Direct multi-scale coupling of a transport code to gyrokinetic turbulence codes

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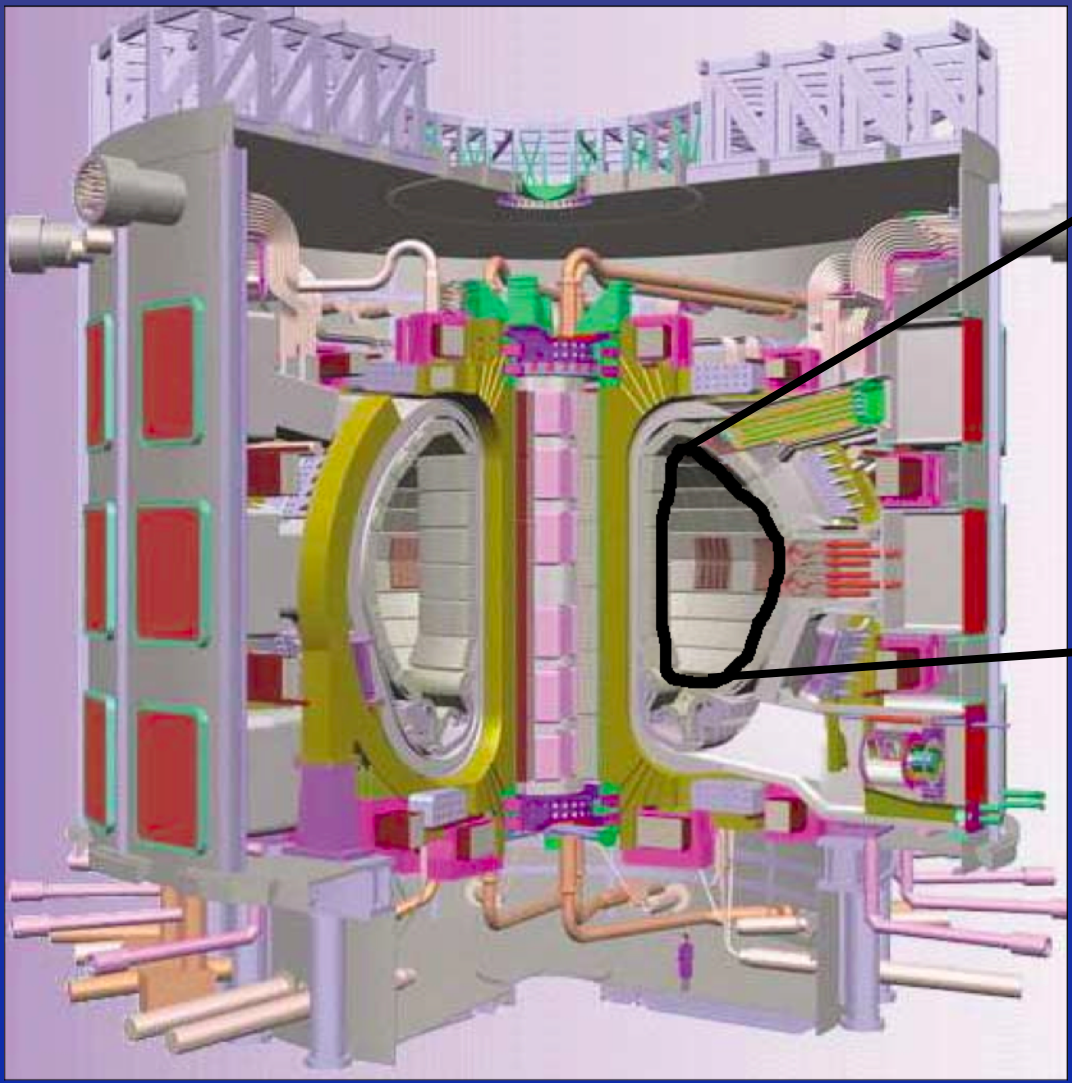
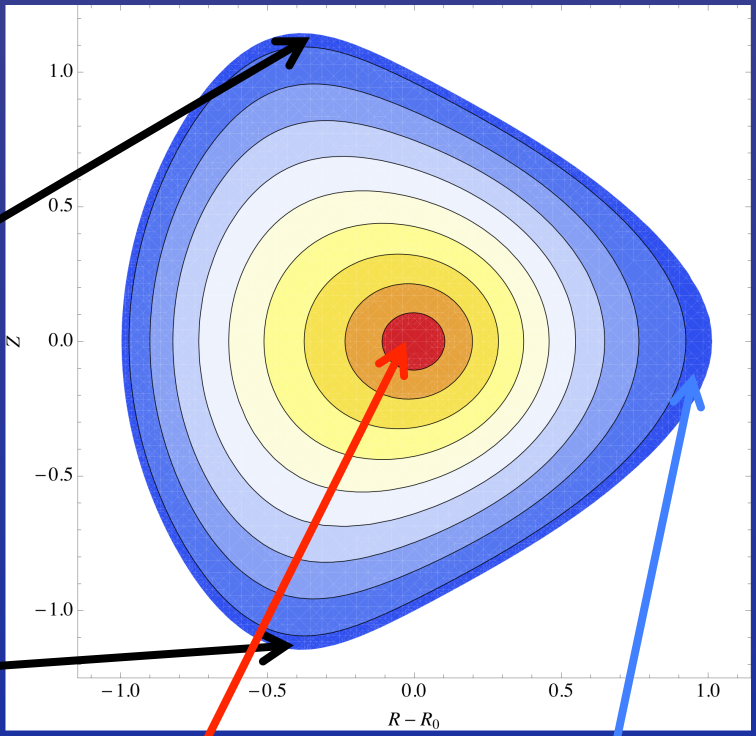
Overview

- Motivation
- Multi-scale model
- TRINITY simulation results
- Future directions

Magnetic confinement fusion



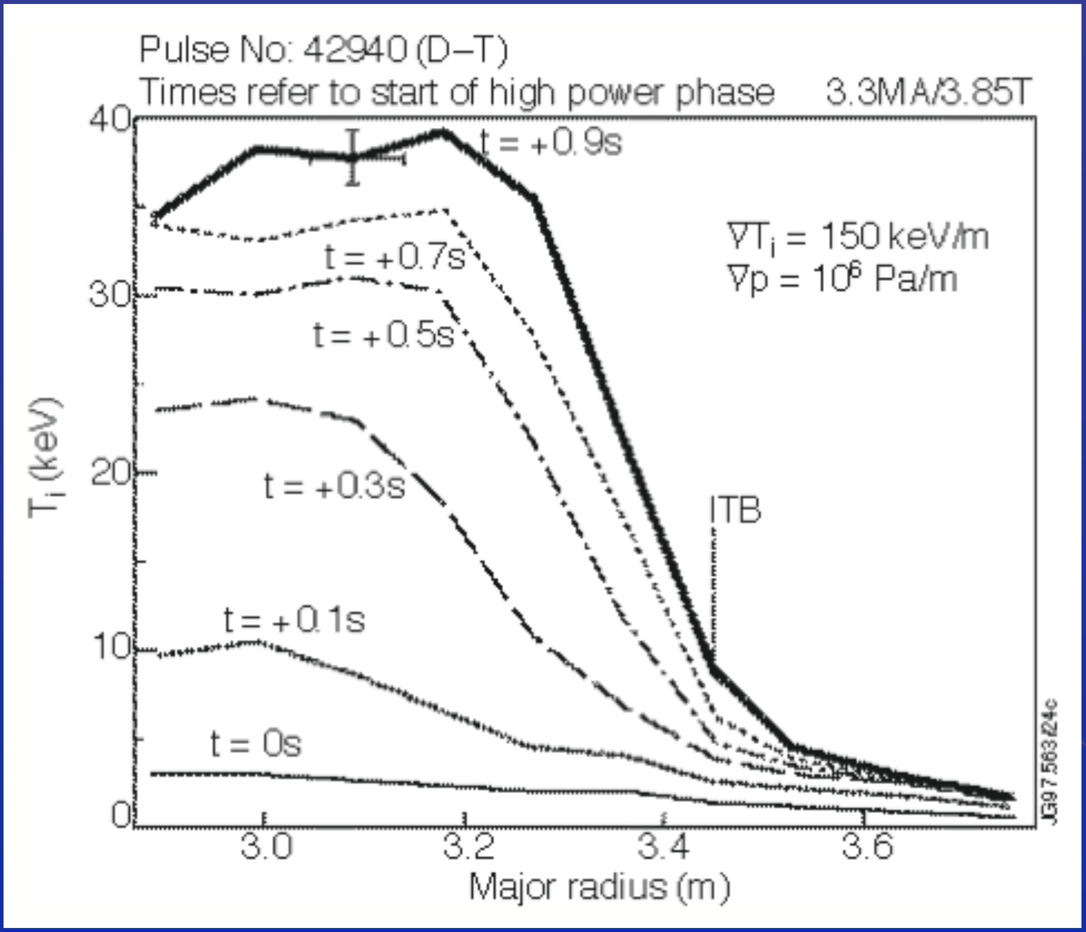
ITER



Hot, dense

Cold, dilute

Objective

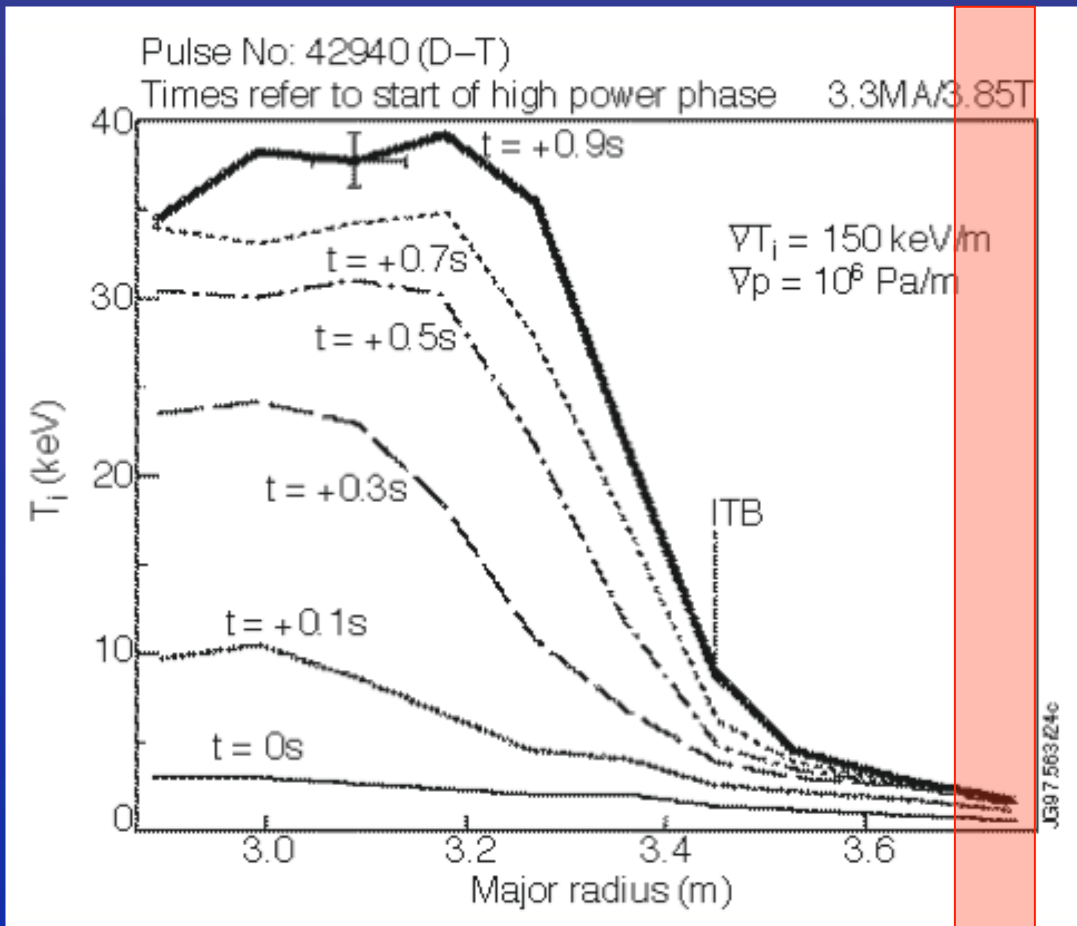


Connor et al. (2004)

Core:
multi-physics,
multi-scale

Edge:
multi-physics,
multi-scale

Objective



Connor et al. (2004)

Core:
multi-physics,
multi-scale

- **kinetic turbulence**
- neoclassical
- sources
- magnetic equilibrium
- MHD

Multiple scale problem

Physics	Perpendicular spatial scale	Temporal scale
Turbulence from ETG modes	$k_\perp^{-1}$ ~ 0.005 – 0.05 cm	ω_* ~ 0.5 - 5.0 MHz
Turbulence from ITG modes	$k_\perp^{-1}$ ~ 0.3 - 3.0 cm	ω_* ~ 10 - 100 kHz
Transport barriers	Measurements suggest width ~ 1 - 10 cm	100 ms or more in core?
Discharge evolution	Profile scales ~ 200 cm	Energy confinement time ~ 2 - 4 s

simulation cost: $(L_\parallel/\Delta_\parallel) \times (L_\perp/\Delta_\perp)^2 \times (L_v/\Delta_v)^2 \times (L_t/\Delta t) \sim 10^{21}$

Major Theoretical & Algorithmic Speedups

Slide from G.W. Hammett

relative to simplest brute force, fully resolved, algorithm, for ITER $1/\rho_* = a/\rho \sim 700$

- Nonlinear gyrokinetic equation
  - ion polarization shielding eliminates plasma freq. $\omega_{pe}/\Omega_{ci} \sim m_i/m_e$ — $x10^3$
  - ion polarization eliminates ρ_e & Debye scales $(\rho_i/\rho_e)^3$ — $x10^5$
  - average over fast ion gyration, $\Omega_{ci} / \omega_* \sim 1/\rho_*$ — $x10^3$
- Continuum or δf PIC, reduces noise, $(f_0/\delta f)^2 \sim 1/\rho_*^2$ — $x10^6$
- Field-aligned coordinates (nonlinear extension of ballooning coord.)

  $\Delta_{||} / (\Delta_\perp q R / a) \sim a / (q R \rho_*)$ — x70
- Flux-tube / Toroidal annulus wedge, ↓ simulation volume
  - $k_\theta \rho_i$ = 0, 0.05, 0.1, …, 1.0

    n = 0, 15, 30, …, 300 (i.e., 1/15 of toroidal direction) — x15
  - $L_r \sim a/5 \sim 140\ \rho \sim 10$ correlation lengths — x5
- High-order / spectral algorithms in 5-D, 2^5 x 2 — x64
- Implicit electrons — x5-50
- Total combined speedup of all algorithms — $x10^{23}$
- Massively parallel computers (Moore's law 1982-2007) — $x10^5$

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Transport equations in GK

Moment equations for evolution of mean quantities:

$$\frac{\partial n_s}{\partial t} = -\frac{1}{V'}\frac{\partial}{\partial \psi}\left(V'\left\langle \mathbf{\Gamma}_s \cdot \nabla\psi\right\rangle\right) + S_n$$

$$\frac{3}{2}\frac{\partial n_s T_s}{\partial t} = -\frac{1}{V'}\frac{\partial}{\partial \psi}\left(V'\left\langle \mathbf{Q}_s \cdot \nabla\psi\right\rangle\right)$$

$$+ \quad T_s\left(\frac{\partial \ln n_s}{\partial \psi} - \frac{3}{2}\frac{\partial \ln T_s}{\partial \psi}\right)\left\langle \mathbf{\Gamma}_s \cdot \nabla\psi\right\rangle + \frac{\partial \ln T_s}{\partial \psi}\left\langle \mathbf{Q}_s \cdot \nabla\psi\right\rangle$$

$$- \quad \left\langle \int d^3v \frac{h_s T_s}{F_{0s}}\left\langle C[h_s]\right\rangle_{\mathbf{R}}\right\rangle + n_s \nu_\epsilon^{su}\left(T_u - T_s\right) + S_p$$

$$\frac{\partial L}{\partial t} = -\frac{1}{V'}\frac{\partial}{\partial \psi}\left(V'\sum_s \left\langle \pi_s\right\rangle\right) + S_L$$

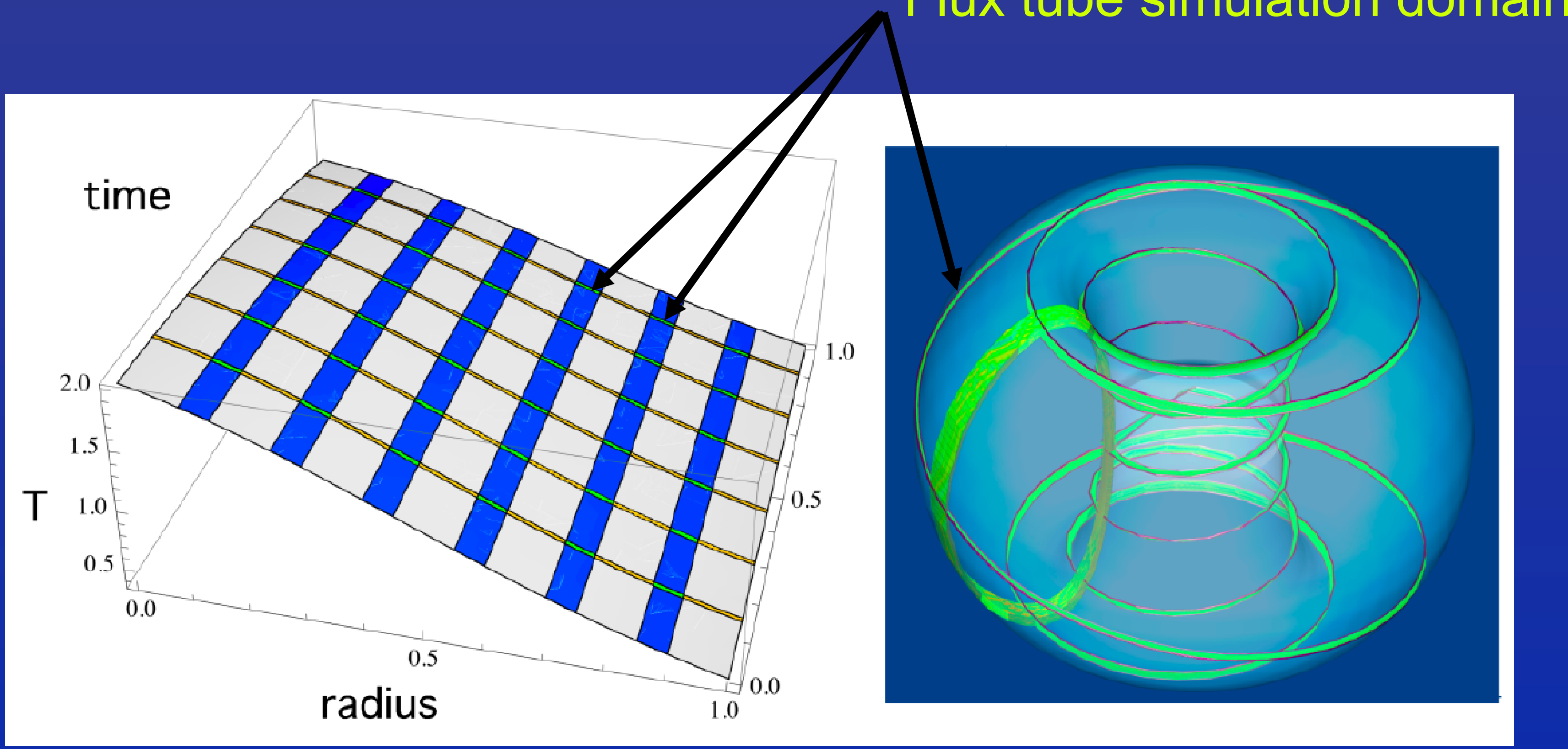
…depend on fluctuations

Sugama (1997)

Multiscale grid

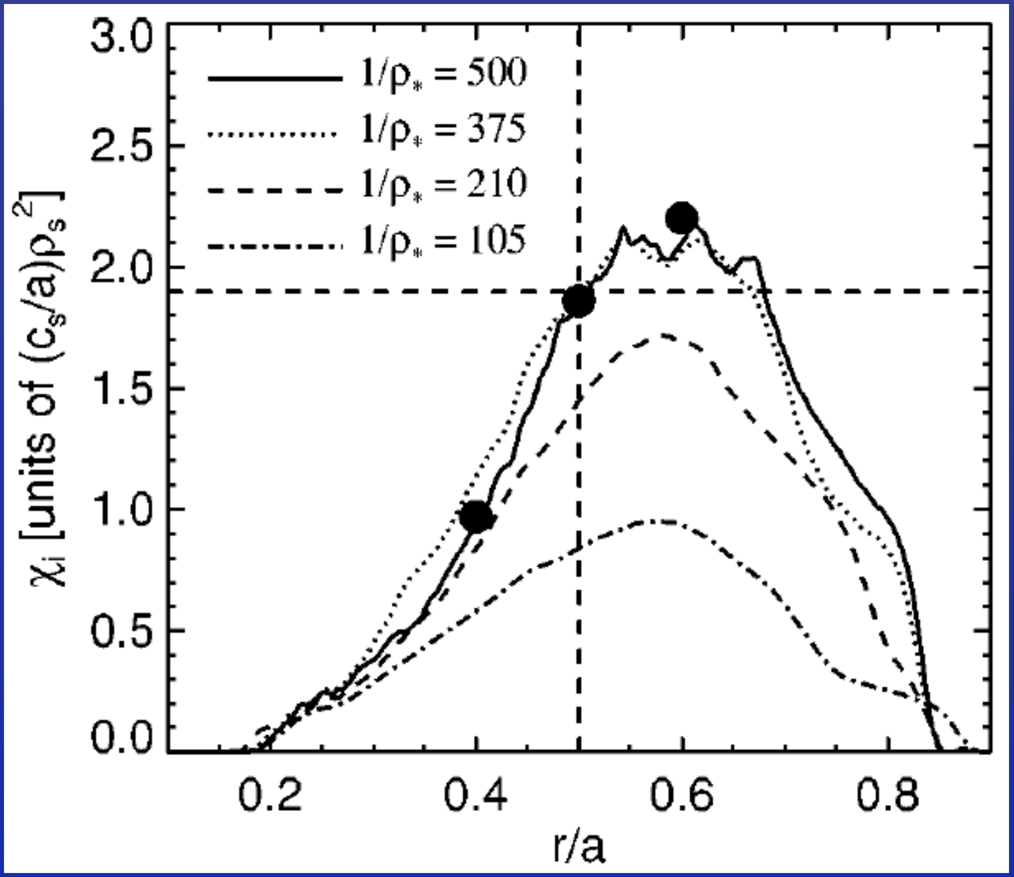
- Turbulent fluctuations calculated in small regions of fine space-time grid embedded in "coarse" grid (for mean quantities)

Flux tube simulation domain



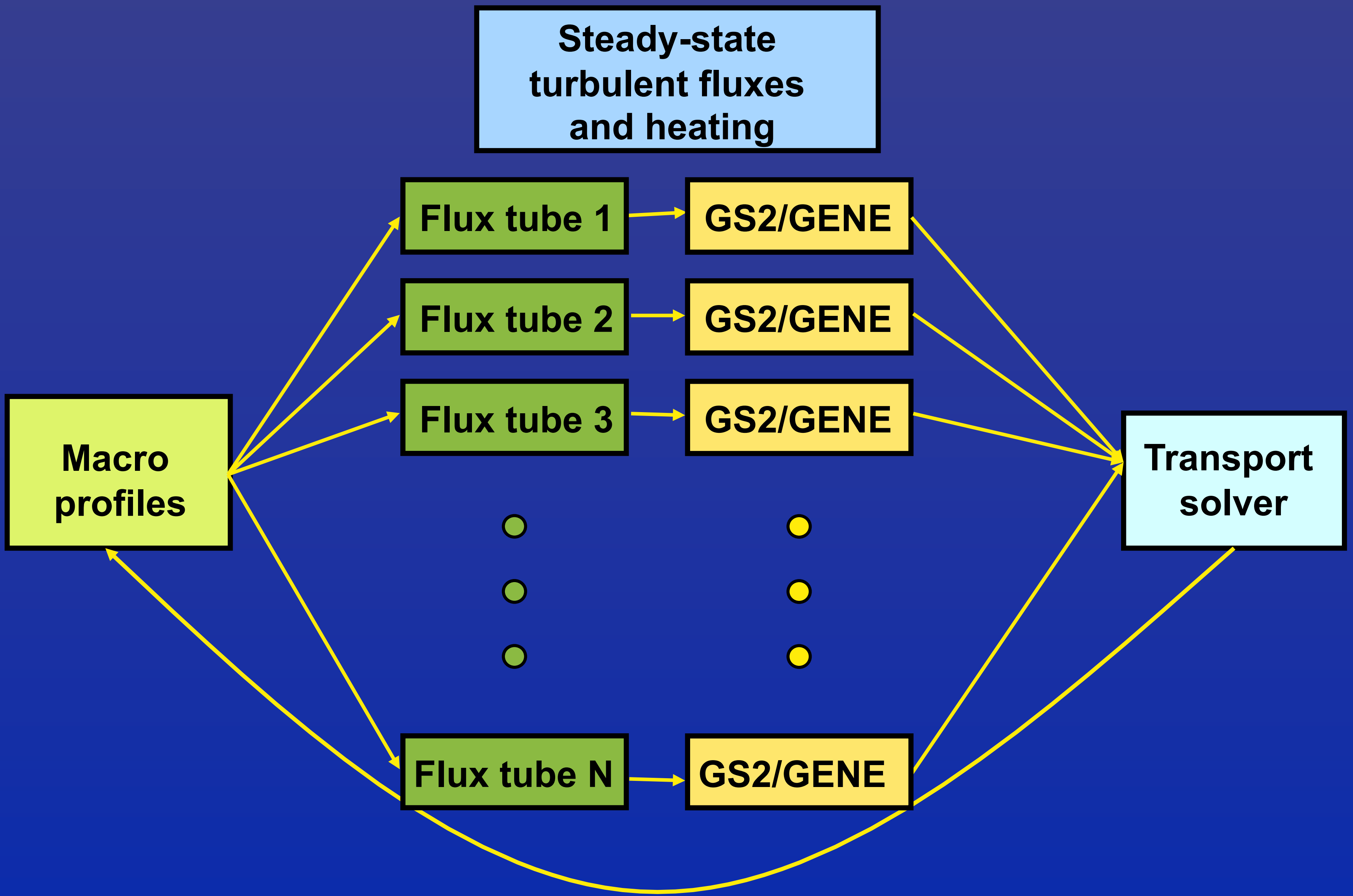
Validity of flux tube approximation

- Lines represent global simulations from GYRO
- Dots represent local (flux tube) simulations from GS2
- Excellent agreement for $\rho_* \ll 1$

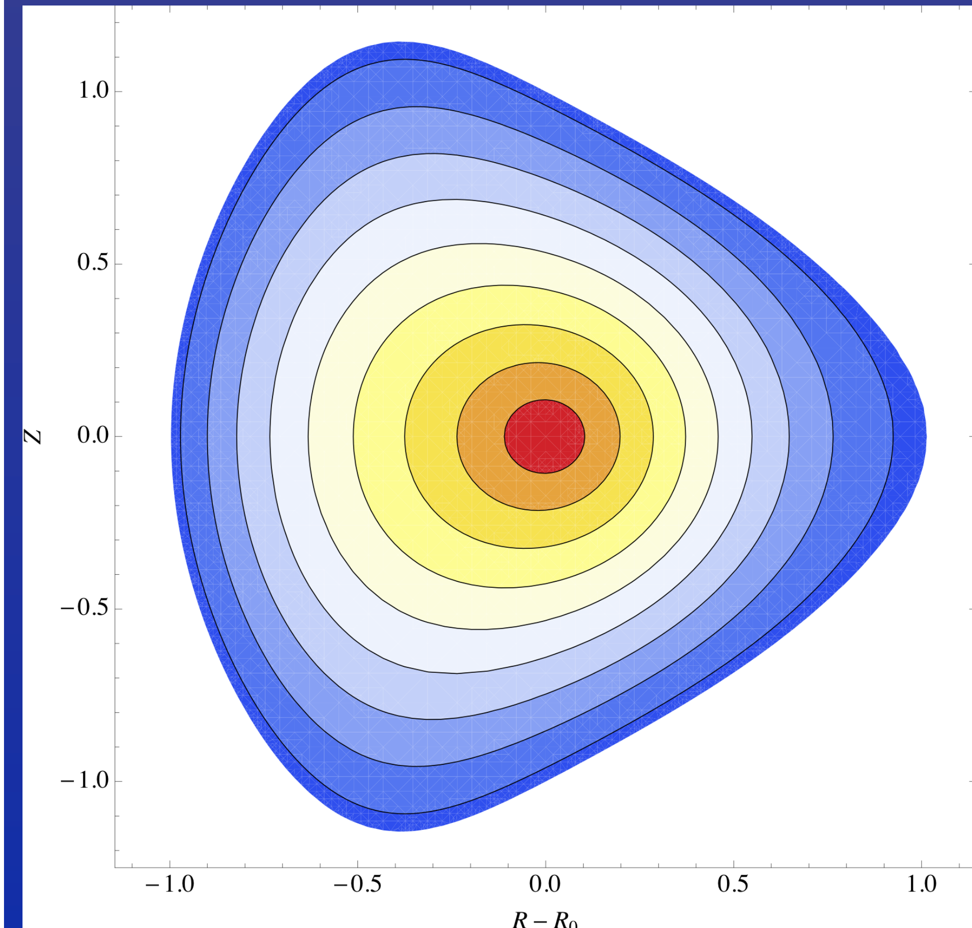


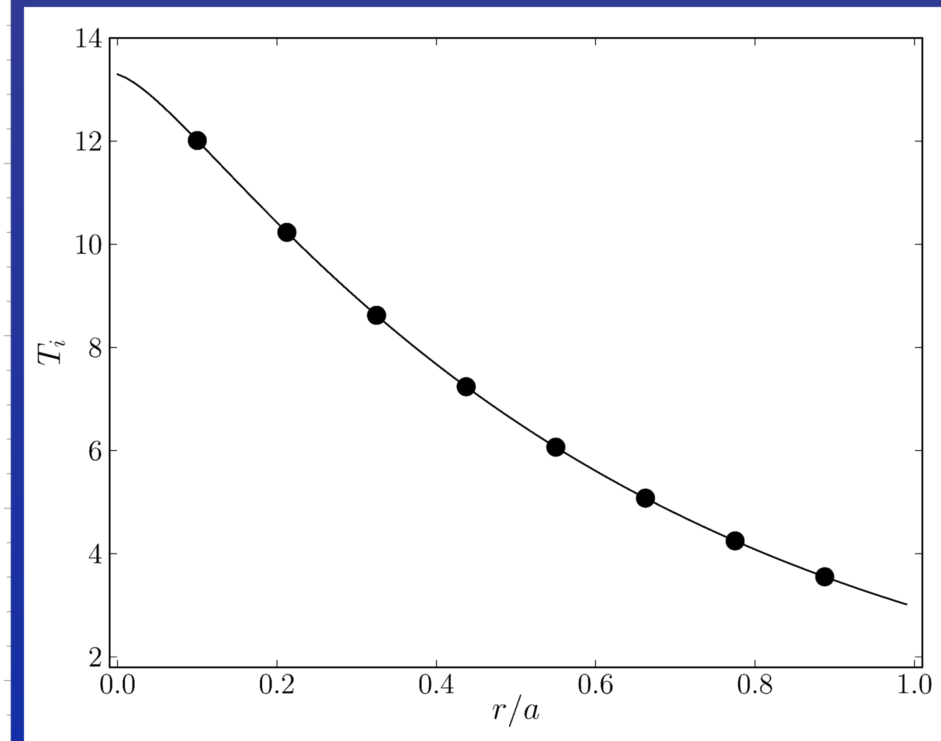
Candy et al (2004)

Trinity schematic



Sampling profile with flux tubes





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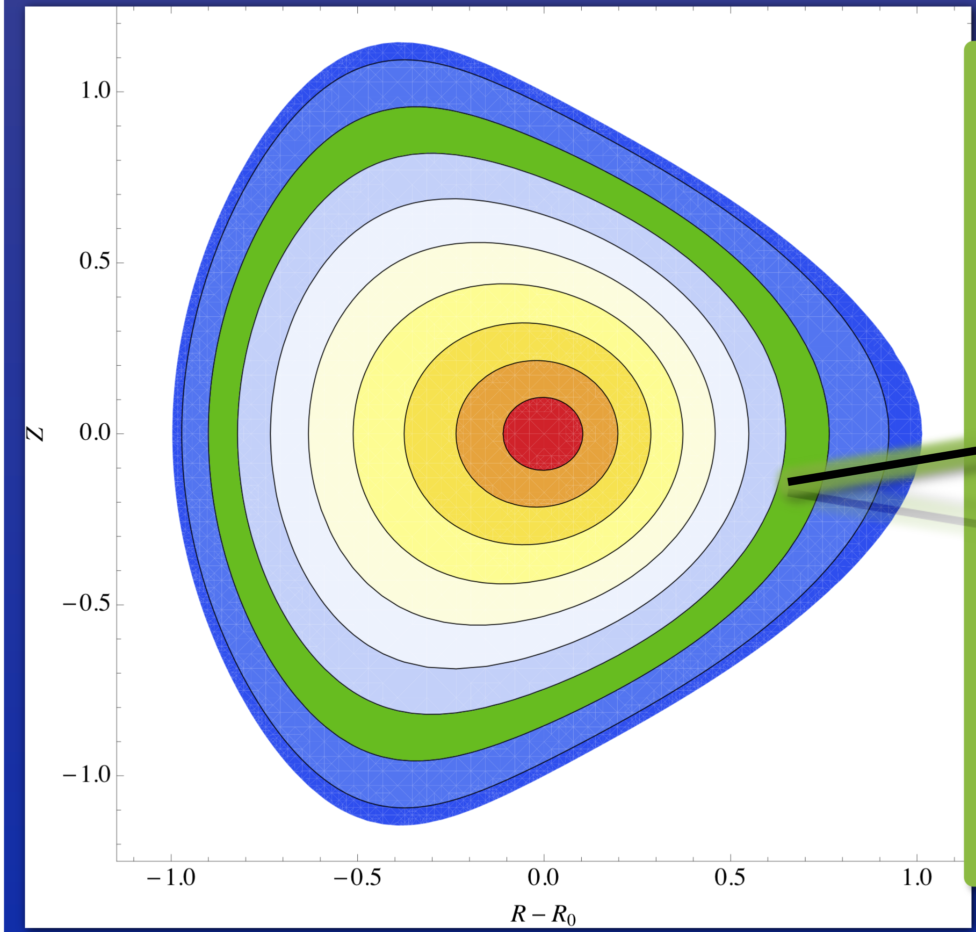
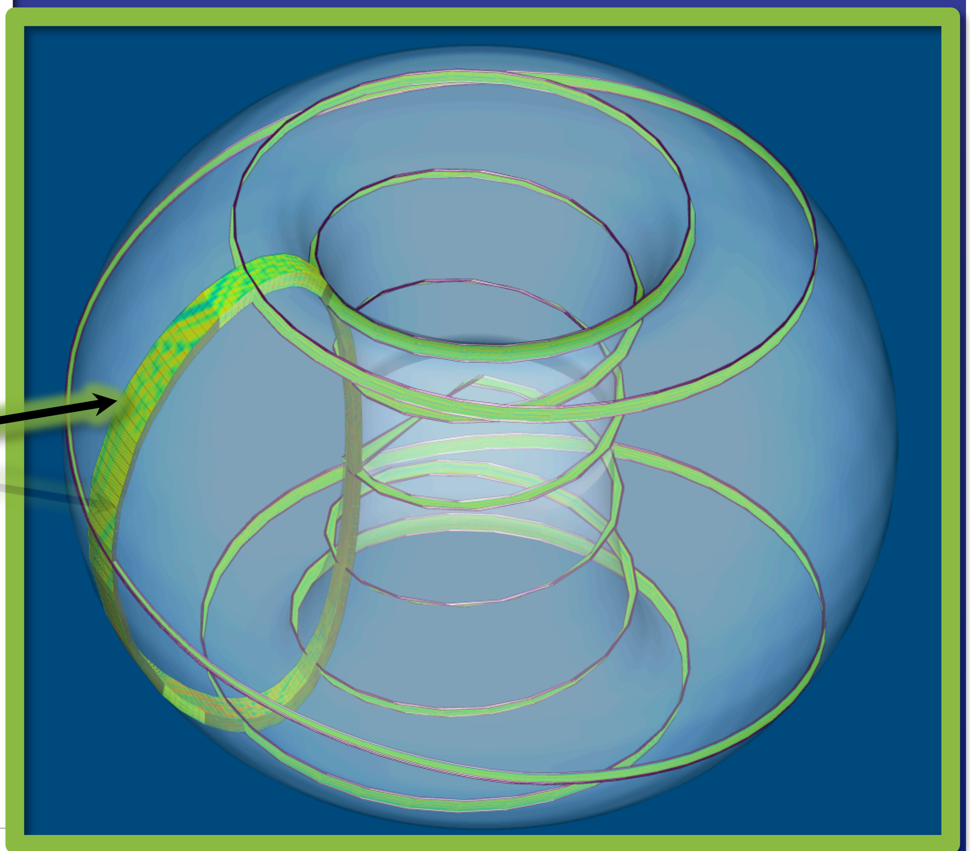




Simulation volume reduced by factor of ~100

Trinity transport solver

- Transport equations are stiff, nonlinear PDEs. Implicit treatment via Newton's Method (multi-step BDF, adaptive time step) allows for time steps ~0.1 seconds (vs. turbulence sim time ~0.001 seconds)
- Challenge: requires computation of quantities like

$$\Gamma_j^{m+1} \approx \Gamma_j^m + \left(\mathbf{y}^{m+1} - \mathbf{y}^m\right) \left.\frac{\partial \Gamma_j}{\partial \mathbf{y}}\right|_{\mathbf{y}^m} \qquad \mathbf{y} = \left[\{n_k\}, \{p_{i_k}\}, \{p_{e_k}\}\right]^T$$

- Local approximation: $\frac{\partial \Gamma_j}{\partial n_k} = \frac{\partial \Gamma_j}{\partial n_j} + \frac{\partial \Gamma_j}{\partial (R/L_n)_j} \frac{\partial (R/L_n)_j}{\partial n_k}$
- Simplifying assumption: normalized fluxes depend primarily on gradient scale lengths

Trinity transport solver

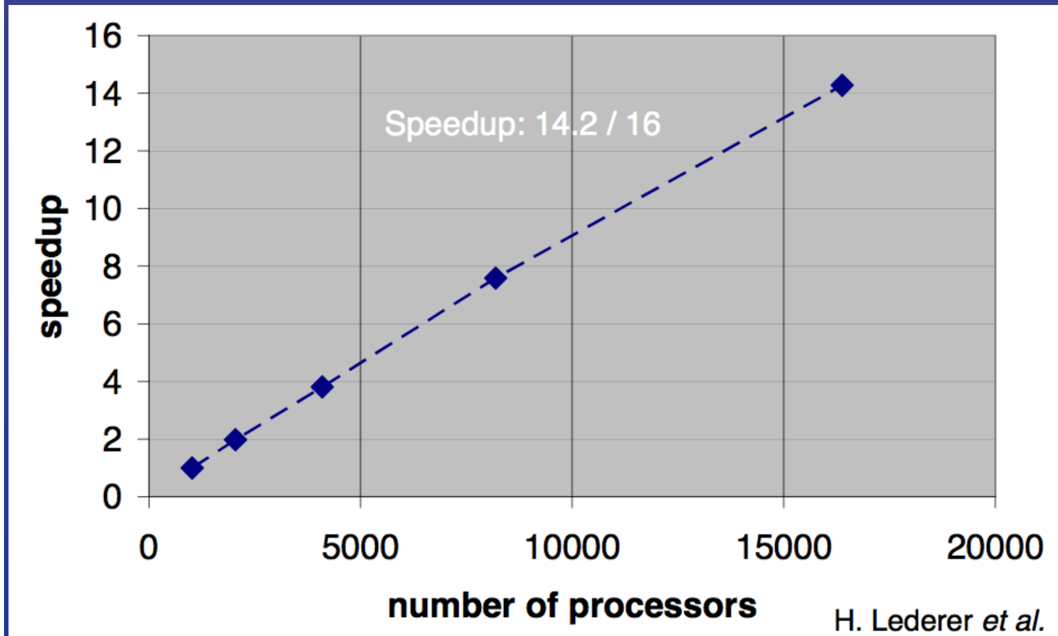
- Calculating flux derivative approximations:
  - at every radial grid point, simultaneously calculate $\Gamma_j[(R/L_n)_j^m]$ and $\Gamma_j[(R/L_n)_j^m + \delta]$ using 2 different flux tubes
  - use 2-point finite differences:

$$\frac{\partial \Gamma_j}{\partial (R/L_n)_j} \approx \frac{\Gamma_j[(R/L_n)_j^m] - \Gamma_j[(R/L_n)_j^m + \delta]}{\delta}$$

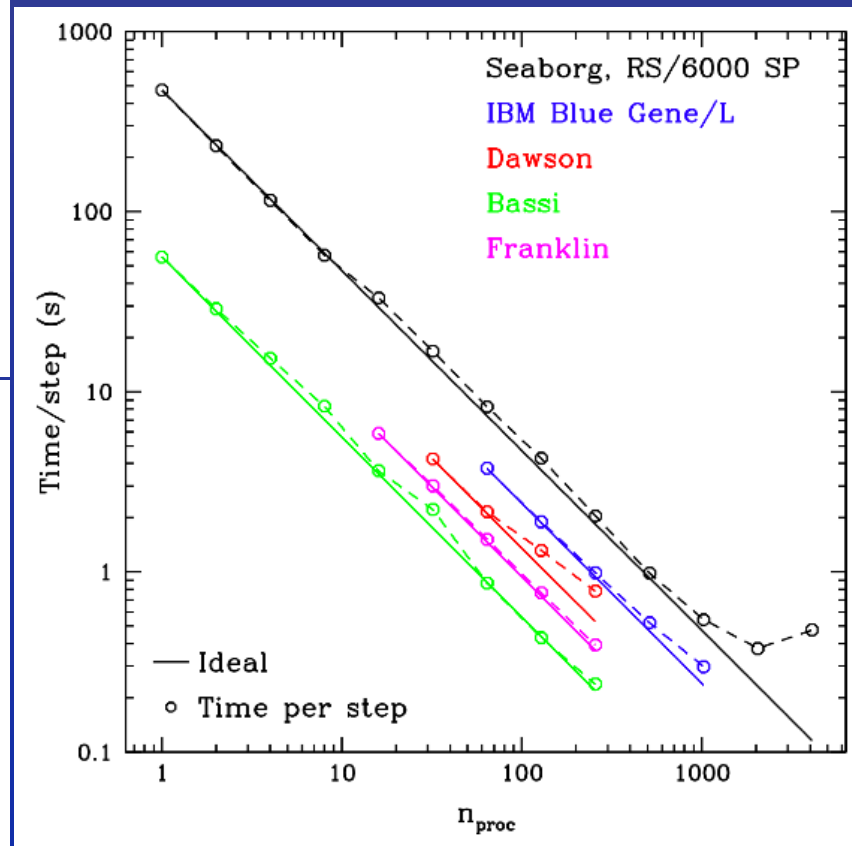
  - possible because flux tubes independent (do not communicate during calculation)
  - perfect parallelization (almost)

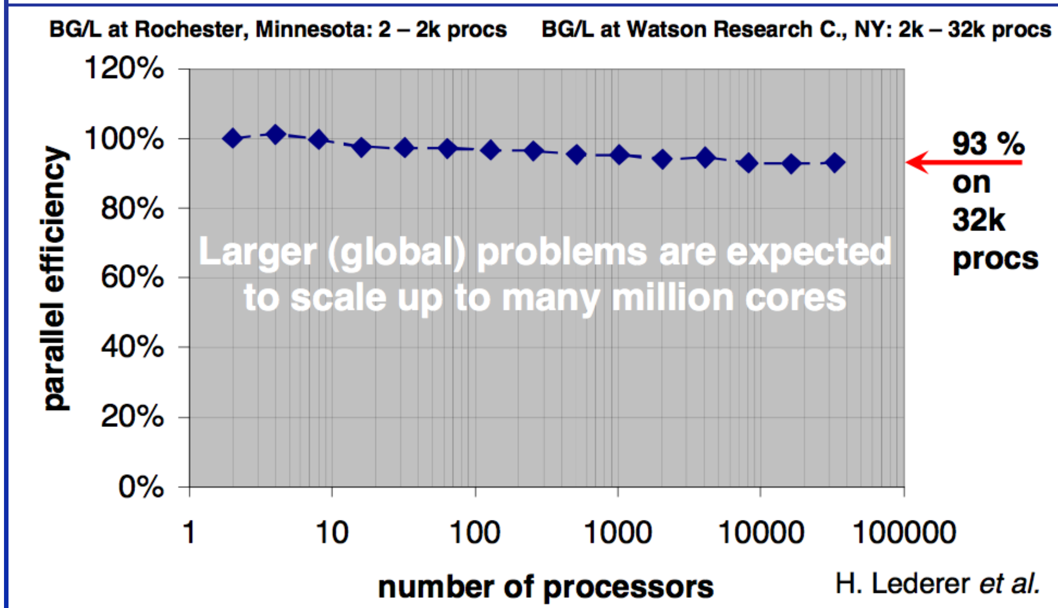
Flux tube scaling

GENE strong scaling



GS2 strong scaling





GENE weak scaling

Trinity scaling

- Example calculation with 10 radial grid points:
  - evolve density, toroidal angular momentum, and electron/ion pressures
  - simultaneously calculate fluxes for equilibrium profile and for 4 separate profiles (one for each perturbed gradient scale length)
  - total of 50 flux tube simulations running simultaneously
  - ~2000-4000 processors per flux tube => scaling to over 100,000 processors with high efficiency
- Adding radial grid points, multiple species, electron space-time scales, and other physics increases weak scaling by up to 10^4

Multi-scale simulation savings

- Statistical periodicity in toroidal direction takes advantage of $k_\perp^{-1} \ll L_\theta$: volume savings factor of ~10-100
- Exploitation of scale separation between turbulence and equilibrium evolution: time savings factor of ~100
- Total saving of ~10^4 + extreme parallelizability: simulation possible on current machines

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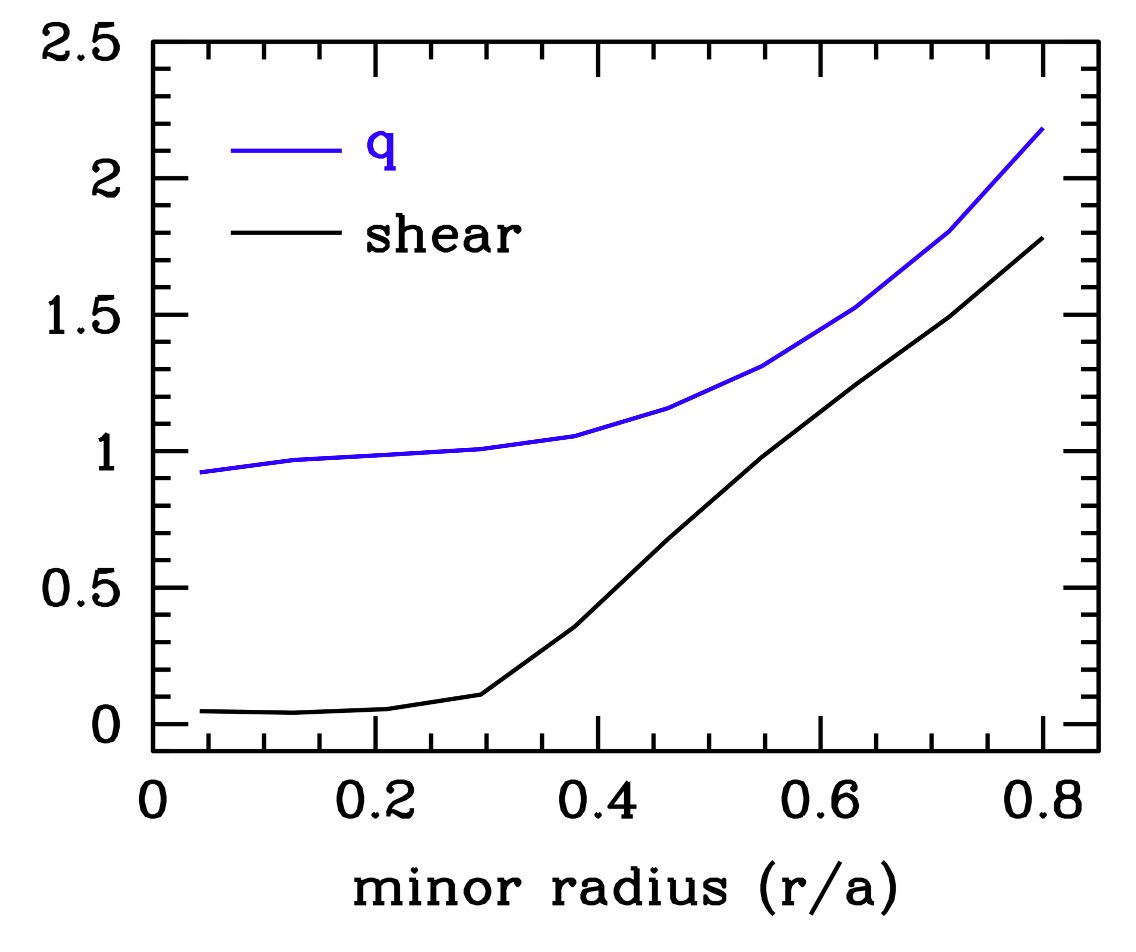
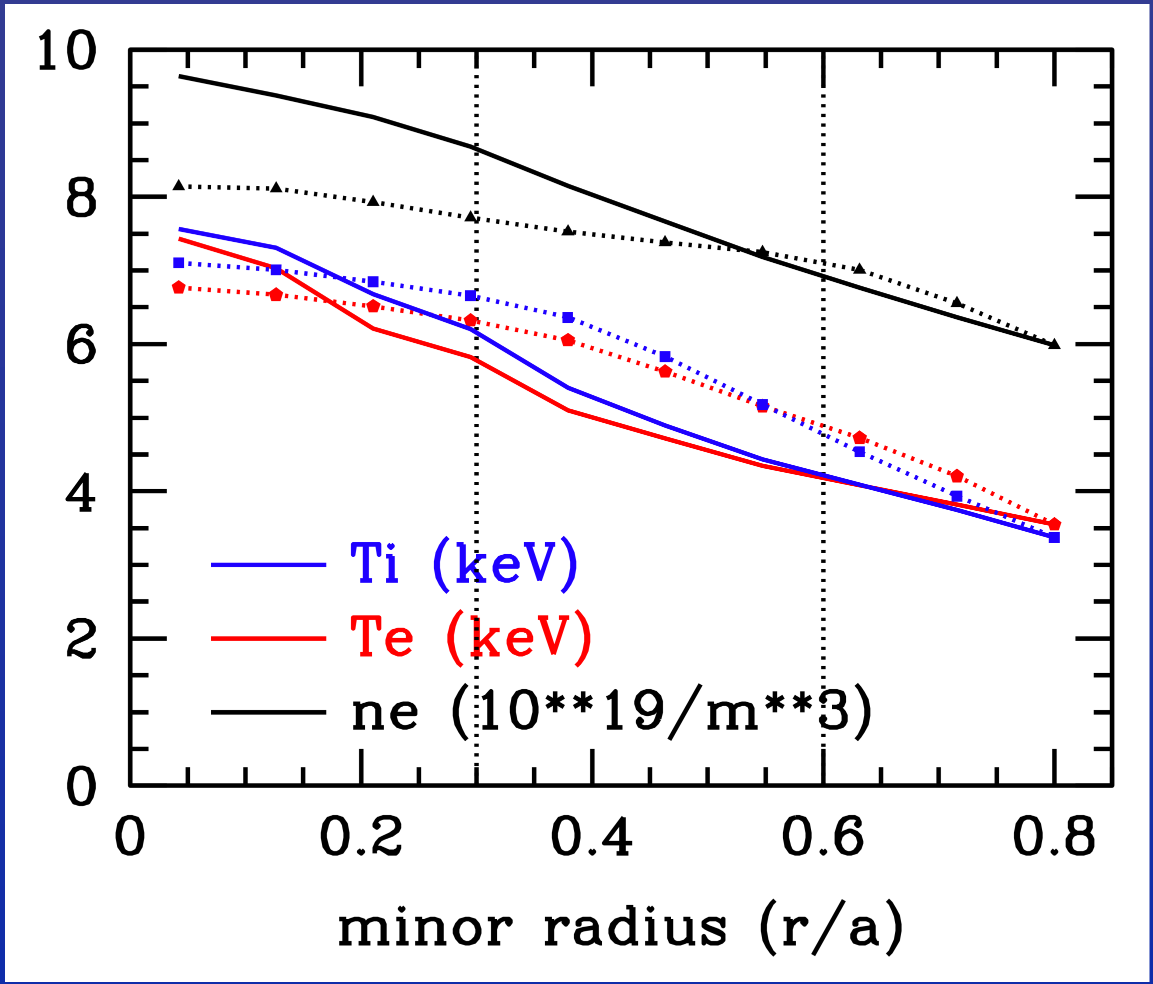
JET shot #42982



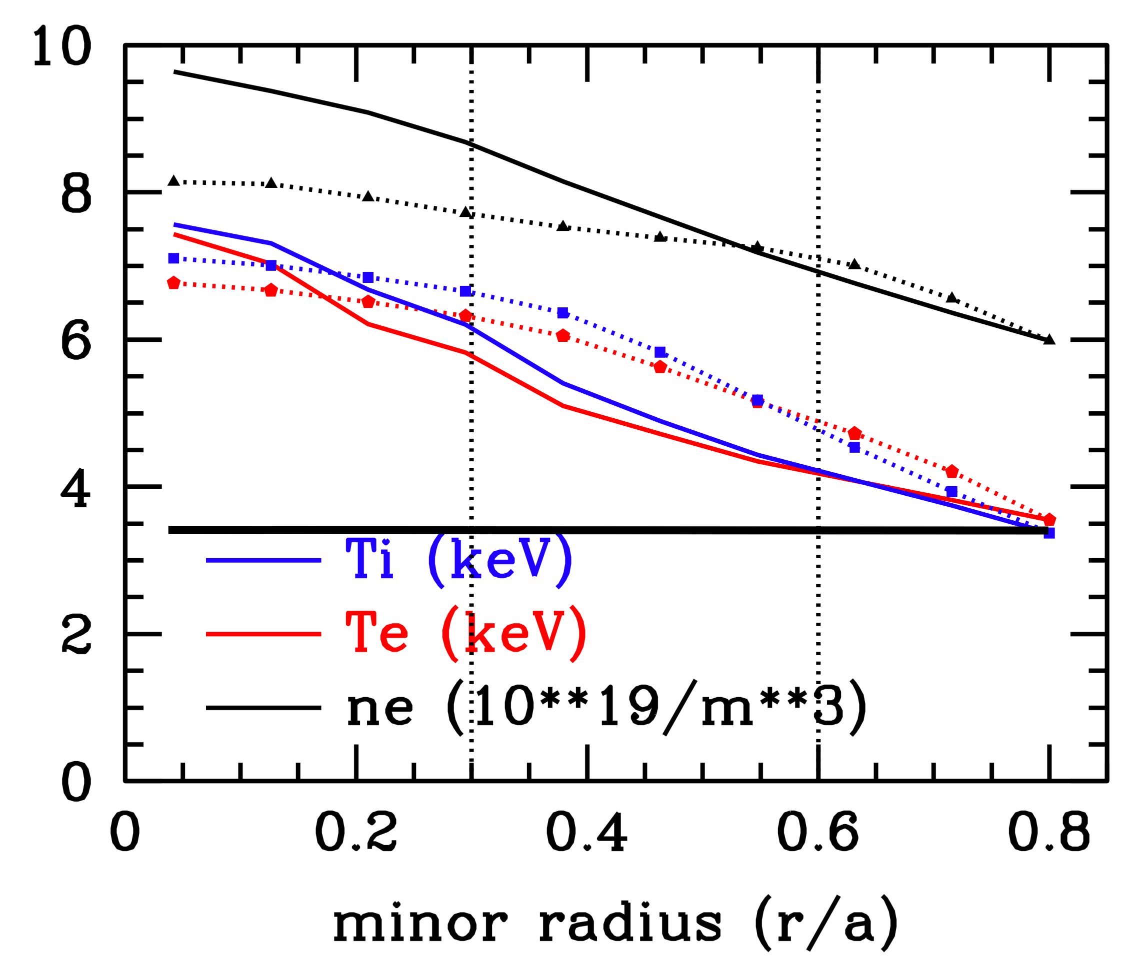
- ITER demo discharge
- H-mode D-T plasma, record fusion energy yield
- Miller local equilibrium model: q, shear, shaping
- B = 3.9 T on axis
- TRANSP fits to experimental data taken from ITER profile database

Evolving density profile



- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%
- Sources of discrepancy:
  - Large error bars
  - Flow shear absent

Evolving density profile



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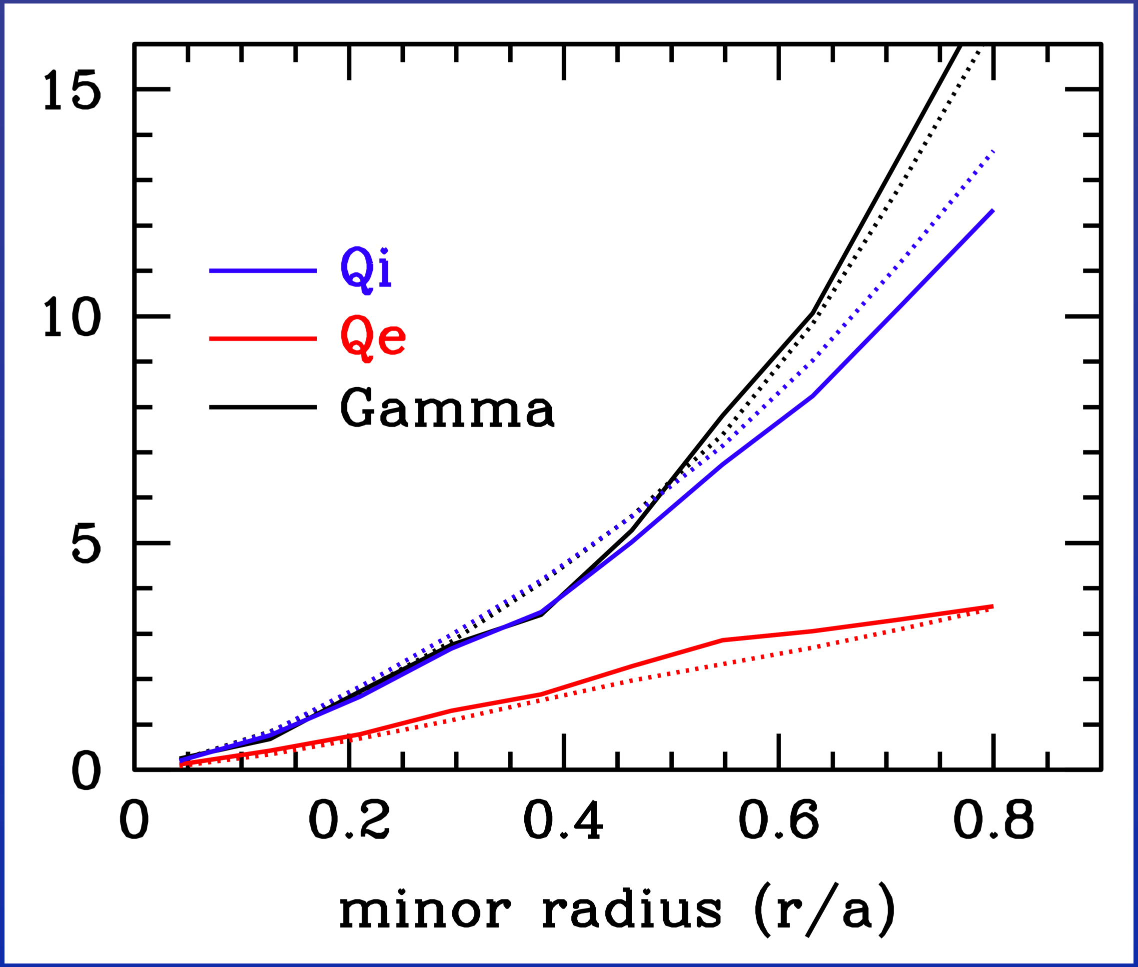
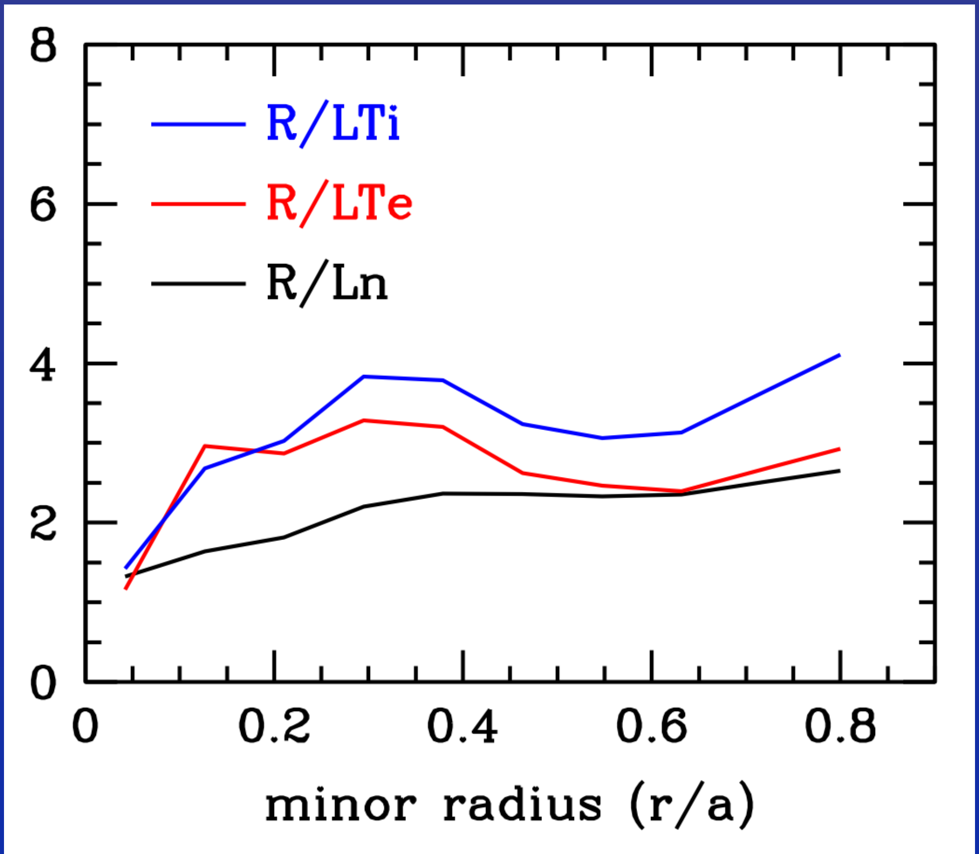
Power balance

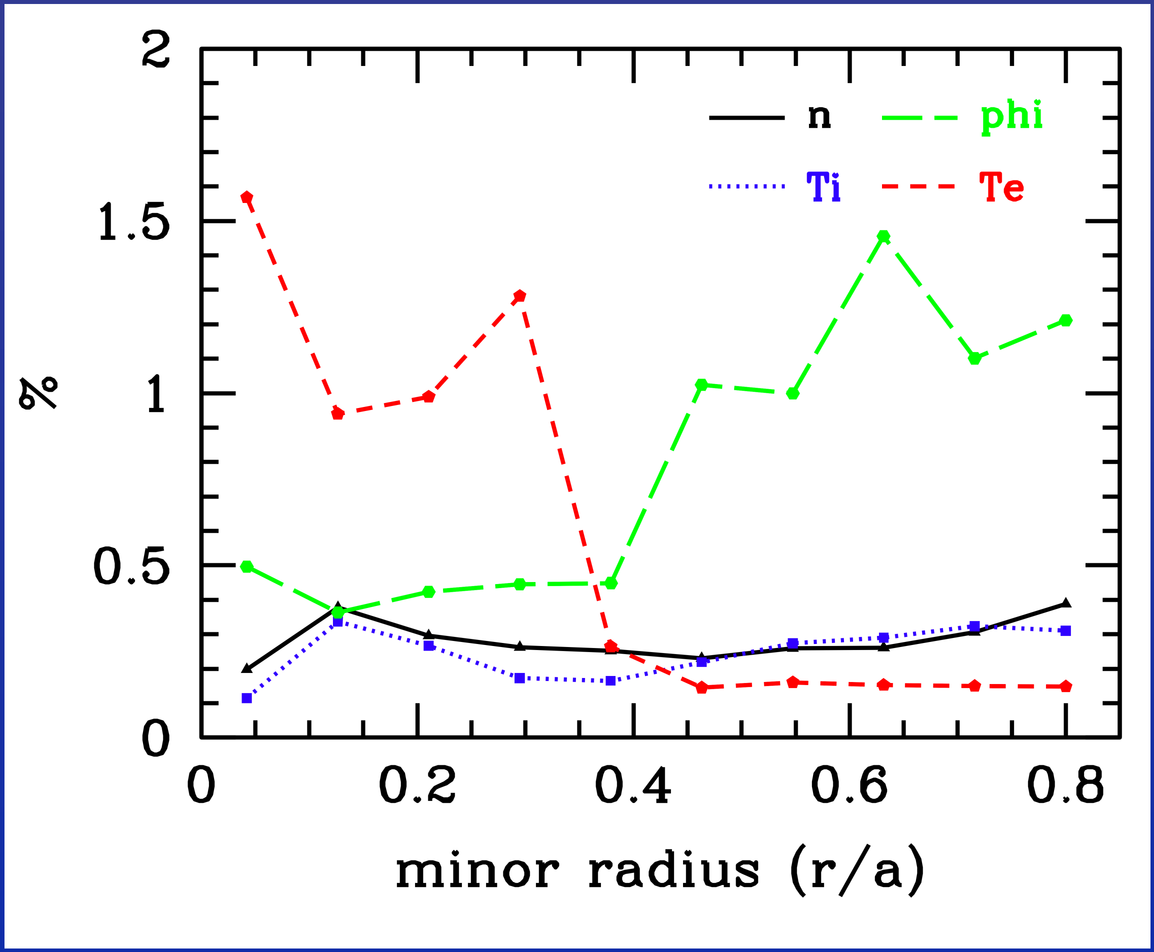


Profile stiffness

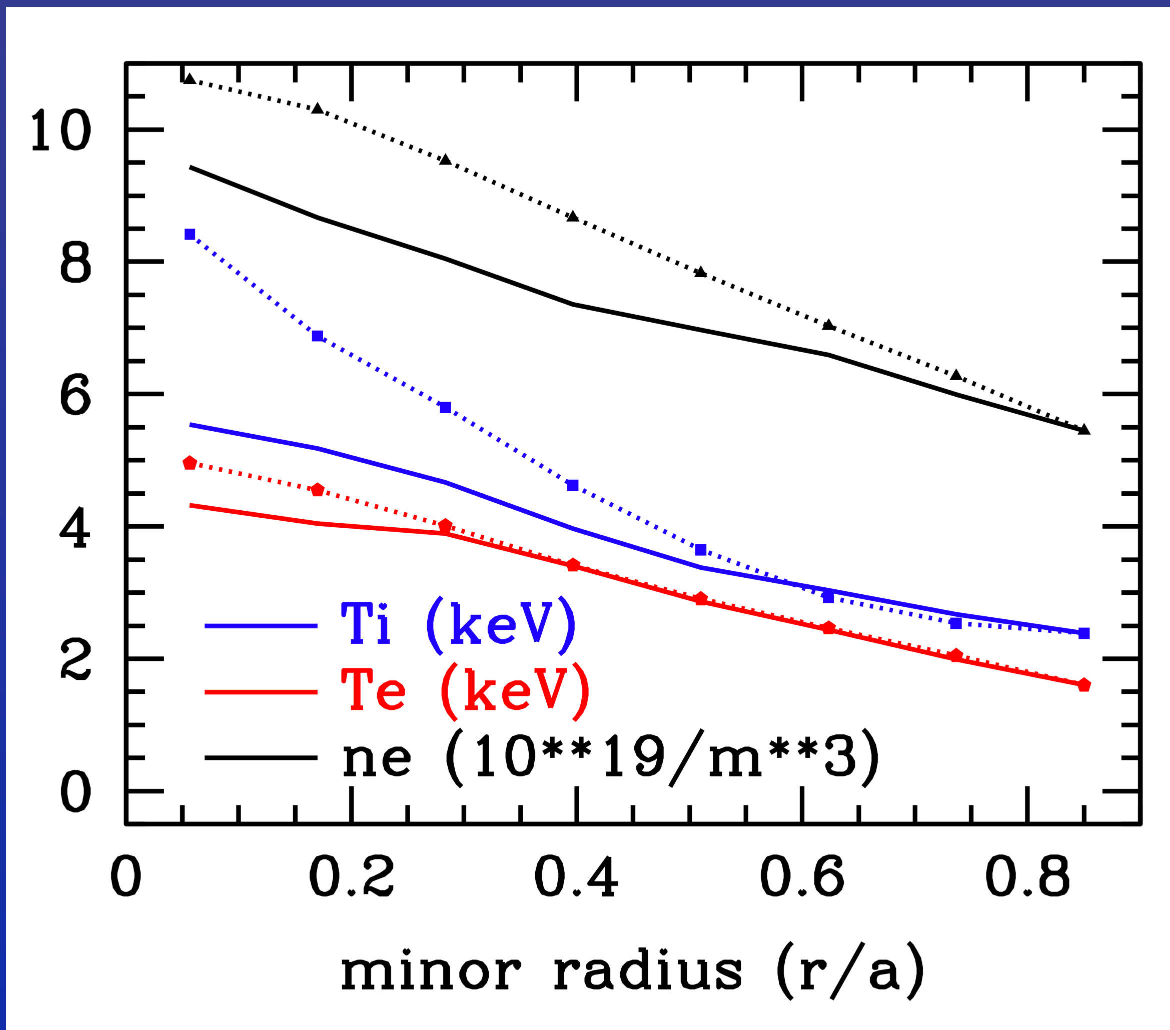
- ~ flat grad scale lengths indicative of stiffness (near critical gradient across most of minor radius)



Fluctuations



AUG shot #13151



- Fluxes calculated with GENE
- 8 radial grid points
- Costs ~400k CPU hrs (<24 clock hrs)
- Dens and electron temp profiles agree within ~10% across device
- Flow shear absent

Future directions

- Capture more physics
  - Magnetic equilibrium evolution
  - MHD stability
- Improve convergence
  - Flux dependences on density, temperature, etc.
- Coupling to global gyrokinetic code (GENE)
  - Address meso-scale spatial structures
- Coupling to GPU-based gyrofluid code (GRYFFIN)
  - Entire calculation in minutes on several GPUs