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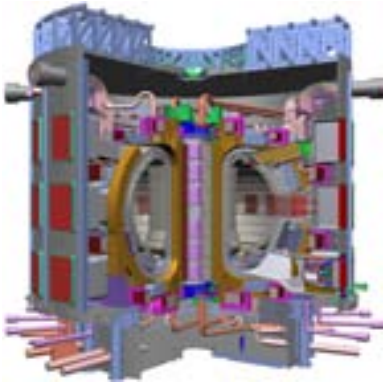
Gyrokinetic global full-f flux-driven simulations

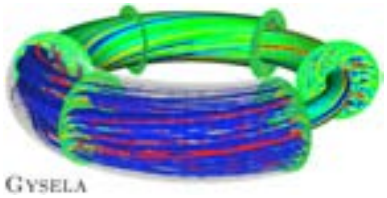
- GYSELA code -

V. Grandgirard, J. Abiteboul, G. Dif-Pradalier, X. Garbet, Ph. Ghendrih
G. Latu, Ch. Passeron, Y. Sarazin, A. Strugarek, D. Zarzoso
Association Euratom-CEA, CEA/DSM/IRFM Cadarache, France

J.P Braeunig, N. Crouseilles, E. Sonnendrücker
IRMA, CNRS-Université Louis Pasteur, 67084 Strasbourg, France.



Joint effort of physics, numerics and computer science supported by ANR EGYPT (2007-2010) + ANR GYPSI (2010-2014)



Association Euratom-Cea

GYSELA code - main characteristics

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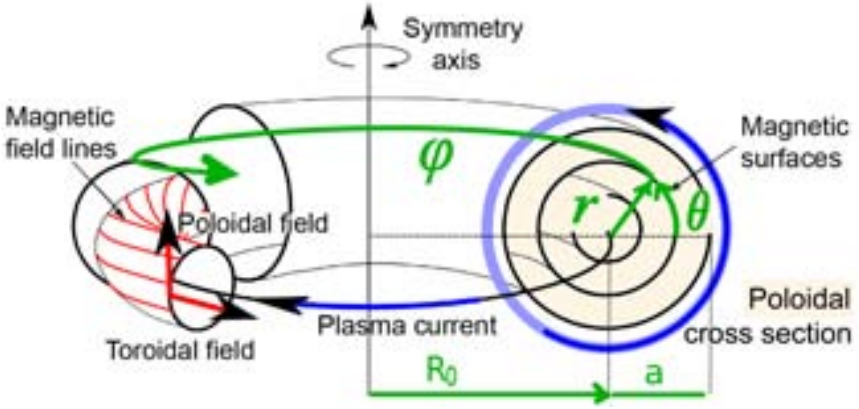
- ✓ Full-f: no scale separation between equilibrium/perturbations
- ✓ Global geometry
  - ➔ Concentric magnetic surface with circular cross-sections



- ✓ Electrostatic ITG driven turbulence
  - ➔ Slab & toroidal branches, trapped & passing ions
- ✓ Adiabatic electrons only ➔ no particle transport, no TEM/ETG
- ✓ Gyroaverage ➠ Bessel function: $J_0(k_\perp \rho_i) \approx \frac{1}{1+\frac{k_\perp^2 \rho_i^2}{4}}$ (Padé)
- ✓ Flux-driven conditions ➔ more realistic source term
- ✓ Semi-Lagrangian approach
  - ➔ GYSELA named for GYrokinetic SEmi-LAgrangian code

Outline

- Flux-driven global full-f non-linear gyrokinetic code as GYSELA are:
  - mature enough to make predictions in terms of turbulence and transport in tokamak plasmas
  - extremely demanding in terms of numerics and require state-of-the art HPC

1. Parallelisation of the semi-lagrangian scheme
2. Delicate boundary conditions for global codes
3. Constraints of the full-f approach
4. Choice of the sources for flux-driven simulations

The GYSELA code - equations

- Time evolution of gyrocenter distribution function $\bar{F}(r, \theta, \varphi, v_{\|}, \mu)$ governed by 5D gyrokinetic Fokker-Planck equation: *[Brizard & Hahm, Rev.Mod.Phys. 2007]*

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

with the equations of motion:

$$B_{\|}^{*} d_t \mathbf{x}_G = v_{G\|}\mathbf{B}^{*} + \frac{1}{e}\mathbf{b} \times \nabla \Lambda$$

$$B_{\|}^{*} m d_t v_{G\|} = -\mathbf{B}^{*} \cdot \nabla \Lambda$$

where $\mathbf{B}^{*} = \mathbf{B} + (m v_{G\|}/e)\nabla \times \mathbf{b}$ and $\Lambda = e\bar{\phi} + \mu B$;

$\mathcal{C}(\bar{F})$ = collision operator and S an additional realistic source

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

$$\tau\left(\phi - \langle \phi \rangle\right) - \frac{1}{n_{eq}}\nabla_{\perp} \cdot \left(n_{eq}\phi \nabla_{\perp}\phi\right) = \frac{1}{n_{eq}}\int J \cdot \left(\bar{F} - F_{eq}\right) d^3 v$$

GYSELA code - global algorithm

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global algorithm of second order in time : predictor-corrector

For each μ: $\Leftarrow$ *N_μ MPI communicators*

- Solving of the non-linear Vlasov equation (4D):
  - Time-splitting of Strang :

  4D $(r, \theta, \varphi, v_\parallel) \Rightarrow$ 2D (r, θ) + 1D (φ) + 1D $(v_\parallel)$

$$\partial_t \bar{F} + u(x)\nabla_x \bar{F} = 0 \quad \Rightarrow \text{Semi-lagrangian}$$

$$+ \quad \partial_t \bar{F} = \mathcal{C}(\bar{F}) + S \quad \Rightarrow \text{Cranck-Nicholson}$$

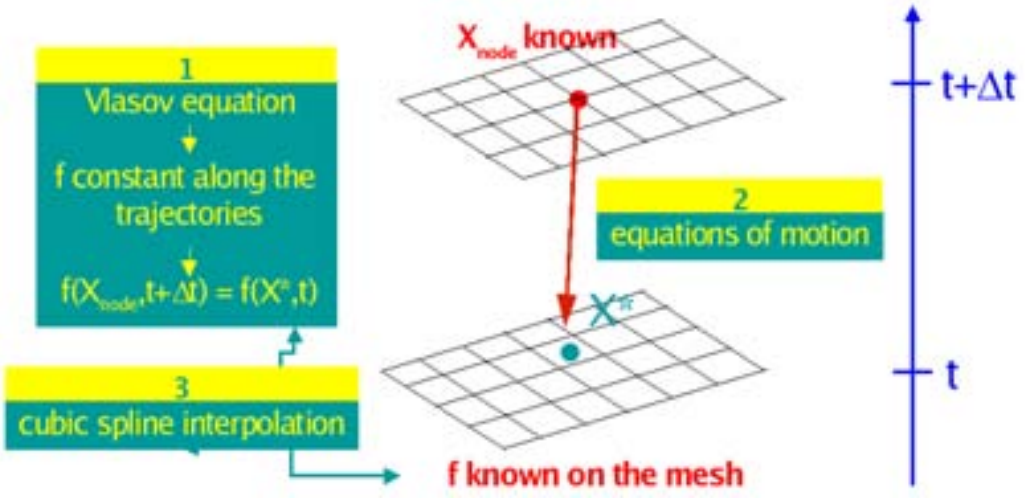
end for

- Computation of $\int J \cdot \bar{F} d^3v$ $\Leftarrow$ *Expensive MPI communication*
- Solving of the quasi-neutrality equation (3D):
  - Fourier in θ and φ + Finite differences in r
- Gyroaverage ($J_0 \Leftrightarrow$ Padé approximation):
  - Fourier in θ + Finite differences in r

The backward semi-lagrangian Method (BSL)

- Solving of advective form of Vlasov equation :

$$\frac{\partial f}{\partial t} + u(x)\frac{\partial f}{\partial x} = 0 \text{ with } \frac{\mathrm{d}x}{\mathrm{d}t} = u(x) \quad \Rightarrow \quad \frac{\mathrm{d}f}{\mathrm{d}t} = 0$$



☺ Noise reduction, good property of conservation

[Grandgirard et al., JOCP 2006]

☹ High order interpolation needed ➔ Cubic splines

- A good compromise between accuracy and simplicity

BSL scheme parallelisation

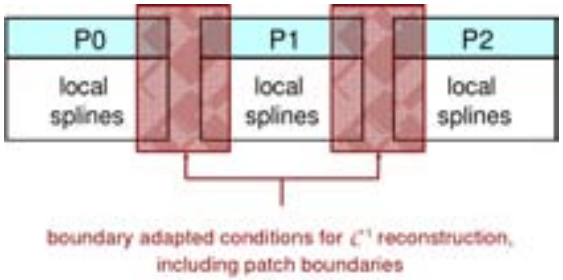
☺ Fixed grid in time ➠ perfect load balancing

☹ Complex parallelization due to **cubic spline interpolation**

- Loss of locality
  (value of f on one grid point requires f over the whole grid)

  ➠ **Not possible to use a simple domain decomposition**

- A new numerical tool has been developed
  ➠ Hermite Spline interpolation on patches *[Latu-Crouseilles 2007]*



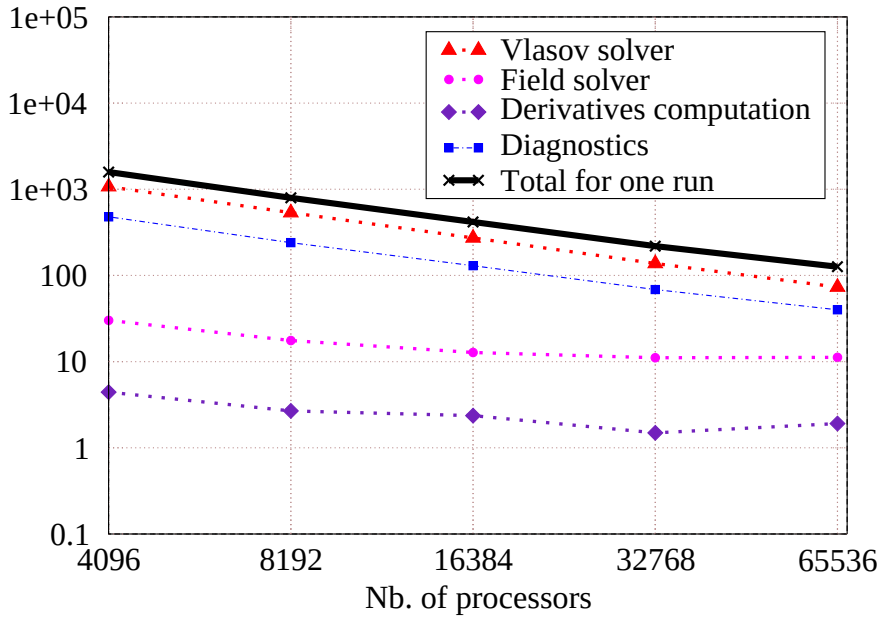
- Local splines on each subdomains with Hermite boundary conditions
- Derivatives are defined so that they match as closely as possible those of global splines

GYSELA : Hybrid MPI/OpenMP parallelisation

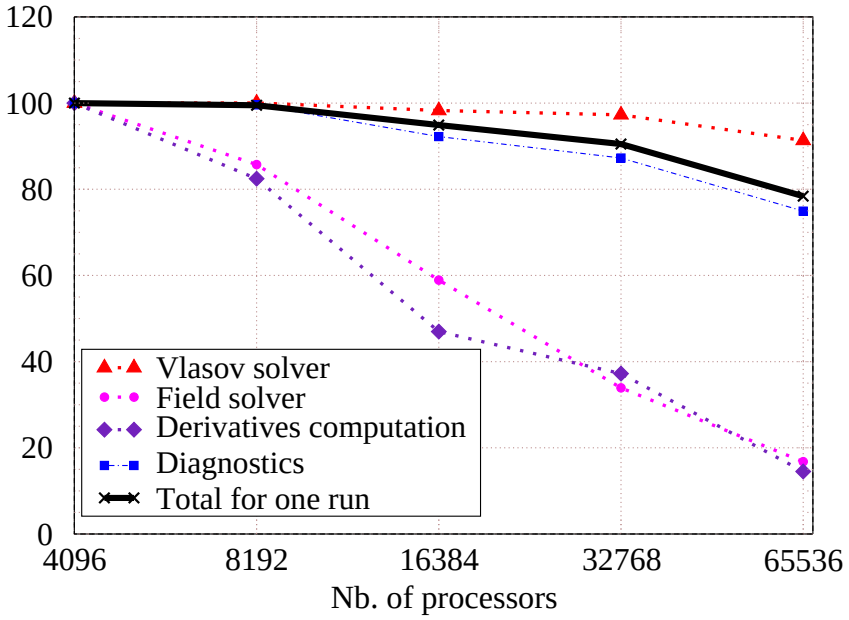
- Four levels of parallelism: r, θ loops , μ loop, OpenMP
- Strong scaling performed on Jaguar machine

$N_r = 512, \quad N_\theta = 512, \quad N_\varphi = 128, \quad N_{v_\parallel} = 128, \quad N_\mu = 32$ (main data = 1 TB)

Execution time for one Gysela run (Strong Scaling)



Relative efficiency for one Gysela run (Strong Scaling)



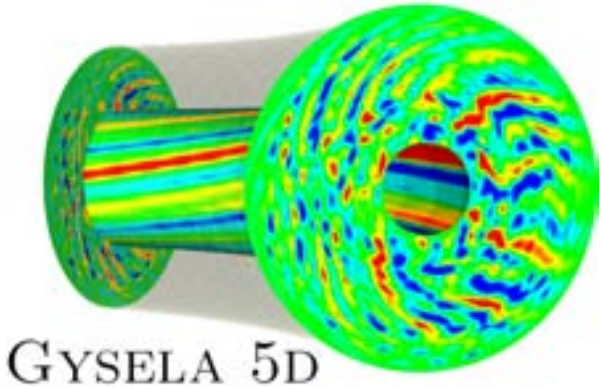
78% of relative efficiency on 65 536 cores

[G. Latu et al., PPAM proceedings 2011]

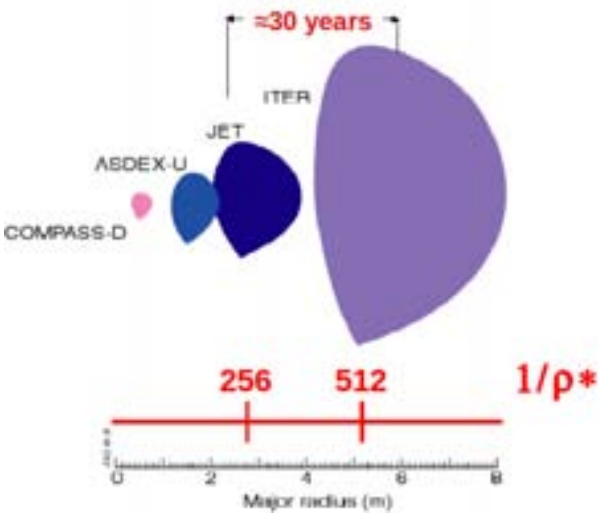
Global codes require huge meshes

- a large fraction of the plasma radius is considered

☺ capture large scale events



☹ Require extremely large 3D meshes



✓ $\rho^* \equiv \frac{\rho_i}{a} \ll 1$

✓ Number grid points $\sim (\rho^*)^{-3}$

⇓

Huge mesh for global simulations

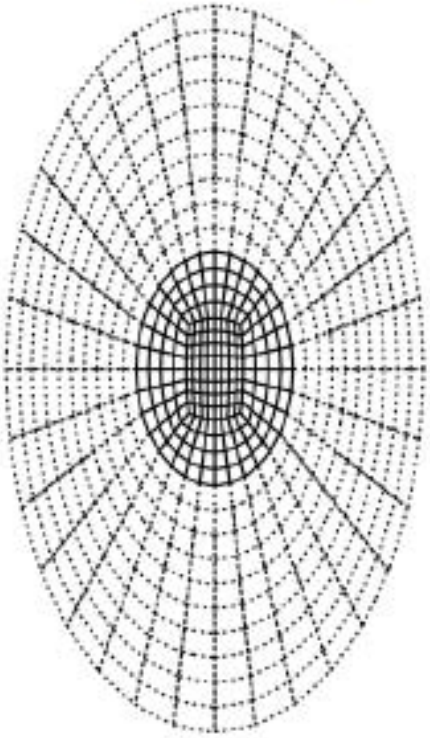
$$\rho^*_{\text{ITER}} = 1/512$$

$\sim 272\ 10^9$ points for 1/4 of torus

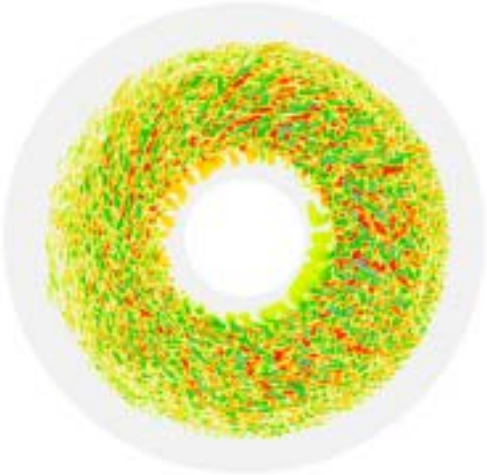
Global codes - problem of boundary conditions

- face delicate problem of radial boundary conditions

- Up to now in the poloidal plane:



  - polar system (r, θ)
  - disc geometry (hole in the center)



- Aim: NURBS or Bezier mapping
  - complex shapes accessible: ellipse, X-point
  - avoid the hole in the center
- Conclusions (on a reduced 2D model)
  - Numerically relevant and accurate
  - Overhead of $\approx$ 200% in the Vlasov solver

[J. Abiteboul, A. Ratnani et al., ESAIM proceedings 2011]

Main issues for full-f gyrokinetic codes

- Full-F code ($F = F_{eq} + \delta F$)
  - ➠ Back reaction of turbulent transport is accounted for in time evolution of the equilibrium

- Main critical issues:
  1. Collision operator : ensures equilibrium Maxwellian & recovers neoclassical theory *[Dif-Pradalier, PRL 2009]*
     - GYSELA : Reduced ion-ion Fokker-Planck collision operator
       $\hookrightarrow$ preferred collisional friction –along $v_{\|}$ *[Garbet, 2008]*
       $\hookrightarrow$ efficient parallelisation (μ remains motion invariant)
  2. Force balance & consistent E_r *[Dif-Pradalier, PoP 2011]*
  3. Source to sustain main profile
     - Turbulence regime is evanescent if no free energy is injected in the system.

Accurate description of the radial force balance

- Force balance $\boxed{E_r - v_\varphi B_\theta + v_\theta B_\varphi = \frac{\nabla p}{ne}}$ primordial for full-f codes
- E_r self-consistently evolved and coupled to the mean profile dynamics (either through thermodynamic force or flows evolution)

$\frac{\nabla p}{ne}$, E_r and $v_\varphi B_\theta$ computed by code

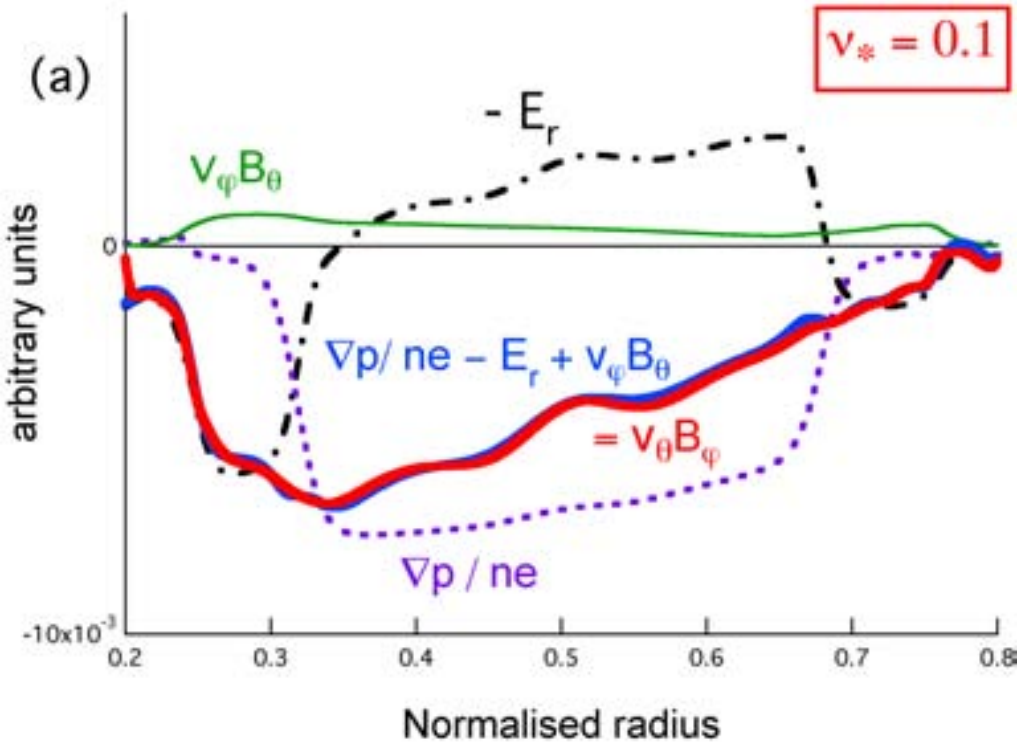
$\Downarrow$

$v_\theta B_\varphi$ deduced from force balance:

$$\boxed{v_\theta B_\varphi = \frac{\nabla p}{ne} - E_r + v_\varphi B_\theta}$$

$\Downarrow$

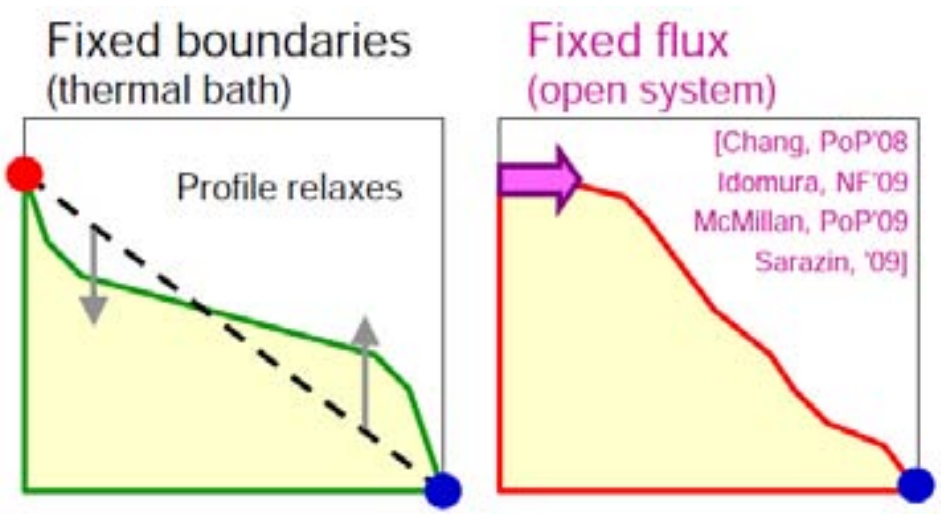
compare to $v_\theta B_\varphi$ given by code



- Accurate description of the force balance in GYSELA

Flux-Driven boundary conditions

☺ Source terms aims at maintaining the equilibrium profiles, which would otherwise relax towards marginal state



- Vanishing gradient boundary conditions at inner boundary $\longrightarrow$ temperature and flows evolve freely
- "Buffer" region (artificial dissipation) near outer boundary
  - acts as energy sink
  - Forces no slip boundary condition for toroidal rotation

Prescribed sources in GYSELA

☹ New degree of freedom ⇒ Source structure in velocity space ?

- In GYSELA : Source = Sum of the product of Hermite and Laguerre polynomials in $v_{G\|}$ and μ

  (in the spirit of pioneering work *[Darmet, CNSNS 2008]*)

- Versatile enough to allow for separate injection of heat, parallel momentum and vorticity.

$$S_{GYSELA} \simeq S_r \left[\left(\frac{v_{G\|}}{v_{Ts}} \right)^2 - 1 \right] \exp\left(- \frac{m_i {v_{G\|}}^2/2 + \mu B}{T_s} \right)$$

(see *[Sarazin, NF 2011]* for more details)

- Recent adding of fast particle source ⇒ EGAMs

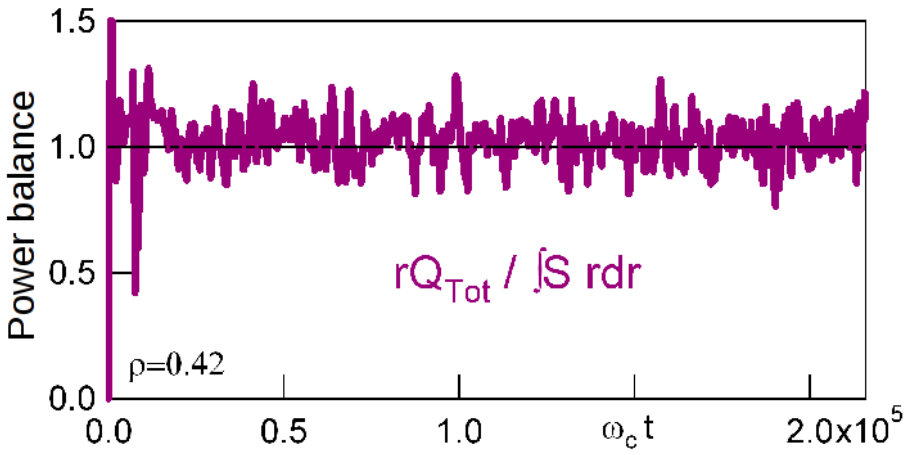
  [Zarsozo, proceedings of IAEA TM 2011]

Flux-Driven simulations extremely time consuming

☺ Flux driven simulations then allow for investigating the impact of heating power on energy confinement time

- total power balance requires that the time averaged total heat flux should balance the integral of the source

☹ Extremely time consuming (several τ_E)



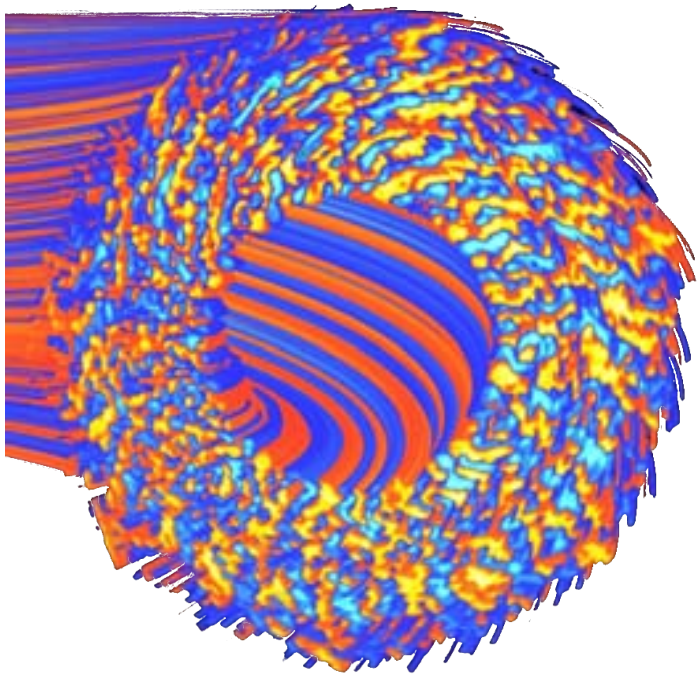
- τ_E scales like ρ_*^{-3}
- Statistical steady-state regime when:

$$r\, Q_{\text{Total}} \,/\, \int S\, d^3x = 1$$

➠ Only reachable for large ρ_* (cf *[Sarazin NF2010]* for $\rho_* = 1/64$)

Biggest simulation ever run with GYSELA

➠ A simulation close to ITER-size scenario ($\rho_* = 1/512$) performed on 1/4 torus with additional heating power of **60 MW during 1 ms**



ion temperature fluctuations in the turbulent saturated phase

✓ A 5D mesh of **272 10^9 points**

$(r, \theta, \varphi, v_{\|}, \mu) = (1024 \times 1024 \times 128 \times 128 \times 16)$

✓ $>$ **6.1 million hours monoproc.**

- $\sim$ 31 days on 8192 processors

⇓

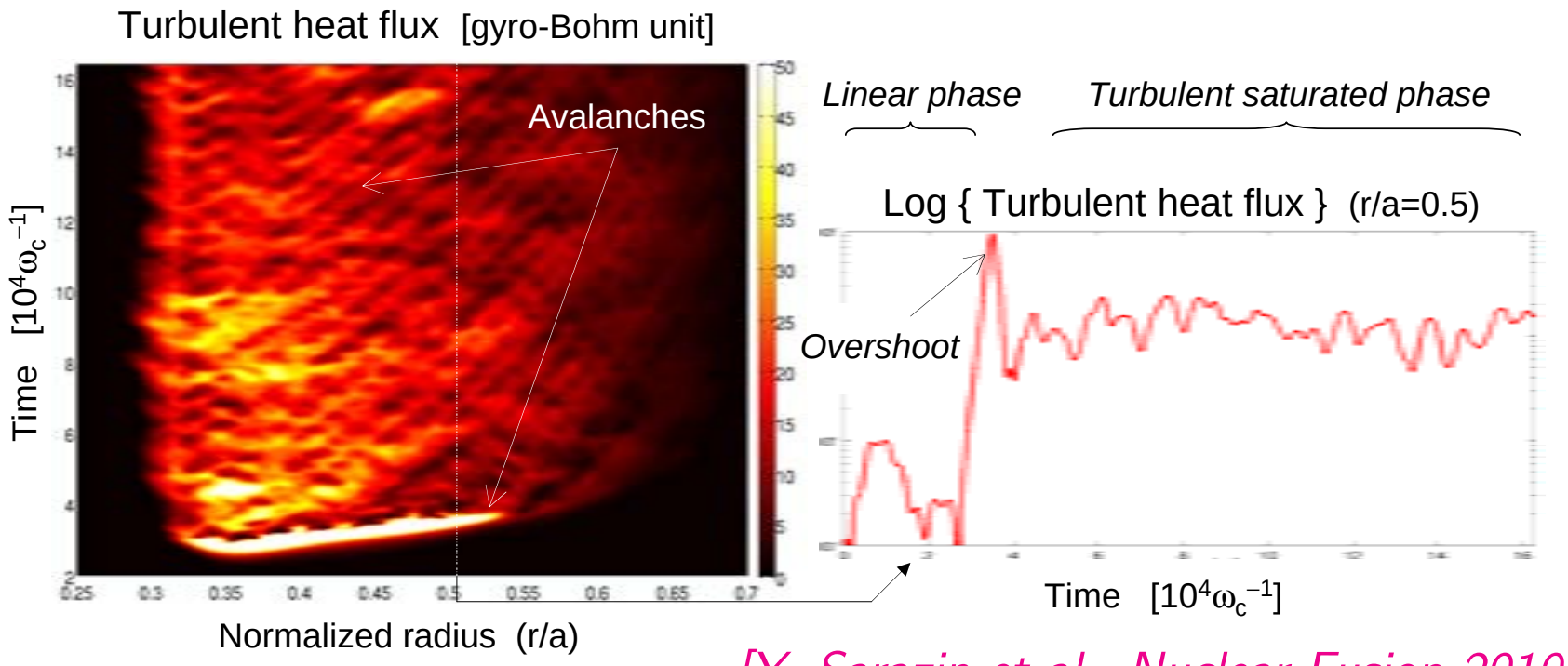
✓ **6.5 TBytes of data** to analyse

- 1.5 TBytes for 2D and 3D savings
- 5 TBytes for restart files

[J. Abiteboul EPS2010, Y. Sarazin IAEA2010]

Large-scale events in turbulent heat transport

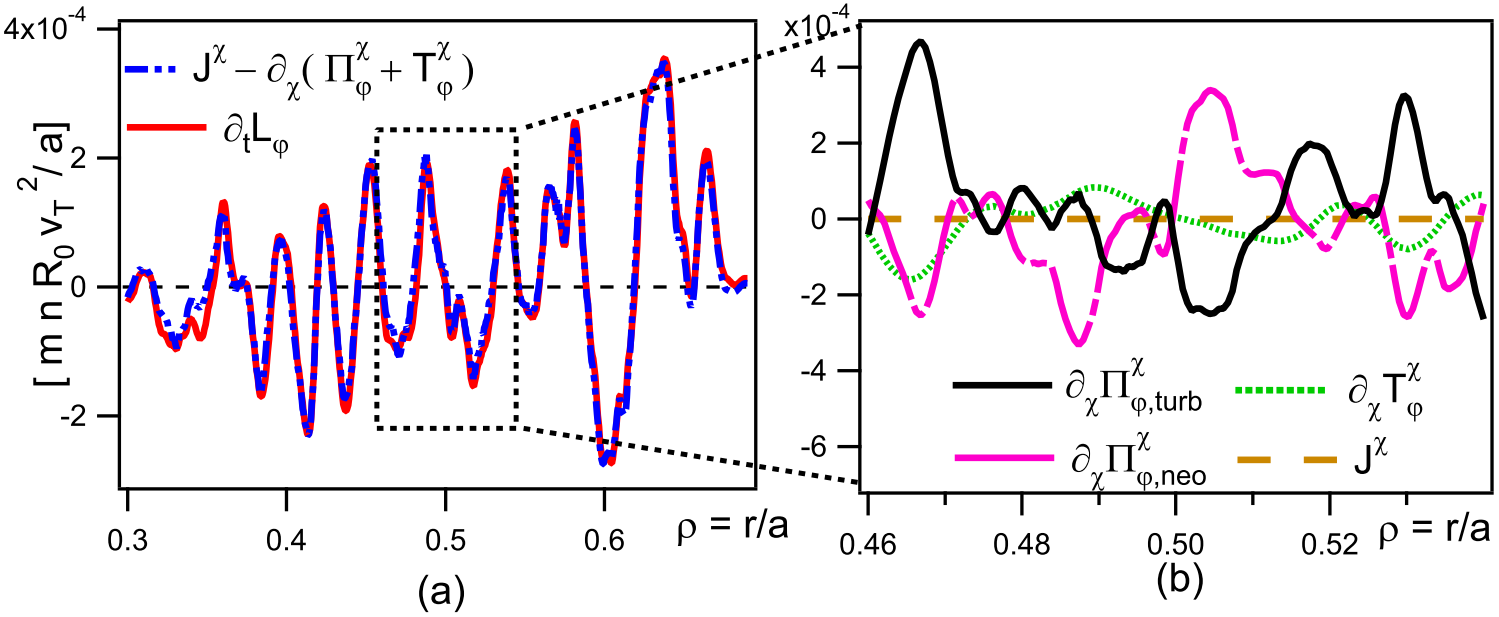
- Intermittent dynamics of turbulent heat flux (always outward)
- Long range ballistic transport events ⇒ inwards & outwards
  - Origin: domino-like effect + transient radially elongated vortices



[Y. Sarazin et al., Nuclear Fusion 2010]

➠ Global + full-f simulations are essential to capture these bursts

Toroidal angular momentum is conserved

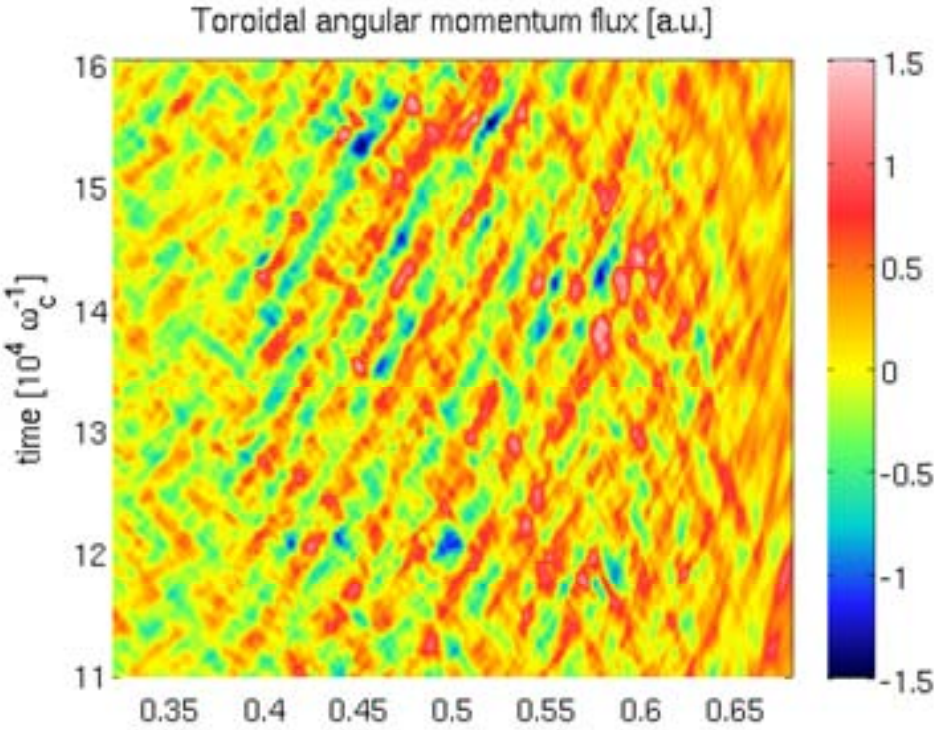


[J. Abiteboul et al., PoP 2011]

- Conservation equation recovered numerically
  despite strong variations (both radially and in time)
- Dominant contribution: Reynolds stress
- Allows to analyse in detail the transport and source/sink of momentum in the absence of injected torque

Momentum transport also displays avalanches

Momentum flux in the saturated non-linear regime



- Momentum flux can be inward and outward ($\neq$heat flux)
- Fronts propagate mostly outward, also inward
- gyro-Bohm scaling also recovered for momentum transport (i.e. Reynolds stress $\sim \rho_*^2$) *[Abiteboul et al., PoP 2011]*

Conclusion

- Semi-lagrangian codes difficult to parallelized but not impossible
  - 78% of relative efficiency on 65 536 cores for strong scaling
- Accurate description of the radial force balance
- Toroidal angular momentum is very well conserved
- GYSELA allows to analyse in detail the transport and source/sink of momentum in the absence of injected torque

➠ Next challenge: Include kinetic electrons

✓ Now ITER-like ion simulation: $272\ 10^9$ points ➠ $6\ 10^6$ hours monoproc.

✓ With electrons: $\rho_{\text{ions}}/\rho_{\text{elec}} = 60$ ➠ mesh size $\times 60^3$ and time step/60 !!!

➠ GYSELA road map

- Huge efforts of parallelisation to scale to more than 100 000 proc.
- Field aligned coordinates ($v_\theta \simeq 100 \times v_r$)
  ➠ Separate slow and fast motion crucial for electrons