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Gyrokinetic turbulence investigations with GENE - the numerics behind and some applications

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Numerical Methods for the Kinetic Equations of Plasma
September 2nd-6th, 2013
Garching

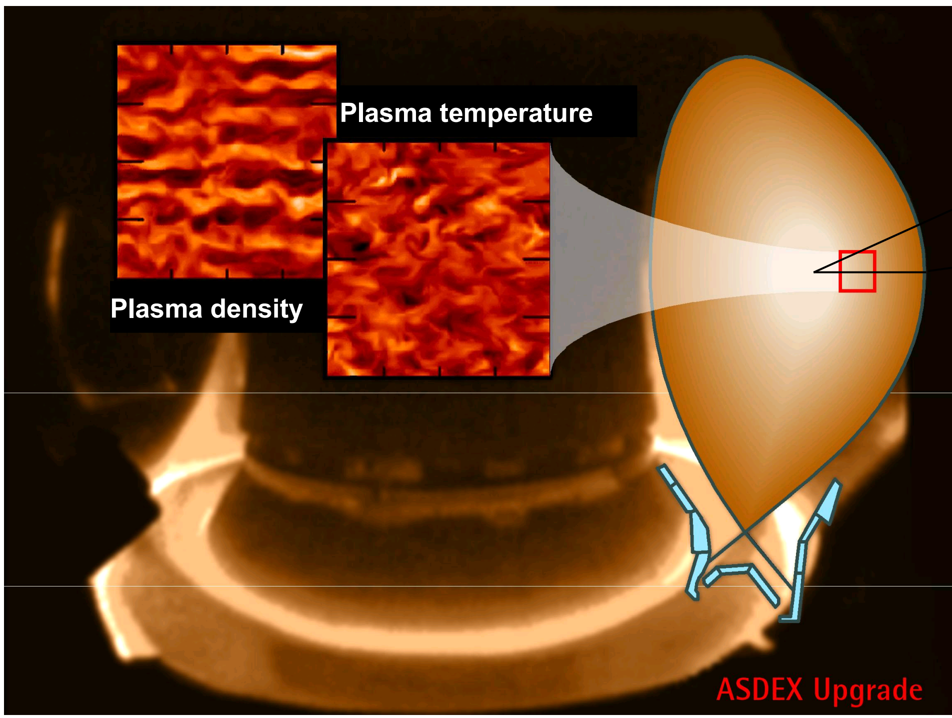
Outline

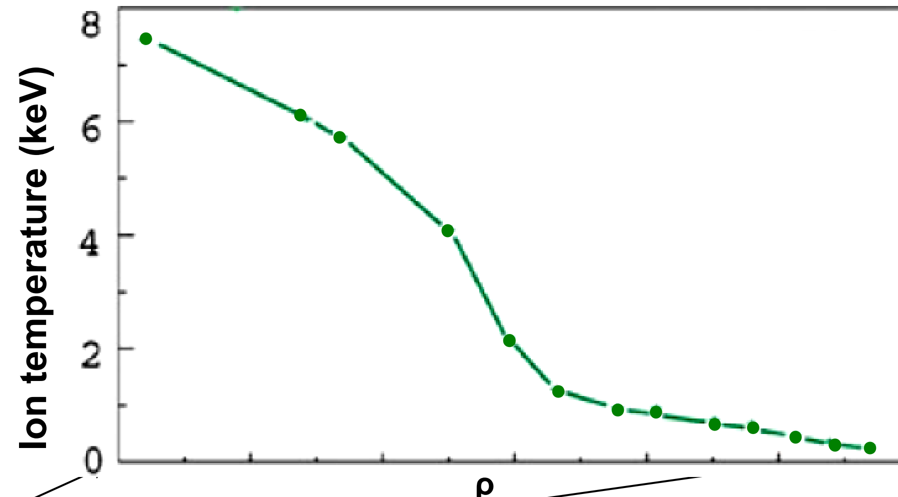
- A brief motivation for and introduction to gyrokinetic theory
- A discussion of a massively parallelized implementation
  - the plasma microturbulence code GENE
- Some selected applications
- Summary & Outlook

Plasma turbulence modeling and gyrokinetic theory in brief

Plasma microturbulence

- **Energy confinement time set by anomalous heat and particle transport → *one of the key physics problems***





- Commonly attributed to plasma microturbulence
  - Microinstabilities driven by strong temperature and density background gradients
  - Quasistationary state far from thermodynamic equilibrium

Theoretical framework: Gyrokinetic theory

Gyrokinetic Vlasov equation

$$\boxed{\frac{\partial f_\sigma}{\partial t} + \dot{\mathbf{X}} \cdot \nabla f_\sigma + \dot{\mu}\frac{\partial f_\sigma}{\partial \mu} + \dot{v}_\parallel \frac{\partial f_\sigma}{\partial v_\parallel} = 0}$$

with gyrocenter position $\mathbf{X}$

$$\dot{\mathbf{X}} = v_\parallel \mathbf{b}_0 + \frac{B_0}{B^*_{0\parallel}}\left(\frac{v_\parallel}{B_0}\bar{\mathbf{B}}_{1\perp} + \mathbf{v}_\perp\right)$$

$$\mathbf{v}_\perp \equiv \frac{c}{B_0^2}\bar{\mathbf{E}}_1 \times \mathbf{B}_0 + \frac{\mu}{m_\sigma \Omega_\sigma}\mathbf{b}_0 \times \nabla B_0 + \frac{v_\parallel^2}{\Omega_\sigma}(\nabla \times \mathbf{b})_\perp$$

parallel velocity $v_\parallel$

$$\dot{v}_\parallel = \frac{\dot{\mathbf{X}}}{m_\sigma v_\parallel} \cdot \left(q_\sigma \bar{\mathbf{E}}_1 - \mu \nabla B_0\right)$$

and magnetic moment μ

$$\dot{\mu} = 0$$

Poisson

$$\begin{aligned} -\nabla^2 \phi(\mathbf{x}) &= 4\pi \sum_\sigma q_\sigma n_\sigma \\ &= 4\pi \sum_\sigma q_\sigma \int \delta(\mathbf{X} + \mathbf{r} - \mathbf{x}) T^* f_\sigma \frac{B^*_{0\parallel}}{m_\sigma} \mathrm{d}^3 X \mathrm{d}v_\parallel \mathrm{d}\mu \mathrm{d}\theta \end{aligned}$$

Ampère’s

$$\begin{aligned} -\nabla^2 A_\parallel(\mathbf{x}) &= \frac{4\pi}{c} j_\parallel \\ &= \frac{4\pi}{c} \sum_\sigma q_\sigma \int \delta(\mathbf{X} + \mathbf{r} - \mathbf{x}) v_\parallel T^* f_\sigma \frac{B^*_{0\parallel}}{m_\sigma} \mathrm{d}^3 X \mathrm{d}v_\parallel \mathrm{d}\mu \mathrm{d}\theta \end{aligned}$$

Nonlinear, 5-dimensional, partial integro-differential system of equations to be solved!

Major theoretical speedups

G.Hammett

relative to original Vlasov/pre-Maxwell system on a naïve grid, for ITER $\rho_* = \rho/a \sim 1/1000$

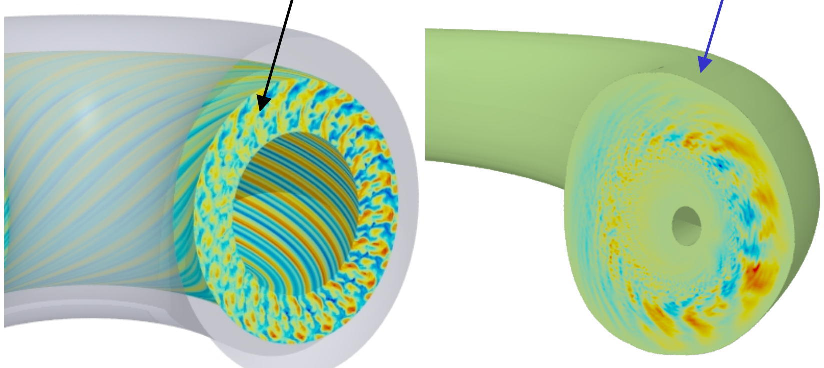
- Nonlinear gyrokinetic equations
  - eliminate plasma frequency: $\omega_{pe}/\Omega_i \sim m_i/m_e$ x10^3
  - eliminate Debye length scale: $(\rho_i/\lambda_{De})^3 \sim (m_i/m_e)^{3/2}$ x10^5
  - average over fast ion gyration: $\Omega_i/\omega \sim 1/\rho_*$ x10^3
- Field-aligned coordinates
  - adapt to elongated structure of turbulent eddies: $\Delta_\parallel/\Delta_\perp \sim 1/\rho_*$ x10^3
- Reduced simulation volume
  - reduce toroidal mode numbers (i.e., 1/15 of toroidal direction) x15
  - $L_r \sim a/6 \sim 160$ r ~ 10 correlation lengths x6
- **Total speedup x10^{16}**
- For comparison: Massively parallel computers (1984-2009) x10^7

The gyrokinetic Vlasov code GENE

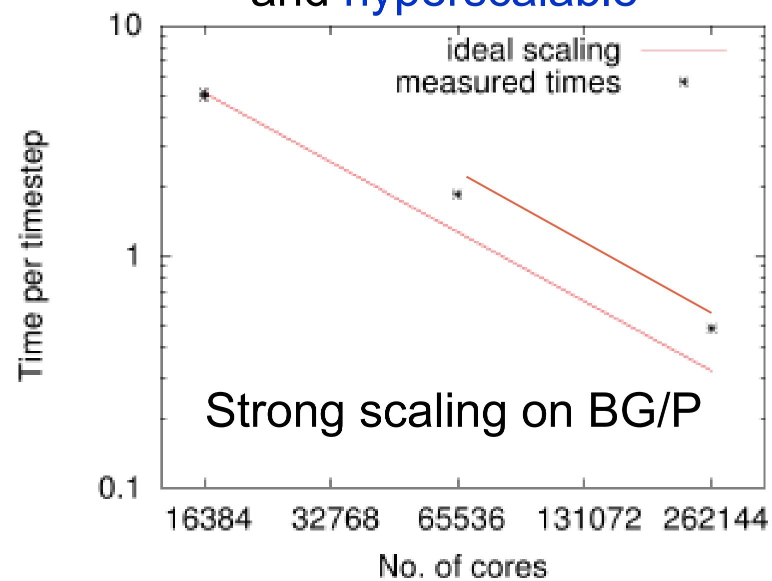
The gyrokinetic code GENE (gene.rzg.mpg.de)

GENE is a physically comprehensive Vlasov code:

- allows for kinetic electrons & electromagnetic fluctuations, collisions, and external ExB shear flows
- is coupled to various MHD codes and the transport code TRINITY
- can be used as **initial value** or **eigenvalue** solver
- supports **local** (flux-tube) and **global** (full-torus), gradient- and flux-driven simulations



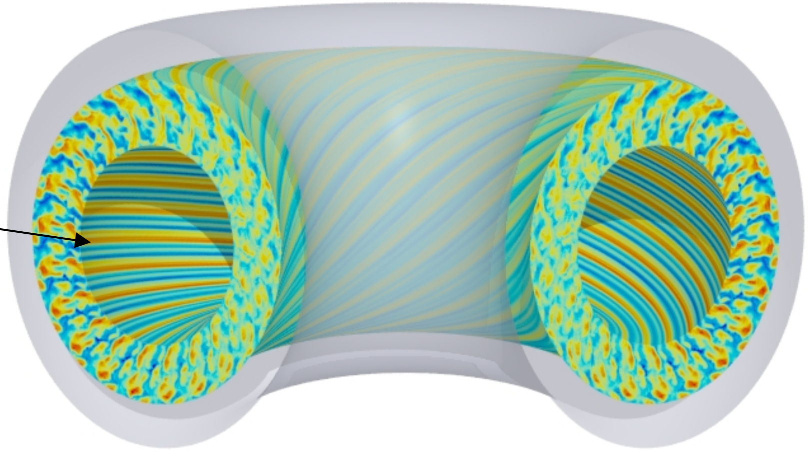
GENE is well benchmarked and hyperscalable



Concepts used within GENE for speed-up

- *field-aligned* (Clebsch-type) coordinate system to exploit the high anisotropy of plasma turbulence;

  parallel (z) derivatives can be taken small compared to perpendicular (x,y) ones(!)



- *δf-splitting:*
  Apply same approach as in the derivation of the GKE and split the distribution function

  $$f = F_0 + \delta f$$

  where
  F_0: stationary background,
  here: local Maxwellian
  δf: fluctuating part with $\delta f/F_0 \ll 1$

Lowest-order nonlinearity kept

$$\sim \frac{\partial \bar{\phi}_1}{\partial x}\frac{\partial f_{1\sigma}}{\partial y} - \frac{\partial \bar{\phi}_1}{\partial y}\frac{\partial f_{1\sigma}}{\partial x}$$

next order

$$-\left\{\frac{q_\sigma}{m_\sigma}\nabla_\parallel \bar{\phi}_1 + c\frac{B_0}{B^*_{0\parallel}} v_\parallel \frac{1}{B_0^2}\left(\mathbf{B}_0 \times \frac{\nabla B_0}{B_0}\right)\cdot \nabla \bar{\phi}_1\right\}\frac{\partial f_{1\sigma}}{\partial v_\parallel}$$

can be switched on for testing

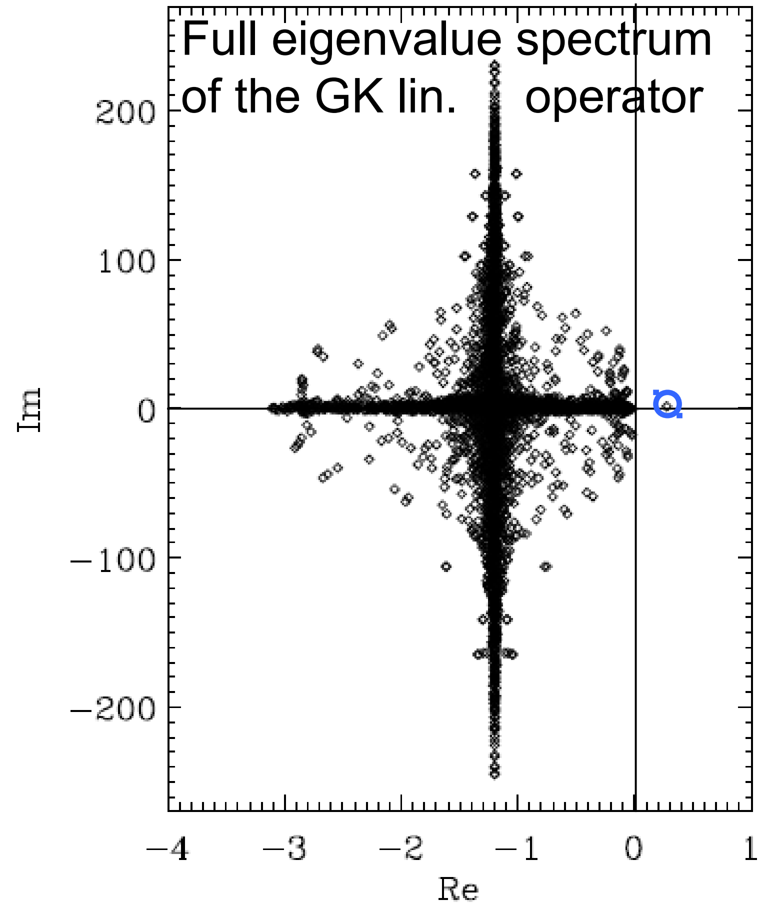
(electrostatic version)

Numerical methods – time scheme I

- *Method of Lines:*
  - turn PDEs into ODEs by discretizing the spatial derivative first
  - solve for the continuous time coordinate

- *Time Solver:*

  - **Linear system:** $$\frac{\partial g}{\partial t} = \mathcal{L}[g]$$
    - *Iterative eigenvalue solver* based on PETSc/SLEPc/Scalapack lib's
      → solve for largest abs/re/im eigenvalues
      → gain insights in linear stability/physics
    - *Explicit Runge-Kutta* (ERK) schemes



Numerical methods – time scheme II

- *Time Solver:*

- (Full) **Nonlinear system:**

$$\frac{\partial g}{\partial t} = \mathcal{V}[g] = Z + \mathcal{L}[g] + \mathcal{N}[g]$$

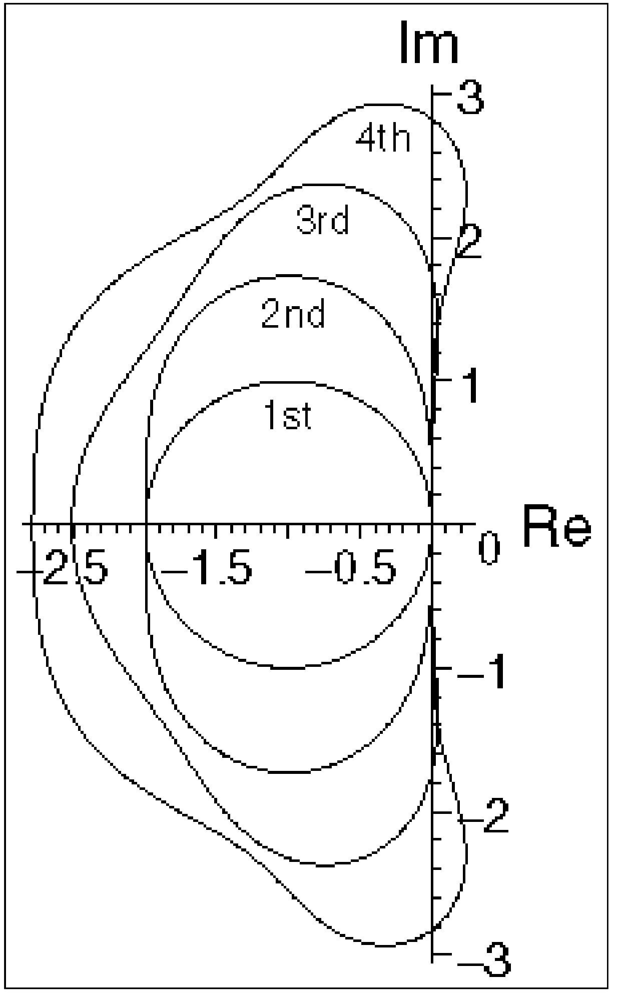
- Several *ERK*-methods, e.g. 4th order

$$g_{n+1} = g_n + \frac{\Delta t}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)$$

$$\begin{aligned} k_1 &= \mathcal{V}(t_n, g_n), \\ k_2 &= \mathcal{V}(t_n + \Delta t/2, g_n + k_1 \Delta t/2), \\ k_3 &= \mathcal{V}(t_n + \Delta t/2, g_n + k_2 \Delta t/2), \\ k_4 &= \mathcal{V}(t_n + \Delta t, g_n + k_3 \Delta t). \end{aligned}$$

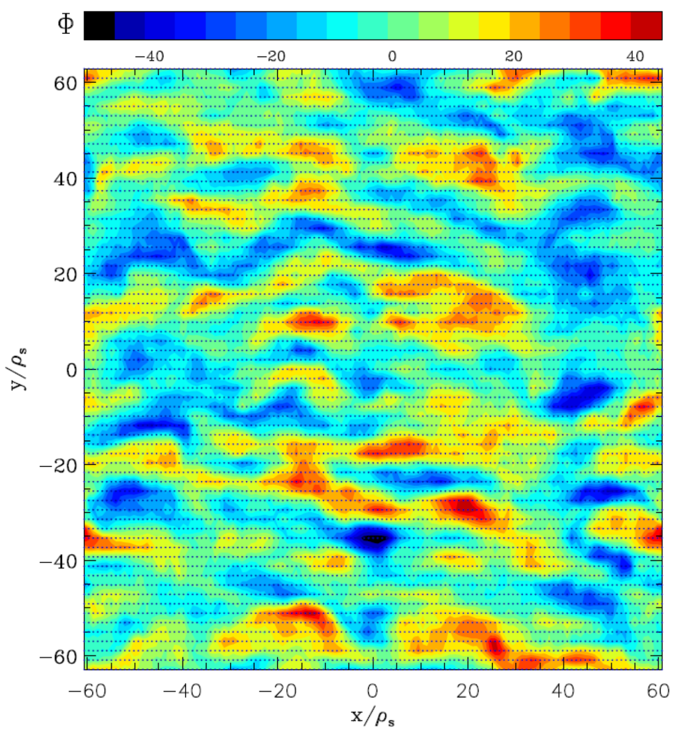
- Optimum linear time step can be precomputed using iterative EV-Solver
- Adaptive CFL time step adaption for nonlinearity

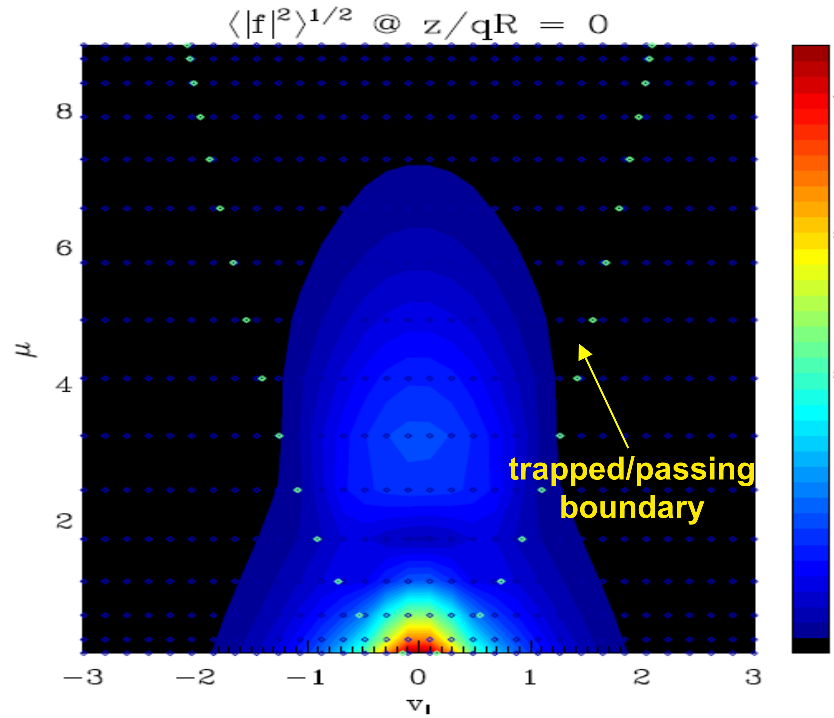
Linear stability regions for low-order RK-schemes



Phase space discretization

- GENE is a *Eulerian* code; thus solving the 5D (δf-splitted) distribution function on a fixed grid in (**x**, $v_\parallel$,μ)





• radial direction x:	equidistant grid (either configuration or Fourier space)
• toroidal direction y:	equidistant grid in Fourier space
• parallel direction z:	equidistant grid points
• $v_\parallel$-velocity space:	equidistant grid
• μ-velocity space:	Gauss-Legendre or Gauss-Laguerre knots

Phase space discretization – finite differences

$$\boxed{\frac{\partial f_\sigma}{\partial t} + \dot{\mathbf{X}} \cdot \nabla f_\sigma + \dot{v}_\parallel \frac{\partial f_\sigma}{\partial v_\parallel} = 0}$$

$$\frac{\partial f}{\partial z} \rightarrow \frac{f\left(z_{(k-2)}\right) - 8f\left(z_{(k-1)}\right) + 8f\left(z_{(k+1)}\right) - f\left(z_{(k+2)}\right)}{12\Delta z}$$

- 4th order finite differences are basic choice
- however, the more elaborate Arakawa-scheme is employed, if possible [A. Arakawa, JCP 135, 103 (1997), reprint]

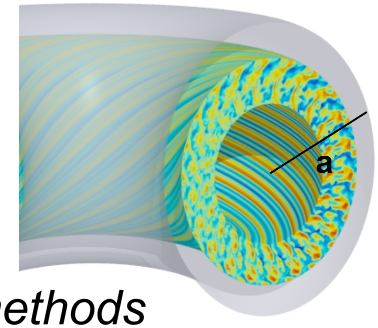
Exception:

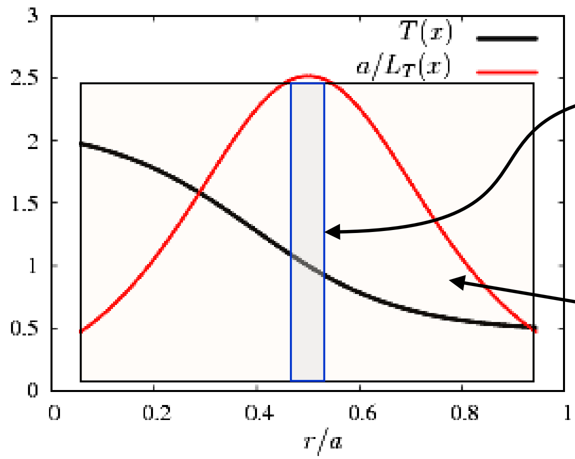
spectral methods are employed in the

- y direction - always
- x direction - depends on the type of operation (local/global)

Local vs. global GENE

- **Local:** in the radial direction
  - Simulation domain small compared to machine size; thus, *constant* temperatures/densities and *fixed* gradients
  - Periodic boundary conditions; allows application of *spectral methods*

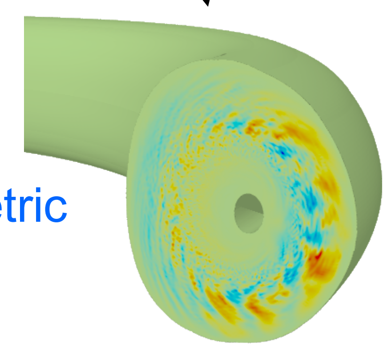




Local sim. domain

$\rho^* = \rho_s/a \ll 1$

Global sim. domain



- **Global:** adding nonlocal features in the *radial* direction
  - Consider full temperature & density profiles; radially varying metric
  - Dirichlet or v. Neumann boundary conditions
  - Heat sources & sinks

Local vs. global GENE – numerical point of view

Local approach:

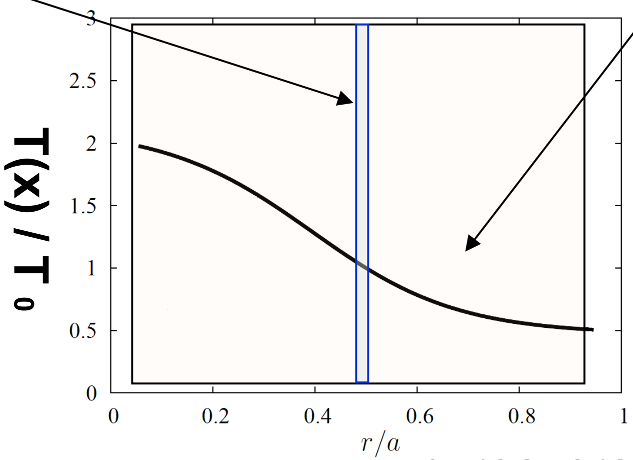
Spectral methods

- derivatives:

$$\frac{\partial f}{\partial x} \rightarrow \mathrm{i}k_x f(k_x)$$

- Gyroaverage & field operators can be given analytically:

$$\langle \phi(\mathbf{x}+\mathbf{r}) \rangle = \sum_{\mathbf{k}_\perp} J_0(k_\perp \rho)\phi(\mathbf{k}_\perp, z)\mathrm{e}^{\mathrm{i}\mathbf{k}_\perp \mathbf{x}}$$



Global approach:

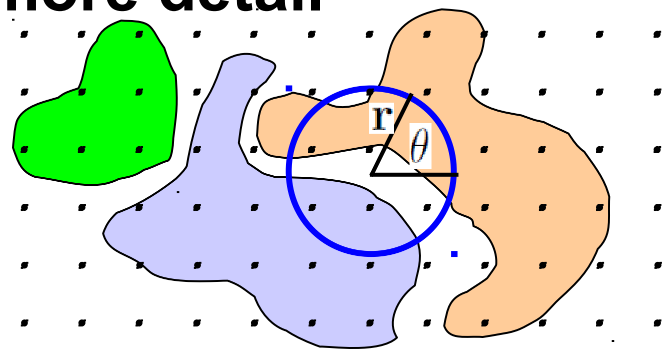
- derivatives: finite difference scheme, typically 4th order
- Use interpolation schemes for gyroaverage & field operators

$$\langle \phi_1(\mathbf{X}+\mathbf{r}) \rangle = \sum_{k_y} \mathrm{e}^{\mathrm{i}k_y Y} \mathcal{G}(X, k_y, z, \mu) \cdot \phi_1(X, k_y, z)$$

with gyromatrix $\mathcal{G}(X, k_y, z, \mu)$

Gyro-averaging procedure in more detail

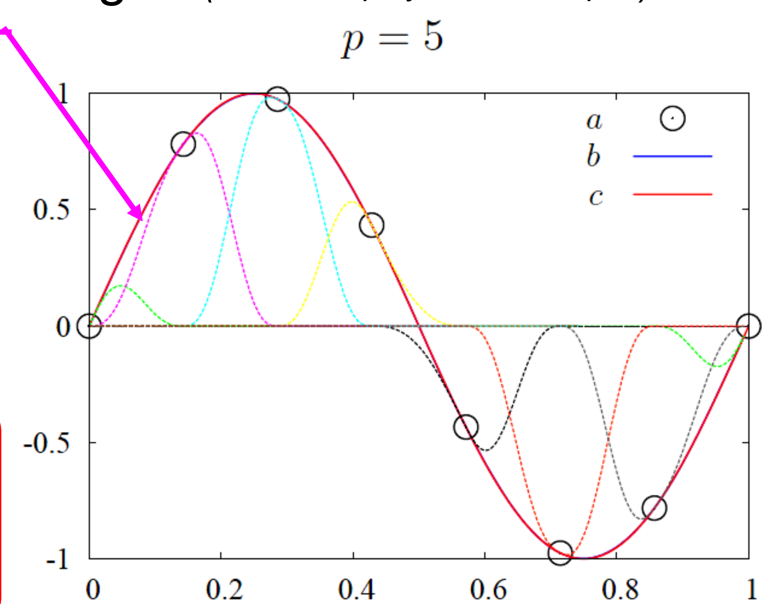
$$\boxed{\bar{f}(\mathbf{x}) \equiv \frac{1}{2\pi}\oint d\theta\, f(\mathbf{x}+\mathbf{r}(\theta))}$$



- discretize gyro-angle integration
- coordinate transform
- interpolation between grid-cells required (!)
  - here: 1-dimensional problem (y remains in Fourier space)
  - use "finite-elements" which allows easy extraction of gyro-averaged quantities on original grid *(~ Hermite polynomial interpol.)*

$$f(x) = \mathbf{\Lambda}(x)\cdot\mathbf{f} = \sum_{m=0}^{(p-1)/2} \mathbf{P}_m(x)\mathcal{D}^m\mathbf{f}$$

$$\frac{\partial^u}{\partial x^u}P_{n,m}(x)\bigg|_{x=x_{(i)}} = \delta_{in}\delta_{um}$$



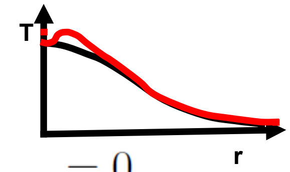
Gyromatrix is constructed at initialization only:

$$\mathcal{G}_{in}(k_y,z,\mu) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\Lambda_n(x_{(i)}+r^x)\,e^{ik_y r^y}$$

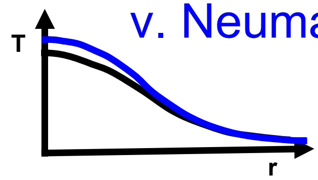
$$\bar{\mathbf{f}}(k_y,z,\mu) = \mathcal{G}(k_y,z,\mu)\cdot\mathbf{f}(k_y,z)$$

Boundary conditions - overview

radial direction x: local: periodic
global: Dirichlet $f(x, y, z)|_{x\in\mathcal{B}} = 0$

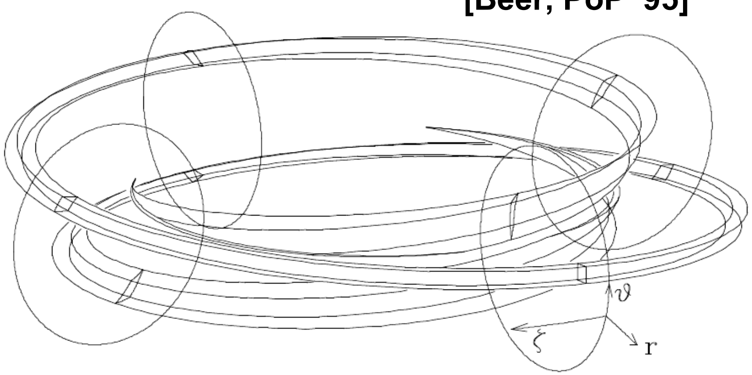


v. Neumann $\partial_x f(x, k_y = 0, z)|_{x\in\mathcal{B}} = 0$



toroidal direction y: periodic

[Beer, PoP '95]



parallel direction z: quasi-periodic

$$f(x, k_y, z + L_z) = f(x, k_y, z)\exp\left(-2\pi i n_0 q(x) j\right)$$

magnetic shear tilts the simulation box → phase factor

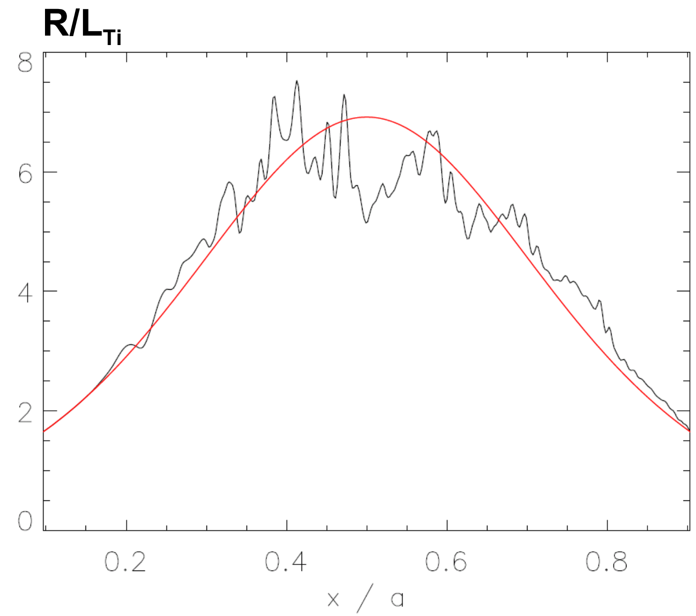
$v_{||}$-velocity space: Dirichlet

μ-velocity space: not required (if collisionless)

Sources/sink models in GENE

- **Localized** heat source *[Görler et al., JCP '11]*

- Full-domain, **radially dep. Krook-type heat source/sink** in *whole* domain *[Lapillonne et al.]*



$$\frac{\mathrm{d}g_{1j}}{\mathrm{d}t} = \mathcal{S}_{\mathrm{KH}} = -\gamma_{\mathrm{KH}} \left[\left\langle f_{1j}^{\mathrm{symm}} \right\rangle_{\mathrm{FS}} - \left\langle F_{0j} \right\rangle_{\mathrm{FS}} \frac{\left\langle \int \mathrm{d}^3 v \left\langle f_{1j}^{\mathrm{symm}} \right\rangle_{\mathrm{FS}} \right\rangle_{\mathrm{FS}}}{\left\langle \int \mathrm{d}^3 v \left\langle F_{0j} \right\rangle_{\mathrm{FS}} \right\rangle_{\mathrm{FS}}} \right]$$

$$f_{1j}^{\mathrm{symm}} \equiv f_{1j}(\mathbf{X}, \left| v_\parallel \right|, \mu) \equiv (f_{1j}(\mathbf{X}, v_\parallel, \mu) + f_{1j}(\mathbf{X}, -v_\parallel, \mu))/2$$

(density and parallel momentum are unaffected)

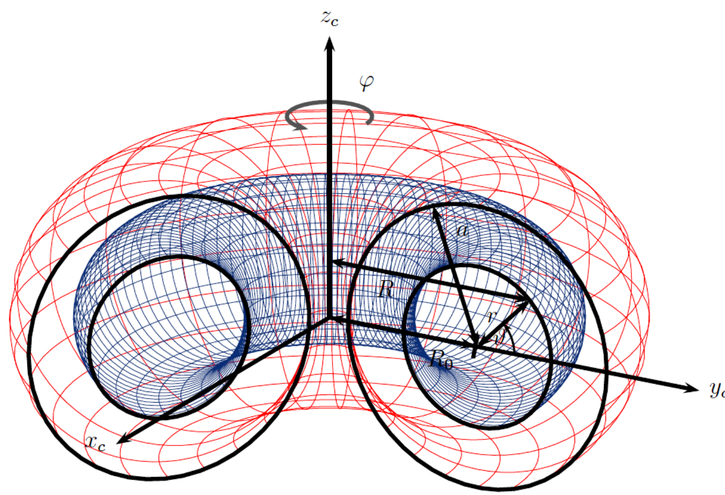
- Required for gradient-driven kinetic electrons sims: **radially dep. Krook-type particle source** *[Told et al.]*

$$\frac{\mathrm{d}g_j}{\mathrm{d}t} = \mathcal{S}_{\mathrm{KP}}^{(1)} = -\gamma_{\mathrm{KP}} \left[\left\langle f_{1j}^{\mathrm{symm}} \right\rangle_{\mathrm{FS}} - \left\langle F_{0j} \right\rangle_{\mathrm{FS}} \frac{\sum_s q_s \left\langle \int \mathrm{d}^3 v \left\langle f_{1s}^{\mathrm{symm}} \right\rangle_{\mathrm{FS}} \right\rangle_{\mathrm{FS}} / n_{\mathrm{spec}}}{q_j \left\langle \int \mathrm{d}^3 v \left\langle F_{0j} \right\rangle_{\mathrm{FS}} \right\rangle_{\mathrm{FS}}} \right]$$

additional heat input is compensated by dynamical γ_{KH} adaptation

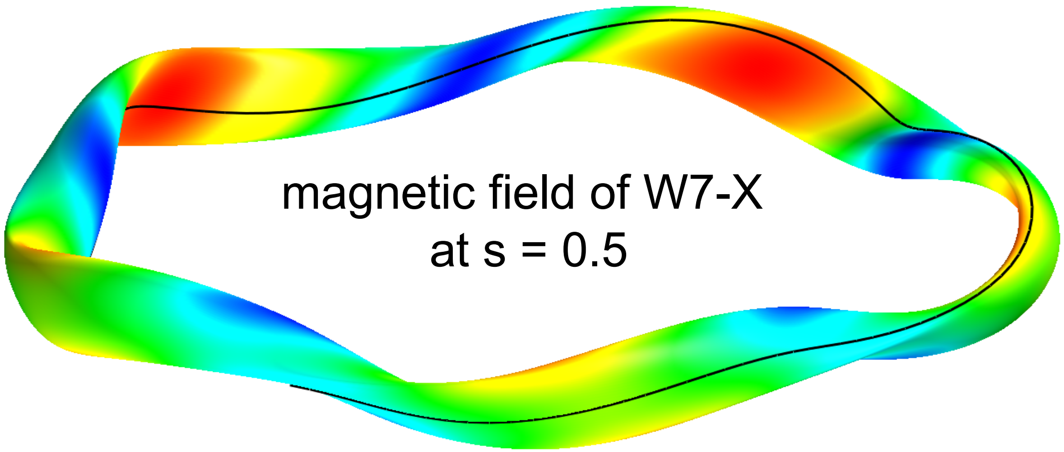
Geometry

- arbitrary flux-surface shapes can be considered as long as the metric $g = (g^{ij}) = (\nabla u^i \cdot \nabla u^j)$ translating to fluxtube coordinates is provided.
  Example: $$\frac{1}{B_0^2}(\mathbf{B}_0 \times \nabla\zeta)\cdot\nabla = \frac{1}{\mathcal{C}}\frac{g^{1i}g^{2j} - g^{2i}g^{1j}}{\gamma_1}\partial_i\zeta\partial_j$$
- internally implemented:
  s-α, Miller (local), circular concentric flux surfaces (local & global)



- Others – even non-axisymmetric ones - can be read via interfaces to TRACER/GIST (field line tracer) and the equilibrium code CHEASE

The full-surface version



Non-axisymmetric equilibria → non-negligible B variations along the flux surface

Approach:

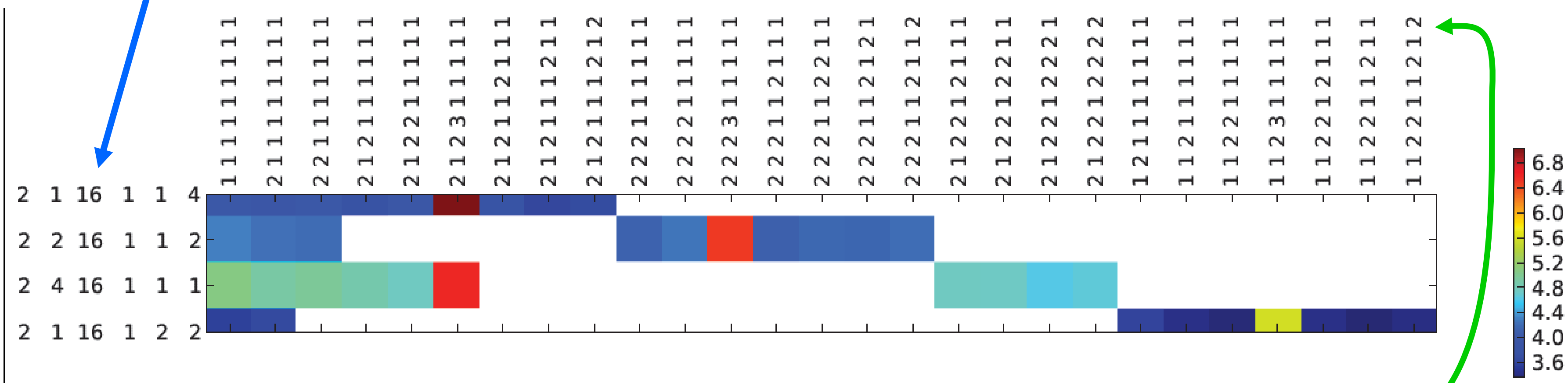
- utilize existing numerical scheme from radially global version
- switch indices (radial ↔ 'toroidal')
- Adapt boundary conditions – flux surface quantities still periodic

Ultimate goal:

- Combine radially and toroidally global version; abandon remaining spectral methods; requires new gyroaveraging schemes etc.

Code parallelization and optimization

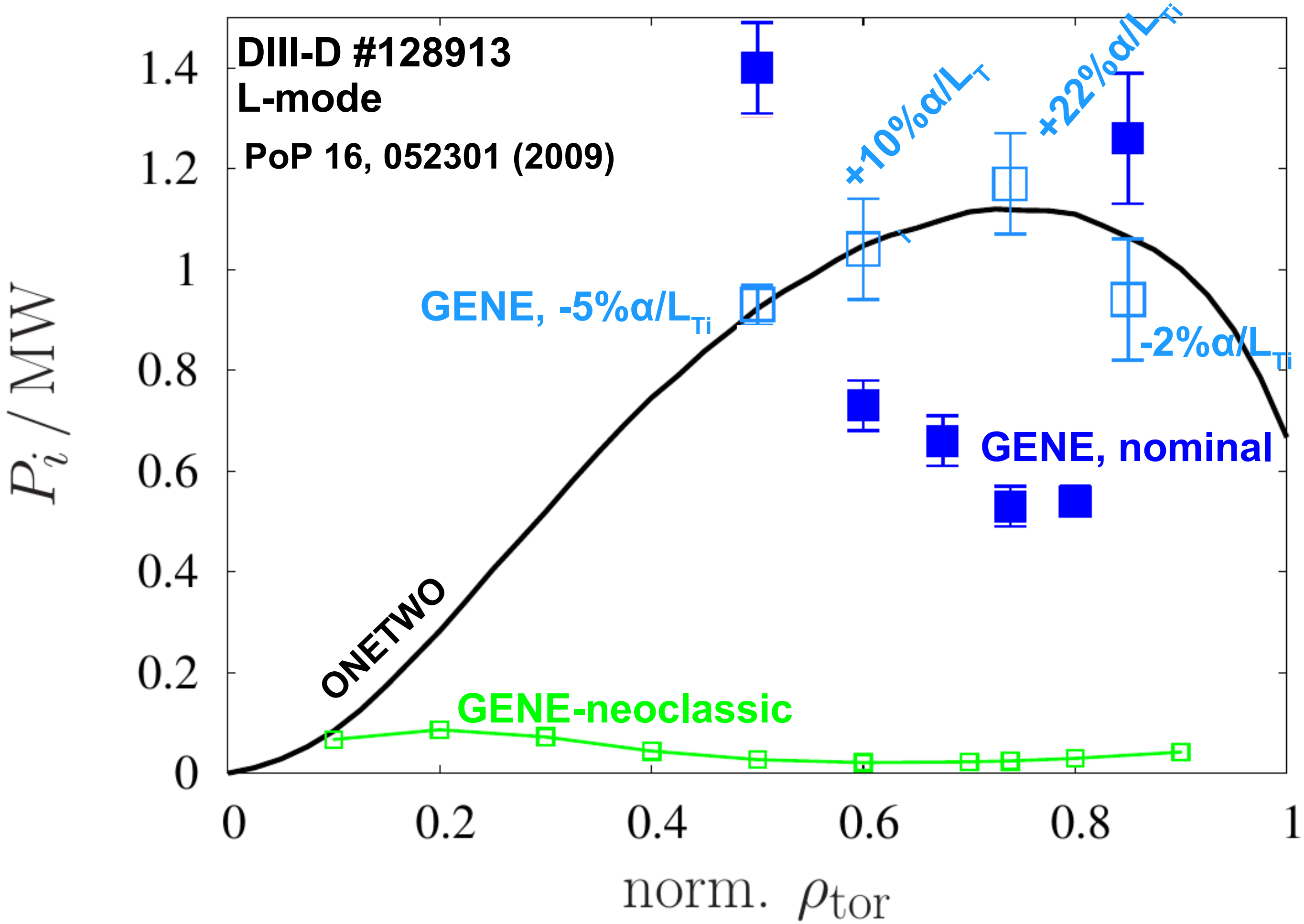
- MPI (message passing interface) parallelization available in all phase space directions + species; however, difficult to estimate interference, especially on large numbers of processors (>1k)
  → automatic comparison at code initialization



- For better utilization of different architectures (different cache sizes!), strip mining techniques and message block adaption
  → FFTW-like performance optimization during initialization

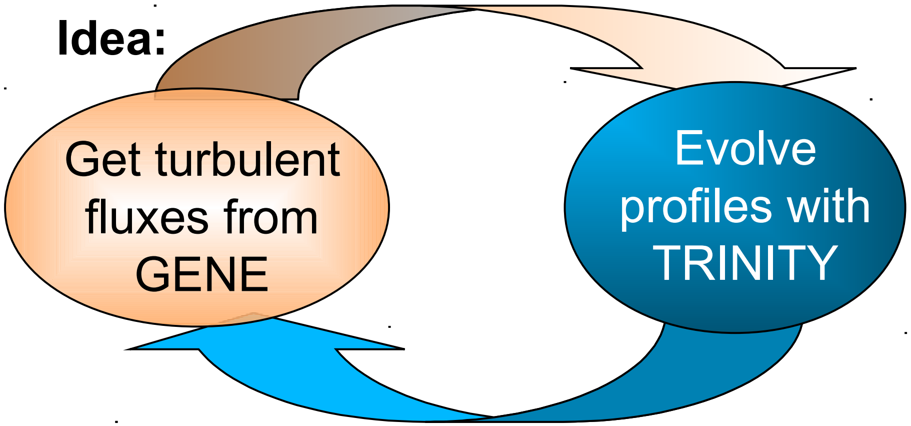
Applications

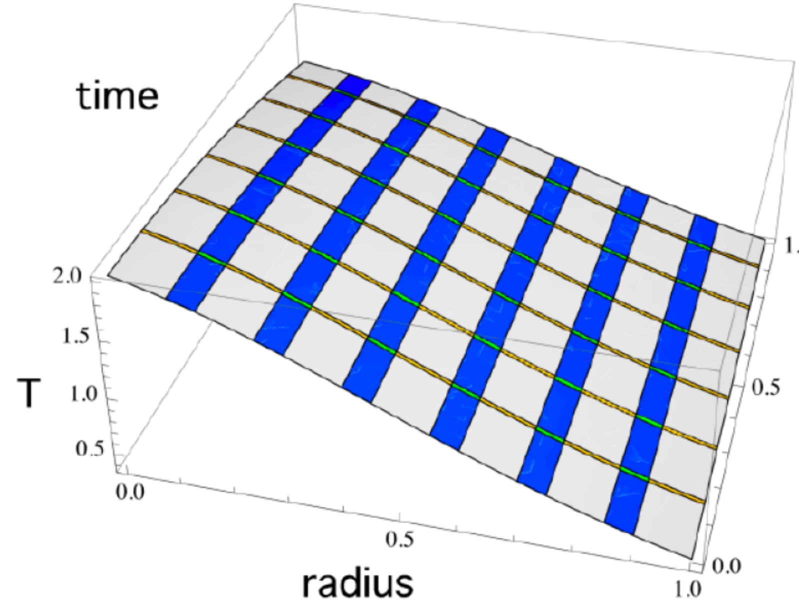
Comparison: local GENE vs. experiment

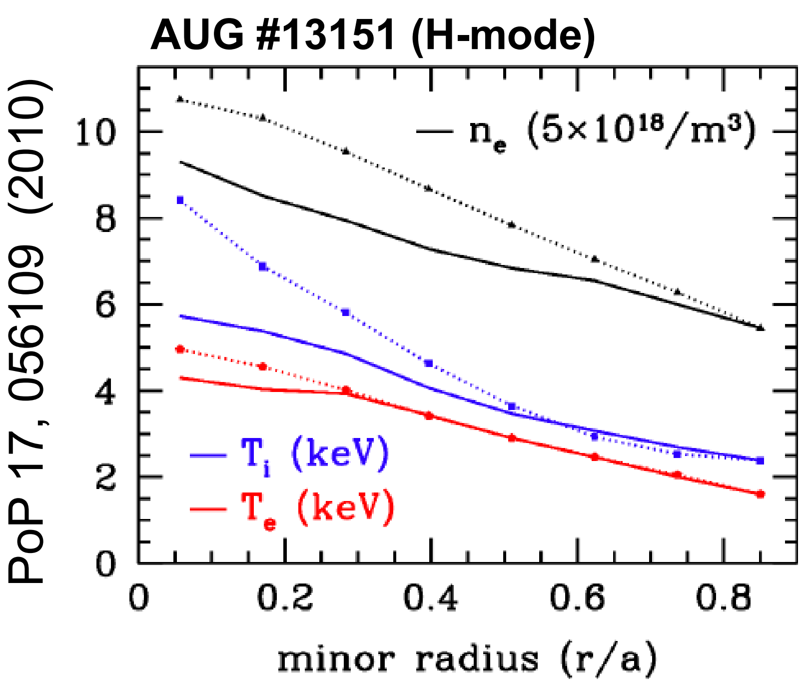


- Simulations: electromagnetic, collisions, ExB flow shear, efit equilibrium, ...
- Heat transfer rate can be matched with ion temperature gradient variations within the error bars → general problem: gradient-driven sims rely on accurate exp. data input

GENE and TRINITY coupling







- Converged results of this turbulence code/transport solver software suite differ on avg. by ~12% from the ASTRA profiles
- Possible explanations:
  - *flow shear*
  - *Here, uncertainties in the q profile*
- ***Coupling to global code?***
- ***Gyrokinetic LES methods?*** [P. Morel et al., PoP 2011, 2012]

Why global?

- Cover a larger radial domain (instead of using several flux tubes)

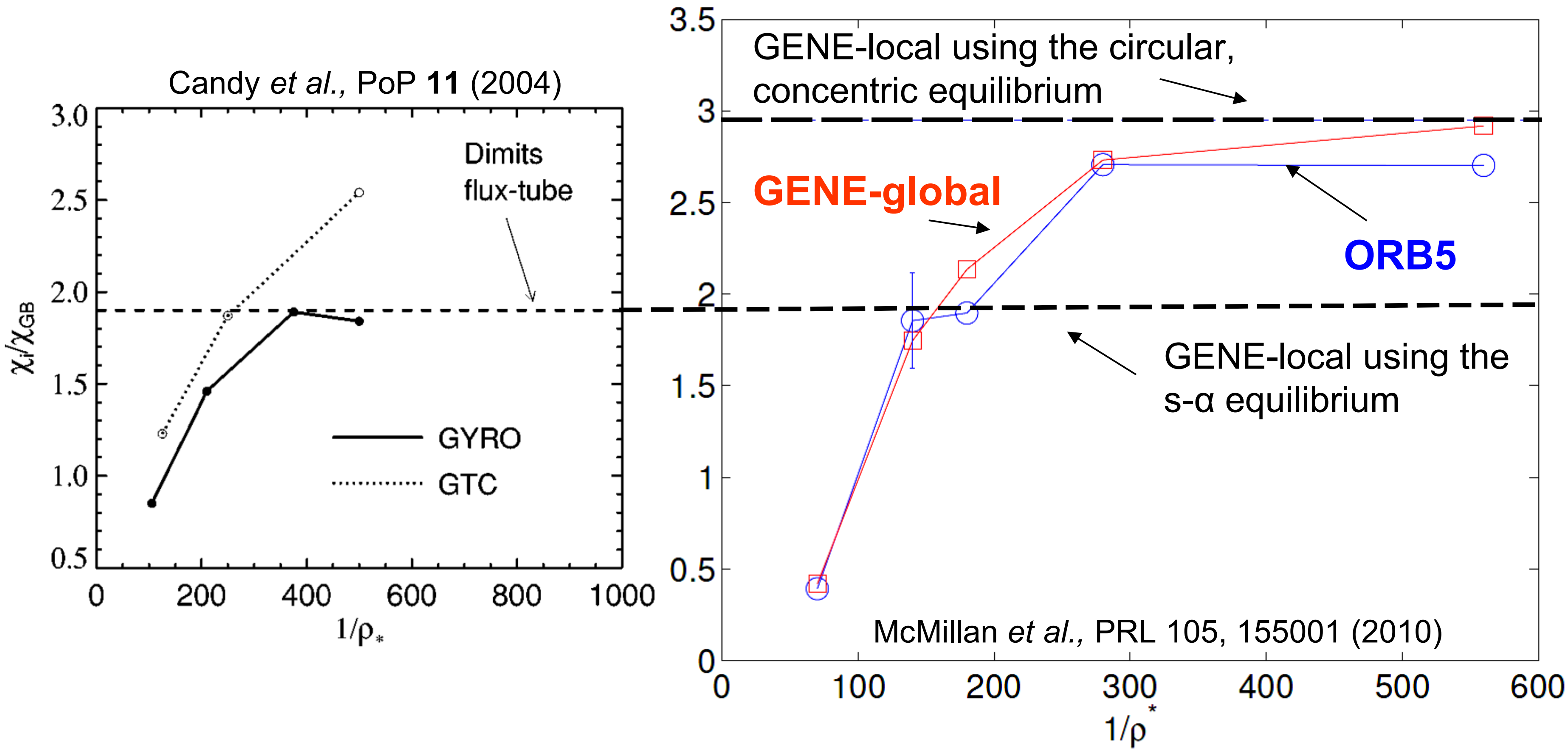
- Check validity of local simulations:
  - When do meso-/large scale events, i.e. avalanches or turbulence spreading, occur?

  - Do they affect the transport scaling?
    - "machine-size" events: Bohm scaling $\chi_B = cT/eB$
    - Gyroradius scale turbulence: Gyro-Bohm scaling $\chi_{\mathrm{GB}} = \rho^* \chi_B$

  - Re-assess earlier results by [Z. Lin et al., PRL, 2002] and [Candy et al., PoP 2004]

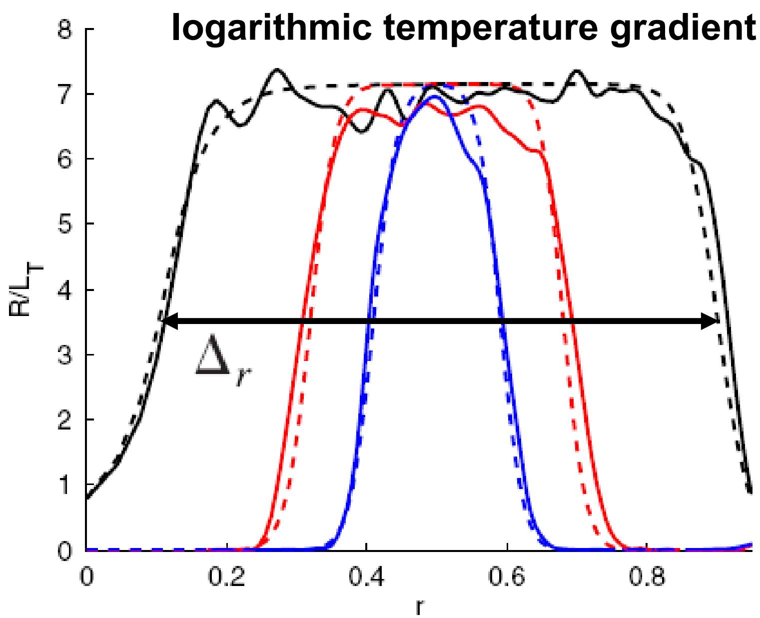
- Allow for flux-driven simulations

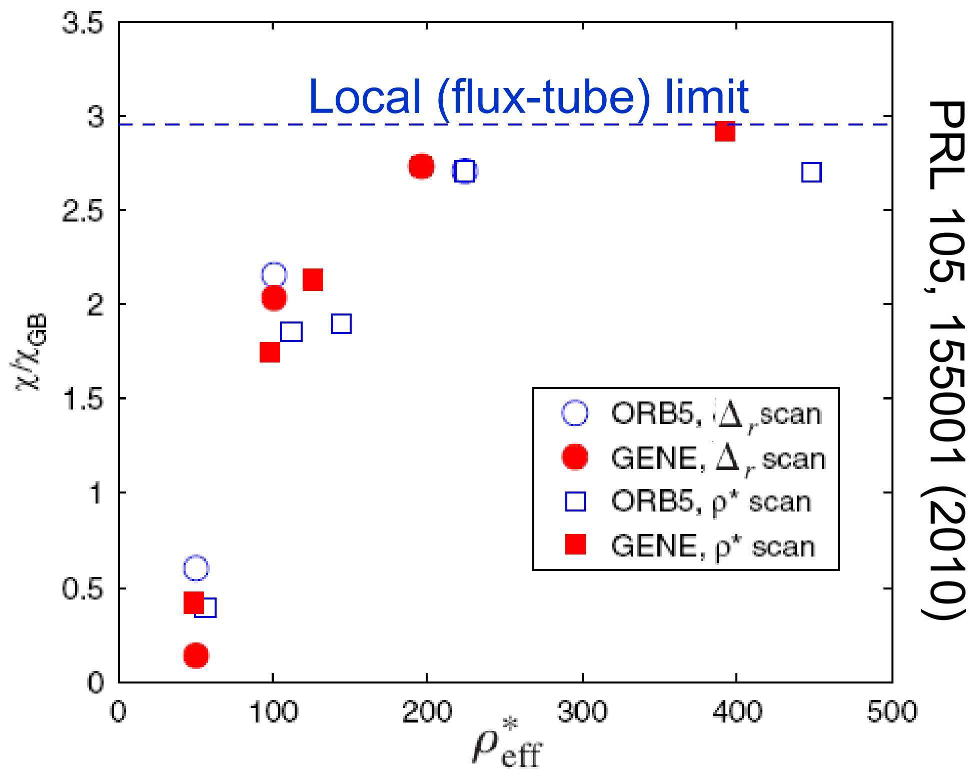
Nonlinear investigation of finite size effects



- ORB5 (Lagrangian) and GENE (Eulerian) agree if the **same geometry** model is used → long lasting controversy probably resolved
- Both, GENE and ORB5 converge towards the local limit
- Deviations (global/local) < 10% at ρ* < 1/300

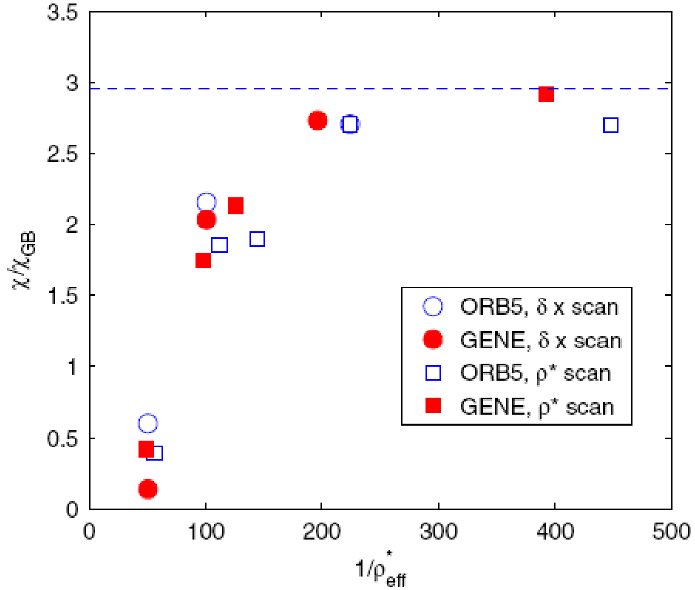
Finite system size: Profile shape matters





- Both codes also show that it is the parameter $\boxed{\rho^*_{\mathrm{eff}} = \rho^*/\Delta_r}$ which really matters – this should be kept in mind when dealing, e.g. with Internal Transport Barriers
- Scaling cannot be explained with profile shearing (only weak Δ_r dependence)
- Turbulence spreading, avalanches?

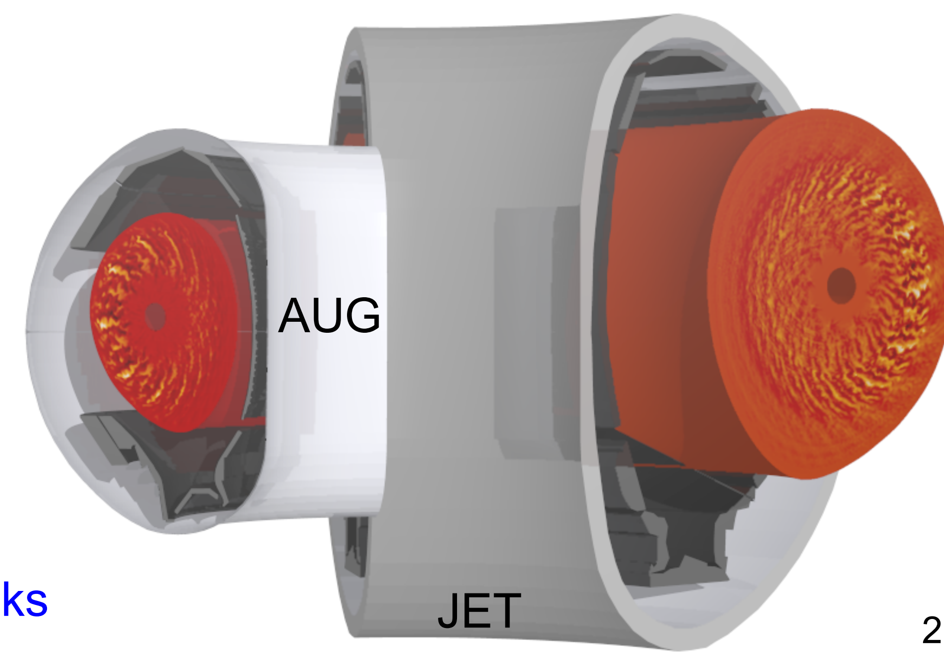
Global simulations of ASDEX-Upgrade & JET



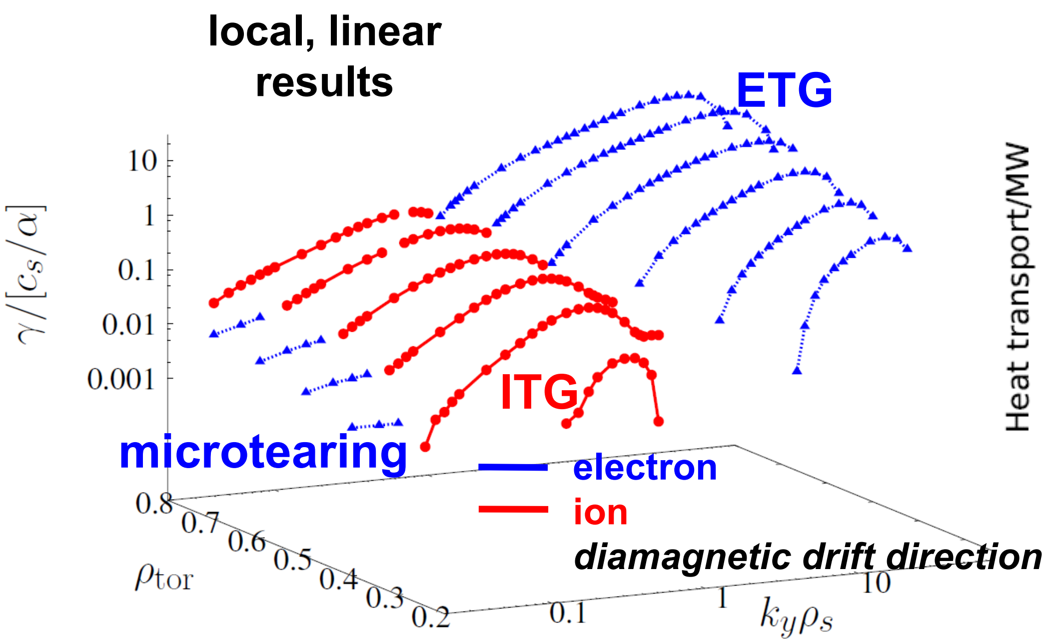
PRL 105, 155001 (2010)

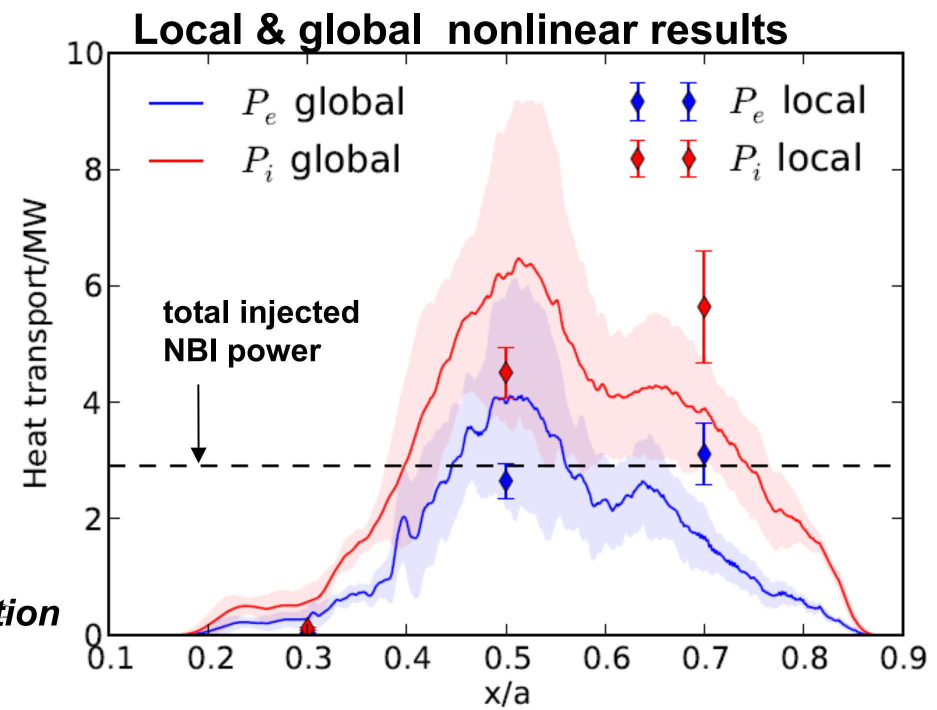
- previous finite-size scaling investigations mostly performed with simplified physics (e.g., adiabatic electrons)
- however, in the absence of barriers, only small deviations are expected for machines like AUG and even smaller ones for JET

- exp. based „size scaling“: global AUG/JET simulations covering ~80% of minor radius including actual profiles and MHD equilibria
- electromagnetic effects
- inter- and intra-species collisions
- perpendicular hyperdiffusion
- gradient-driven using appropriate Krook-type heat & particle sources/sinks



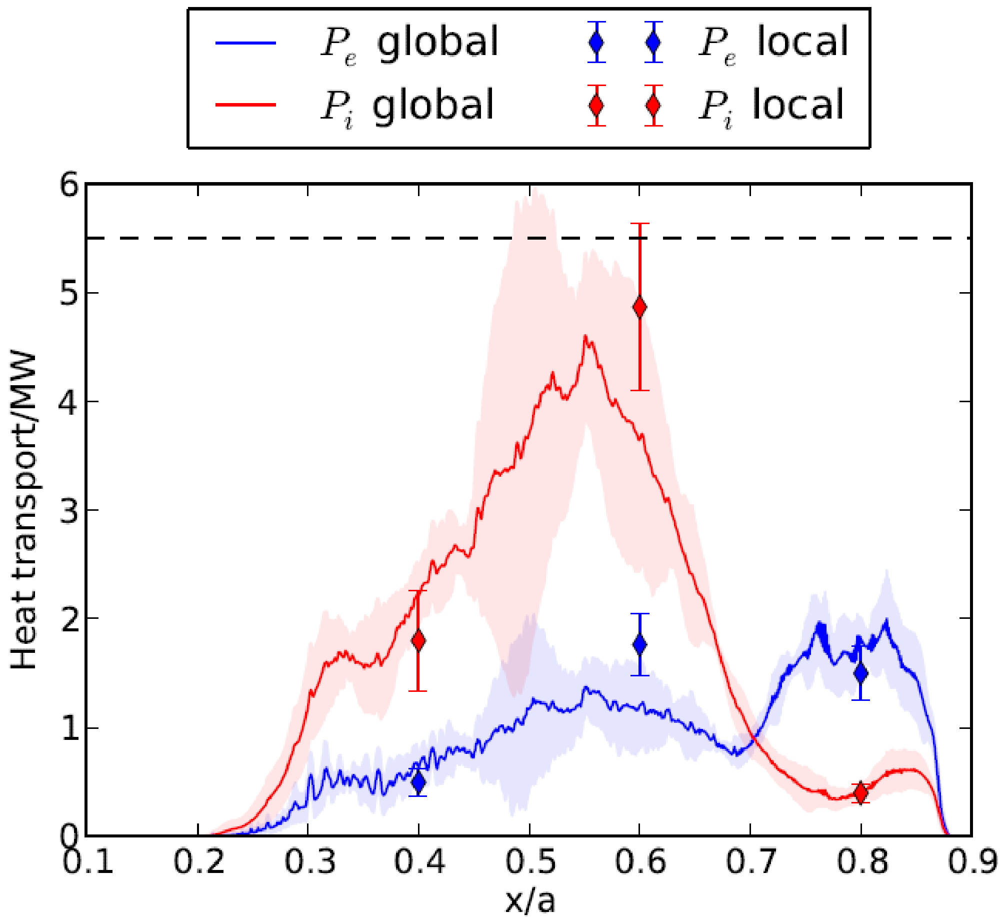
ASDEX-Upgrade #22009, L-mode regime (NBI heated)





- Nonlinear results restricted to (dominant) ITG region -> Q_e most likely underpredicted at radially outer positions
- Reasonable agreement between local and global heat fluxes
- Heat flux level comparable to experiment

JET #70084, L-mode regime

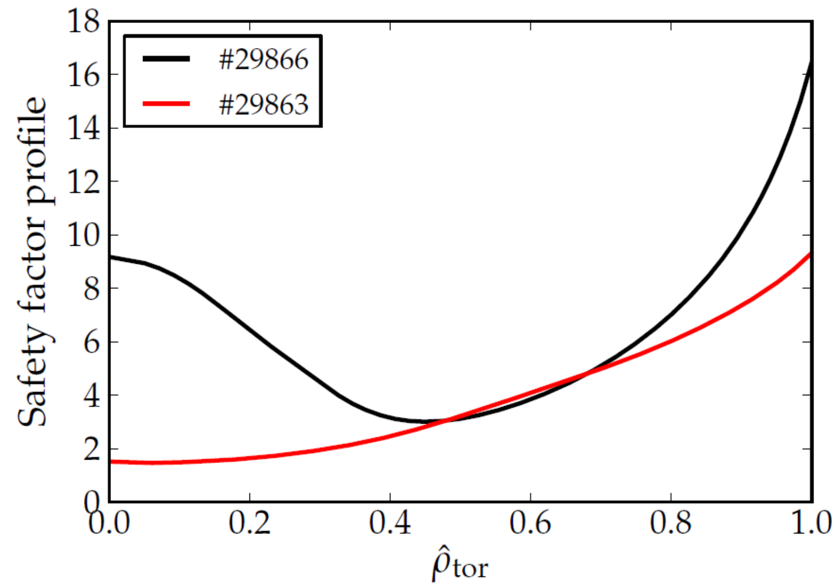


- Local and global results agree well – finite-size effects negligible here!
- Heat flux in the right ballpark compared to experiment
- Edge heat transport underprediction due to uncertainties in T_i
- ETG again cut off – real Q_e thus larger near edge

Finite-size effects in real life: TCV with eITB *(Told et al.)*

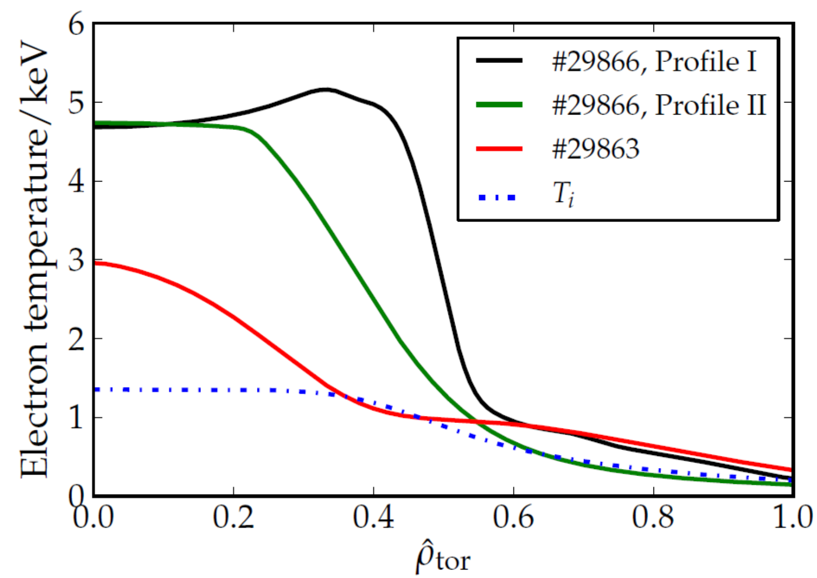
Experimental background:

- Non-inductive discharges in the TCV tokamak with electron ITB
- Current driven solely by EC heating + bootstrap (<~ 70%)
- Add minor inductive currents (co/ctr) → smooth variation of barrier strength [O.Sauter 2005]



Study two discharges with GENE

- Co-current inductive component → monotonic q-profile (#29863)
- Counter-current inductive component → strongly reversed q-profile (#29866)
- **Global simulations required as $\rho^*=\rho_i/a \sim 1/80$ and $L_{Te} \sim 5\rho i$**



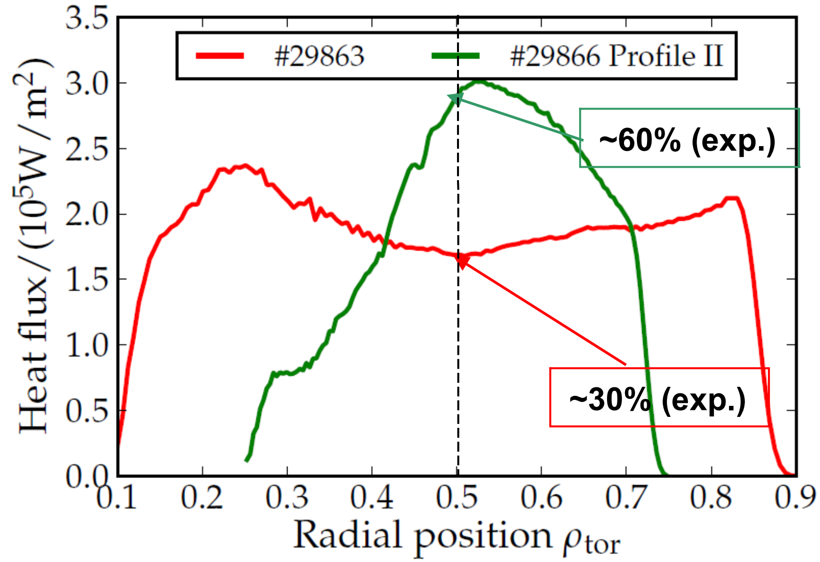
Finite-size effects in real life: TCV with eITB *(Told et al.)*

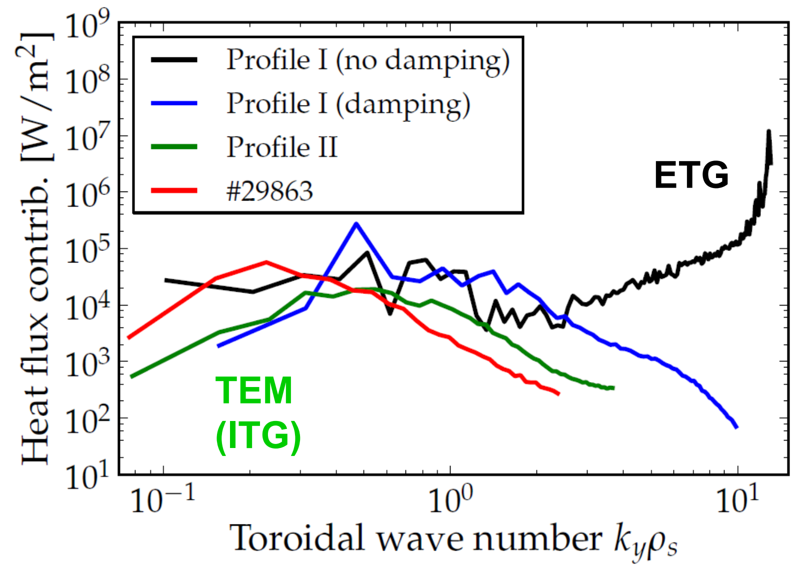
Nonlinear, *global* results:

- **For weak barrier cases** (and low T_i),
  - TEMs dominate
  - Heat fluxes at mid-radius comparable to the experimentally found levels
    #29863: Q_{es} ~ 0.17 MW/m²
    #29866 II: Q_{es} ~ 0.29 MW/m²
    (local result: Q_{es} ~ 5 MW/m² !!!)

- **For steep barrier**
  - ETG strongly unstable, dominate transport

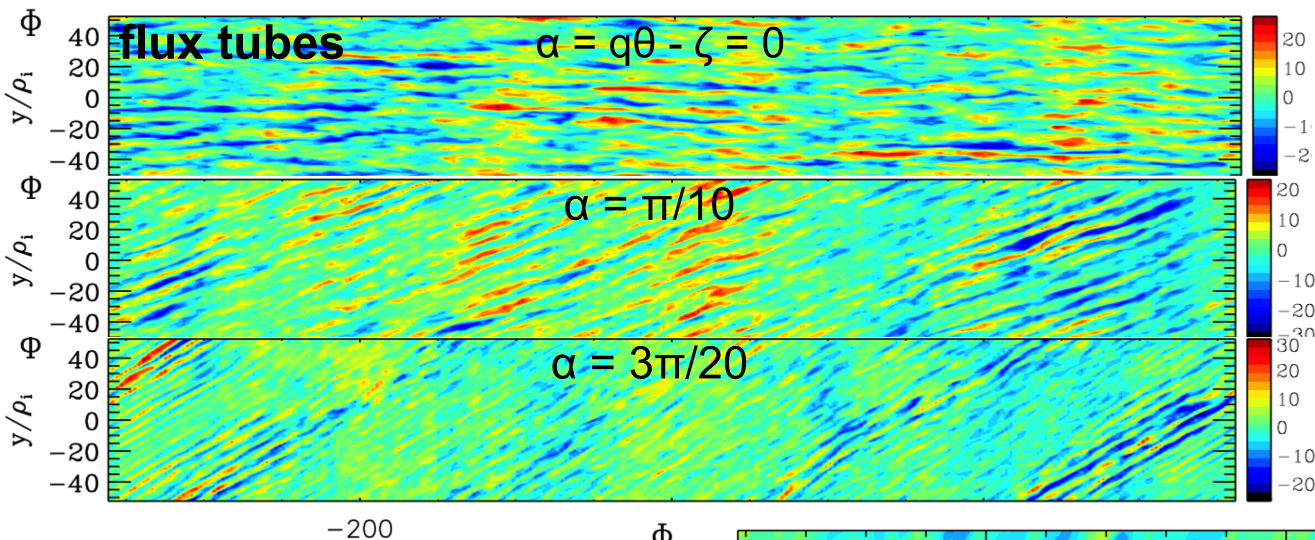
- Considering robustness, ETG might be relevant in limiting barrier steepness





The full-surface version

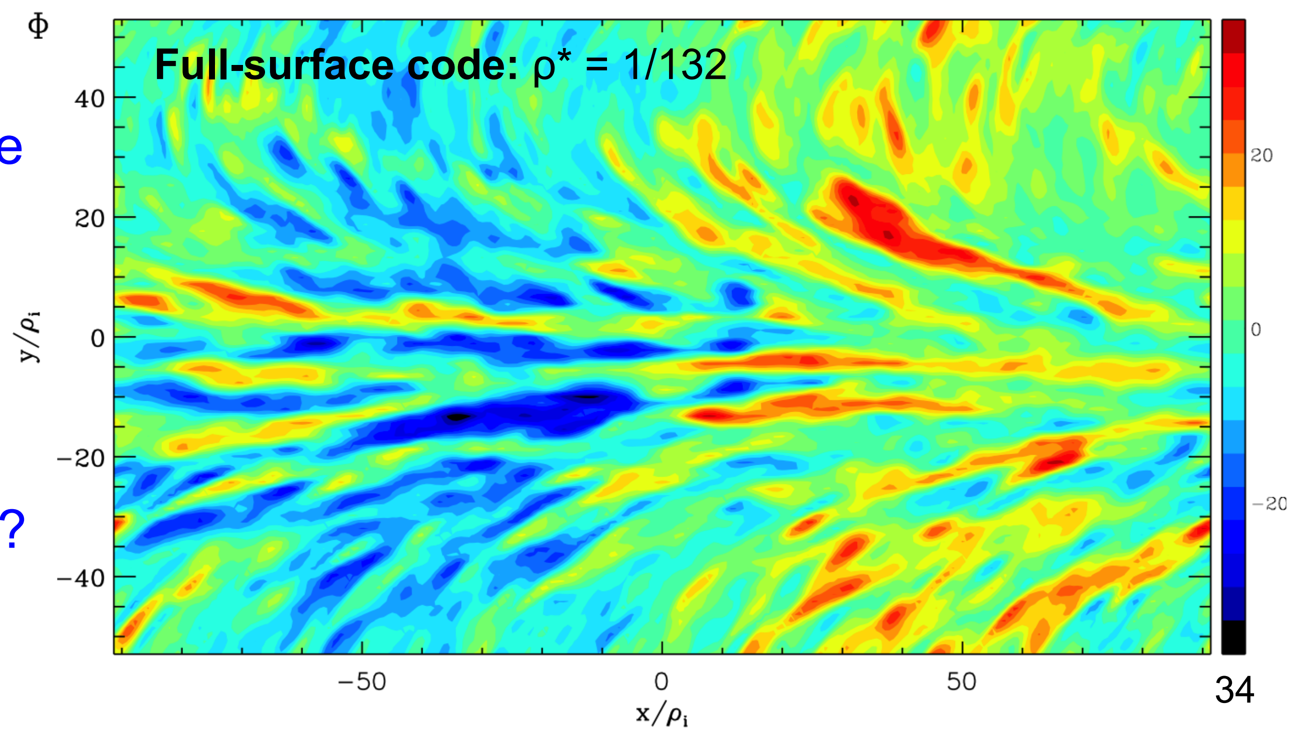
Comparison: W7-X, local flux tube vs. flux-surface



In stellarators, the region of negative normal curvature differs between field lines → turbulence aligns, different eddy tilting

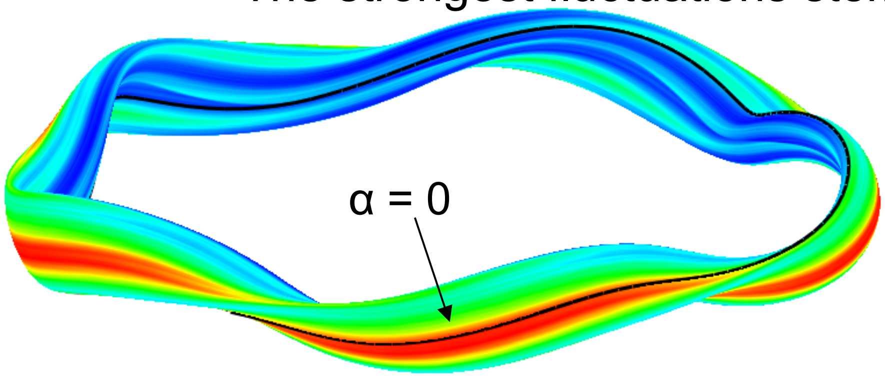
In the full surface code, the turbulence propagates across the whole surface and the eddies tilt smoothly.

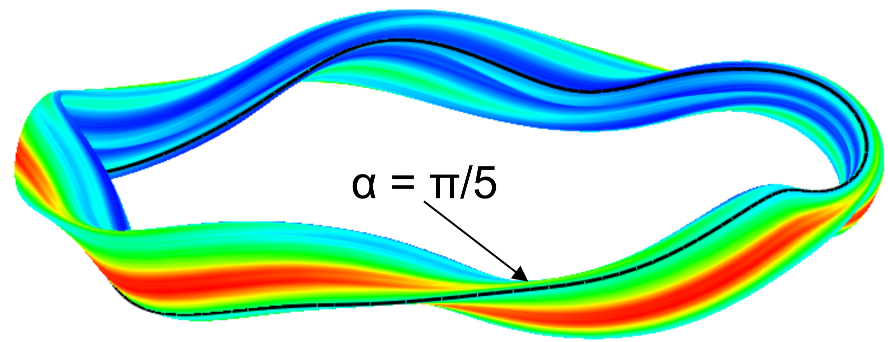
→ effect on total transport?



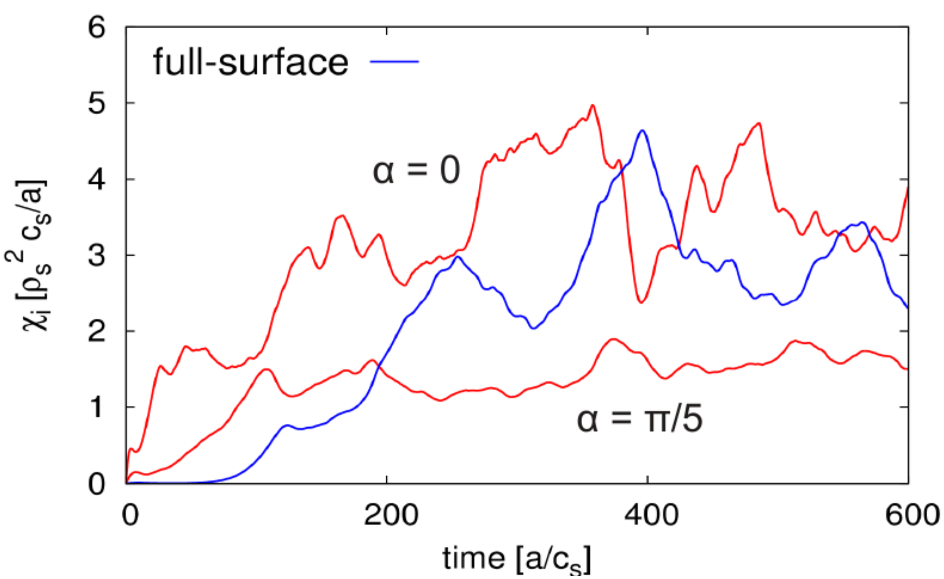
Understanding the spatial variation of ITG turbulence on a surface for stellarator configurations: W7-X

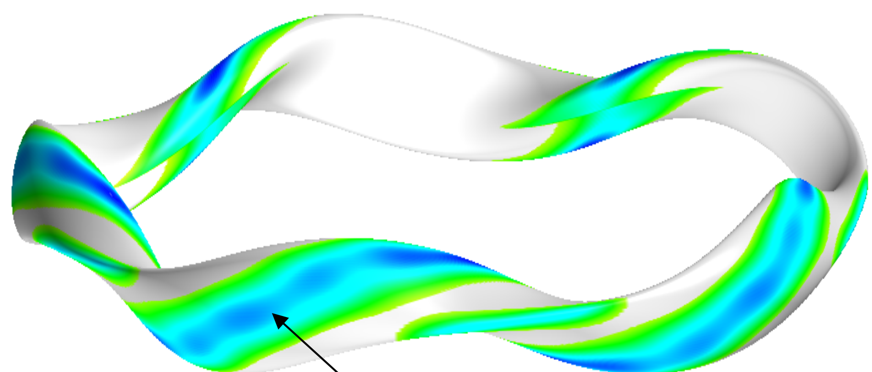
The strongest fluctuations stem from the bean plane ($\alpha = 0$)





The full-surface outcome averages out the flux-tube results

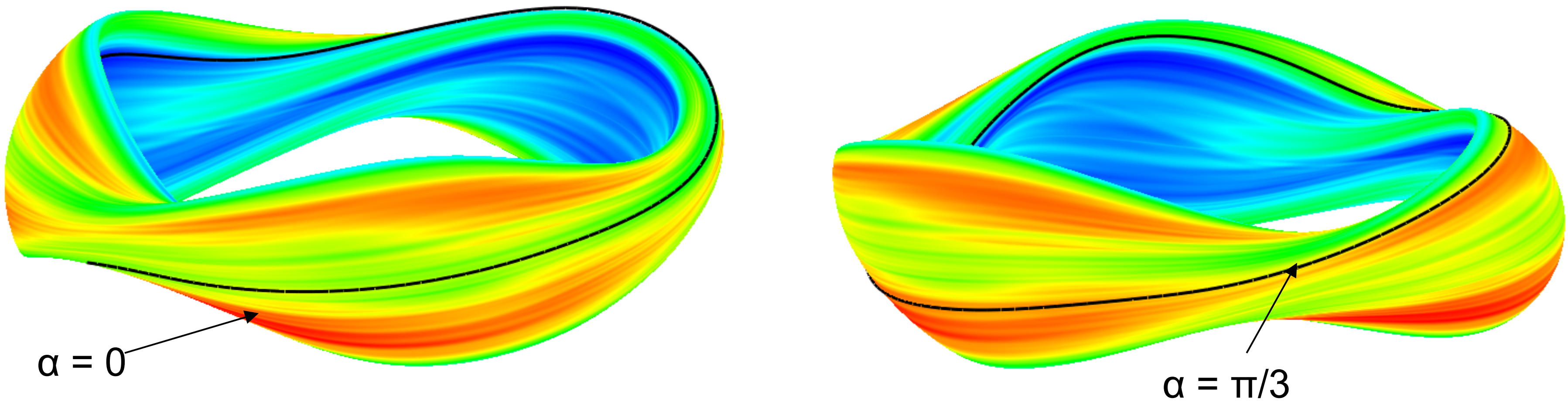




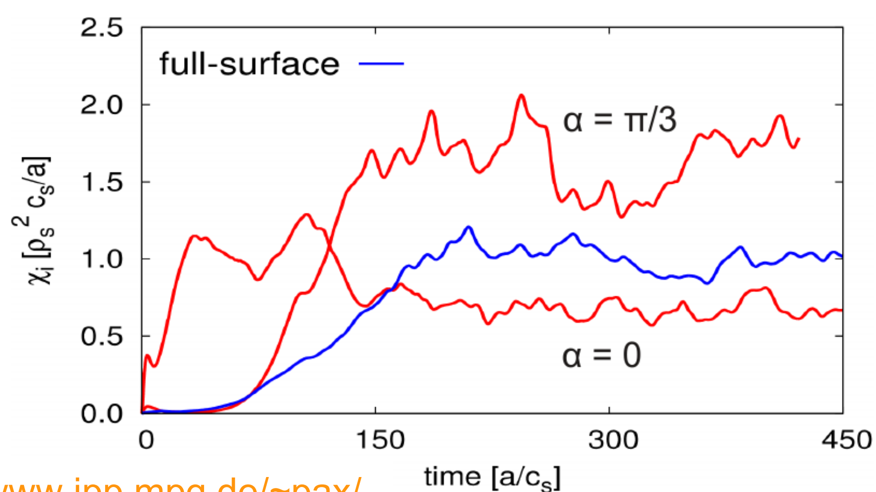
The worst curvature is at bean plane (α=0)

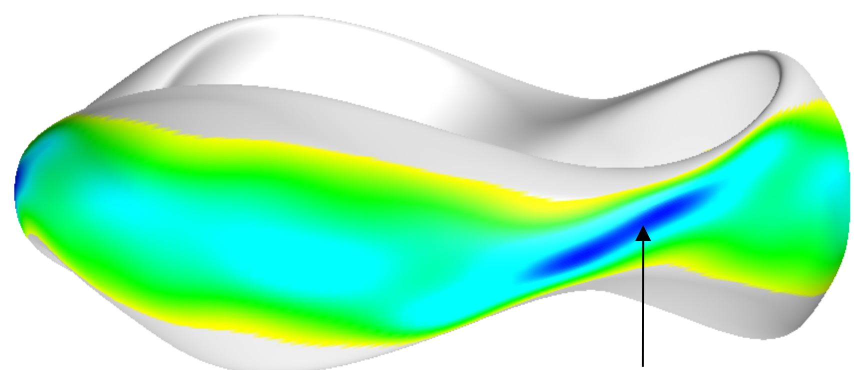
Understanding the spatial variation of ITG turbulence on a surface for stellarator configurations: NCSX

The strongest fluctuations stem from the bullet plane ($\alpha = \pi/3$)



The full-surface outcome averages out the flux-tube results





The worst curvature is at bullet plane ($\alpha = \pi/3$)

Conclusions

Summary & Outlook

- The nonlinear gyrokinetic plasma turbulence code *GENE* has been introduced and its features and recent extension to a nonlocal code have been discussed;

- GENE offers three different options, all of them massively parallelized:
  - Local: Quick, robust and relatively simple assessment of transport in larger machine
  - Global: Small devices or steep gradient regimes
    Transition from nonlocal to local turbulence ($\rho^* \rightarrow 0$) has been revisited cooperatively via Lagrangian & Eulerian codes; linear driving region important
  - Flux-surface: Non-axisymmetric equilibria (stellarators, tokamak-ripples); modes average over individual 'fluxtubes'

- Next major step to be taken:
  - Combine radially global and flux-surface code (“3D-global”)
    → smaller stellarators,
    tokamak outer-core to edge regime

References:

- **http://gene.rzg.mpg.de (→ publications)**
- **[Görler et al., JCP 230, 7053 (2011)]**

Thank you very much for your attention!

Global Gyrokinetic Simulation of

Turbulence in

ASDEX Upgrade

GENE

gene.rzg.mpg.de