Advanced gyrokinetic numerical simulations of turbulence in fusion plasmas

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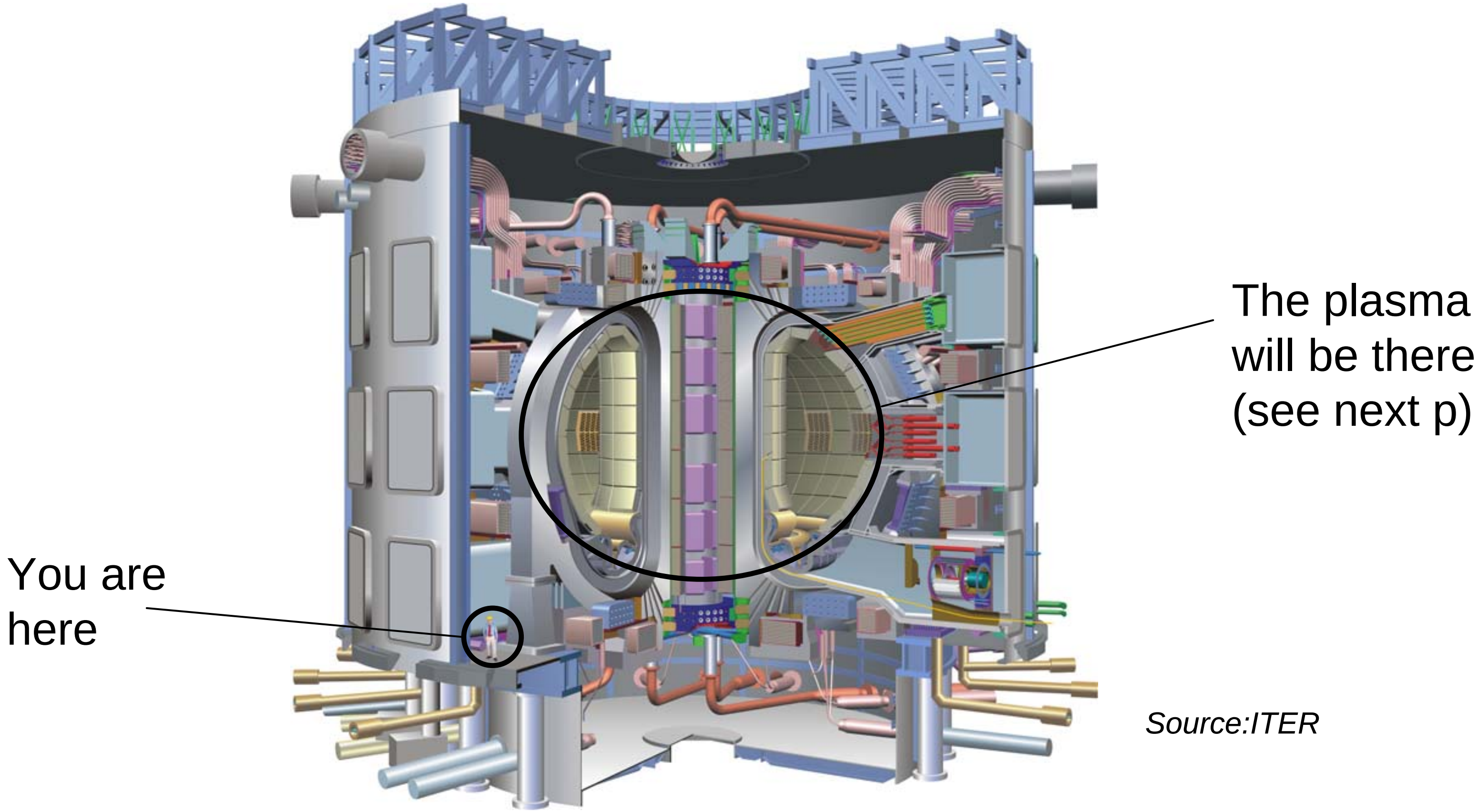
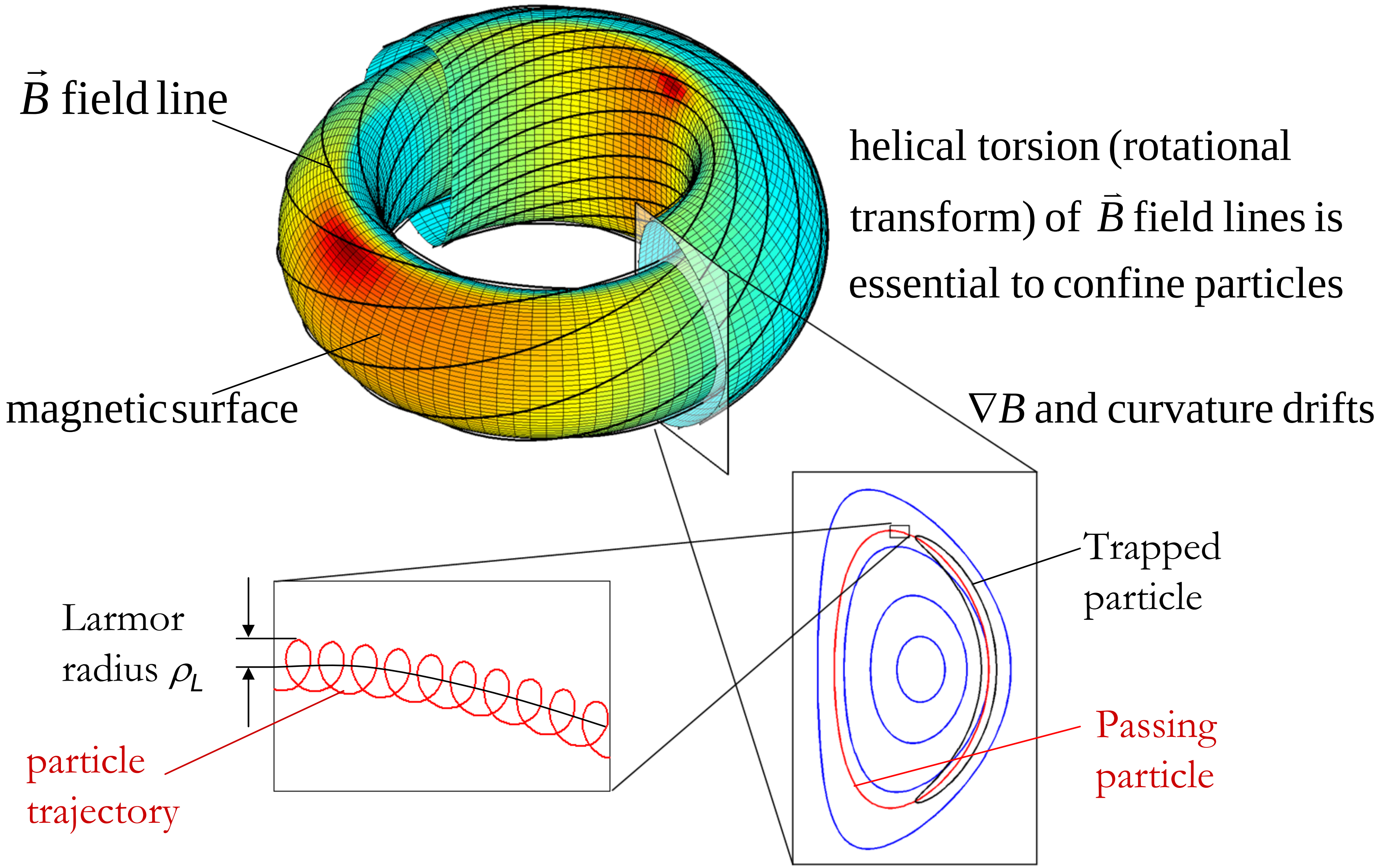
ITER: the way to fusion

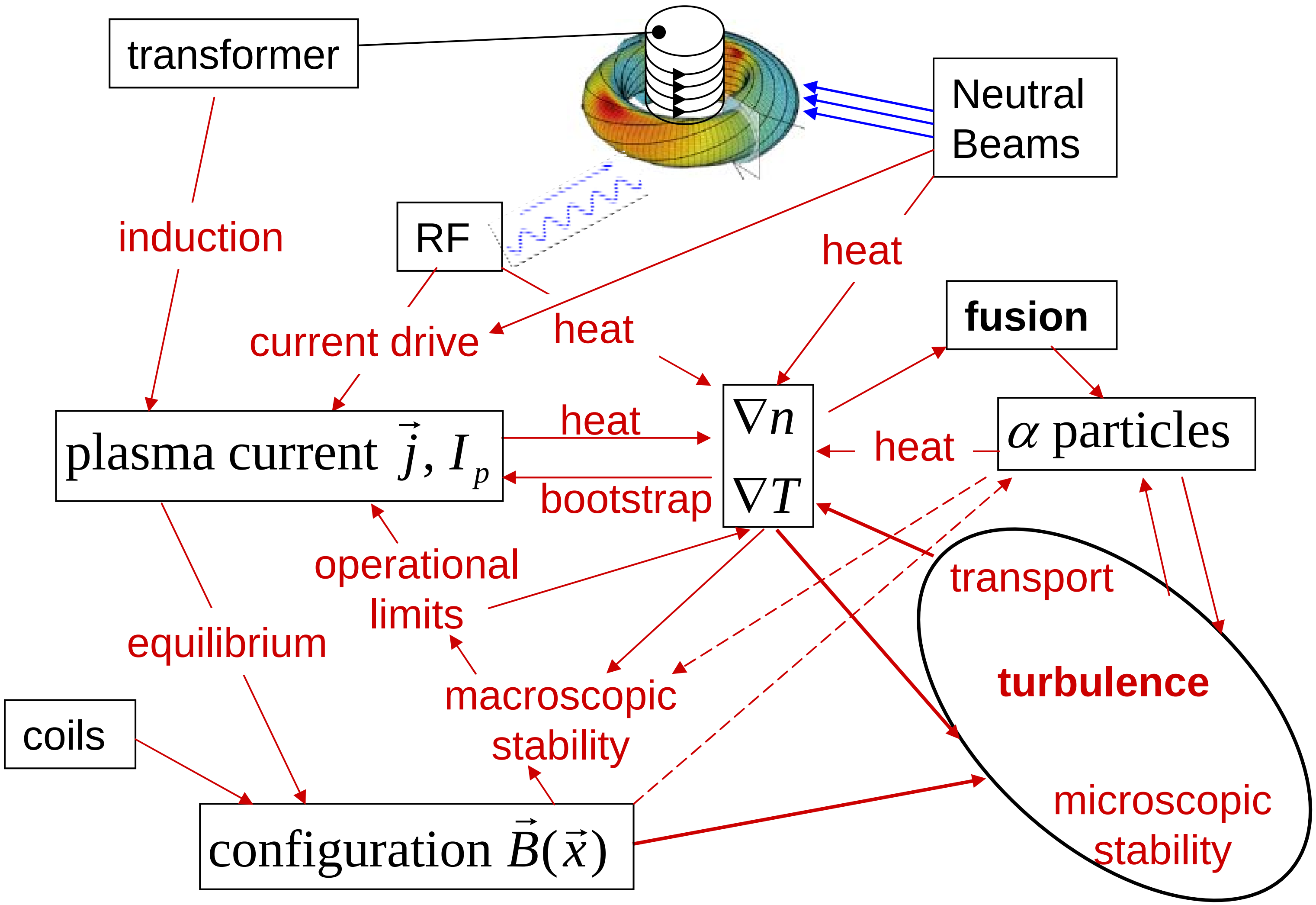


- EU, Japan, USA, China, India, South Korea, Russian Federation
- > 5.3G€ construction cost (1/3 G € /y = 0.06% of world overall R&D)
- Virtually inexhaustible, environmentally benign source of energy:
  - from Deuterium and Lithium; gives Helium. (Tritium is recycled)

Magnetic confinement: tokamak

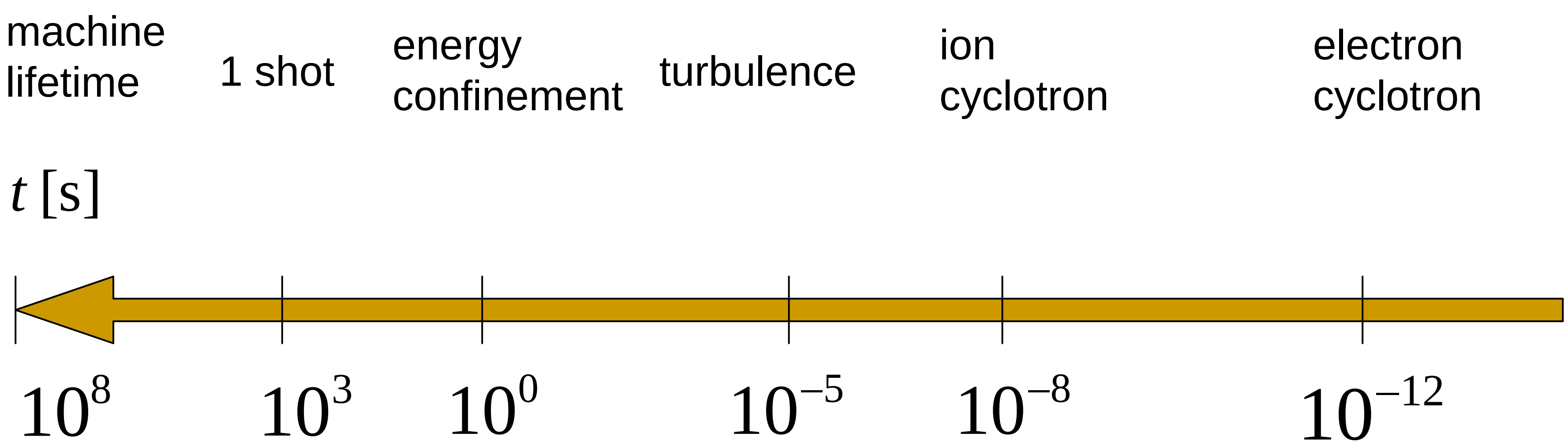


Complexity: many nonlinearities



- Geometry of magnetic configuration is an essential feature of fusion plasma physics

Timescales in the ITER plasma



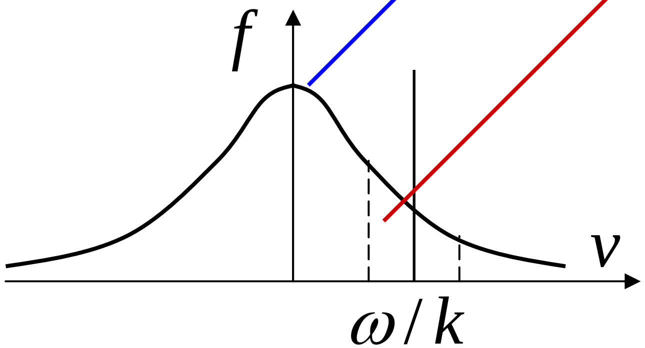
- Physics spans several orders of magnitude
- Direct Numerical Simulation (DNS) of “everything” is unthinkable
  - Need to separate timescales using approximations

Kinetic effects: wave-particle interaction

Surfers with velocity too different from the phase velocity of the wave will not ride the wave

Surfers with velocity just below the phase velocity of the wave will be accelerated

-> momentum and energy transfer



Net energy transfer from the wave to the particles if $\partial f / \partial v < 0$

Collisionless Landau damping

- General: distribution function in 6D phase space $f(\vec{x}, \vec{v}; t)$
- To be solved with consistent electromagnetic fields $\vec{E}(\vec{x}, t), \vec{B}(\vec{x}, t)$

Gyrokinetic-Maxwell: summary

- Assuming frequencies << cyclotron frequencies, analytical phase space reduction from 6D to 5D

- A time evolution partial differential equation (PDE) describing the advection-diffusion in 5D phase space of the distribution function *f*
- A set of 5 nonlinear, coupled ordinary differential equations (ODEs) for the characteristics
- A set of integral – partial differential equations for the perturbed fields (potentials ϕ, A) in 3D real space

Gyrokinetic equations

$f_s(\vec{R}, v_{//}, \mu)$ distribution function of species *s* in 5D phase space

$$\frac{\partial f_s}{\partial t} + \frac{d\vec{R}}{dt} \cdot \frac{\partial f_s}{\partial \vec{R}} + \frac{dv_{//}}{dt} \frac{\partial f_s}{\partial \vec{R}} = C(f_s, f_{s'})$$

advection-diffusion

$$\frac{d\vec{R}}{dt} = \ldots \mathrm{fct}(\phi, \vec{A}), \quad \frac{dv_{//}}{dt} = \ldots \mathrm{fct}(\phi, \vec{A})$$

equations of motion
(characteristics)
(orbits)

$(\phi, \vec{A})$ solution of Maxwell's equations,
with ρ, $\boldsymbol{j}$ obtained as moments of f_s

Solving GK: numerical approaches

- **Lagrangian: Particle In Cell (PIC), Monte Carlo**
  - Sample phase space with markers and follow their orbits
  - Noise accumulation is difficult to control in long simulations
- **Semi-Lagrangian**
  - Fixed grid in phase space, trace orbits back in time
  - Multi-dimensional interpolation is difficult
- **Eulerian**
  - Fixed grid in phase space, finite differences for operators
  - CFL condition; overshoot versus dissipation
- **Common to all three: Poisson (+Ampere) field solver**
  - Various methods: finite differences, finite elements, FFT,…

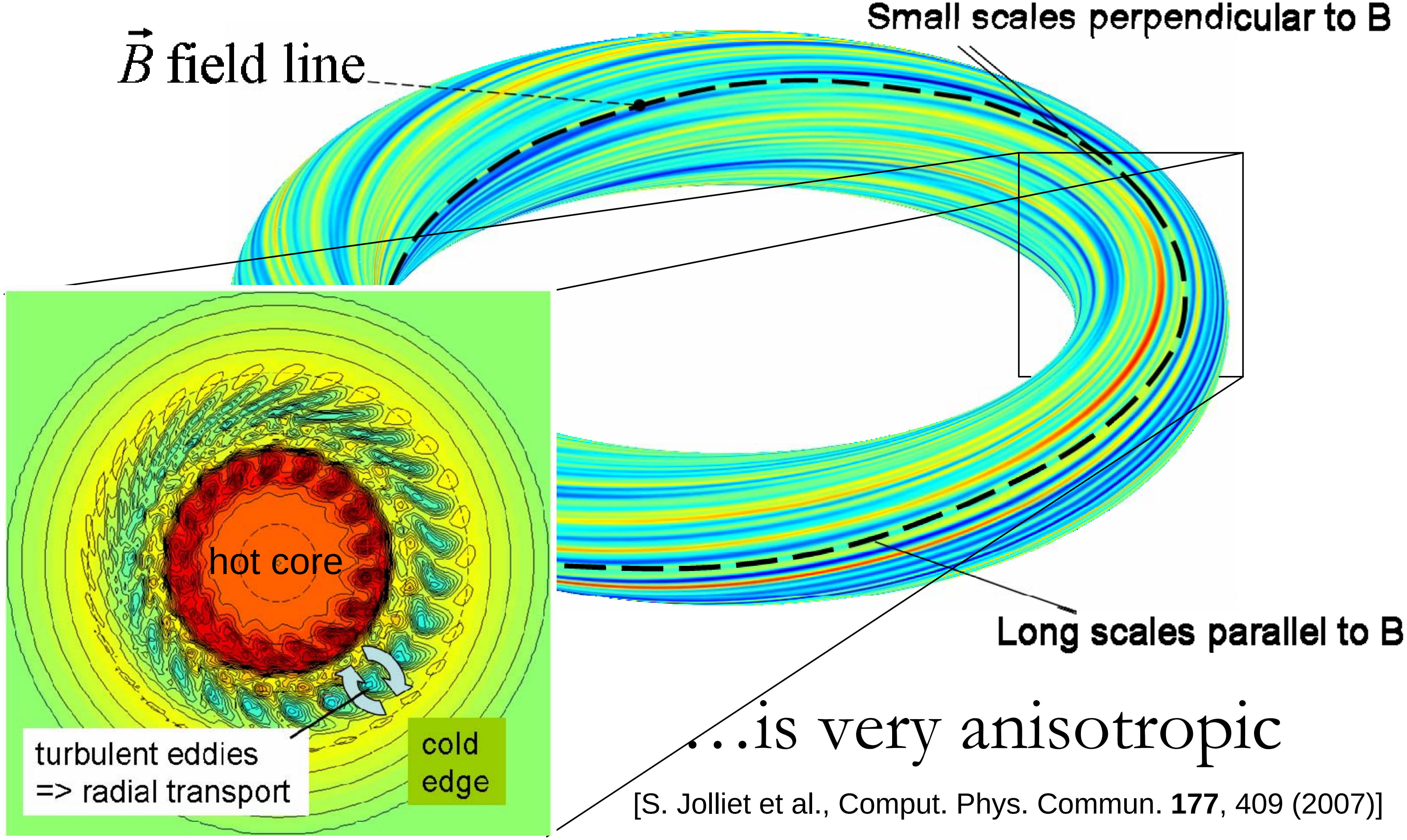
ORB5 (Lagrange-PIC) code: in-house (CRPP) + Max-Planck-IPP

GENE (Euler) code: Max-Planck-IPP + CRPP

ITER global gyrokinetic turbulence simulation: computational requirements

- Turbulence spatial scales down to gyroradius $\rho_s = c_s/\Omega_i$ $c_s=(T_e/m_i)^{1/2}$
- Normalized size = system size / gyration radius : $1 / \rho^* = a / \rho_s$
  - ITER: $1 / \rho^* = \sim 1000$
- Relevant scales: resolve up to $k_\perp \rho_s \leq 1$
- 3D field solver: min 4 pts/wavelength
  - ➔ 7'000'000'000 grid cells
- Velocity space resolution: ~ 300 / cell
  - ➔ 2'000'000'000'000 phase space cells (or markers)
- Time until statistical steady-state: ~ 2000 a / c_s
  - ➔ ~10^6 time steps
- This is clearly unfeasible!
- Cost of algorithm ~ $(1 / \rho^*)^4$

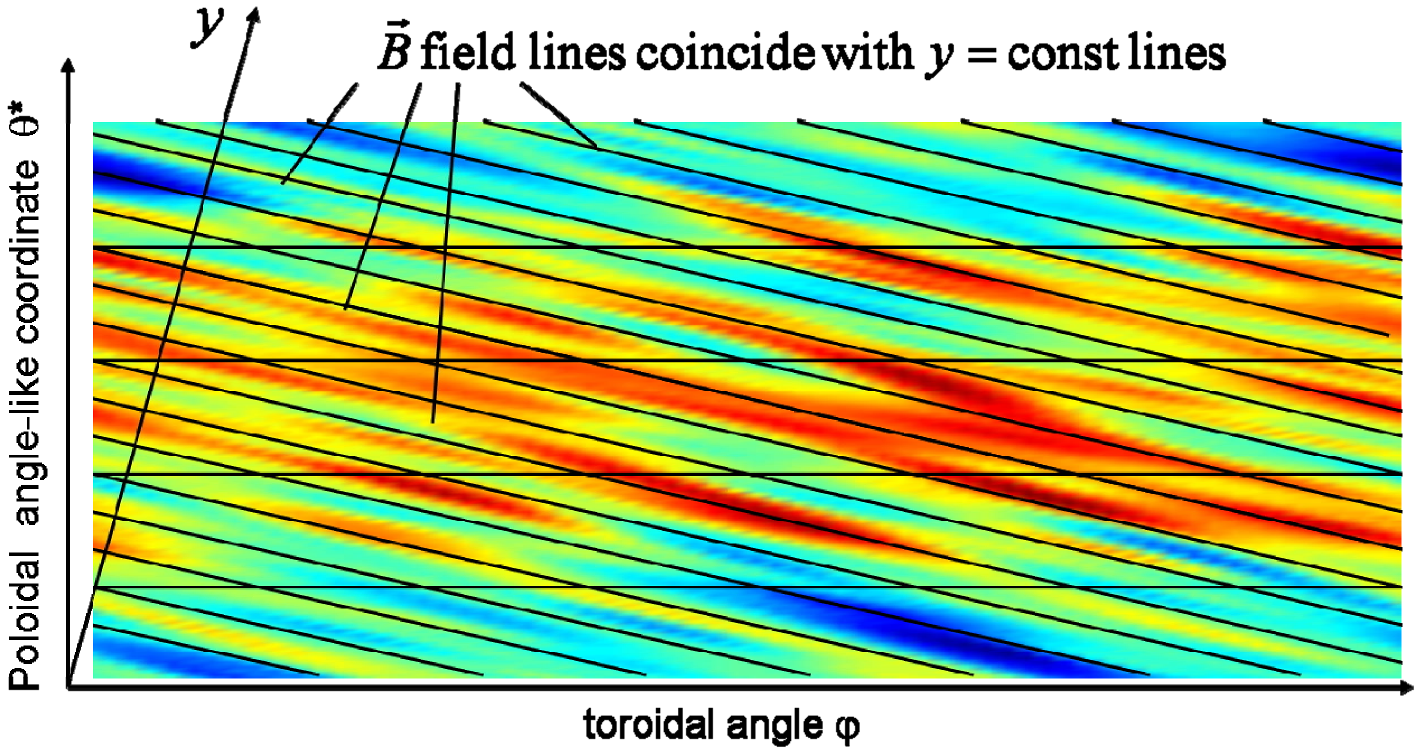
Turbulence in magnetized plasmas…



…is very anisotropic

[S. Jolliet et al., Comput. Phys. Commun. **177**, 409 (2007)]

At the heart of the HP2C proposal: Field-aligned coordinates



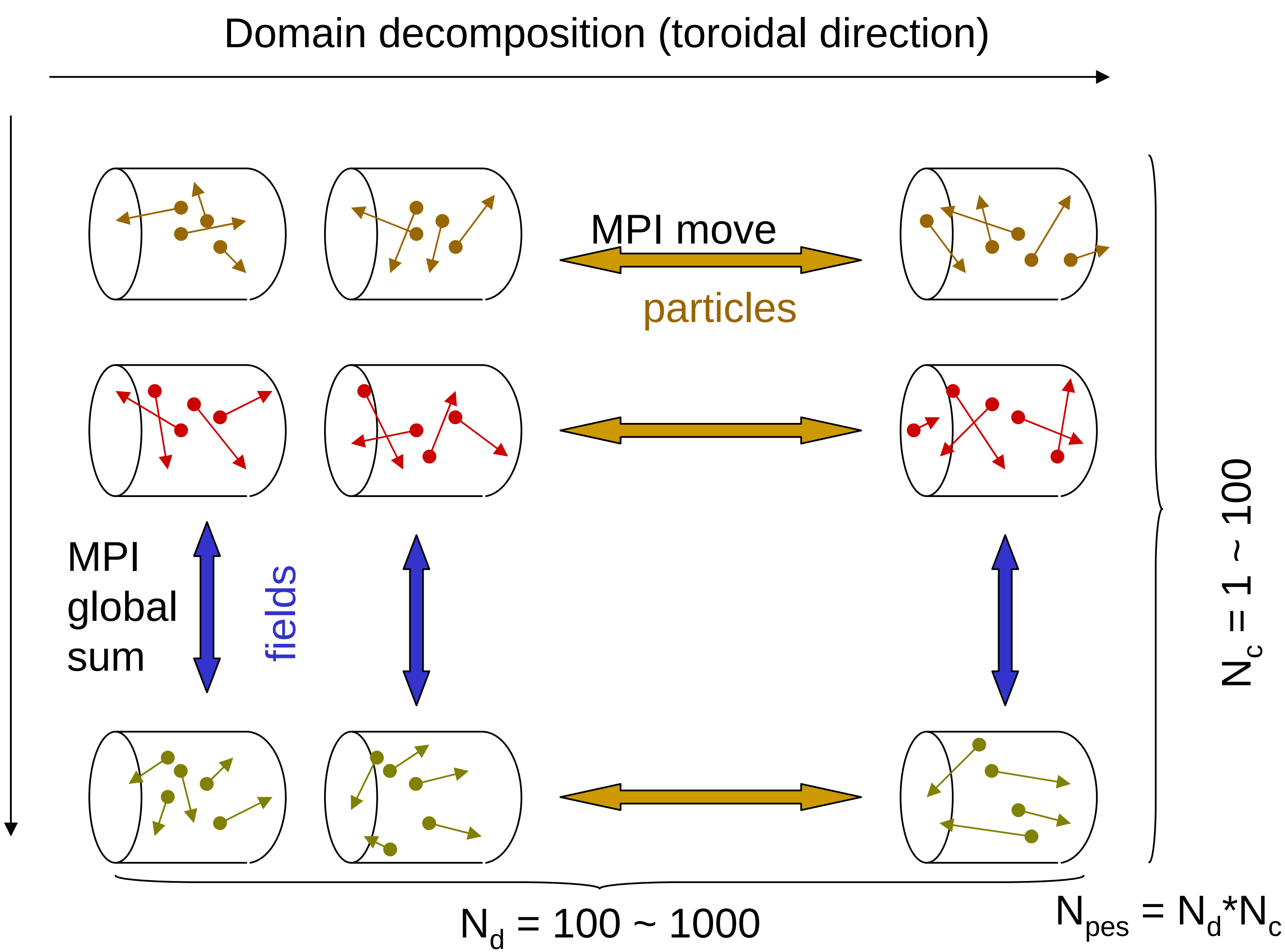
- ➔ reduction of 3D grid by factor ~ $1/\rho^*$ (1000 for ITER)
- ➔ requires major refactoring of existing codes (ORB5, GENE) and/or new code development (semi-Lagrangian)

Parallelization scheme – ORB5 code

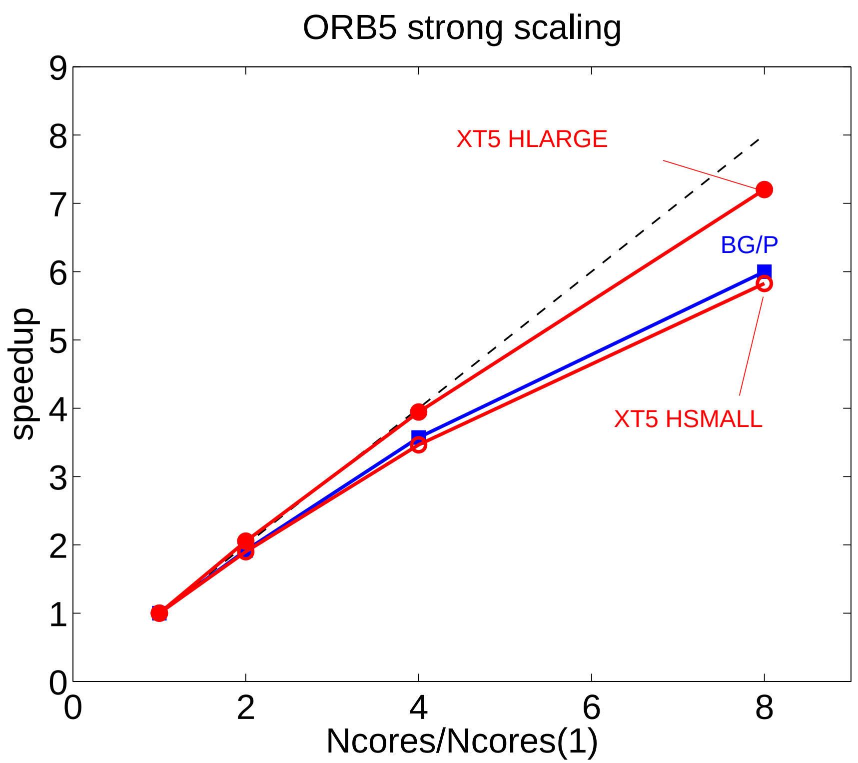
Aim: solve very large problems
=> huge nr of procs

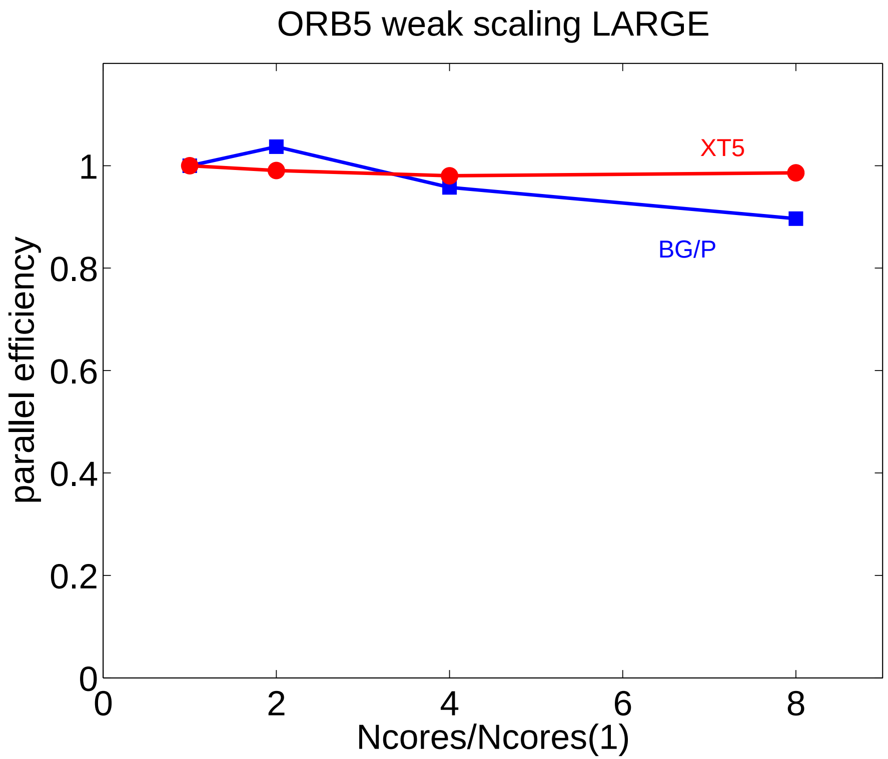
=> huge nr of domains !?!!!?

Domain Cloning: field quantities (density, potential) are replicated



Massive parallelism - Scalability





- IBM BG/P (Idris) (Deisa Extreme Computing Initiative)
  - 8192 to 32768 cores
- Cray XT-5 (CSCS) (thanks to Tim Stitt)
  - 1024 to 8192 cores

Bottlenecks to further scalability

- Recent strong scaling tests up to 64'000 cores (on a BG/P JUGENE, Juelich) of ORB5 code scalability have revealed a saturation of the parallel efficiency
- The problem comes from parallel data transpose operations (FFT and domain decomposition in the toroidal direction) which start to dominate cpu time
- With the use of field-aligned coordinates, the amount of data to be transposed will be reduced by orders of magnitude (~ $1/\rho^*$) (typically 100-1000)
- Requires major code refactoring
- Other changes envisaged:
  - Domain decomposition in the radial direction
  - Hybrid MPI/OpenMP parallelization scheme

ITER global gyrokinetic turbulence simulation: computational requirements

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  - ITER: $1 / \rho^* = \sim 1000$
- Relevant scales: resolve up to $k_\perp \rho_s \leq 1$
- 3D field solver: min 4 pts/wavelength → **60'000'000**
  - ➔ 7'000'000'000 grid cells
- Velocity space resolution: ~ 300 / cell → **18'000'000'000**
  - ➔ 2'000'000'000'000 phase space cells (or markers)
- Time until statistical steady-state: ~ 2000 a / c_s
  - ➔ ~2×10^6 time steps → **2×10^4**
- This is clearly ~~unfeasible!~~ → **feasible**
- Cost of algorithm ~ $(1 / \rho^*)^4$ → **$(1 / \rho^*)^2$**

Timeline

- 2010
  - Formulation of the equations in field-aligned coordinates
  - Field solver code module development
  - First scalability tests of the solver
  - Implementation of the solver in the ORB5 code
- 2011
  - Implementation of the solver in the GENE code
  - Parallel scalability tests
  - Review further modifications of parallelization scheme (e.g. MPI+OpenMP)
  - Start the development of a new semi-Lagrangian code, in simplified geometry
- 2012
  - ITER-size simulations of ITG turbulence
  - Scalability tests with physical system size
  - Benchmark ORB5 vs GENE
  - Simulations including more physical effects
  - Assess potential of semi-Lagrangian code vs Lagrange-PIC (ORB5) and Euler (GENE) approaches

Staff

- CRPP-funded staff
  - Laurent Villard (PI), Stephan Brunner (co-PI), Trach-Minh Tran (co-PI)
  - Ben F. McMillan (Post-Doc), Sohrab Khosh Aghdam (PhD)
- International collaborators
  - Alberto Bottino, Max-Planck IPP, Garching, Germany
  - Sébastien Jolliet, JAEA, Tokyo, Japan
- HP2C-funded staff at CRPP
  - 1 Post-Doc: Alessandro Casati, started 1st March 2010
  - 1 PhD: T. Vernay (50%); 50%: open
- Competence profile to be developed on both the physics side (turbulence, plasma physics, magnetic confinement) and the computational side (large codes, HPC, …)
- Help from and interaction with CSCS will continue (and is deeply appreciated!)
  - Porting, I/O, libraries, code profiling, diagnostics (e.g. visualization), …

Conclusion

- Thanks to this HP2C project, it is expected that we shall be in an ideal position in the scientific community of fusion plasma physics to address crucial issues related to the transport of heat, particles and momentum, and hence the quality of confinement, in ITER-like plasmas.

- By anticipating our needs in terms of increasing physical system size and physical complexity and exploring the future evolution of HPC, this project will enable us to be ready to use the next generation of HPC platforms when they become available.

- *Many thanks to Prof Thomas Schulthess for driving this wonderful HP2C initiative. Thank you for your attention!*
- *For a recent overview: X. Garbet, Y. Idomura, L. Villard, T.H. Watanabe, Nucl. Fusion **50**, 043002 (2010)*

Gyrokinetic model: basic assumptions

- Small parameter ε_g , with

characteristic frequency of perturbations

$\mathbf{E} \times \mathbf{B}$ drift velocity

perturbed density

perturbed magnetic field

Larmor radius

$$\frac{\omega}{\Omega_s} \sim \frac{k_{||}}{k_{\perp}} \sim \frac{v_E}{v_{ts}} \sim \frac{\delta n_s}{n_0} \sim \frac{B_1}{B_0} \sim \frac{\rho_s}{L_n} \sim \mathcal{O}(\epsilon_g)$$

cyclotron frequency

thermal velocity

equilibrium density

equilibrium magnetic field

characteristic length scale of equilibrium n_0

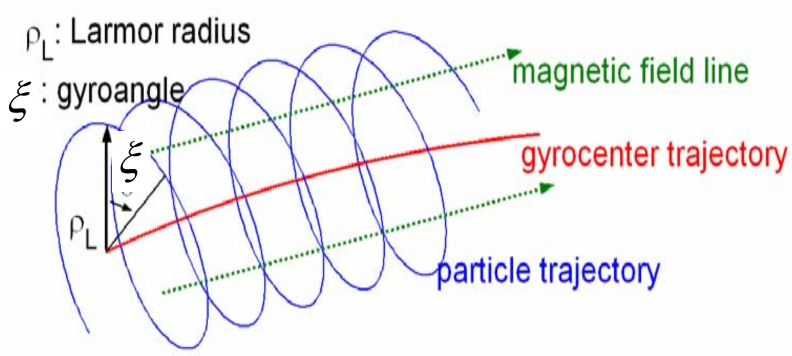
wave vector components in perpendicular and parallel directions w.r.t **B** field

- Small parameter $\epsilon_B = \rho_s / L_B$

characteristic length scale of equilibrium B

Gyrokinetic model

- Assume $\omega_{\text{turbulence}} << \omega_{\text{ion cyclotrc}}$
- Average out the fast motion of the particle around the guiding center
- Fast parallel motion, slow perpendicular motion (drifts)
- Strong anisotropy of turbulent perturbations (// vs perp to **B**)



phase space dimension reduction

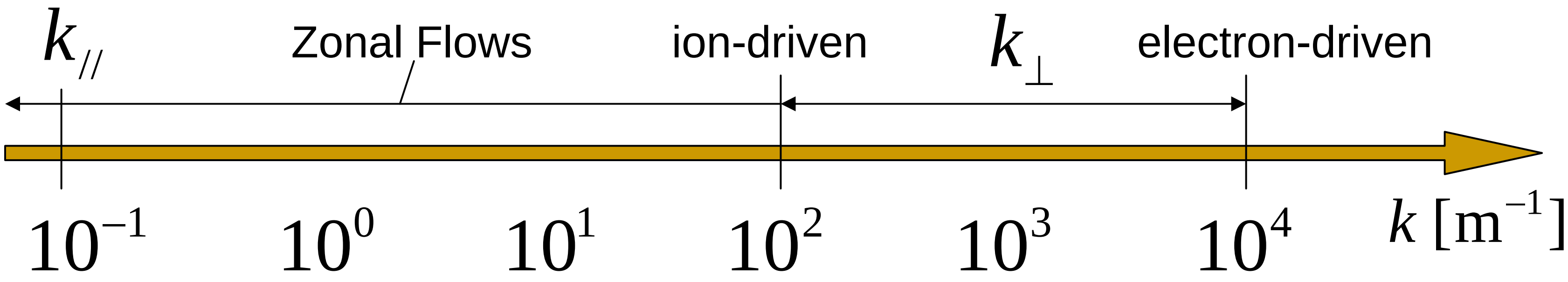
6D ***---> 5D***

$$f_s(\vec{q},\vec{p};t) \rightarrow \bar{f}_s(\bar{\vec{R}},\bar{u},\bar{\mu};t)$$

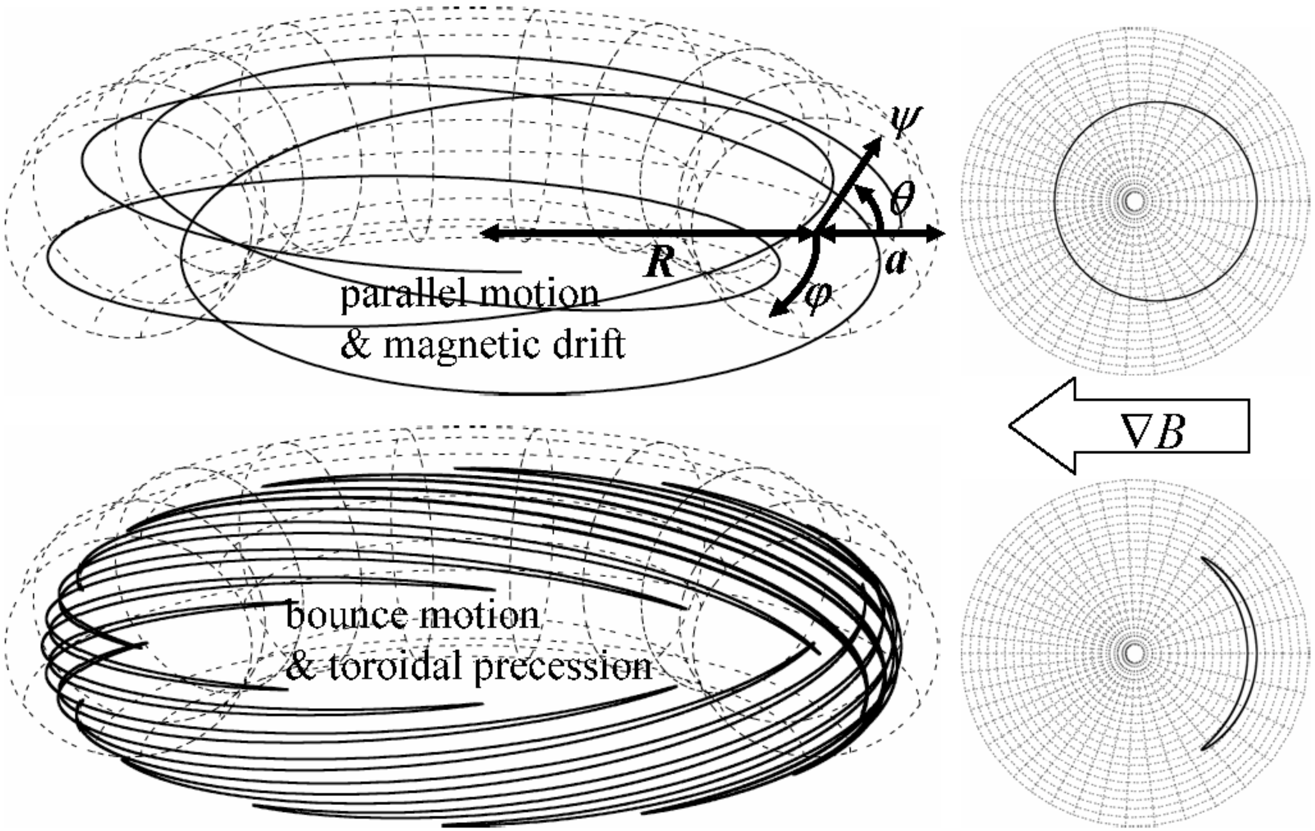
$$\vec{R} = \vec{q} - \vec{\rho}_s$$

$$u = v_{\|} + (e_s/cm_s)A_{\|}$$

$$\mu = m_s v_{\perp}^2/2B_0$$



Guiding center motion in a tokamak



"Passing" (top) and "trapped" (bottom) particle orbits: the guiding centres almost follow the equilibrium magnetic field.
Left: 3D view. Right: projection on the poloidal plane

Y. Idomura et al., C.R. Physique 7 (2006) 650-669

Gyrokinetic equations

$$\frac{D\bar{f}_s}{Dt} = \frac{\partial \bar{f}_s}{\partial t} + \frac{d\bar{\mathbf{R}}}{dt}\cdot\frac{\partial \bar{f}_s}{\partial \bar{\mathbf{R}}} + \frac{d\bar{u}}{dt}\frac{\partial \bar{f}_s}{\partial \bar{u}} = 0$$

It is an advection equation along nonlinear characteristics:

$$\frac{d\bar{\mathbf{R}}}{dt} = \bar{u}\mathbf{b} - \frac{e_s}{cm_s}\langle A_\|\rangle_{\bar{\xi}}\frac{\mathbf{B}^*}{B_\|^*} + \frac{c}{e_s B_\|^*}\mathbf{b}\times\left(e_s\nabla\langle\Psi\rangle_{\bar{\xi}} + m_s\bar{u}^2\mathbf{b}\cdot\nabla\mathbf{b} + \bar{\mu}\nabla B_0\right)$$

parallel motion (FAST)

magnetic and ExB nonlinearities

curvature and grad-B

drifts (SLOW)

parallel velocity nonlinearity

$$\frac{d\bar{u}}{dt} = -\frac{\mathbf{B}^*}{m_s B_\|^*}\cdot\left(e_s\nabla\langle\Psi\rangle_{\bar{\xi}} + \bar{\mu}\nabla B_0\right)$$

mirror term

$\frac{d\bar{\mu}}{dt} = 0$: conservation of the magnetic moment

$$\mathbf{B}^* = \mathbf{B}_0 + (B_0\bar{u}/\Omega_s)\nabla\times\mathbf{b}$$

$\Psi(\mathbf{R}, u, \mu, \xi, t) = \phi - uA_\|/c$: generalized potential

Gyrokinetic perturbed field equations

- Poisson (or: quasi-neutrality) equation, here with Boltzmann electrons, linearized ion polarization density, long wavelength approx. $\sim O(k_\perp \rho_{Li})^2$

$$\underbrace{\frac{en_0}{T_e}\left(\delta\phi - \overline{\delta\phi}\right)}_{\delta n_e} \underbrace{- \nabla_\perp \cdot \left(\frac{n_0}{B\Omega_i} \nabla_\perp \delta\phi \right)}_{\delta n_i^{pol}} = \langle \delta n_i \rangle$$

gyro-center perturbed ion density

$$\overline{\delta\phi} = \frac{\int \delta\phi \, J \, d\theta^* d\varphi}{\int J \, d\theta^* d\varphi}$$: flux-surface-averaged potential

- Ampère's law, here neglecting $\delta B_{//}$ and expanding $\sim O(k_\perp \rho_{Li})^2$

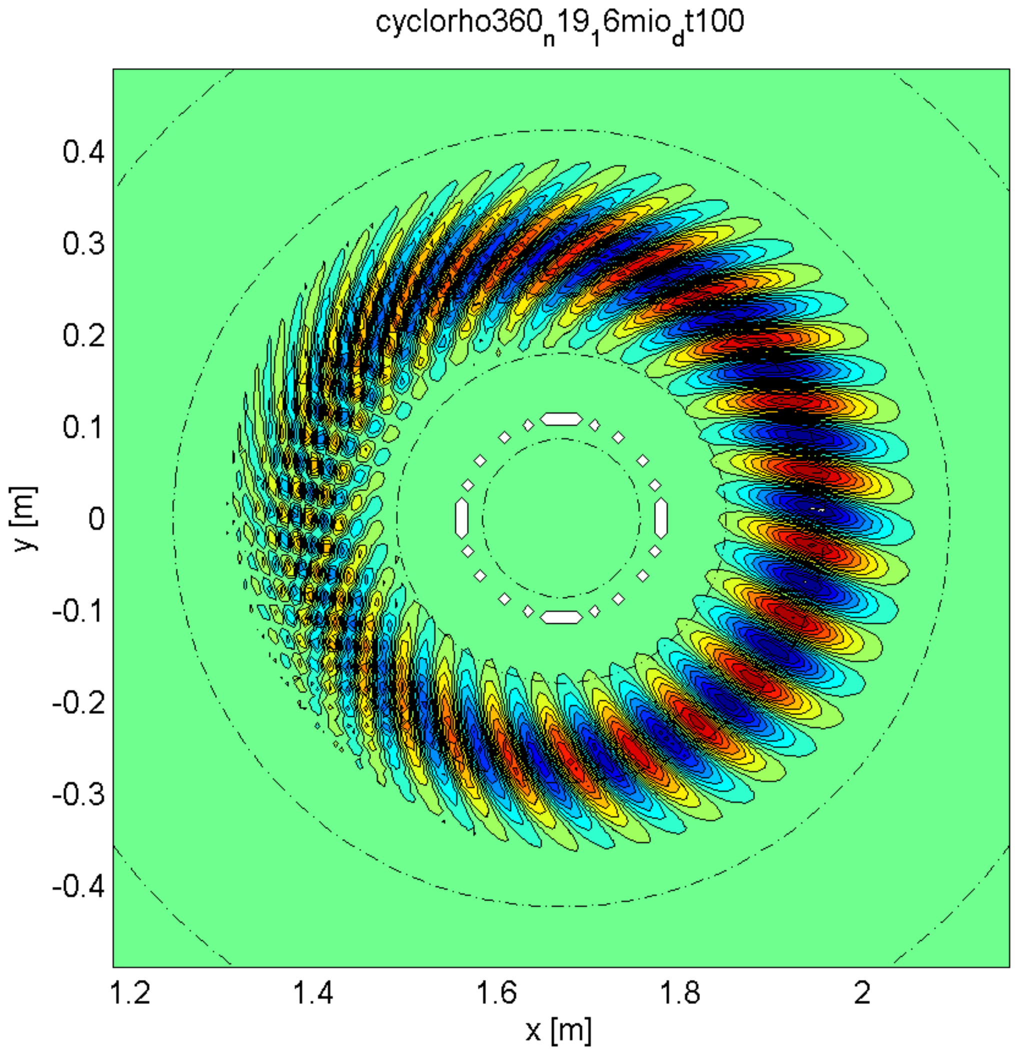
$$\left(\frac{\beta_i}{\rho_{Li}^2} + \frac{\beta_e}{\rho_{Le}^2} \right) \delta A_{//} - \nabla_\perp \cdot \left((1-\beta_i) \nabla_\perp \delta A_{//} \right) = \mu_0 \left(\langle \delta j_{//i} \rangle + \langle \delta j_{//e} \rangle \right)$$

gyro-center perturbed ion and electron currents

Integral – partial differential system of equations, inhomogeneous, linear

ITG gyrokinetic global linear simulation

Linearised δf

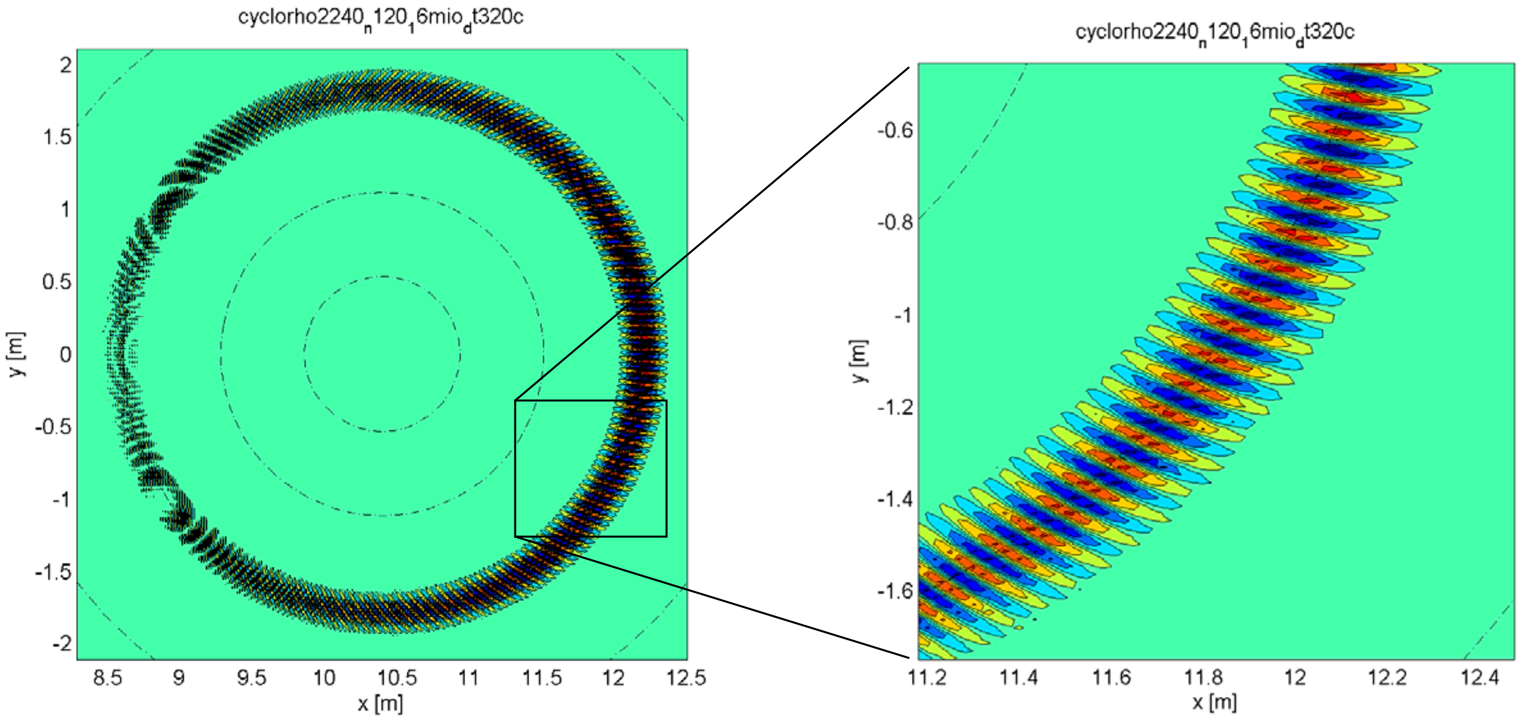


Contours of perturbed potential

- "CYCLONE" base case 1/ρ*=180. GYGLES code *[M. Fivaz et al, CPC 111 (1998) 27]*

ITG gyrokinetic global linear simulation

- ITER-size “cyclone” case $1/\rho^* = 1120$



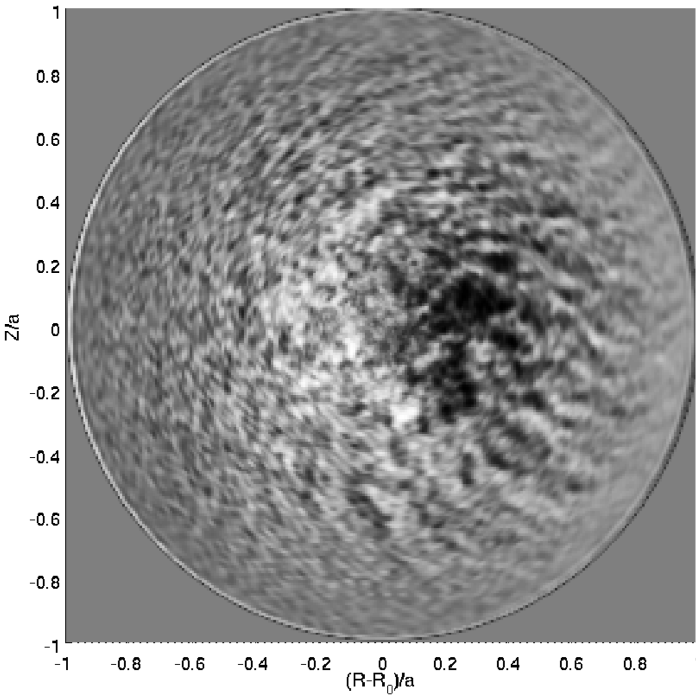
- m~170 wavelengths, solved with N_θ=64 grid points: how is it possible?

Resolving a longstanding problem: numerical noise in Lagrange-PIC simulations

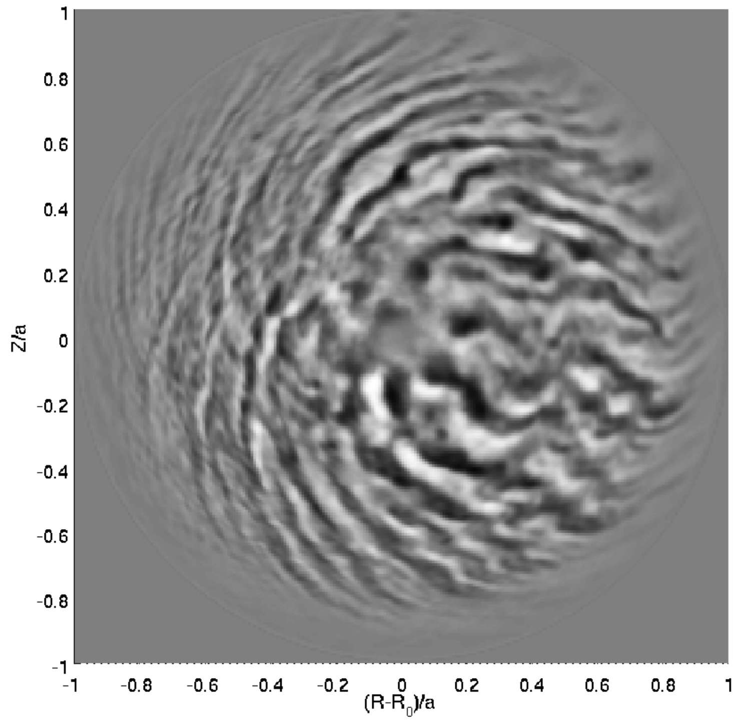
- A numerical noise control algorithm has been developed, introduced in the ORB5 code, and successfully tested

Contours of non-zonal perturbed potential $\phi - <\phi>$

Without noise control



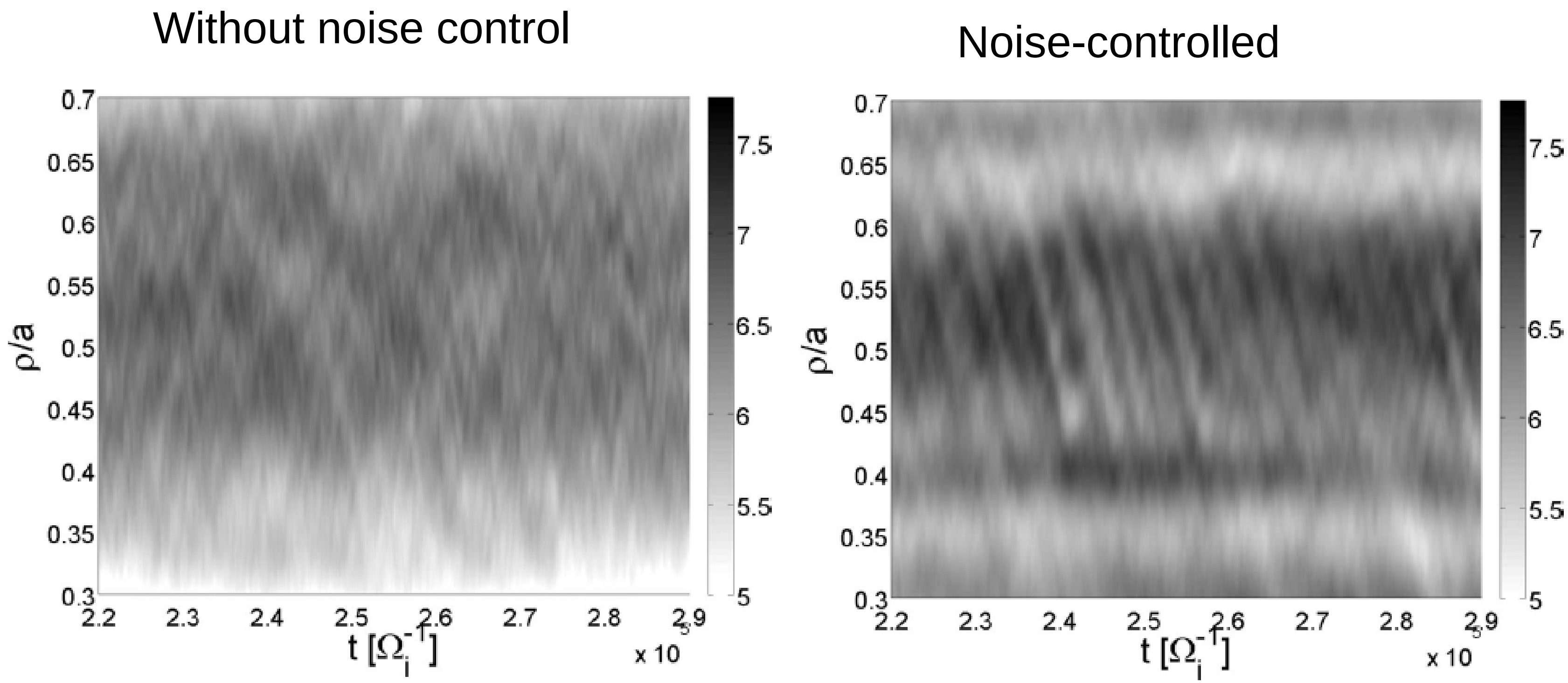
Noise-controlled



[B.F. McMillan, et al., Phys. Plasmas 15, 052308 (2008)]

Noise destroys the avalanches and bursts

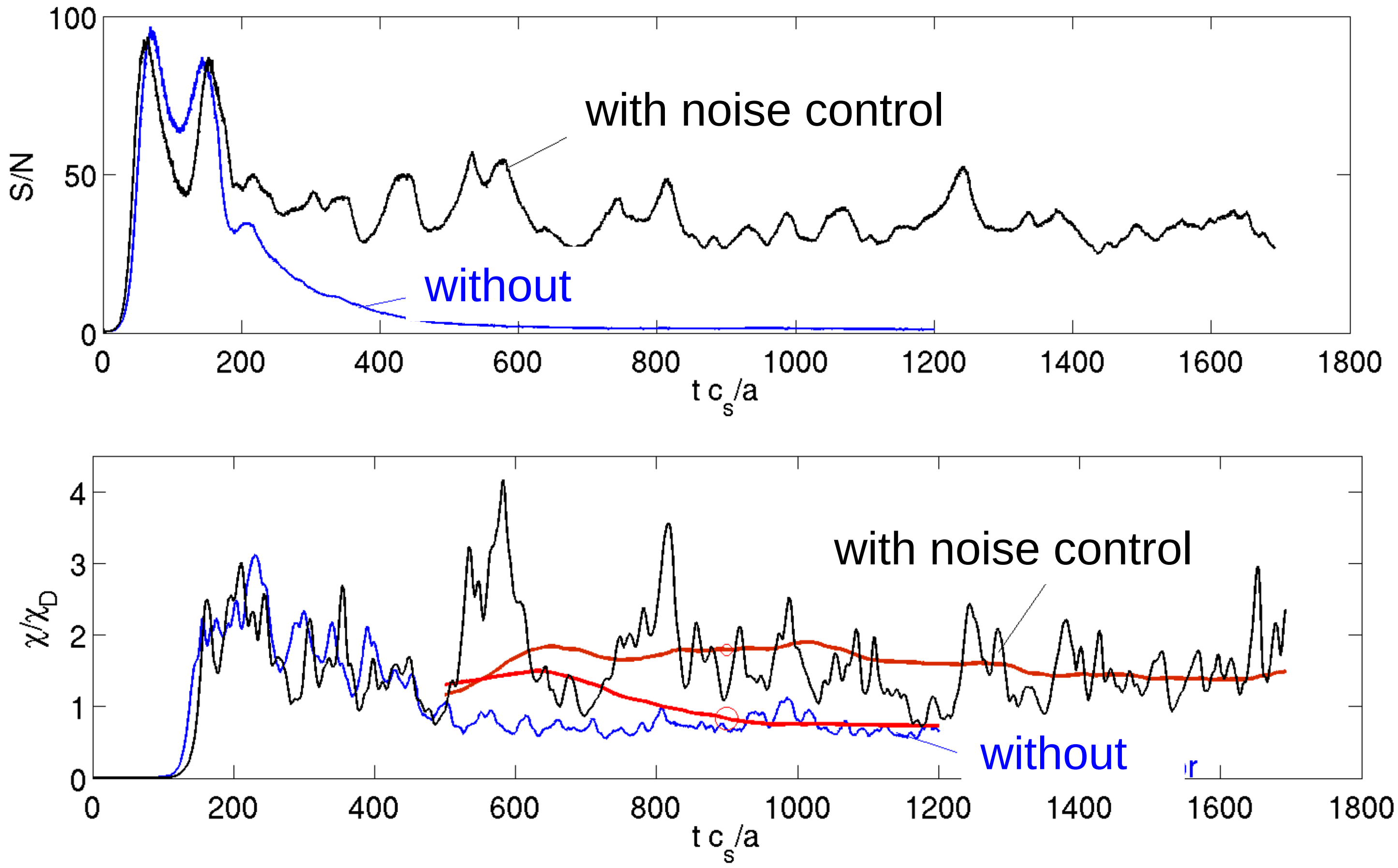
Contours of R/L_{Ti} vs time and radius



[S. Jolliet, et al., Phys. Plasmas 16, 052307 (2009)]

The development and implementation of statistical numerical noise operators in the Lagrange-PIC global code ORB5 has been successful in allowing for truly statistical-steady-state numerical simulations with sources

Noise control



[B.F. McMillan, et al., Phys. Plasmas 15, 052308 (2008)]

- When Signal/Noise ratio is lost, there is a *decrease in transport* and the *bursty nature of transport is suppressed*