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Recent GENE developments and finite-size effects

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4th Fusion theory working group meeting

March 19th-30th, 2012
Wolfgang Pauli Institute, Vienna

- Follow-ups on previous Vienna meetings
  - Recent GENE developments

    - Neoclassical solver
    - Parallel magnetic fluctuations

- Finite-size effects in ASDEX-Upgrade

- Summary

Recent developments in GENE - partially Vienna inspired

Collisions in GENE

Neoclassical transport in GENE

- Solve for k_y=0 (local: k_x=0, as well) component of

$$\boxed{\begin{aligned}&\frac{\partial g_{1\sigma}}{\partial t}+\frac{B_0}{B^*_{0\|}}\left(\mathbf{v}_{\nabla B_0}+\mathbf{v}_c\right)\cdot\left(\nabla F_{0\sigma}+\mu\frac{F_{0\sigma}}{T_{0\sigma}}\nabla B_0\right)+\\&\quad\left(v_\|\mathbf{b}_0+\frac{B_0}{B^*_{0\|}}\left(\mathbf{v}_{\nabla B_0}+\mathbf{v}_c\right)\right)\cdot\mathbf{\Gamma}_\sigma-\frac{\mu}{m_\sigma}\mathbf{b}_0\cdot\nabla B_0\frac{\partial f_{1\sigma}}{\partial v_\|}=\langle C_\sigma(f)\rangle\end{aligned}}$$

with $\mathbf{\Gamma}_\sigma=\nabla f_{1\sigma}+\frac{F_{0\sigma}}{T_{0\sigma}}\left(q_\sigma\nabla\bar{\phi}_1+\mu\nabla\bar{B}_{1\|}\right)$

either by

  - **explicit solve** or
  - **algebraic solver** based on PETSc (Krylov subspace methods)

- Collision operator: Linearized Landau-Boltzmann [F. Merz, PhD, 2009] with improvements to conservation terms by H. Doerk et al. (2011/2012)

Collision operator

- Landau-Boltzmann operator: $C(F_j, F_{j'}) = \frac{\partial}{\partial \vec{v}} \cdot (\mathbf{D} \cdot \frac{\partial}{\partial \vec{v}} - \vec{R}) F_j$

  with diffusion tensor $\mathbf{D}$ and dynamical friction $\vec{R}$

- Linearization: $C_{\sigma\sigma'}[f_\sigma] = C[f_\sigma, f_{0\sigma'}] + C^F_{\sigma\sigma'}[f_{\sigma'}]$

- Test particle part: $C^T_{\sigma\sigma'\perp} = \frac{\gamma_{\sigma\sigma'} n_{\sigma'} T_{0\sigma'}}{m_\sigma^2 m_{\sigma'}} \frac{1}{v^5} \left(v^2 F_1 + \frac{3\mu B_0}{m_\sigma} F_2 \right) \nabla_\perp f_\sigma$

$$C^T_{\sigma\sigma'\mathbf{v}} = \frac{\mathrm{d}}{\mathrm{d}\mathbf{v}} \cdot \frac{\gamma_{\sigma\sigma'} n_{0\sigma'}}{m_\sigma m_{\sigma'}} f_{M\sigma} \left(\frac{T_{0\sigma'}}{m_\sigma v^5} \begin{bmatrix} \frac{2\mu B_0}{m_\sigma} F_1 + v_\parallel^2 F_2 & 6\mu v_\parallel F_2 \\ 6\mu v_\parallel F_2 & \frac{2m_\sigma}{B_0} v_\parallel^2 \mu F_1 + 4\mu^2 F_3 \end{bmatrix} \cdot \frac{\mathrm{d}}{\mathrm{d}\mathbf{v}} \right) \frac{f_\sigma}{f_{M\sigma}}$$

$$+ \frac{\gamma_{\sigma\sigma'} n_{0\sigma'}}{m_\sigma m_{\sigma'}} f_{M\sigma} \left(1 - \frac{T_{0\sigma'}}{T_{0\sigma}} \right) \frac{F_3}{v^3} \begin{bmatrix} v_\parallel \\ 2\mu \end{bmatrix} \frac{f_\sigma}{f_{M\sigma}}.$$

with:

$$F_1(x_\sigma) = x_\sigma \frac{\mathrm{derf}(x_\sigma)}{\mathrm{d}x_\sigma} + (2x_\sigma^2 - 1)\,\mathrm{erf}(x_\sigma)$$

$$F_2(x_\sigma) = (1 - \frac{2}{3} x_\sigma^2)\mathrm{erf}(x_\sigma) - x_\sigma \frac{\mathrm{derf}(x_\sigma)}{\mathrm{d}x_\sigma} \qquad x_\sigma = v/v_{T\sigma}$$

$$F_3(x_\sigma) = F_1(x_\sigma) + 3F_2(x_\sigma)$$

Collision operator

- Field part constructed to conserve particles, momentum, energy & be self-adjoint [Doerk, Brunner et al.]

$$C^F_{\sigma\sigma'}(\delta f_\sigma) = \frac{F_{0\sigma}}{n_{0\sigma}(x)}\frac{\sqrt{2\pi}}{4}(1+\frac{m_{\sigma'}}{m_\sigma})^{3/2}\left[6H(\hat{x}_{\sigma'})\frac{v_\parallel}{v_{t\sigma'}(x)}\frac{\delta\mathcal{P}_{\parallel\sigma'\sigma}}{m_{\sigma'}v_{t\sigma'}(x)}\right.$$

$$\left.+\left\{\left[(1+\frac{m_\sigma}{m_{\sigma'}})\hat{x}^2_{\sigma'}-1\right]H(\hat{x}_{\sigma'})-K(\hat{x}_{\sigma'})\right\}\frac{\delta\mathcal{E}_{\sigma'\sigma}}{m_{\sigma'}v^2_{t\sigma'}(x)}\right\}\right]$$

- Abbreviations:

$$H(x_{\sigma'}) = \frac{1}{x^3_{\sigma'}}\left[\mathrm{erf}(x_{\sigma'}/\sqrt{2}) - \sqrt{\frac{2}{\pi}}x_{\sigma'}e^{-x^2_{\sigma'}/2}\right]$$

$$K(x_{\sigma'}) = \frac{1}{x^3_{\sigma'}}(x^2_{\sigma'}-1)\mathrm{erf}(\mathrm{x}_{\sigma'}/\sqrt{2}) + \sqrt{\frac{2}{\pi}}\mathrm{x}_{\sigma'}e^{-x^2_{\sigma'}/2}$$

- Momentum correction term: $\delta\mathcal{P}_{\parallel\sigma'\sigma} = -\int m_{\sigma'}v_\parallel C^T_{\sigma'\sigma}(\delta f_{\sigma'})\mathrm{d}^3v$

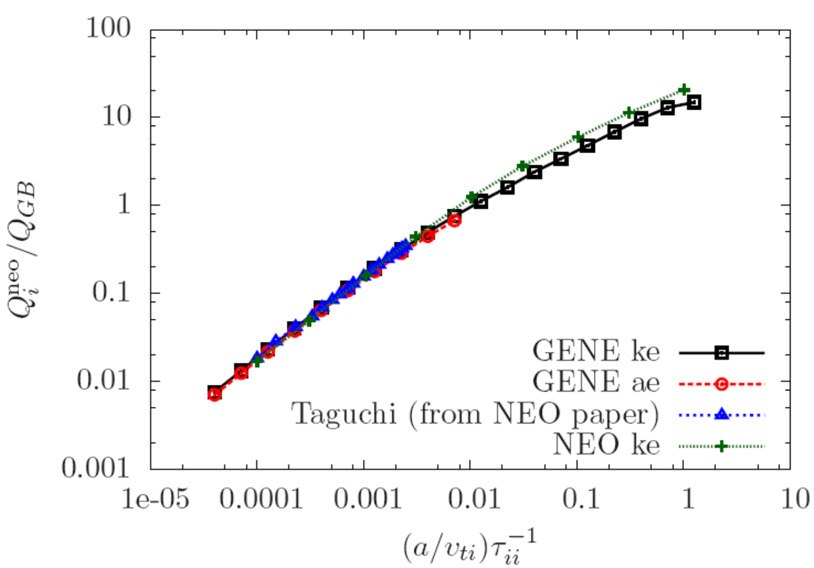
- Energy correction term: $\delta\mathcal{E}_{\sigma'\sigma} = -\int m_{\sigma'}v^2 C^T_{\sigma'\sigma}(\delta f_{\sigma'})\mathrm{d}^3v$

Neoclassical transport - benchmarks

Neoclassical ion heat transport

- local simulations vs Taguchi
- global simulations vs ORB5

Doerk, Vernay *et al.*



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Global results will be published soon
in H. Doerk, PhD thesis
summer 2012

Parallel magnetic fluctuations

Parallel magnetic fluctuations

- Three field equations:

$$\nabla_\perp^2 \phi_1 = -4\pi \sum_\sigma q_\sigma n_{1\sigma}$$

$$\nabla_\perp^2 A_{1\|} = -\frac{4\pi}{c} \sum_\sigma j_{1\|\sigma}$$

$$B_{1\|} = -4\pi \sum_\sigma \frac{p_{1\perp,\sigma}}{B_0}$$

… with the following moments

$$n_{1\sigma,\mathbf{k}} = \frac{2\pi B_0}{m_\sigma} \int \mathrm{d}v_\| \mathrm{d}\mu \left[J_0 h_{1\sigma,\mathbf{k}} - q_\sigma \phi_{1,\mathbf{k}} \frac{F_{0\sigma}}{T_{0\sigma}} \right]$$

$$j_{1\|\sigma,\mathbf{k}} = q_\sigma \frac{2\pi B_0}{m_\sigma} \int \mathrm{d}v_\| \mathrm{d}\mu \; v_\| \left[J_0 h_{1\sigma,\mathbf{k}} - q_\sigma \phi_{1,\mathbf{k}} \frac{F_{0\sigma}}{T_{0\sigma}} \right]$$

$$p_{1\perp\sigma,\mathbf{k}} \equiv \frac{2\pi B_0}{m_\sigma} \int \mathrm{d}v_\| \mathrm{d}\mu \; \mu B_0 I_1 h_{1\sigma,\mathbf{k}}$$

and abbreviations

$$h_{1\sigma} \equiv f_{1\sigma} + \left[q_\sigma J_0 \phi_1 + \mu I_1 B_{1\|} \right] \frac{F_{0\sigma}}{T_{0\sigma}}$$

$$J_0 = J_0(k_\perp \rho)$$

$$I_1 = I_1(k_\perp \rho) = 2 J_1(k_\perp \rho)/(k_\perp \rho)$$

Parallel magnetic fluctuations: particle flux

- Basic definition:

$$\boldsymbol{\Gamma}_\sigma(\mathbf{x}) = \int \mathrm{d}^3X \mathrm{d}v_\parallel \mathrm{d}\mu \mathrm{d}\theta \; \delta(\mathbf{X}+\mathbf{r}-\mathbf{x}) \frac{B_0}{m_\sigma} \left\{ h_{1\sigma}(\mathbf{X}) - \frac{q_\sigma F_{0\sigma}}{T_{0\sigma}} \phi_1(\mathbf{x}) \right\} \mathbf{v}_D(\mathbf{x})$$

- Radial component, keeping ExB drift

$$\langle \Gamma^x_\sigma \rangle_\perp = \sum_{\mathbf{k}} \frac{c}{\mathcal{C}} (-\mathrm{i}k_y) \left[n^*_{1\sigma,\mathbf{k}} \phi_{1,\mathbf{k}} - \frac{1}{q_\sigma c} j^*_{1\parallel\sigma,\mathbf{k}} A_{1\parallel,\mathbf{k}} + \frac{1}{q_\sigma} \frac{p^*_{1\perp\sigma,\mathbf{k}}}{B_0} B_{1\parallel,\mathbf{k}} \right] \equiv \sum_{\mathbf{k}} \Gamma^x_{\sigma,\mathbf{k}}$$

- Ambipolarity can easily be shown:

$$\sum_\sigma q_\sigma \langle \Gamma^x_\sigma \rangle_\perp = -\frac{1}{4\pi} \frac{c}{\mathcal{C}} \sum_{\mathbf{k}} \mathrm{i}k_y \left[k_\perp^2 \left|\phi_{1,\mathbf{k}}\right|^2 - k_\perp^2 \left|A_{1\parallel,\mathbf{k}}\right|^2 - \left|B_{1\parallel,\mathbf{k}}\right|^2 \right] = 0$$

- Implementation based on f instead of h:

$$\Gamma^x_{\sigma,\mathbf{k}} = -\frac{c}{\mathcal{C}} \frac{2\pi B_0}{m_\sigma} \int \mathrm{d}v_\parallel \mathrm{d}\mu \; (\mathrm{i}k_y) \Bigg\{ \left(f^*_{1\sigma,\mathbf{k}} + \left[q_\sigma J_0 \phi^*_{1,\mathbf{k}} + \mu I_1 B^*_{1\parallel,\mathbf{k}} \right] \frac{F_{0\sigma}}{T_{0\sigma}} \right)$$
$$\left[J_0 \phi_{1,\mathbf{k}} - \frac{v_\parallel}{c} J_0 A_{1\parallel,\mathbf{k}} + \frac{1}{q_\sigma} \mu I_1(k_\perp \rho) B_{1\parallel,\mathbf{k}} \right]$$
$$- \frac{q_\sigma F_{0\sigma}}{T_{0\sigma}} \phi^*_{1,\mathbf{k}} \left[\phi_{1,\mathbf{k}} - \frac{v_\parallel}{c} A_{1\parallel,\mathbf{k}} \right] \Bigg\}$$

Ambipolarity is numerically preserved in GENE

Parallel magnetic fluctuations: heat flux

- Basic definition:

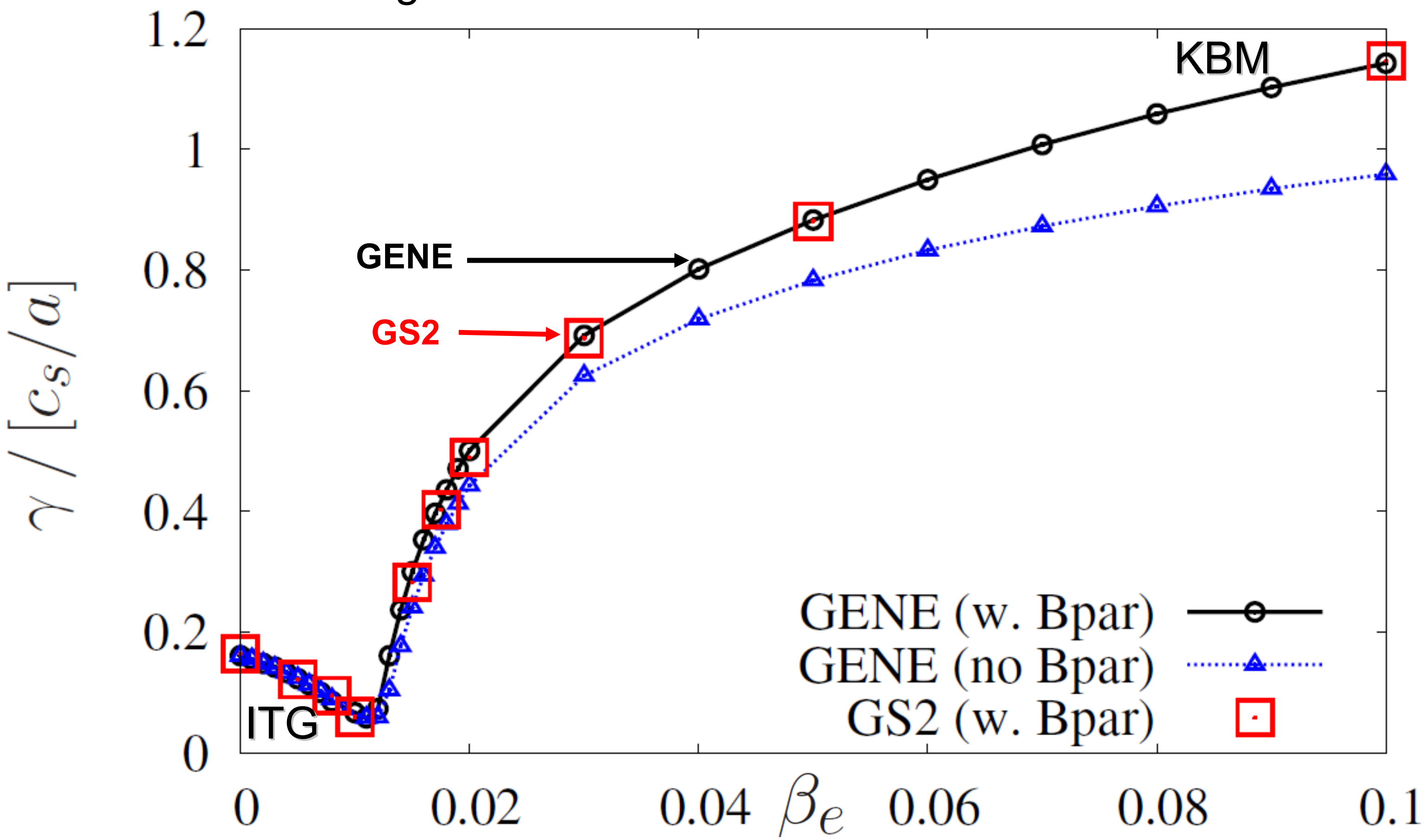
$$\mathbf{Q}_\sigma(\mathbf{x}) = \int \mathrm{d}^3 v \; \frac{1}{2} m_\sigma v^2 f^{(pc)} \; \mathbf{v}_D$$

- Radial component, keeping ExB drift

$$\begin{aligned}\langle Q_\sigma^x \rangle_\perp = & -\frac{c}{\mathcal{C}} \sum_{\mathbf{k}} (\mathrm{i}k_y) \frac{2\pi B_0}{m_\sigma} \int \mathrm{d}^3 v_\parallel \mathrm{d}\mu \; \frac{1}{2} m_\sigma \left(v_\parallel^2 + \frac{2B_0}{m_\sigma}\mu \right) \Bigg\{ \\ & \left(f_{1\sigma,\mathbf{k}}^* + \left[q_\sigma J_0 \phi_{1,\mathbf{k}}^* + \mu I_1 B_{1\parallel,\mathbf{k}}^* \right] \frac{F_{0\sigma}}{T_{0\sigma}} \right) \left[J_0 \phi_{1,\mathbf{k}} - \frac{v_\parallel}{c} J_0 A_{1\parallel,\mathbf{k}} \right. \\ & \left. + \frac{1}{q_\sigma} \mu I_1(k_\perp \rho) B_{1\parallel,\mathbf{k}} \right] - \frac{q_\sigma F_{0\sigma}}{T_{0\sigma}} \phi_{1,\mathbf{k}}^* \left[\phi_{1,\mathbf{k}} - \frac{v_\parallel}{c} A_{1\parallel,\mathbf{k}} \right] \Bigg\}\end{aligned}$$

Parallel magnetic fluctuations – GENE/GS2 benchmark

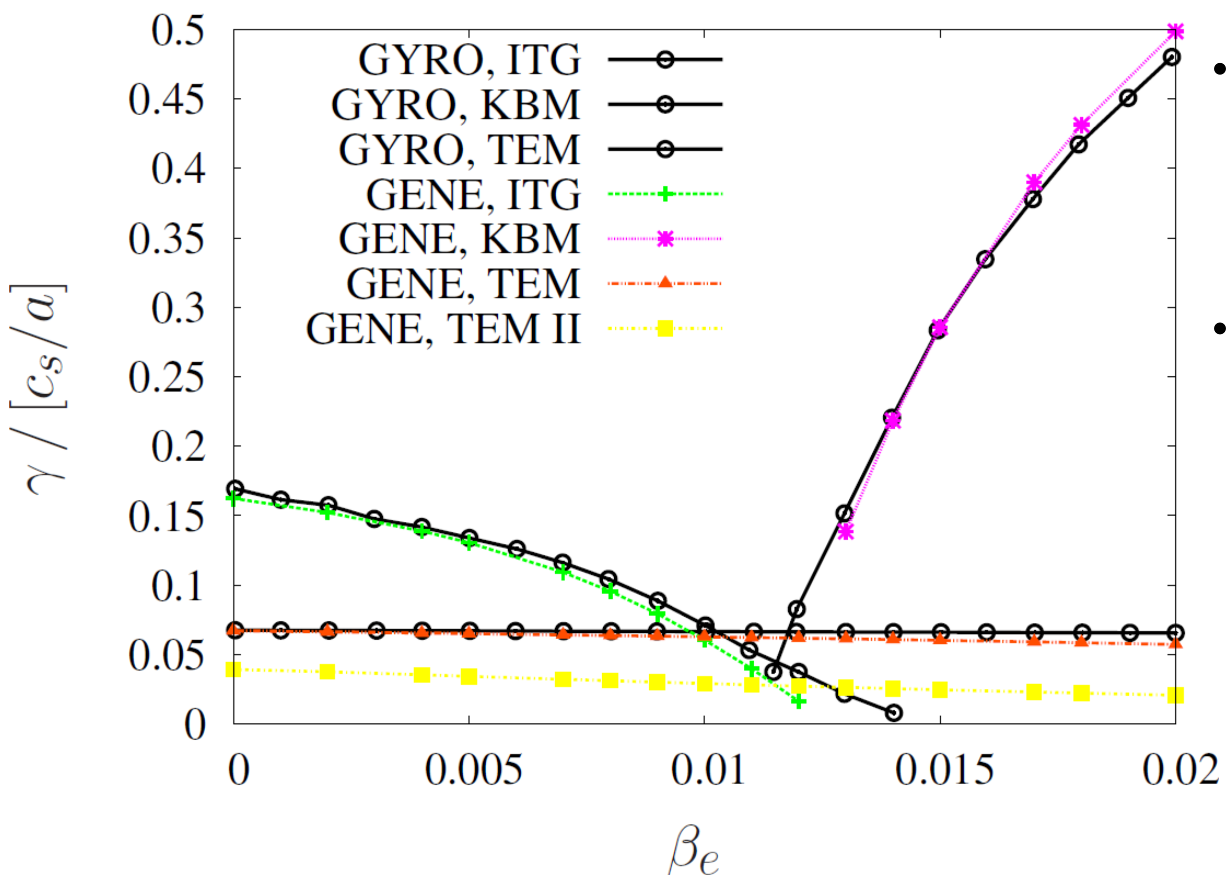
- Cyclone parameters at $k_y\rho_s = 0.25$
- *here:* no Shafranov shift, no pressure gradient in curvature term for benchmarking reasons



Excellent agreement between both codes – even at high β (~10%)!

Parallel magnetic fluctuations & Eigenvalue Solver

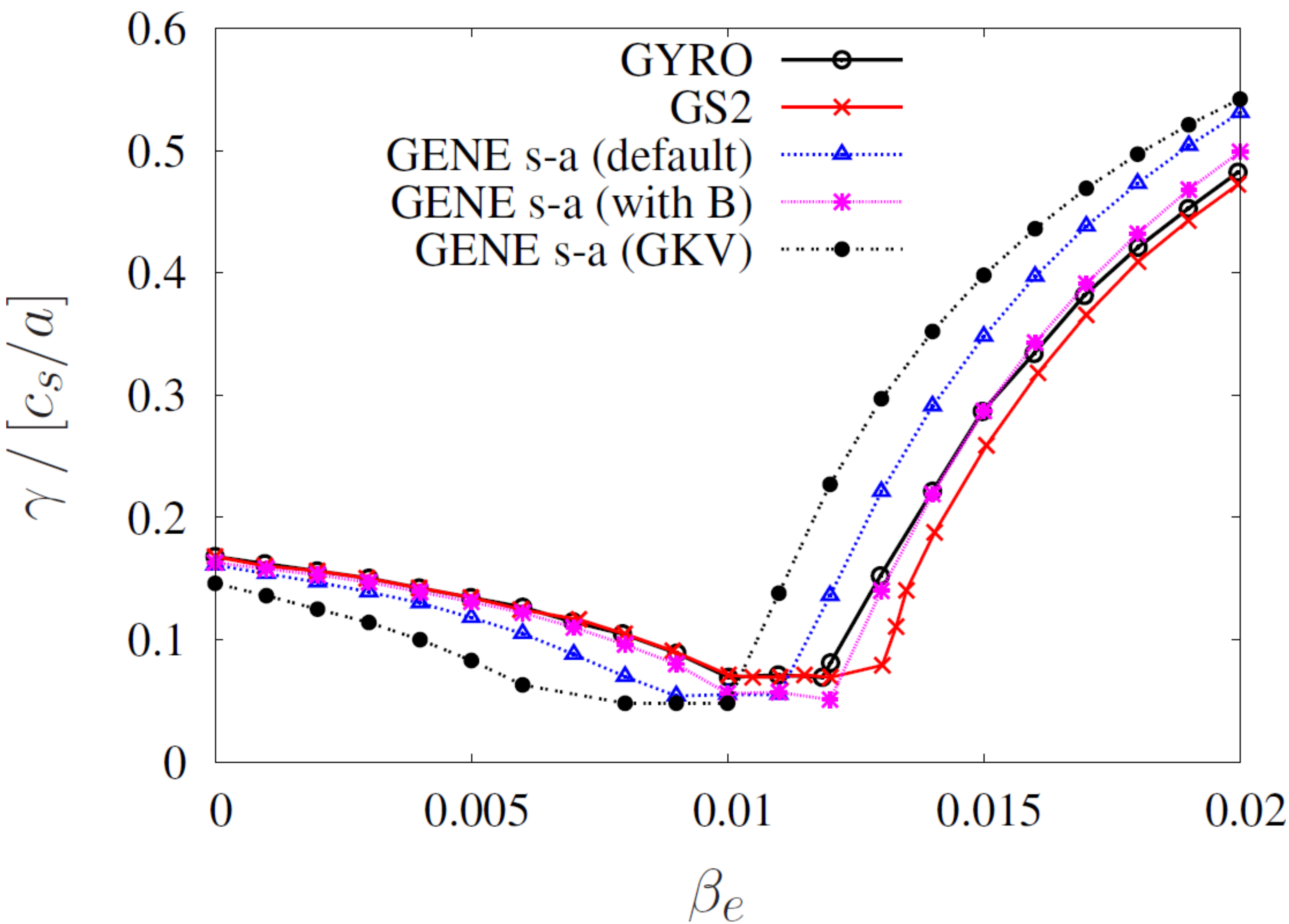
- Cyclone parameters at $k_y \rho_s = 0.25$, no Shafranov shift



- Both codes show remarkably good agreement even for subdominant modes

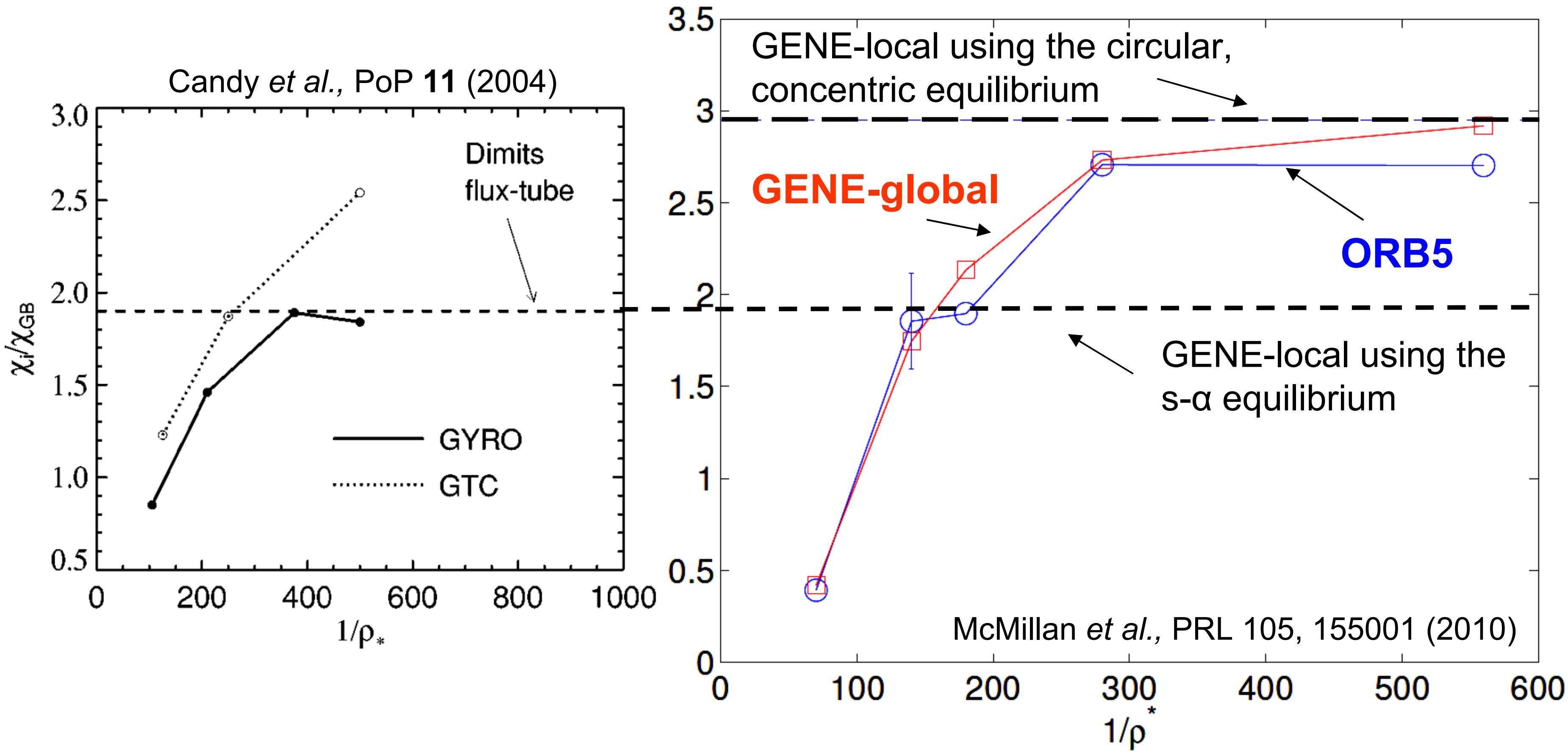
- New **eigenvalue solvers** in GENE in collaboration with the SLEPc team (www.grycap.upv.es/slepc) → efficiency greatly improved (up to 10x faster) by appropriate *preconditioning*

Why we shouldn‘t use s-α …



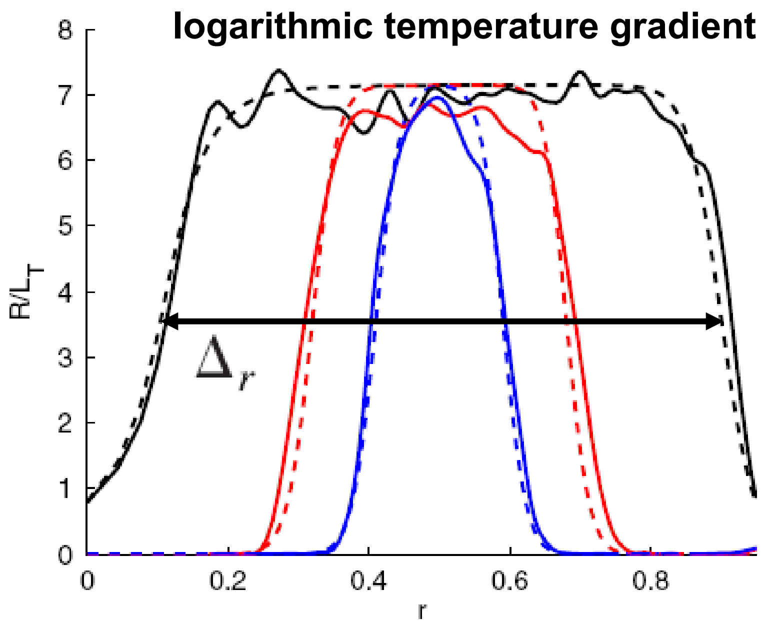
Finite-size effects in real life

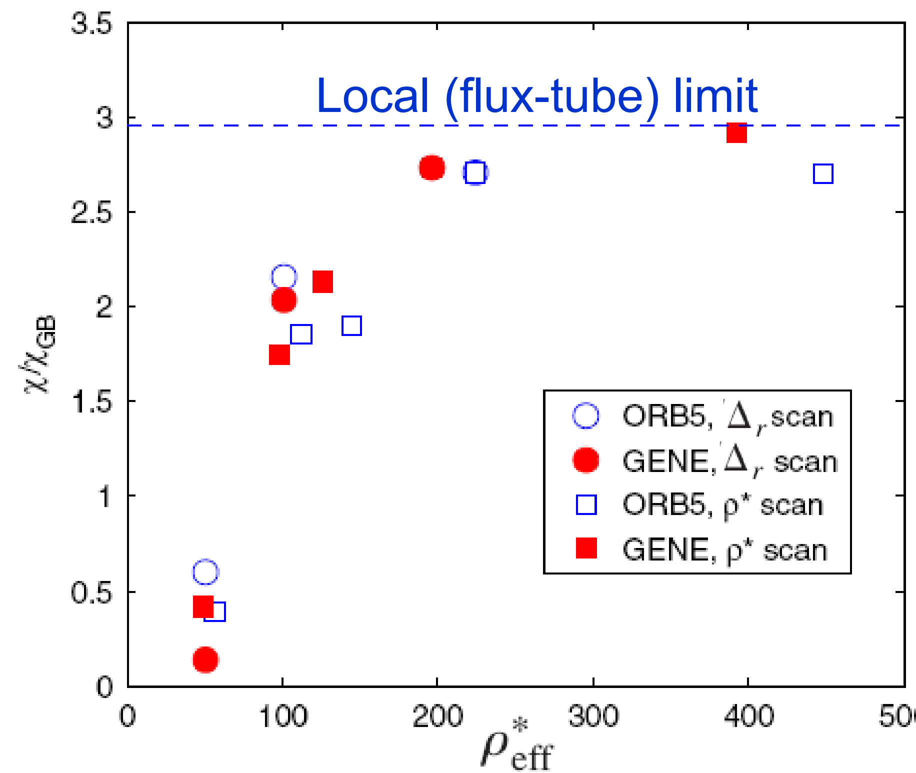
Reminder: discussion of finite size effects



- 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





PRL 105, 155001 (2010)

- 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

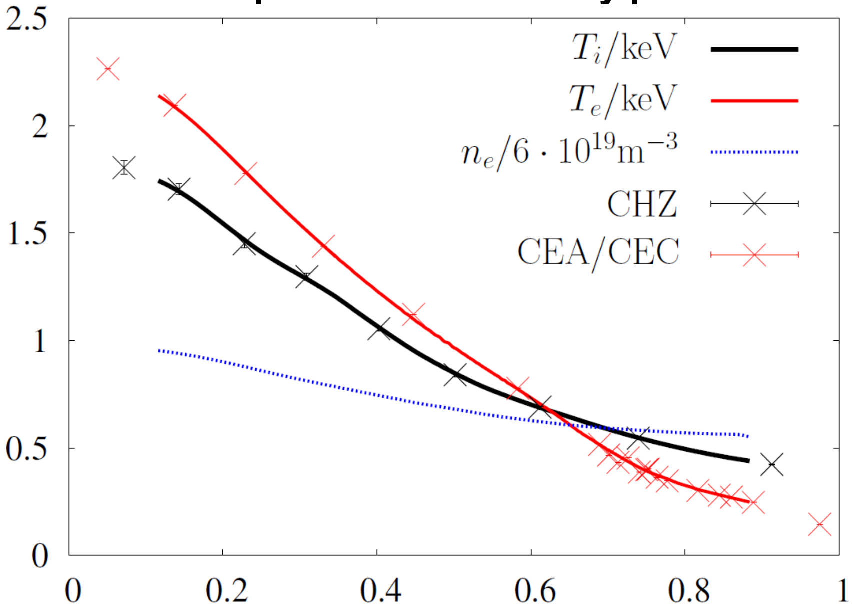
So far simplified physics, e.g.,

- **adiabatic electrons, collision-free, simple geometry, …**

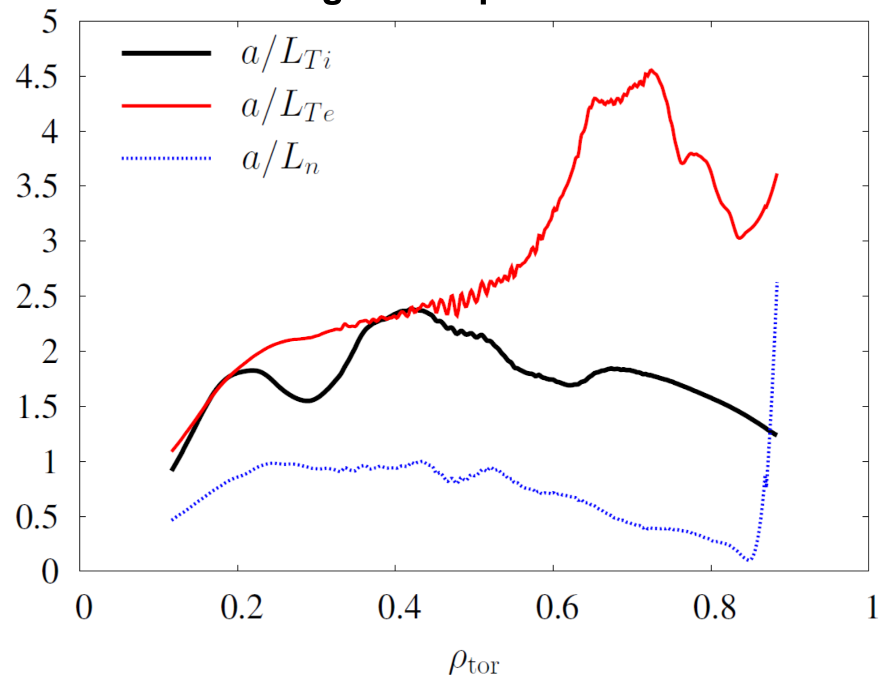
→ **What about real-life parameters & more comprehensive physics?**

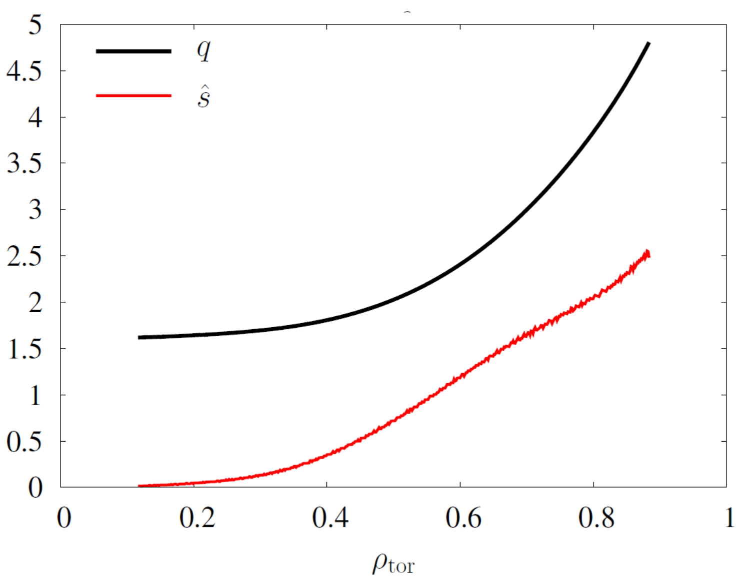
ASDEX-Upgrade L-mode plasma

temperature and density profiles



gradient profiles

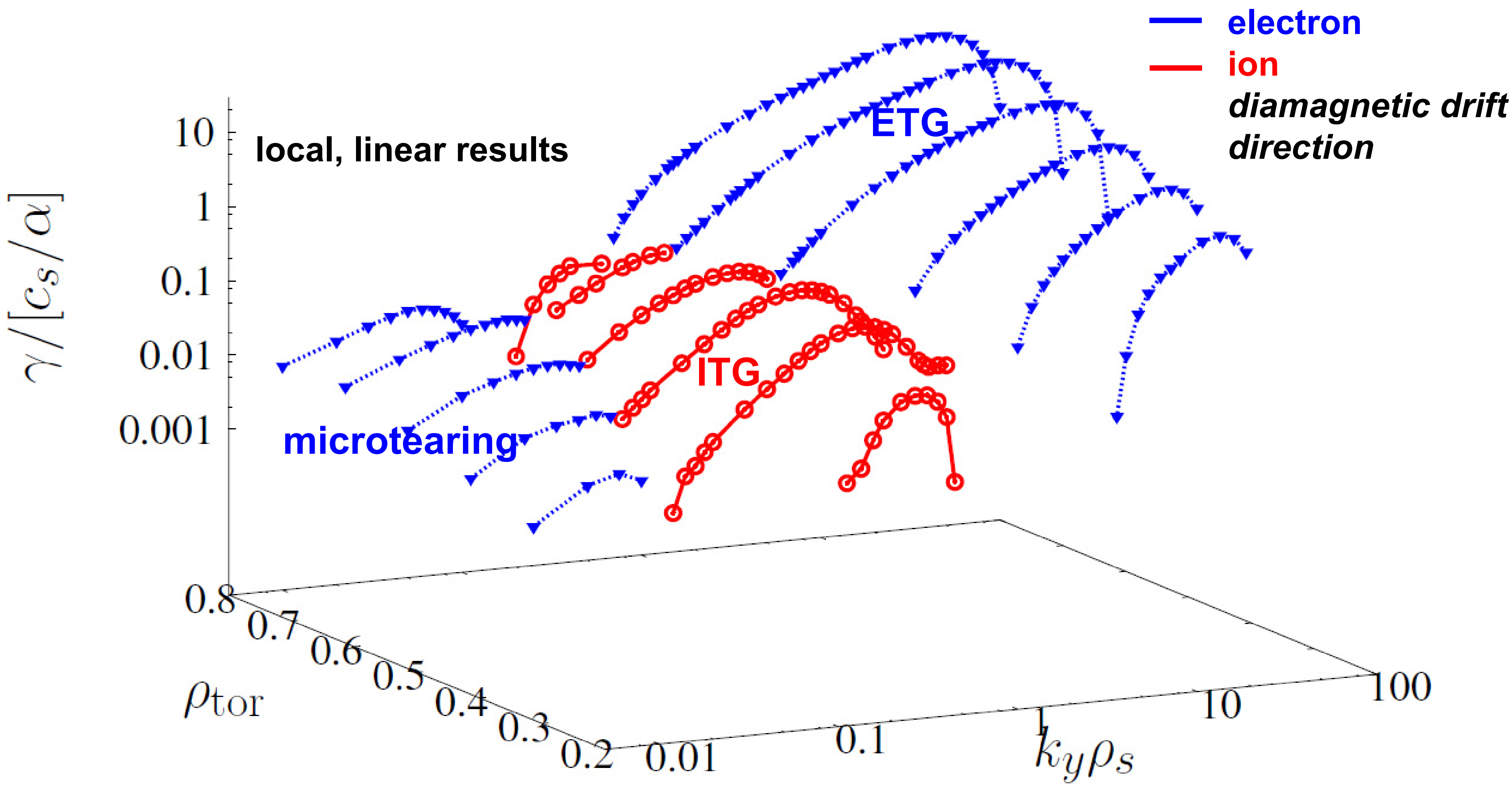




Here:

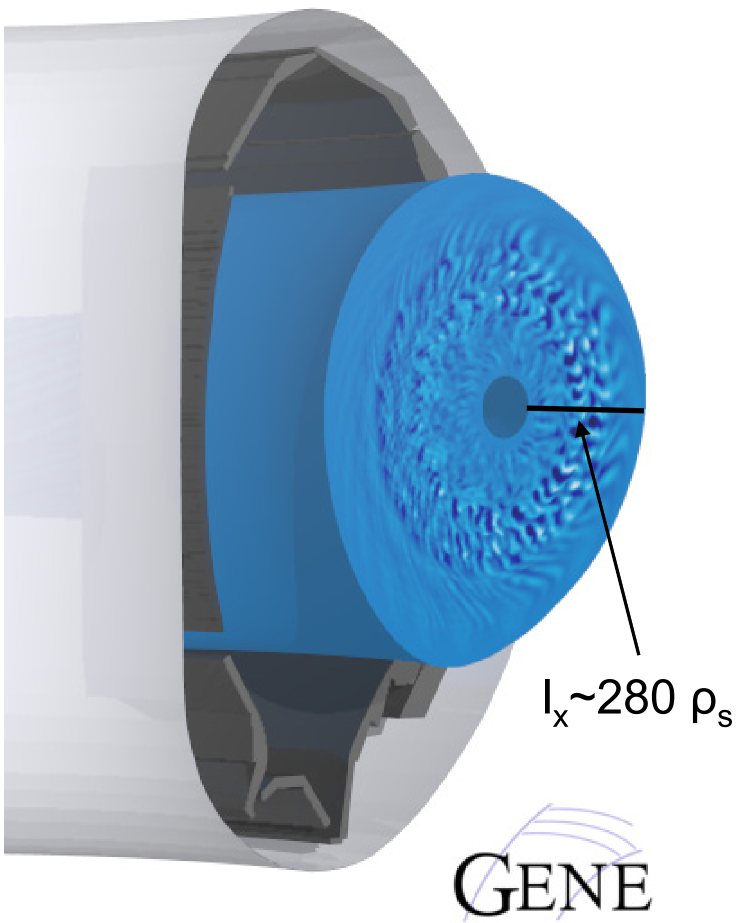
- application to #22009, t=4.1s (L-mode; ~3 MW power deposition)
- shear flow neglected

ASDEX-Upgrade #22009, L-mode regime



- Huge variety of modes – *triple-scale problem*!
- high-k modes become more important at larger radii

ASDEX-Upgrade L-mode plasma - simulation



- radial box covering 80% of minor radius (neglecting pedestal) $\Delta x \sim 0.5\ \rho_s$
- minimum toroidal mode number: $n_0 = 5$
  32 modes in total
  (extending to $k_y\rho_s \sim 1.7$ at ref. flux surface)
- 24 parallel grid points
- velocity space:
  $(n_{v||} \times n_\mu) = 96 \times 32$
  with box sizes $(l_{v||} \times l_\mu) = (4\ v_{th,j},\ 12\ T_{0,j}/B_0)$
- kept collisions and electromagnetic effects
- perpendicular hyperdiffusion to suppress sub-ion-gyroradius-scale turbulence
- gradient-driven using appropriate Krook-type heat & particle sources/sinks

ASDEX-Upgrade #22009, L-mode regime

(removed unpublished content for web upload)

publication is expected in the next months

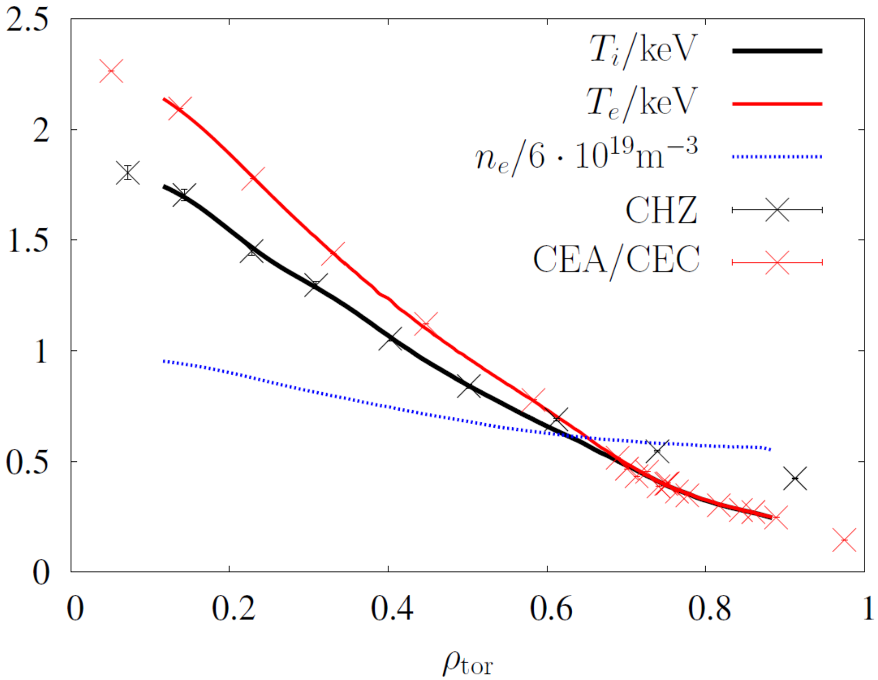
- Heat flux in the right ballpark compared to experiment
- Local and global results agree well – finite-size effects negligible here!
- Peak evolving in transport profile due to missing external ExB shear?
- However: transport level too low at larger radii … high-k? Exp. data?

ASDEX-Upgrade #22009, L-mode regime II

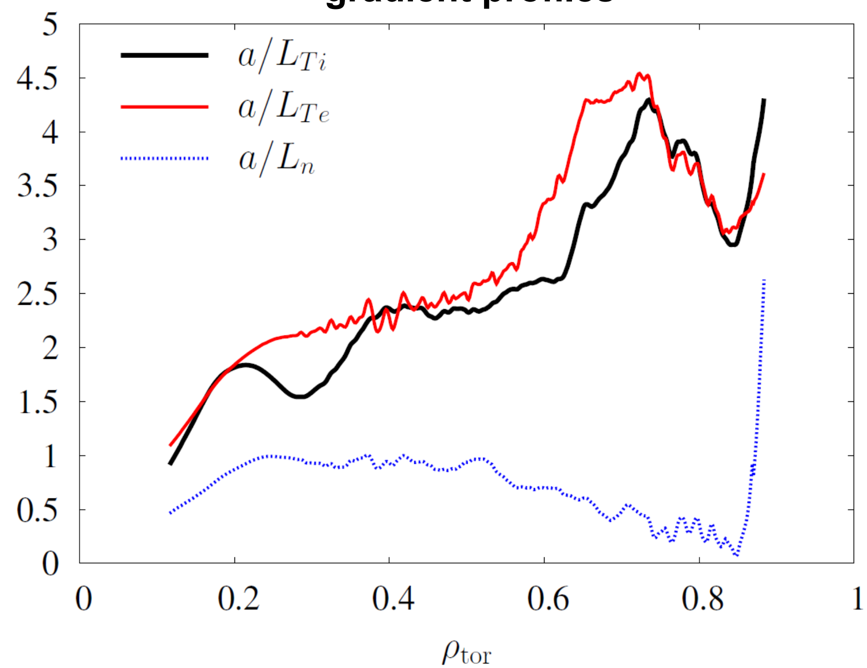
- **CHZ might be overestimating T_i**

  → alternative assumption: $T_i \sim T_e$ at $\rho_{tor} > 0.7$

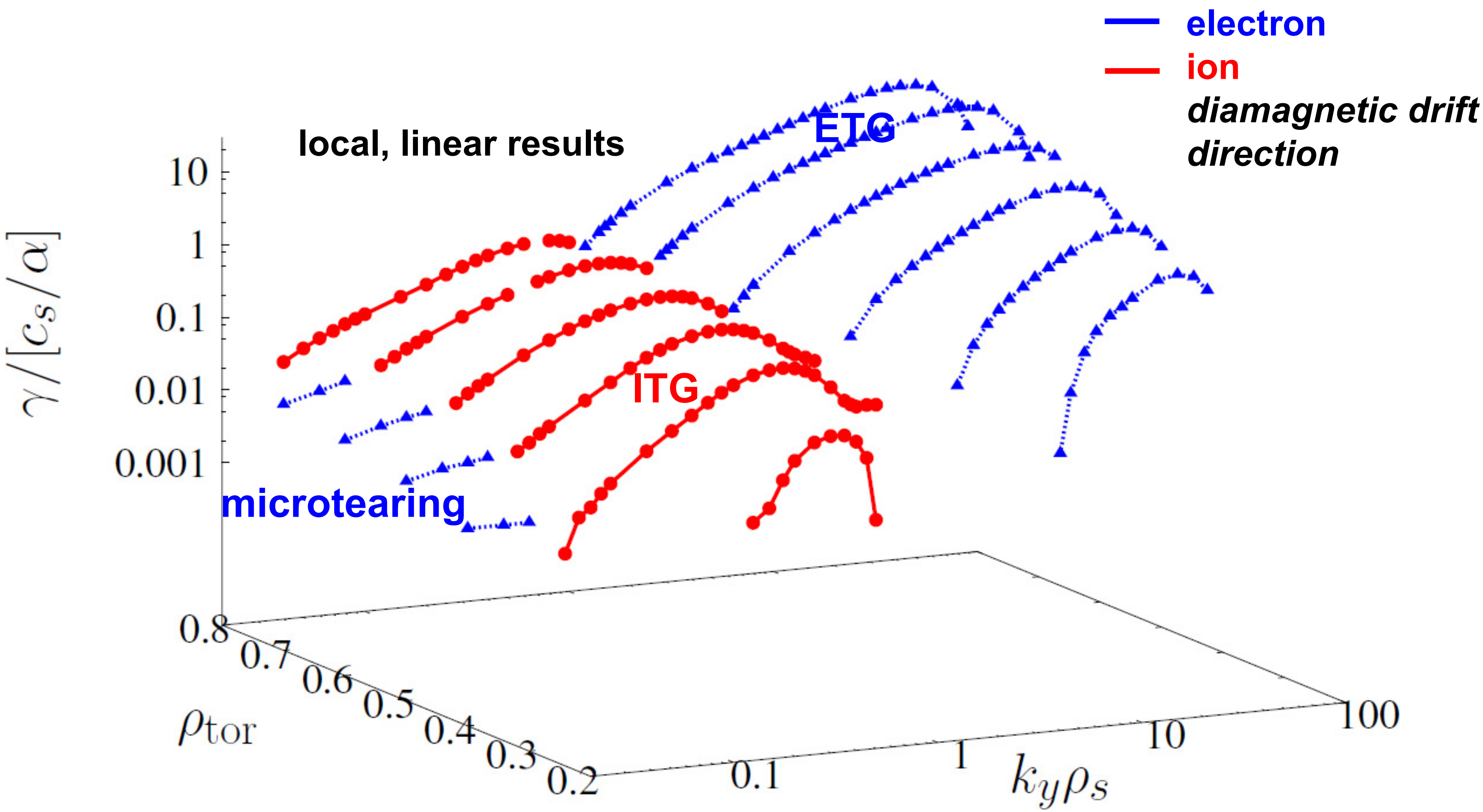
temperature and density profiles



gradient profiles



ASDEX-Upgrade #22009, L-mode regime II



- ITG much more pronounced
- However, high-k modes still considerably excited

ASDEX-Upgrade #22009, L-mode regime II

(removed unpublished content for web upload)

publication is expected in the next months

- Heat flux again in the right ballpark compared to experiment
- Local and global results agree reasonably well
- Transport level fall-off less pronounced at larger ρ_{tor}

Conclusions

Summary

New GENE features

- Local and global neoclassical solvers
- Consideration of parallel magnetic field fluctuations

Measuring finite-size effects in ASDEX-Upgrade L-mode discharges

- Profiles & equilibrium directly from experiment
- Differences local/nonlocal (gradient-driven) not pronounced here
  → compare to TCV (Daniel's talk), H-mode plasmas (upcoming)
- Approx. heat flux matching
- However, the radial profiles either indicate an overestimated ion temperature or might point to contribution from scales not being covered here (ETG?)