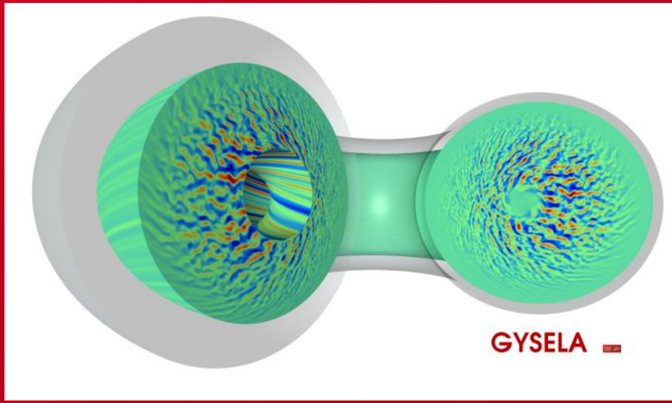
DE LA RECHERCHE À L'INDUSTRIE

GYROKINETIC SIMULATIONS OF MAGNETIC FUSION PLASMAS: NUMERICAL CHALLENGES



V. Grandgirard, Y. Asahi[1], J. Bigot[2], E. Caschera, G. Dif-Pradalier, P. Donnel, X. Garbet, Ph. Ghendrih, G. Latu, Ch. Passeron, J. Richard, Y. Sarazin

CEA, IRFM, 13108 Saint-Paul-lez-Durance Cedex, France
[1] National Institutes for Quantum and Radiological Science and Technology, 039-3212, Rokkasho, Aomori, Japan
[2] Maison de la simulation, CEA Saclay, FR-91191 Gif sur Yvette

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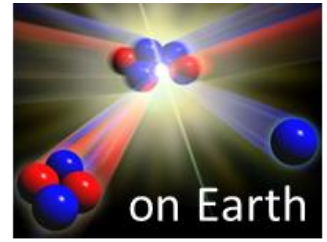
Main challenges for Magnetic Fusion

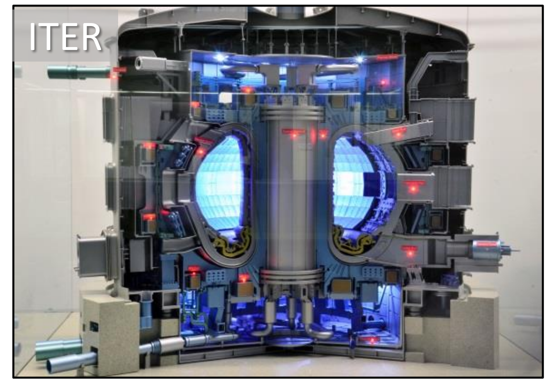
- **Goals of fusion researches**: To control fusion reactions on earth that occur naturally in sun for instance
  - Fusion reactions only at high temperatures (~150 Million °C)
  - How to confine turbulent plasmas ?
  - Most advanced concept = Tokamak



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

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.



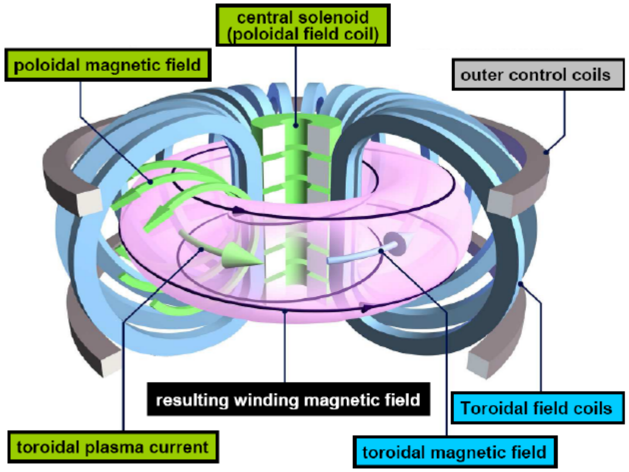
Plasma volume: 840 m^3

- 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

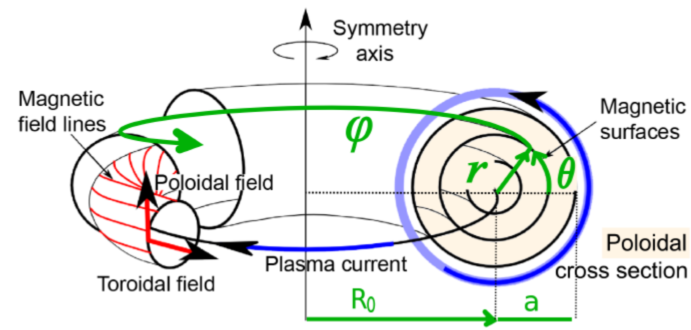
Plasma volume ~ 20 m^3

ITER building site at Cadarache

Plasma turbulence simulations
→ Kinetic approach mandatory



magnetic toroidal geometry (r, θ, φ)



- 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 ?
   - Increase code Parallelization
     → Prepare GYSELA to Exascale machine
   - Separation of dynamics (//, ⊥)
     → Weak discretization in // direction
   - Heavy electrons
     → spatial / temporal discretization x $(m_i/m_e)^2$

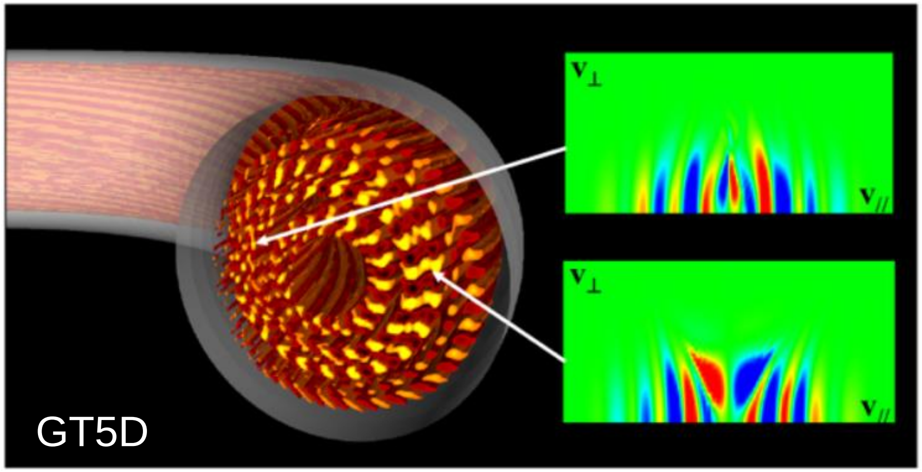
3. GYSELA-X future code: Exascale core-edge simulations in X-point magnetic configuration
   - Numerical challenges

Gyrokinetic plasma turbulence simulations

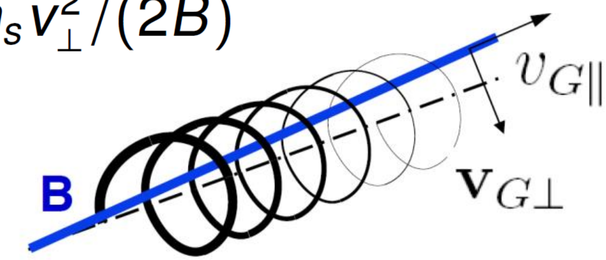
- Kinetic theory: 6D distribution function of particles (3D in space + 3D in velocity) $F_s(r,\theta,\varphi,v_\parallel,v_\perp,\alpha)$

- 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.

- N. Tronko et al., *Hierarchy of second order gyrokinetic Hamiltonian models for particle-in-cell codes*, Plasma Physics and Controlled Fusion (2017)

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 $\tau_E \sim 10s$

GK codes already use Petascale capabilities

- 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]

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

- Various simplifications in terms of physics: — *complex* $\longrightarrow$ +

- 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: $\mathbf{B} = \text{const}$	$\neq$	Electromagnetic

→ None of the codes cover all physical aspects

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

→ ITER simulations without any assumptions are unreacheable

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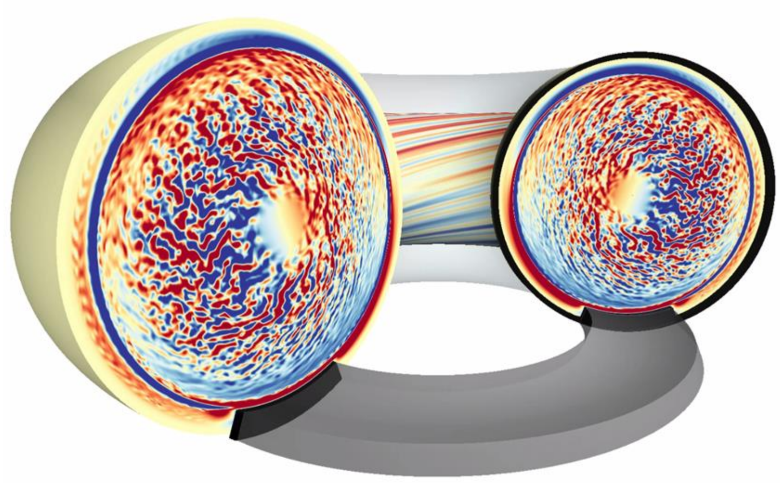
GYSELA = GYrokinetic SEmi LAgrangian code

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

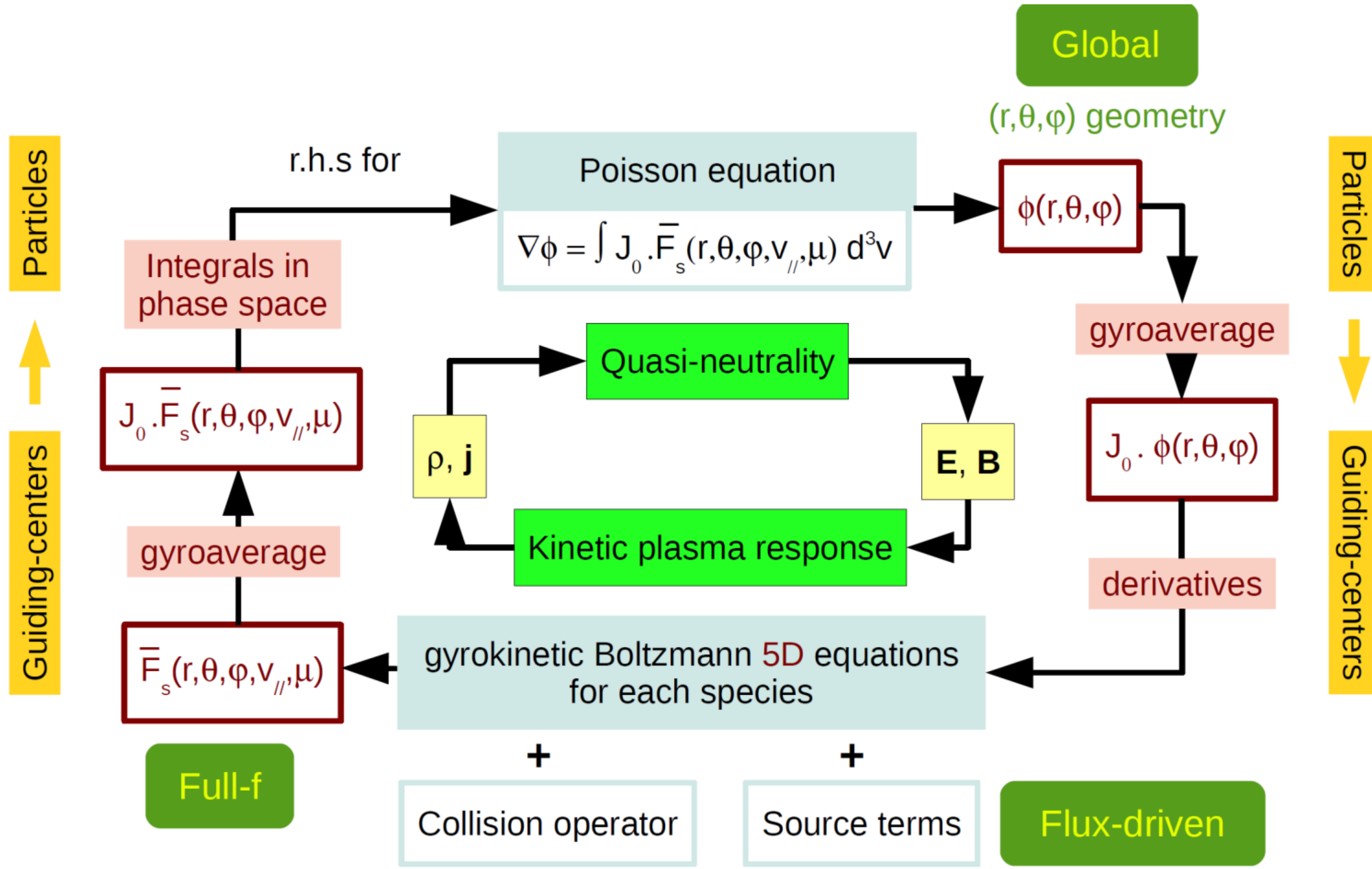
- GYSELA strength:
  - Global: simulate entire tokamak
    $\rightarrow$ boundary conditions (SOL-like, limiter)
  - Full-f: multi-scale physics
  - Flux-Driven (heat, momentum, … sources)
    $\rightarrow$ steady state on τ_E
  - Multi-ion species $\rightarrow$ impurity transp.
  - Collision operator $\rightarrow$ synergy between neoclassical & turbulent transports
  - Full-kinetic or trapped kinetic electrons



- Present GYSELA limitations:
  - Circular magnetic configuration
  - Electrostatic

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



Small scales & gyro-average operator

- Gyro-average → Finite Larmor Radius effects

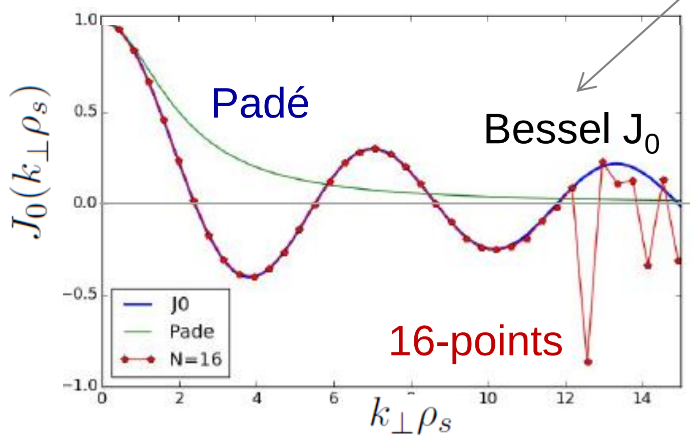
$$\bar{g}(\mathbf{x}_G, v_\perp) = \oint_0^{2\pi} \frac{d\varphi_c}{2\pi} g(\mathbf{x}) = \int_{-\infty}^{+\infty} \frac{d^3\mathbf{k}}{(2\pi)^3} J_0(k_\perp \rho_s) \hat{g}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}_G}$$

- From **Padé** to **N-point average**

Padé: $1 / [1+(k_\perp \rho_c/2)^2]$

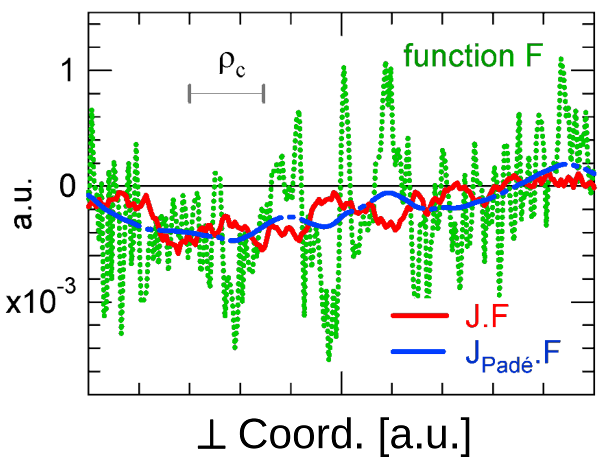
small scales filtered out

$$\begin{cases} \lim_{x\to\infty} J_0(x) = \sqrt{\frac{2}{\pi}} \frac{\cos(x-\pi/4)}{x^{1/2}} \\ \lim_{x\to\infty} J_{\text{Padé}}(x) = \frac{4}{x^2} \end{cases}$$

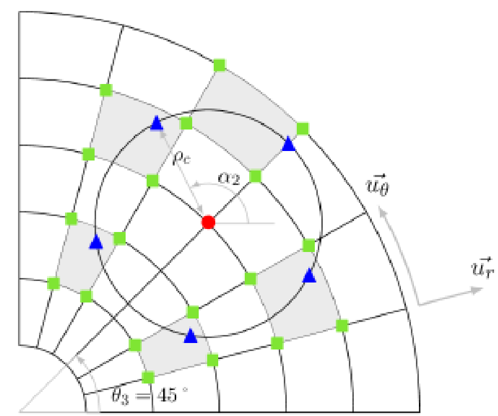


N-point average (Hermite):

- Convergence reached for N=8 points (ion turb.)
- Issue: boundary condition?



[Steiner, EJP 2015; Rozar, ESAIM 2016; Bouzat, 2016]



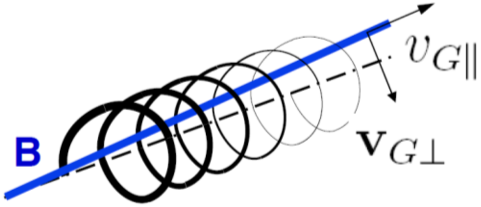
5D Boltzmann eq. + 3D quasi-neutrality eq.

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

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

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

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.

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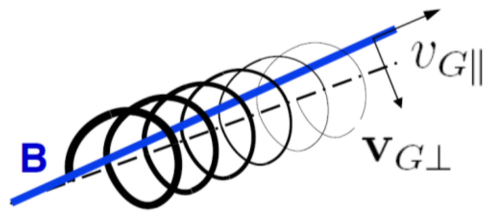
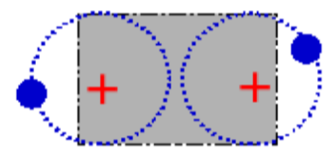


$\mathbf{E} = \nabla\left(J_0\cdot\phi\right)$ with $\phi(\mathbf{x})$ electrostatic potential and J_0 the gyroaverage operator.

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



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

Time-splitting for Boltzmann equation

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

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

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

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

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

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

➠ Semi-Lagrangian scheme

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

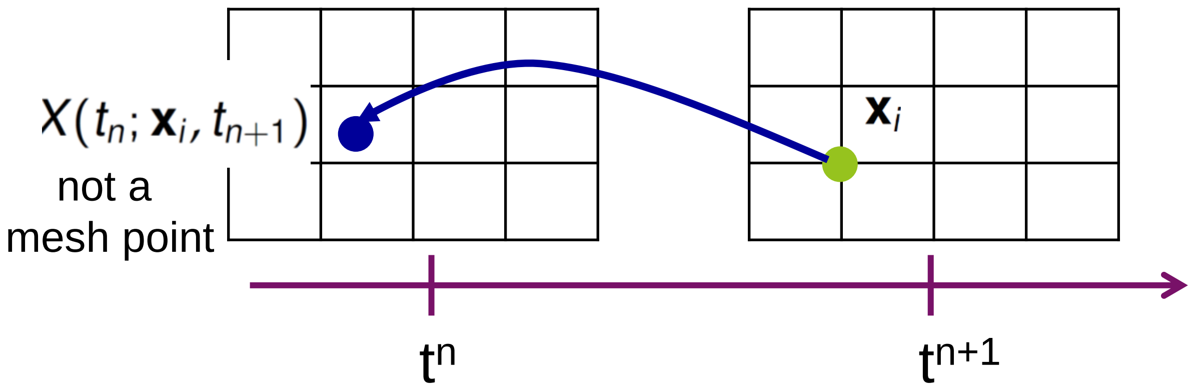
$$(\tilde{\mathcal{B}}) \equiv \left(\frac{\tilde{\mathcal{S}}}{2}, \frac{\tilde{\mathcal{C}}}{2}\right)\left(\frac{\tilde{v_{G\|}}}{2}, \frac{\tilde{\varphi}}{2}, \tilde{\mathcal{X}}_G, \frac{\tilde{\varphi}}{2}, \frac{\tilde{v_{G\|}}}{2}\right)\left(\frac{\tilde{\mathcal{C}}}{2}, \frac{\tilde{\mathcal{S}}}{2}\right)$$

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

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

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]*
    $\hookrightarrow$ 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 modelling 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

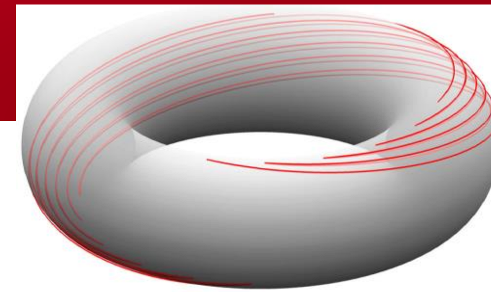
- Idea: Replace cubic splines used for interpolation in semi-Lagrangian scheme by high-order Lagrange polynomials
  - Lagrange are more local than cubic splines
  - Lagrange polynomials degree 5 → best compromise (accuracy)

- **But** Lagrange involves extra operations

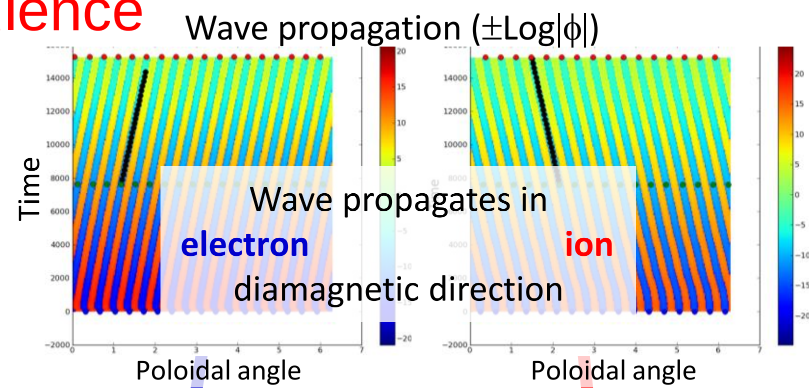
Kind of interpolation	Mem. load	Mem. store	Multiply	Add	Divide
1D spline	1	1	26	16	1
1D Lagrange 6-pts	1	1	30	25	0
2D spline	1	1	60	40	2
2D Lagrange 6-pts	1	1	90	74	0

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

Trapped kinetic electrons → Hybrid model



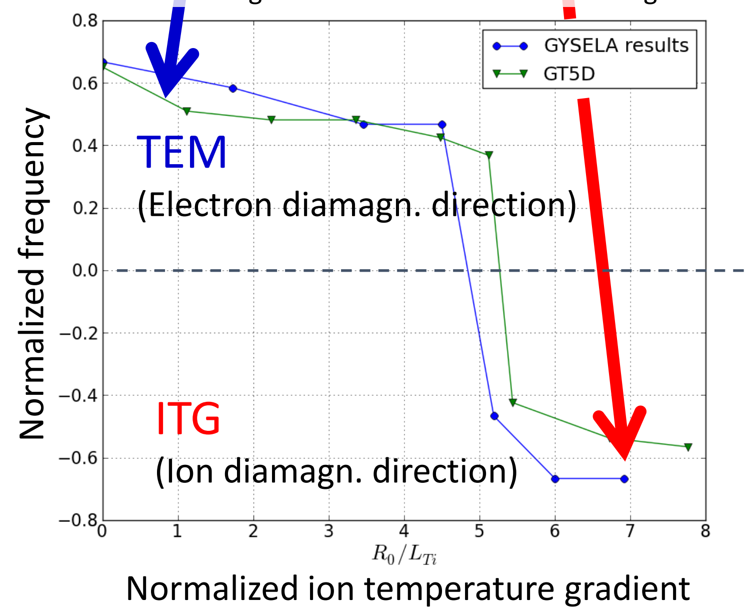
- **Associated physics is relevant for ITER**
  - Allow for particle turbulent transport
  - Account for trapped electron driven turbulence (expected at the edge)



- Small electron inertia → **Numerical issue**

  $v_{Te}/v_{Ti} \sim (m_i/m_e)^{1/2} \sim 60$

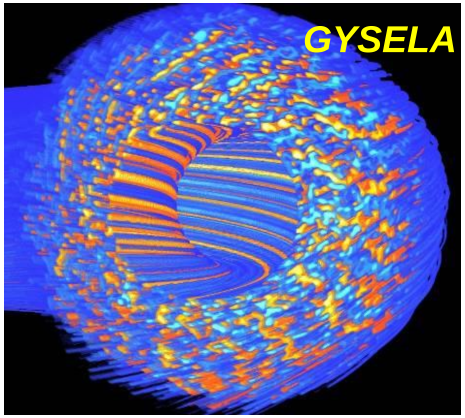
  Solutions:
  - Consider artificially large electron mass → OK for trapped particles
  - Field aligned approach to cope with transport anisotropy



- **Linear benchmarks OK** (TEM & GAMs)
- Still issues in nonlinear regime

Taking benefit of the strong anisotropy

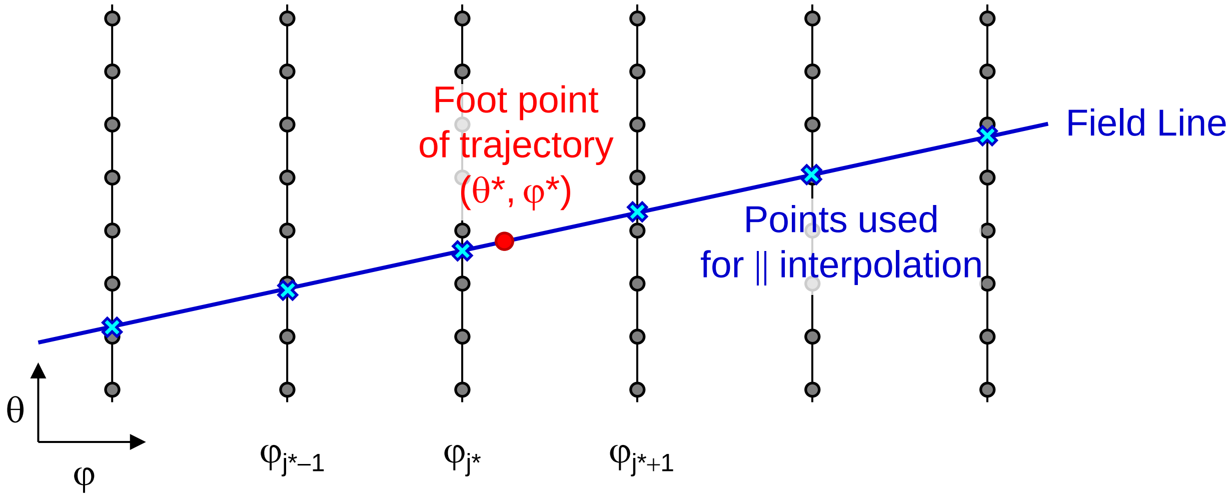
Objective: take benefit of strong anisotropy (// vs. ⊥) to reduce nb. of grid points in 1direction



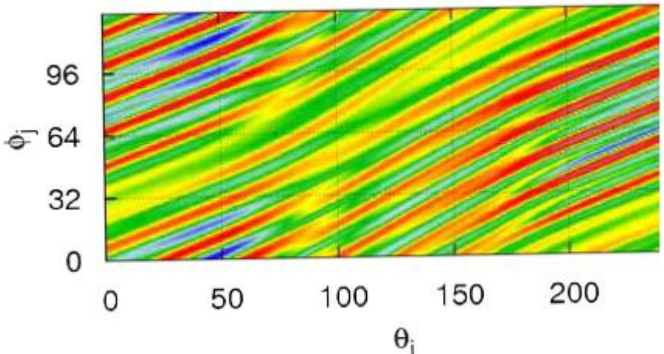
- Drawbacks of using aligned coordinates:
  - GYSELA uses (r,θ,φ) coord. system
    → would require complete rewritting
  - Not periodic → loss of natural double periodicity of torus

- 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]

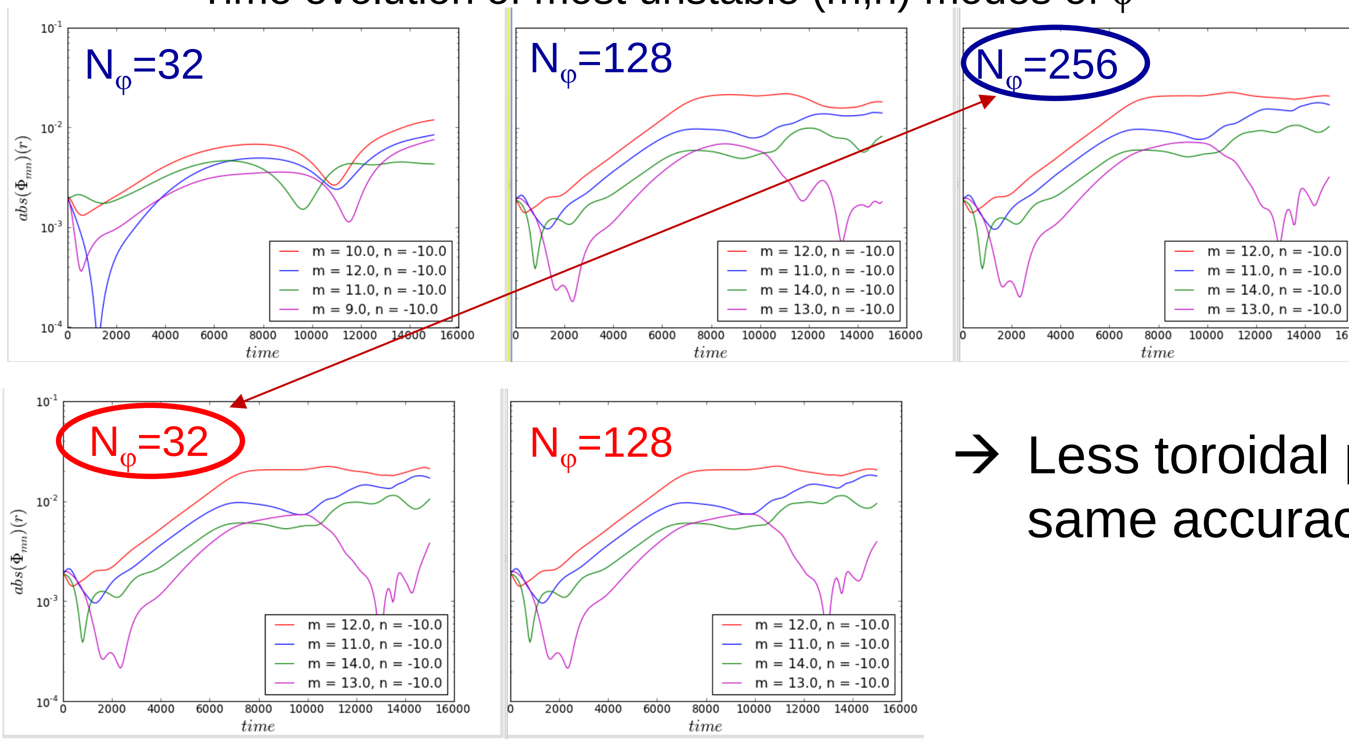
- Standard method → Nb of grid points ~ ρ_*^{-3}
- New "aligned-coordinates" method = take advantage of weak $\nabla_{//}$
  - Decouples // & ⊥ dynamics → Nb of grid points ~ ρ_*^{-2} → crucial for kinetic e$^-$

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

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Pushing gyrokinetic modelling towards the edge region

- Core transport studies in tokamak plasmas have now reached maturity
- However, despite their numerous successes to date, their predictive capabilities are still constrained with respect to the energy content in particular in optimized discharges.
- Challenging this gap requires pushing gyrokinetic modelling towards the edge region of the container vessel
  → If possible, addressing edge and core transport on an equal footing

↓

Long-term aim for GYSELA:

→ Exascale core-edge simulations in X-point magnetic configuration

- To many parts need to be changed in the current GYSELA code

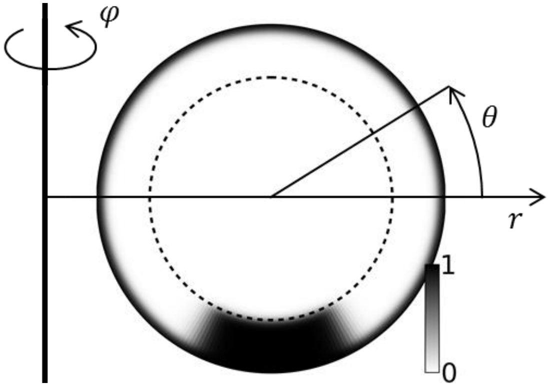
  → Development of a new code: GYSELA-X

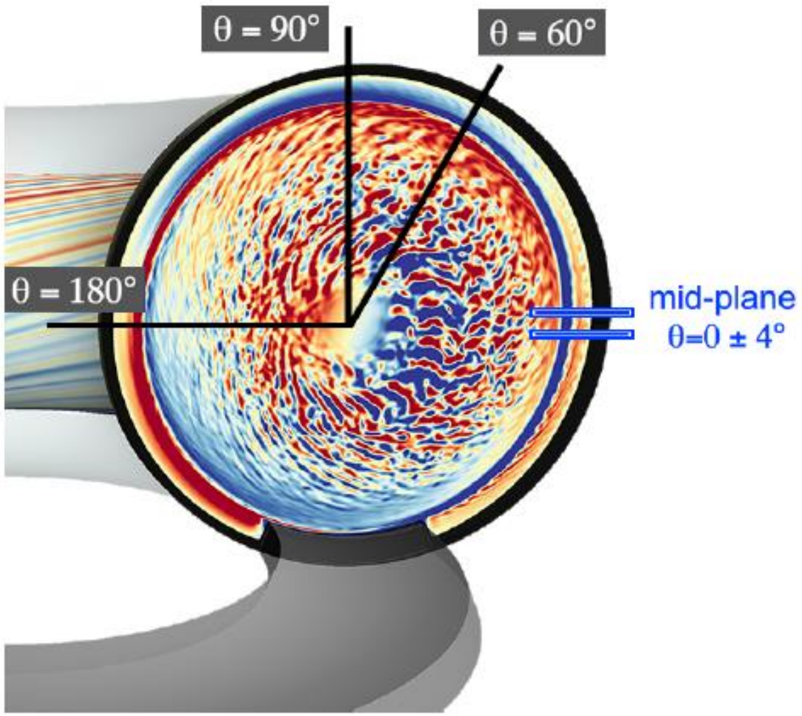
EoCoE-II European project (2019-2022)

Already more physically relevant boundary conditions in GYSELA

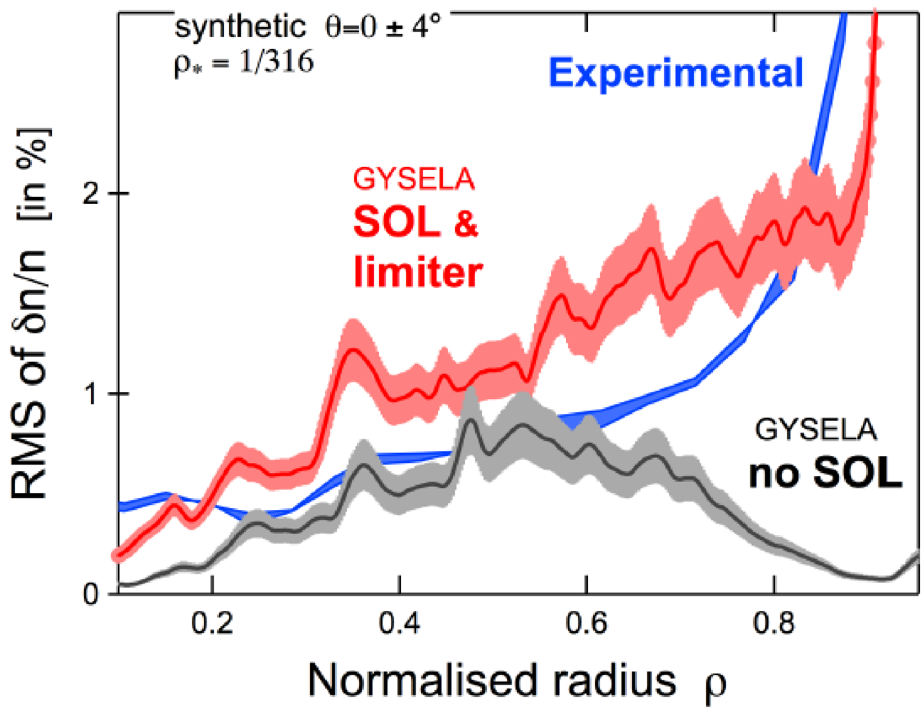
Radial domain extended to r/a>1 in GYSELA

- **Simplified** original **unconfined (SOL) region**
  - Limiter → immersed boundary (penalization technique)
  - Prescribed divertor-plasma interaction in // direction



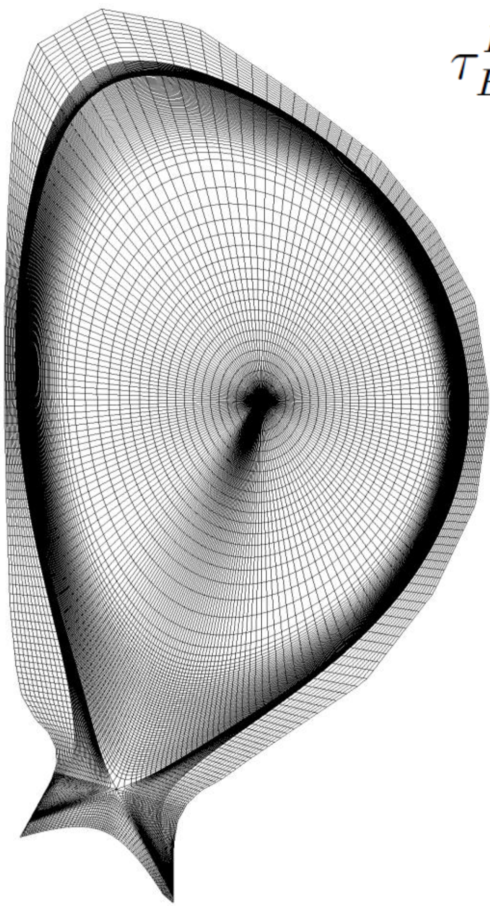


[Caschera PhD (2018), Dif-Pradalier (2018)]



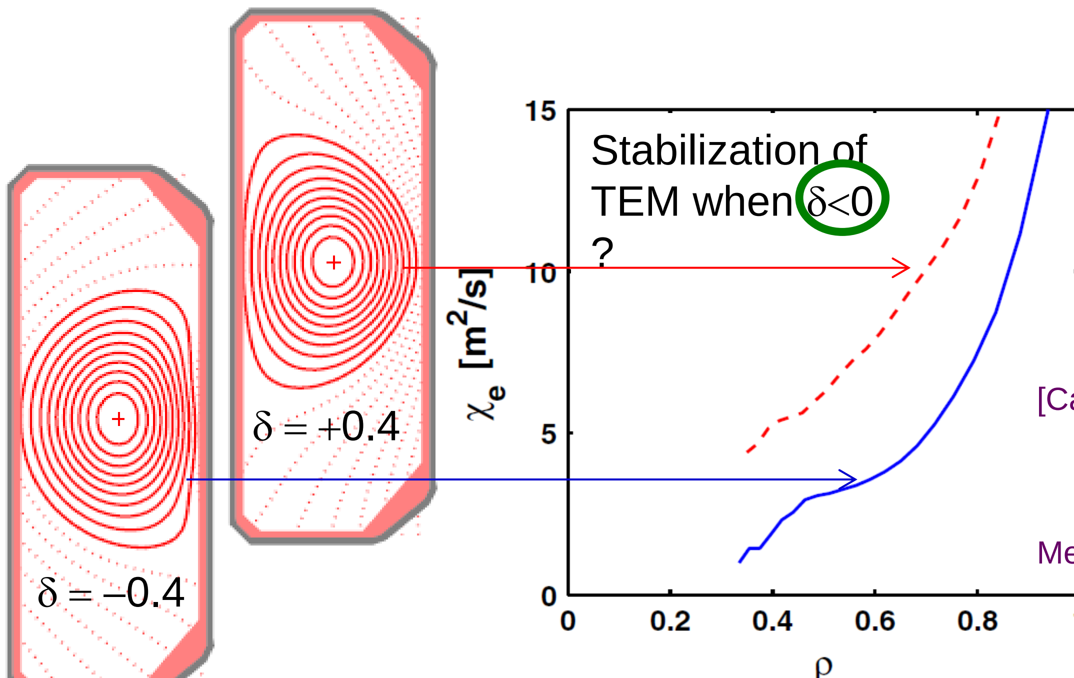
Physical Challenge for EoCoE-II → Impact of magnetic geometry

- **Arbitrary & consistent (G-S) magnetic equilibrium**
  - Impact of magnetic geom. (elongation κ, triangularity δ) on confinement



$$\tau_{E,th}^{ELMy} \propto \tau_B \rho_*^{-0.83} \beta^{-0.50} \nu_*^{-0.10} \times M^{0.97} q^{-2.52} \varepsilon^{-0.55} \kappa^{2.72}$$

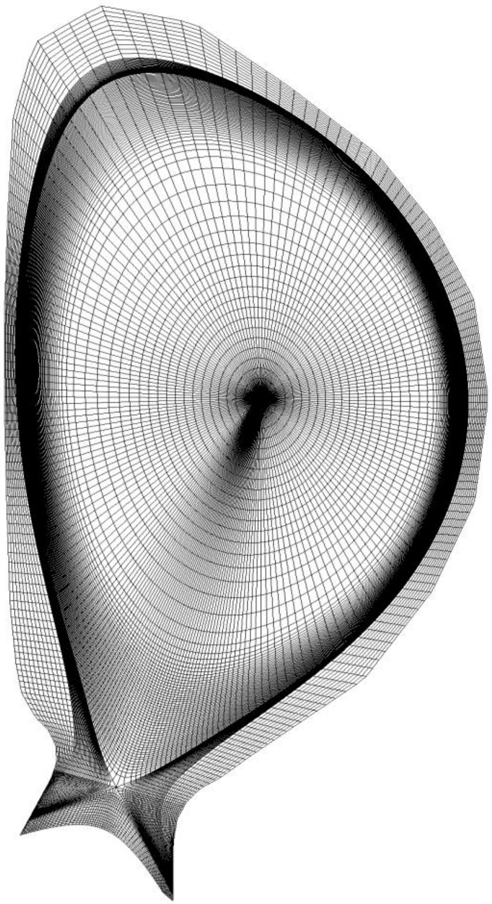
[ITER Physics Basis (1999)]



[Camenen NF (2007); Marinoni PPCF (2009); Sauter PoP (2014); Medvedev NF (2015)]

Numerical challenges → Choice of the coordinates

- **Arbitrary & consistent (G-S) magnetic equilibrium**



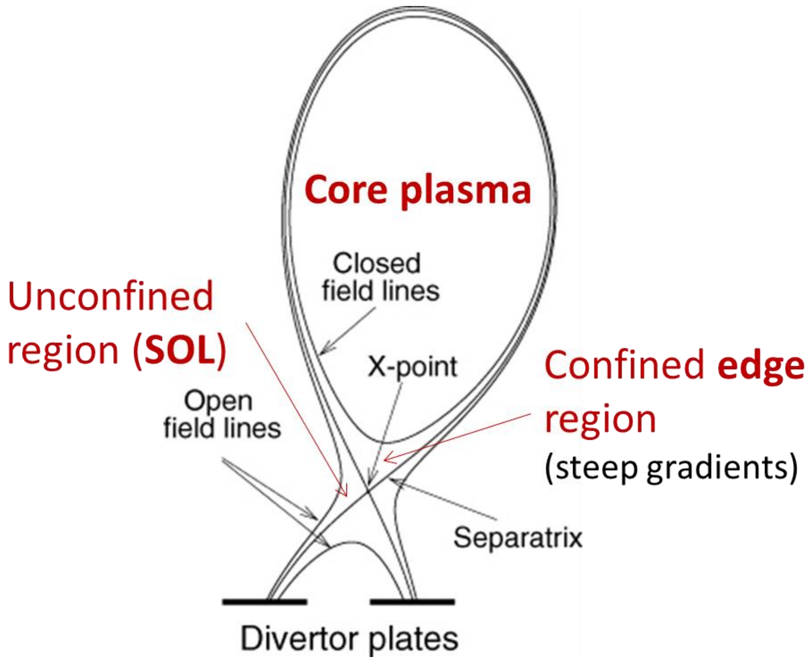
- Generalized metric
- Choice of ⊥ coordinates:

  → flux-aligned (ψ,θ) vs. (R,Z) for Vlasov?
- X-point singularity (B_θ=0) → avoided in (R,Z)
- Diagnostics

  → Flux-surface average not straightforward in (R,Z) coordinates

Physical Challenge for EoCoE-II → Core-edge interplay

- **From the plasma core to the Scrape-Off Layer**
  - "No man's land" issue: core turbulence spreading into the edge or SOL turbulence invading the edge?
  - Core turbulence & confinement much sensitive to boundary C^ons
  - Transition from Low- to High-confinement regime: power threshold? control scheme?



Pecularities of the edge:

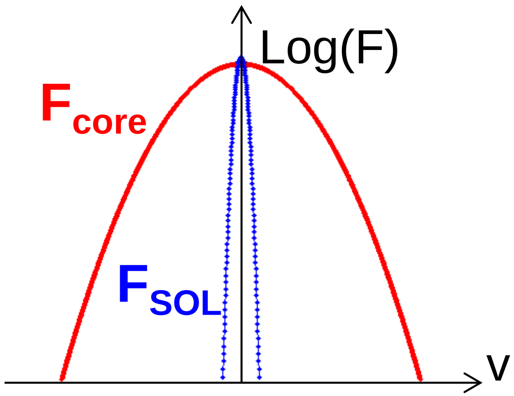
- **Large fluctuations**: $\delta n/n=O(1)$
  $\Rightarrow$ full-F + non linear polarization term ?
- **Steep gradients** $\Rightarrow$ equilibrium & fluctuation scales merge (no scale separation)

❑ From the plasma core to the Scrape-Off Layer

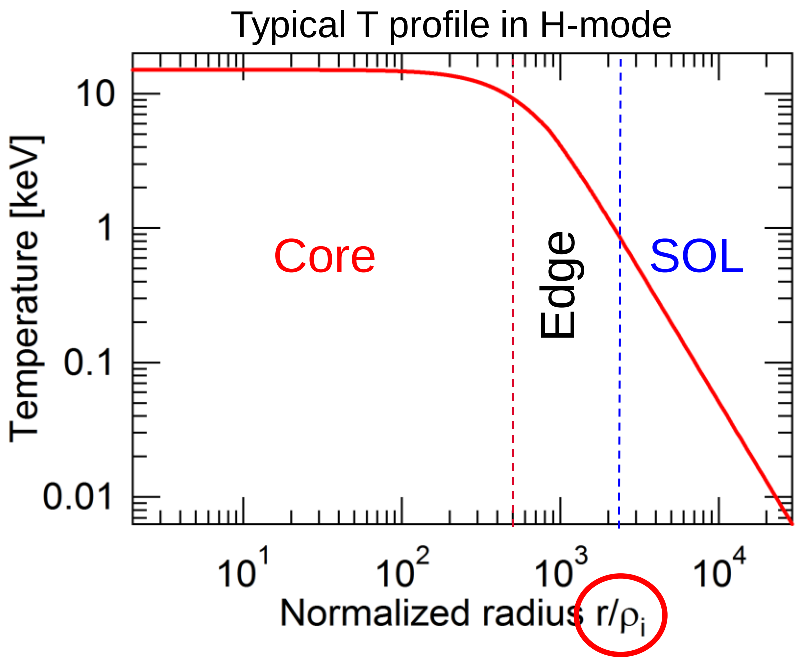
- Cope with large variation of temperature → 5D patches?

- Temperature varies by orders of magnitude from core to edge

- Turbulence scales like $\rho_i \sim T_i^{1/2}$



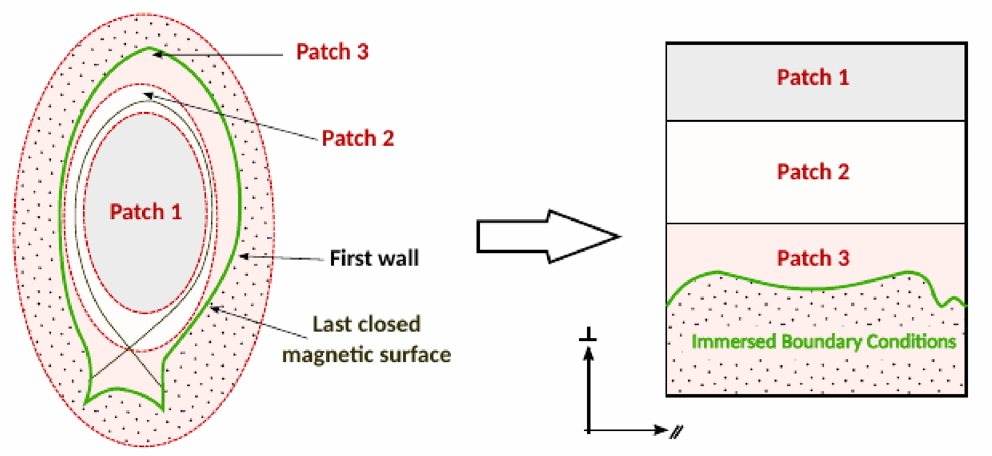
Cf. e.g. [Jarema CPC (2017)]



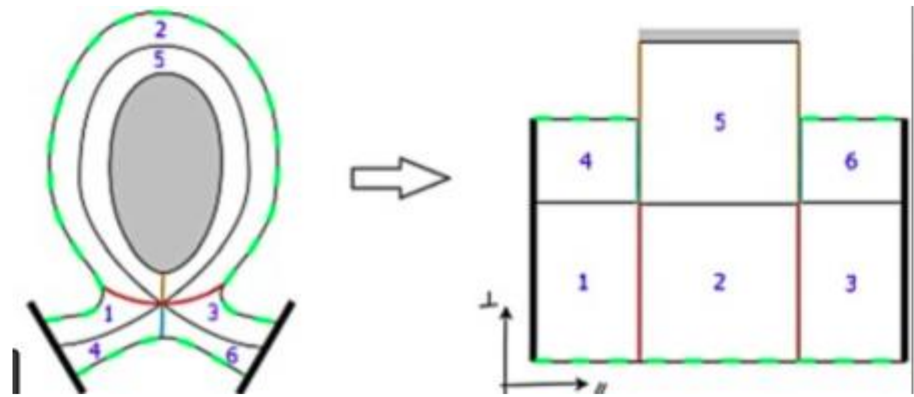
Stable numerical schemes able to treat steep gradients ?

Numerical Challenges
→Mesh: Three approaches considered

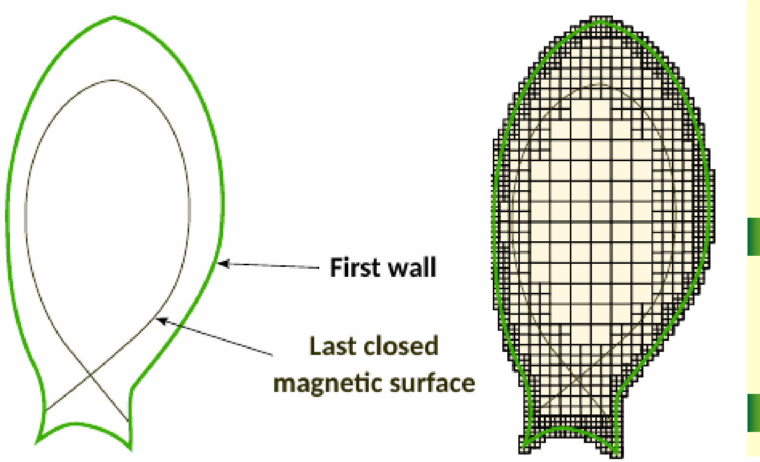
1. Mapped grid



2. Aligned mapped grid



3. Cartesian grid

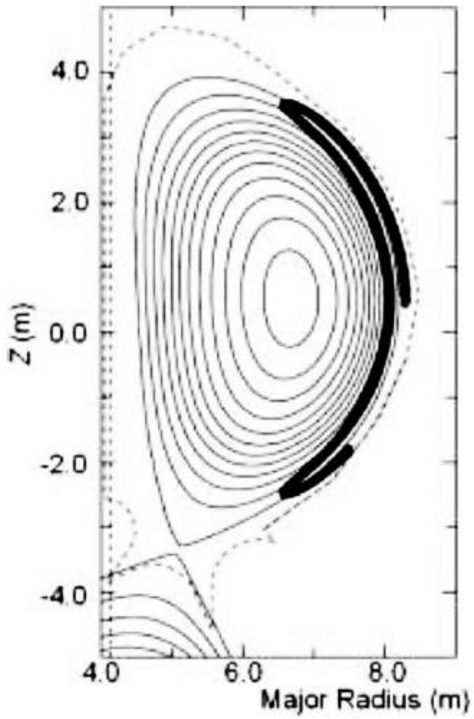


- New semi-Lagrangian methods for Vlasov:
  - Hybrid method with multi-patches ?
  - Semi-Lagrangian method on cartesian grid
- Scalable schemes up to several thousands of nodes → block-structured mesh
- Multigrid 2D poisson solver

How to treat boundary conditions ?

- **Boundary conditions at the outer edge**
  - // plasma-wall interaction ⇒ Bohm condition at sheath entrance constraints potential ($e\phi/T_e \sim 3$), density decay & Mach number ($|M_{||}| \geq 1$)
  - Fast ion orbit losses (banana orbits hitting the wall → also relevant for stellerators) ⇒ edge polarization

Alpha particle orbit in ITER
[Funaki 2008]



- // : ensuring Bohm criterion with immersed boundaries
  → with & without kinetic electron physics
- ⊥ : accounting for ion orbit losses with semi-Lagrangian scheme

Kinetic electrons & electromagnetic effects

Kinetic electrons & Electromagnetic effects

- Optimal filtering in velocity space: loss cone $v_{//}=(2\varepsilon)^{1/2}\,v_\perp$ or $v_{//}=Cst$?
- Passing electrons mandatory for electromagnetic effects
  → important at the edge where $\beta(L_s/L_T)^2$ is large O(1)
- All electrons are kinetic in the SOL

- Different time steps for electrons & ions ?
  (Δt governed by core electrons)
- Ampère equation on A// → Magnetic cancellation issue ($\exists$ solutions)

$$\nabla_\perp^2 A_\parallel + \frac{\omega_p^2}{c^2} A_\parallel = -\mu_0 J_\parallel$$

small huge ~ counterpart

Cf. e.g. [E. Sonnendrücker (2018)]

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

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

- EoCoE-II project: Development of a new code GYSELA-X
  - Coupling between core and edge turbulence
  - Big challenges for semi-Lagrangian scheme for Vlasov equation
  - Multigrid 2D Poisson solver
  - Choice of numerical schemes strongly linked to exascale objective

Back-up slides

Linearized collision operator without FLR effects

$$C_{ab}(F_a, F_b) = C^0_{ab}(F_{M0a}, F_{M0b}) + C^1_{ab}(F_a, F_b)$$

$$F_{M0a} = N_a \left(\frac{1}{2\pi v_{Ta}^2}\right)^{3/2} \exp\left(-\frac{v^2}{2v_{Ta}^2}\right)$$

$$C^0_{ab}(F_{M0a}, F_{M0b}) = \frac{T_b - T_a}{T_b}\frac{m_a v^2}{2T_a}\nu_{E,ab}F_{M0a}$$

[D.Esteve, POP(2015)]

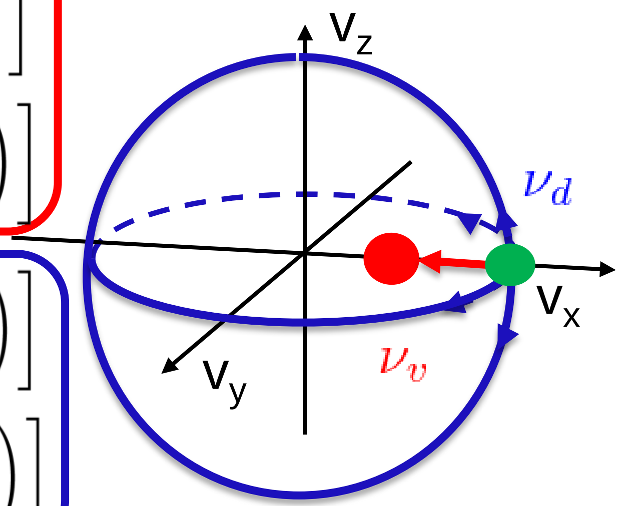
$$C^1_{ab}(F_a, F_b) = C_{v,ab}(F_a) + C_{d,ab}(F_a) + C_{\parallel,ab}(F_a, F_b)$$

$$C_{\parallel,ab}\left(F_a, F_b\right) = -\nu_{s,ab}(v)\frac{m_a}{T_a}v_\parallel\left(U_{\parallel d,a} - U_{\parallel ba}\right)F_{M0a}$$

$$g_a = f_a - \frac{m_a v_\parallel U_{\parallel d,a}}{T_a}$$

$$C_{v,ab}\left(F_a\right) = \frac{1}{2B^\star_\parallel v_\perp}\frac{\partial}{\partial v_\perp}\left[B^\star_\parallel F_{M0a}\nu_{v,ab}v_\perp^2\left(v_\perp\frac{\partial g_a}{\partial v_\perp} + v_\parallel\frac{\partial g_a}{\partial v_\parallel}\right)\right] + \frac{1}{2B^\star_\parallel}\frac{\partial}{\partial v_\parallel}\left[B^\star_\parallel F_{M0a}\nu_{v,ab}v_\parallel\left(v_\perp\frac{\partial g_a}{\partial v_\perp} + v_\parallel\frac{\partial g_a}{\partial v_\parallel}\right)\right]$$

$$C_{d,ab}\left(F_a\right) = \frac{1}{2B^\star_\parallel v_\perp}\frac{\partial}{\partial v_\perp}\left[B^\star_\parallel F_{M0a}\nu_{d,ab}v_\perp v_\parallel\left(v_\parallel\frac{\partial g_a}{\partial v_\perp} - v_\perp\frac{\partial g_a}{\partial v_\parallel}\right)\right] + \frac{1}{2B^\star_\parallel}\frac{\partial}{\partial v_\parallel}\left[B^\star_\parallel F_{M0a}\nu_{d,ab}v_\perp\left(-v_\parallel\frac{\partial g_a}{\partial v_\perp} + v_\perp\frac{\partial g_a}{\partial v_\parallel}\right)\right]$$



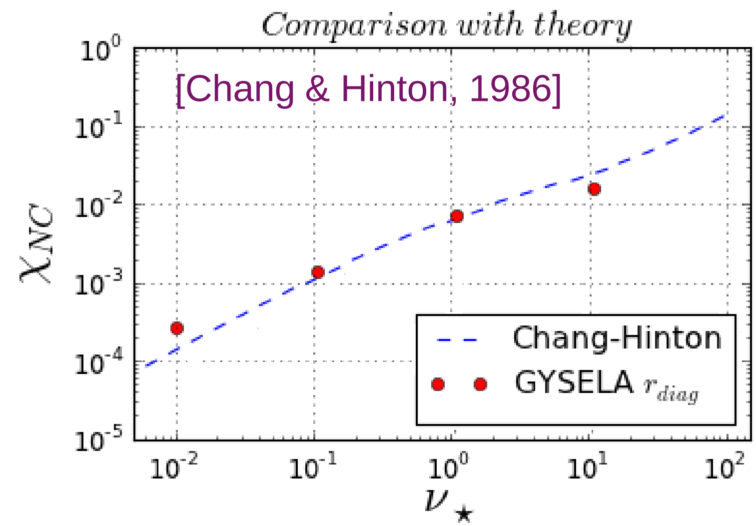
Close to Sugama operator [Sugama, POP(2009)]

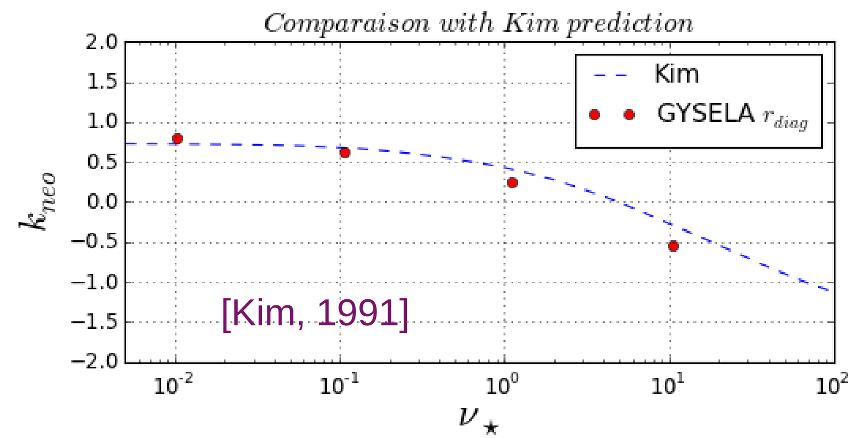
New collision operator validation

Conservations after one collision time

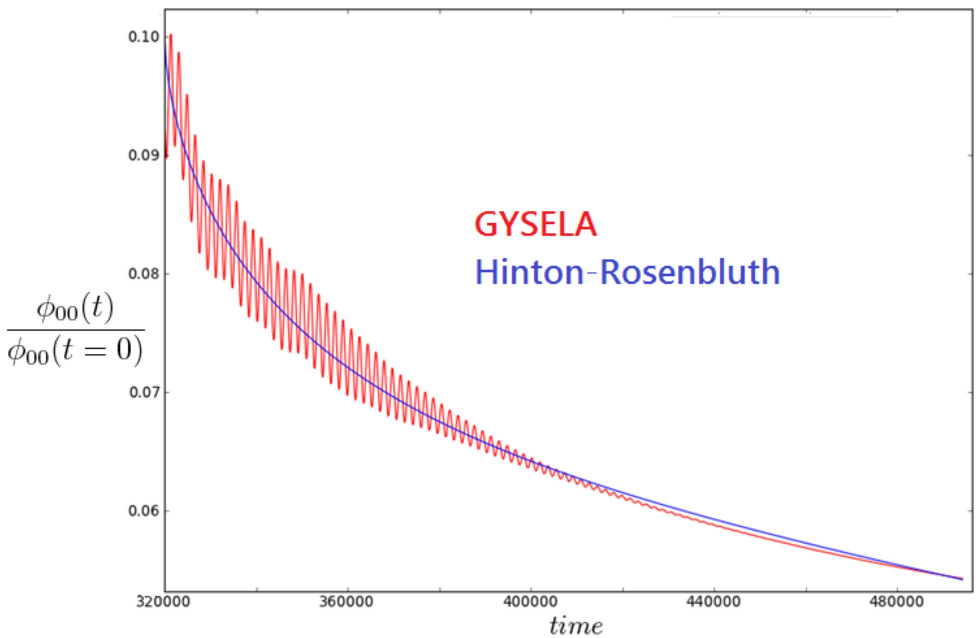
$$\frac{\Delta n}{n} \simeq 7 \cdot 10^{-7} \quad \Delta p_{\|} \simeq 10^{-9} \quad \frac{\Delta E}{E} \simeq 6 \cdot 10^{-6}$$

Neoclassical benchmarks





Zonal flow damping

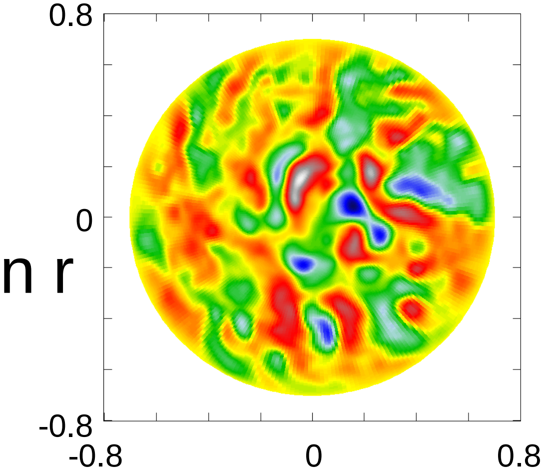


[Hinton & Rosenbluth , 1999]

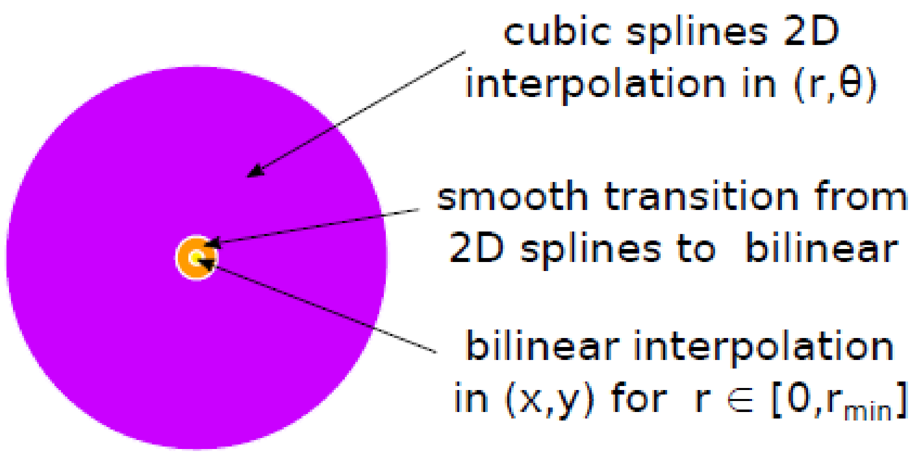
Removing Inner Boundary Condition: r = 0

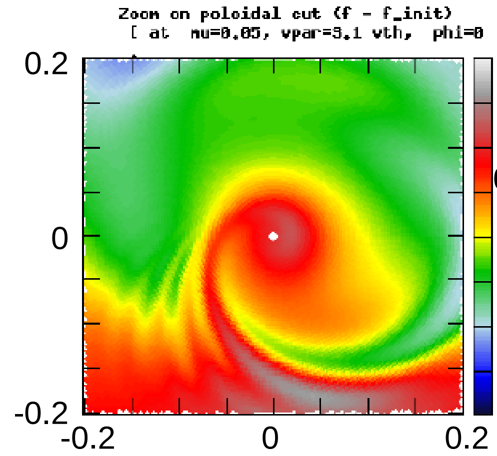
Issue at r=0: divergence of metric (1/r) + too many θ points

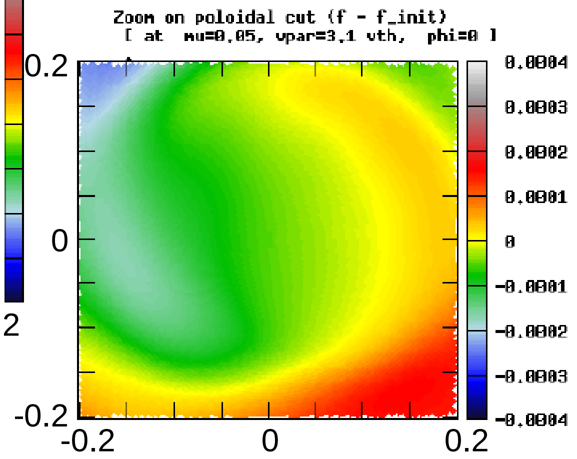
- Previously: $r_{min}>0$ $\rightarrow$ | Dirichlet for ϕ_{mn} / Neumann for ϕ_{00}
- Upgrade:
  - Poisson (trick): $r_{min}=\Delta r/2 \Rightarrow$ no BC required in r
  - Vlasov: bilinear interpolation in $0<r<r_{min}$



[Latu-Mehrenberger, 2016]







Kinetic electrons & spurious ω_H modes

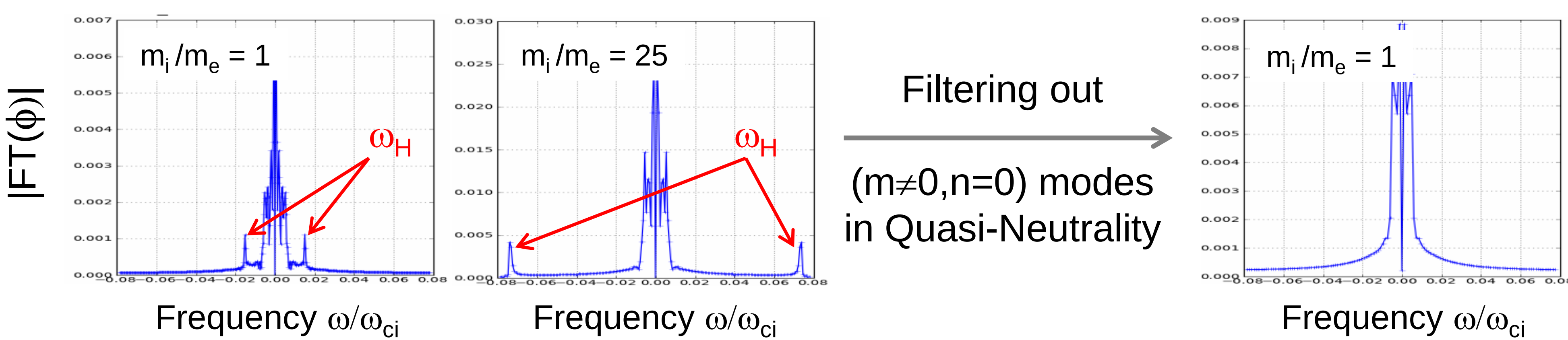
- Electrostatic limit $\rightarrow$ spurious "ω_H" modes: $\omega_H / \omega_{ci} = (k_{//} / k_\perp)(m_i/m_e)^{1/2}$
  - Correspond to hydro-dynamical limit ($\omega \gg k_{//} v_{th}$) of ITG disp. rel. [Lee 1987]
  - Also: electrostatic limit (β=0) of kinetic Alfvén wave

$$\omega_{KAW}^2 = k_\parallel^2 v_A^2 \frac{1+k_\perp^2\rho_i^2}{1+k_\perp^2 d_e^2} = \frac{k_\parallel^2\rho_i^2 \;\; \omega_{ci}^2}{k_\perp^2\rho_i^2(m_e/m_i)+\beta/2}\,(1+k_\perp^2\rho_i^2)$$

[Scott 1997]

$\Rightarrow$ Should disappear in electromagnetics (for $\beta > (k_\perp\rho_i)^2 m_e/m_i \sim 2.10^{-5}$)

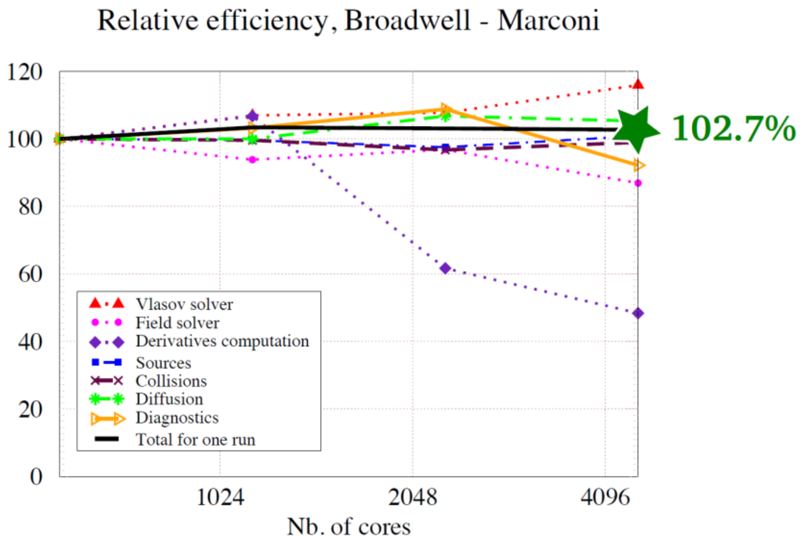
- Trick: disappear when filtering out ($m \neq 0, n=0$) modes in QN eq. [Idomura 2016]

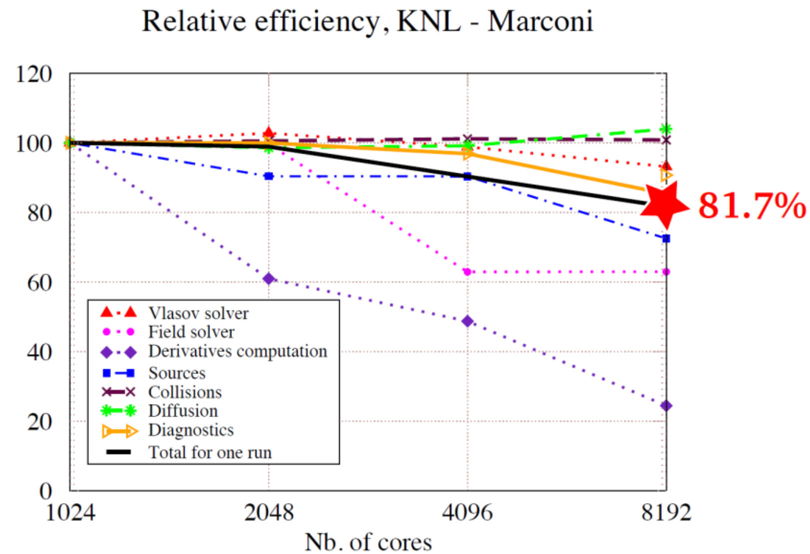


[Ehrlacher 2016]

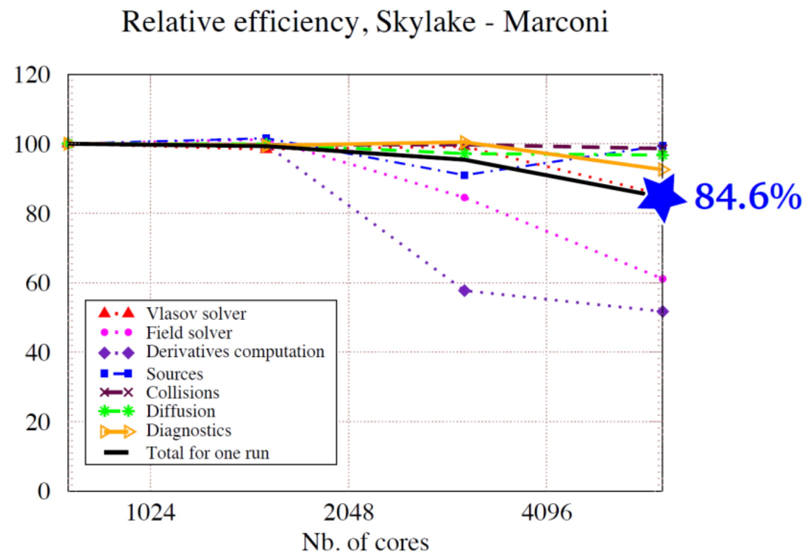
Strong scaling – Relative efficiency Broadwell / KNL / Skylake

- From 16 up to 128 nodes. Domain size $512 \times 256 \times 128 \times 128 \times 16$ - Medium case





- *Good* efficiencies
- *Pb* to scale:
  - Field solver
  - Derivatives comp.



G. Latu & al.

Towards Scrape-Off Layer physics r>a

- Coupling core (r/a<1) – SOL (r/a>1) is important: H-mode, impurities & neutrals

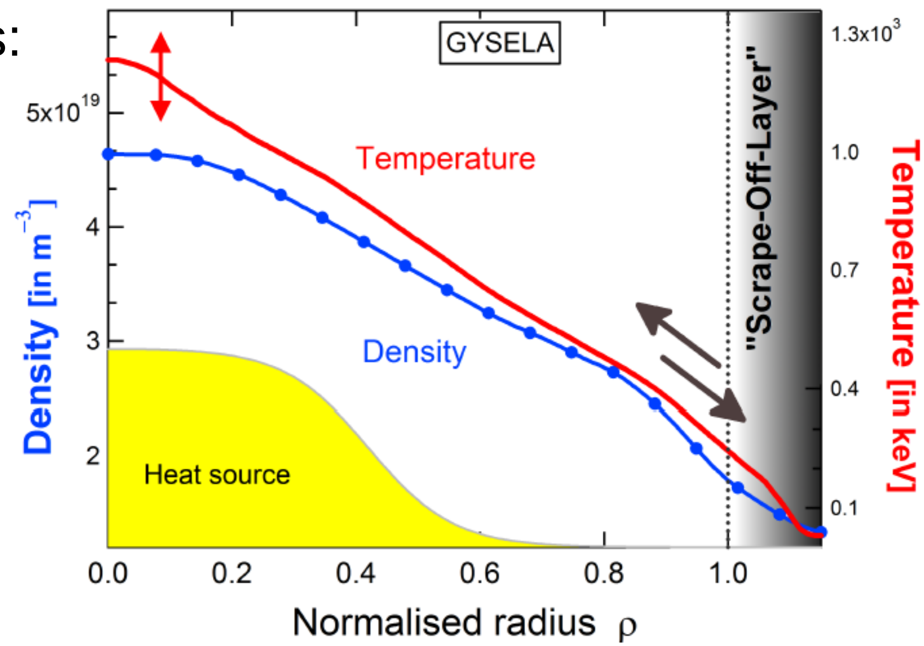
  Critical challenges:
  - close/open magnetic surfaces (periodicity; plasma-surface interaction)
  - relative fluctuation levels
  - particle sources/sinks

[Dif-Pradalier, 2016]

- Forced relaxation towards SOL-like profiles:

$$\underbrace{\frac{DF}{Dt} = \mathcal{C}(F) + \mathcal{S}(F)}_{\text{core — edge}} - \underbrace{\nu(F - F_{SOL})}_{\text{“SOL-like”}}$$

  - Smooth transition towards vanishing fluctuations
  - Some evidence of SOL → core interplay



- Possible alternatives: penalization and/or transition towards fluid description?

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