal points for same accuracy : ~ N_φ / 8

- Gain of a factor 4 in time and memory including calcul. + comm. overhead

Trapped kinetic electrons : Hybrid model

Trapped Electron Modes : one of the main contributor in heat transport

[Bottino, PPCF, 2011]



$$\omega_{de} \sim q \frac{\rho_e}{4R} \frac{v_{th,e}}{R} < \frac{v_{th,e}}{R} \qquad \delta_{be} \sim 2q\rho_e \sqrt{2R/r} > \rho_e$$

Idea : Capture physics of TEM at low cost (ω_{de} and δ_{be} resolved)

- **Trapped electrons** : Kinetic
- **Passing electrons** : Adiabatic

(response close to adiabaticity in ITG-TEM turbulence)

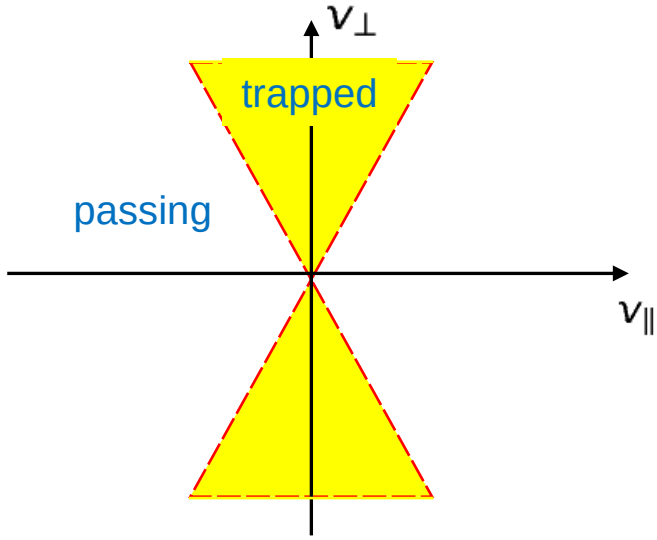
[Idomura, PoP 2016]

$$n_e = \int_{trap.} f_e d^3v + (1-\alpha_t)\langle n_e \rangle_{FS} \exp\left\{\frac{e}{T_e}\left(\phi - \langle \phi \rangle_{FS}\right)\right\}$$

Kinetic — Adiabatic

with $\alpha_t = \dfrac{n_e^{trap.}}{n_e}$

Fraction of trapped electrons



Advantage :

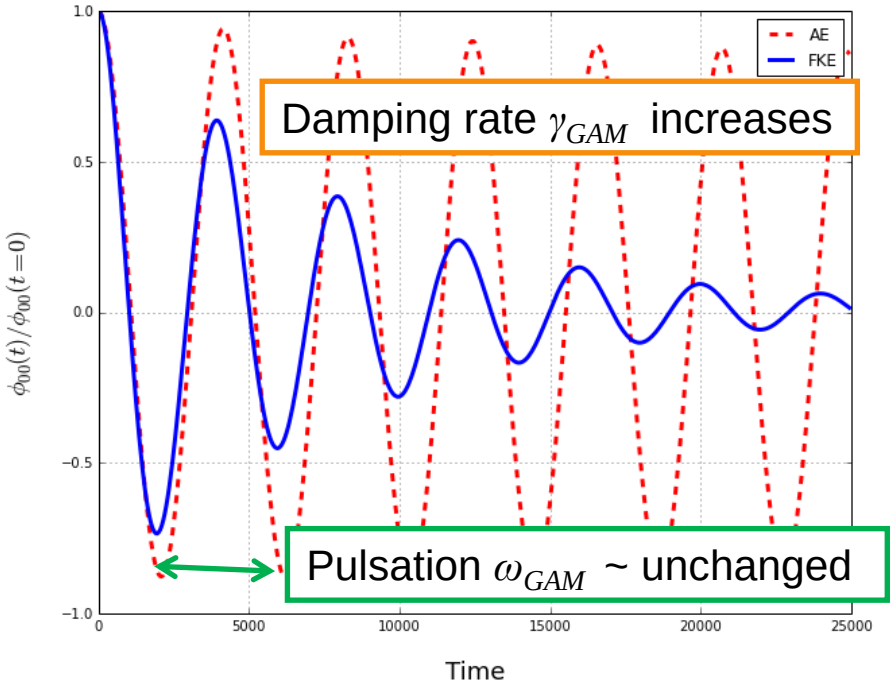
- Impact of trapped electrons on transport (TEM)
- Passing electrons well described at low m_i / m_e

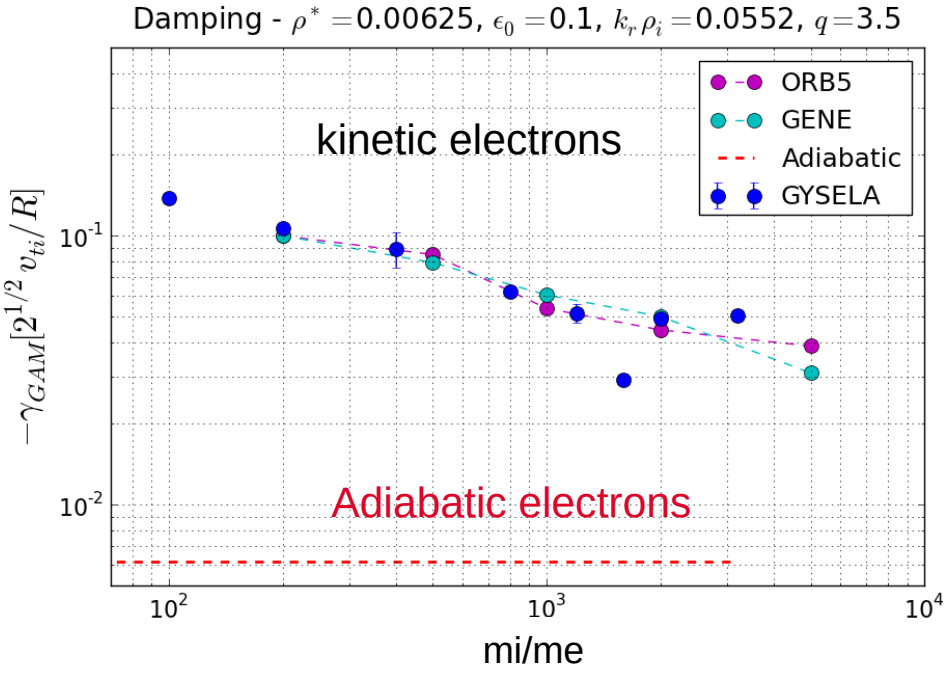
Damping of GAM due to kinetic electrons

- Standard benchmark: Damping of Geodesic Acoustic Mode (GAM)
  - Thermodynamic equilibrium : flat n and T profiles $\rightarrow$ no instabilities
  - Comparison with ORB5 and GENE codes performed via EUROfusion project "GK code benchmarks" (2015-2017)
- Successful comparison with adiabatic electrons [Biancalani, PoP 2017]

Damping of GAM due to kinetic electrons

- Standard benchmark: Damping of Geodesic Acoustic Mode (GAM)
  - Thermodynamic equilibrium : flat *n* and *T* profiles → no instabilities
  - Comparison with ORB5 and GENE codes performed via EUROfusion project "GK code benchmarks" (2015-2017)
- Kinetic electrons : Good agreement - influence of the mass ratio m_i / m_e



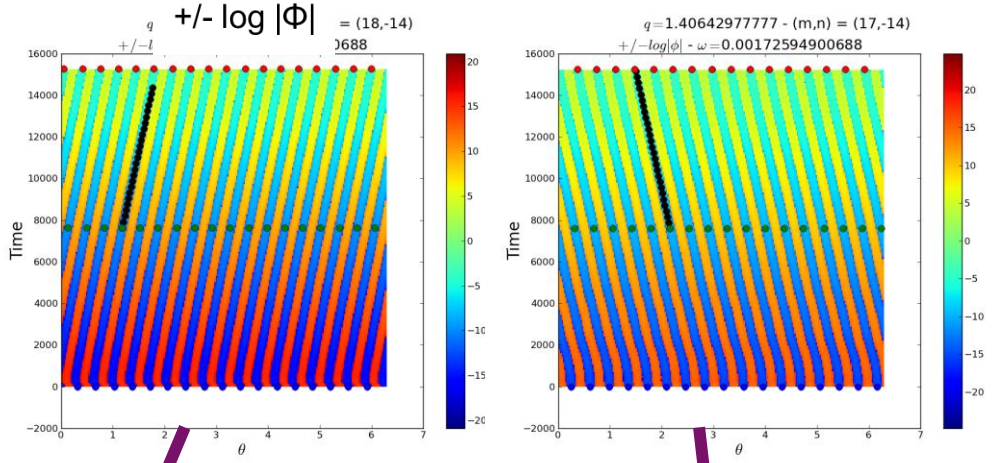


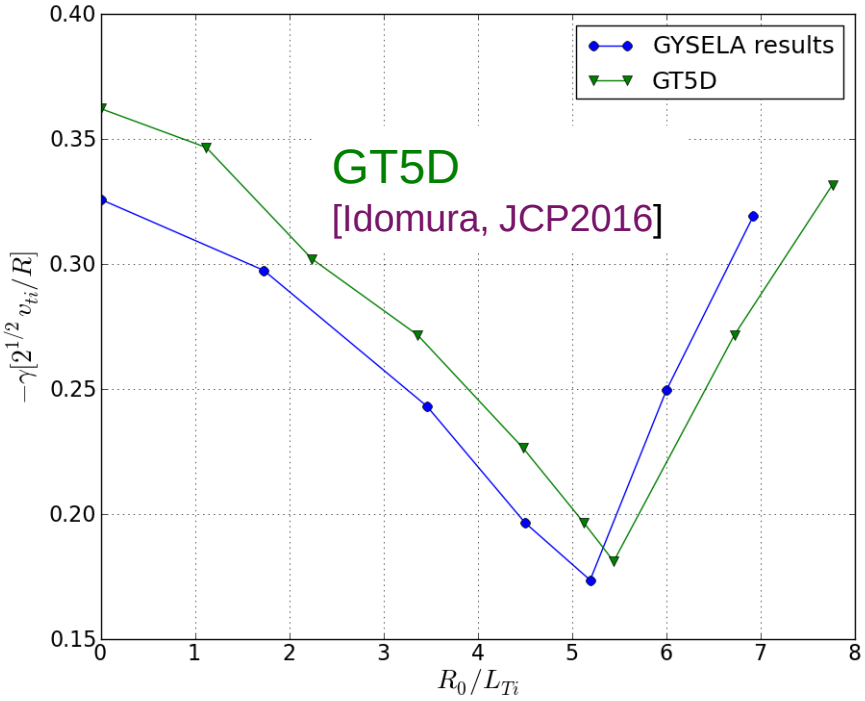
Transition ITG/TEM versus ion temperature gradient

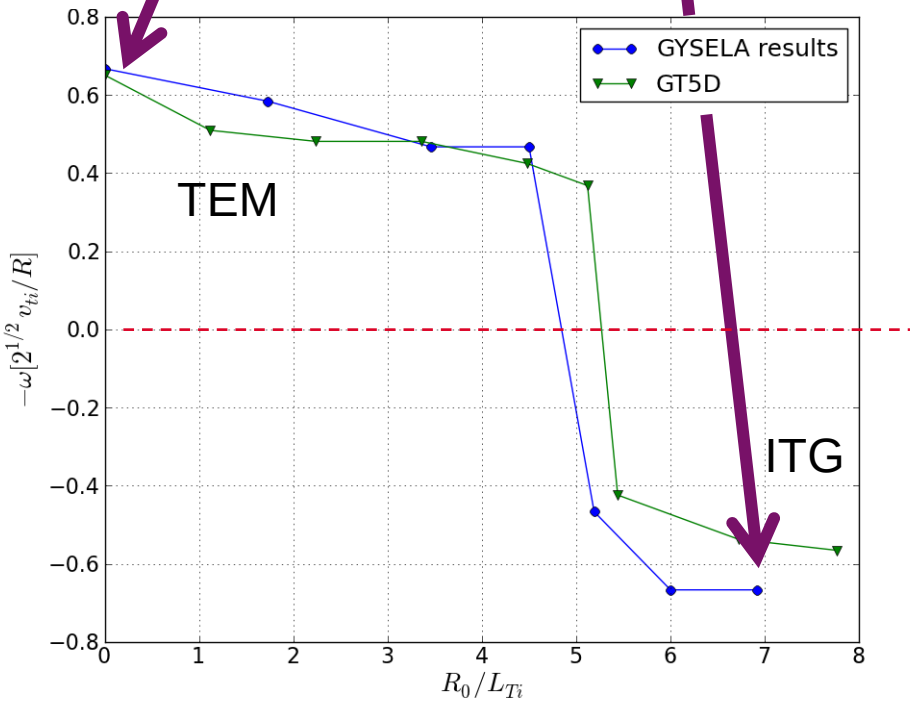
- Comparison with gyrokinetic GT5D code [Idomura, CPC 2008]
  - Via Japan/France collaboration [post-doc. Y. Asahi]
  - Successful comparison for flux-driven full-f global simulations with adiabatic electrons [Asahi, submitted 2017]

Transition ITG/TEM versus ion temperature gradient

- Comparison with GT5D code
  - Cyclone Base Case with $R_0/L_{Te} \sim 6.92$
- Kinetic electrons: Agreement Transition ITG/TEM for $R_0/L_{Ti} \sim 5.2$

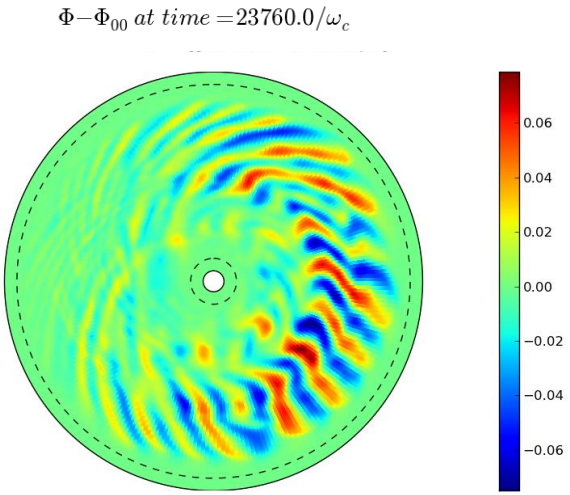




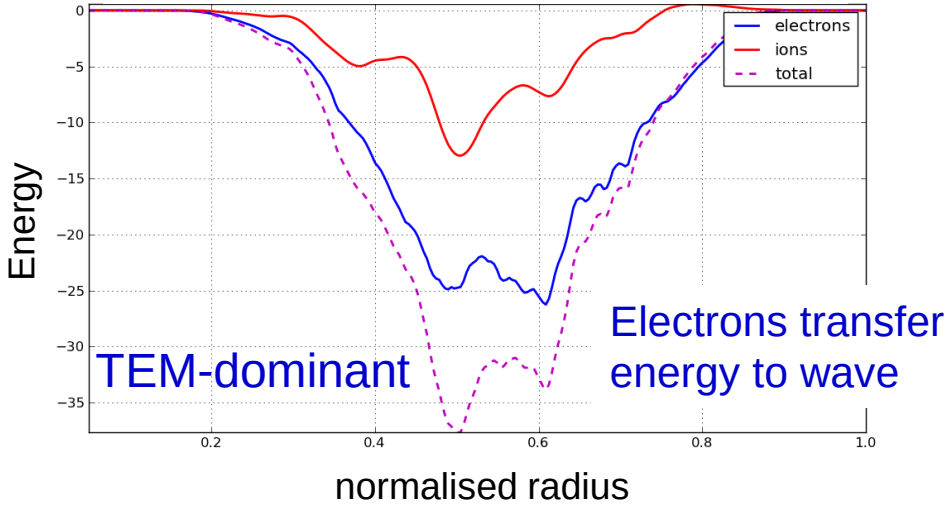


Preliminary non-linear results

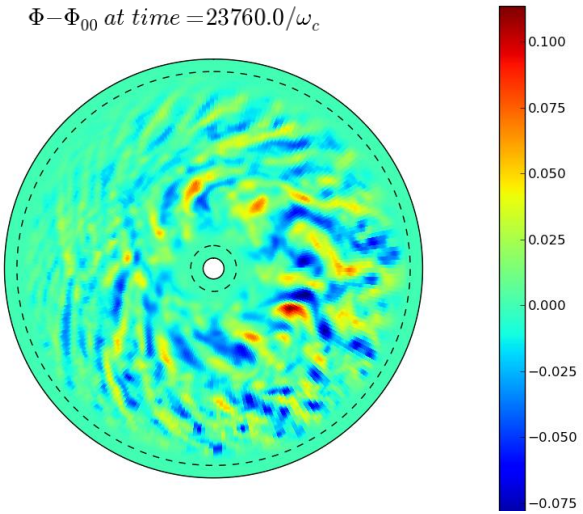
Cyclone Base Case, R/L_{Te}=6.92, R/L_{Ti}=0.5



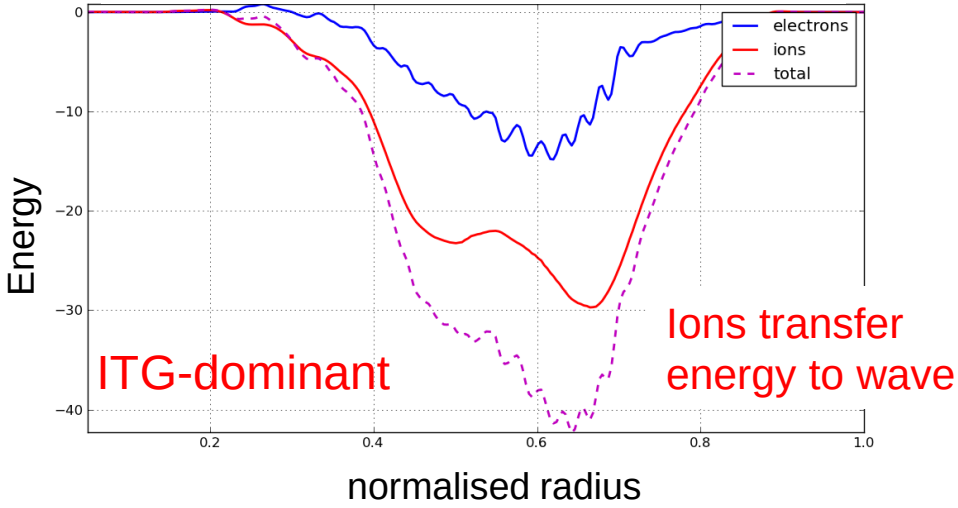
Energy transfer: wave to particle



R/L_{Ti}=6.92



Energy transfer: wave to particle



Conclusion & Perspectives

- Kinetic electrons recently implemented in the gyrokinetic global full-f flux-driven code GYSELA.
  - Hybrid model → Kinetic trapped electrons for non linear simulations
  - Goal: Particle and energy transport (role of TEM) studies

- <u>Perspectives for GYSELA:</u> [PhD, E. Caschera]
  - More realistic boundary conditions → penalisation techniques
  - Complex geometries → develop hybrid semi-Lagrangian schemes
  - Electromagnetic effects [EuroFusion project]

- Gyrokinetic global codes will require exascale capabilities for ITER simulations with kinetic electrons

- <u>Future challenges for gyrokinetic codes:</u>
  - Coupling between core and edge turbulence