

# TRINITY: local gyrokinetics + global transport = predictive modeling of ITER-like plasma performance

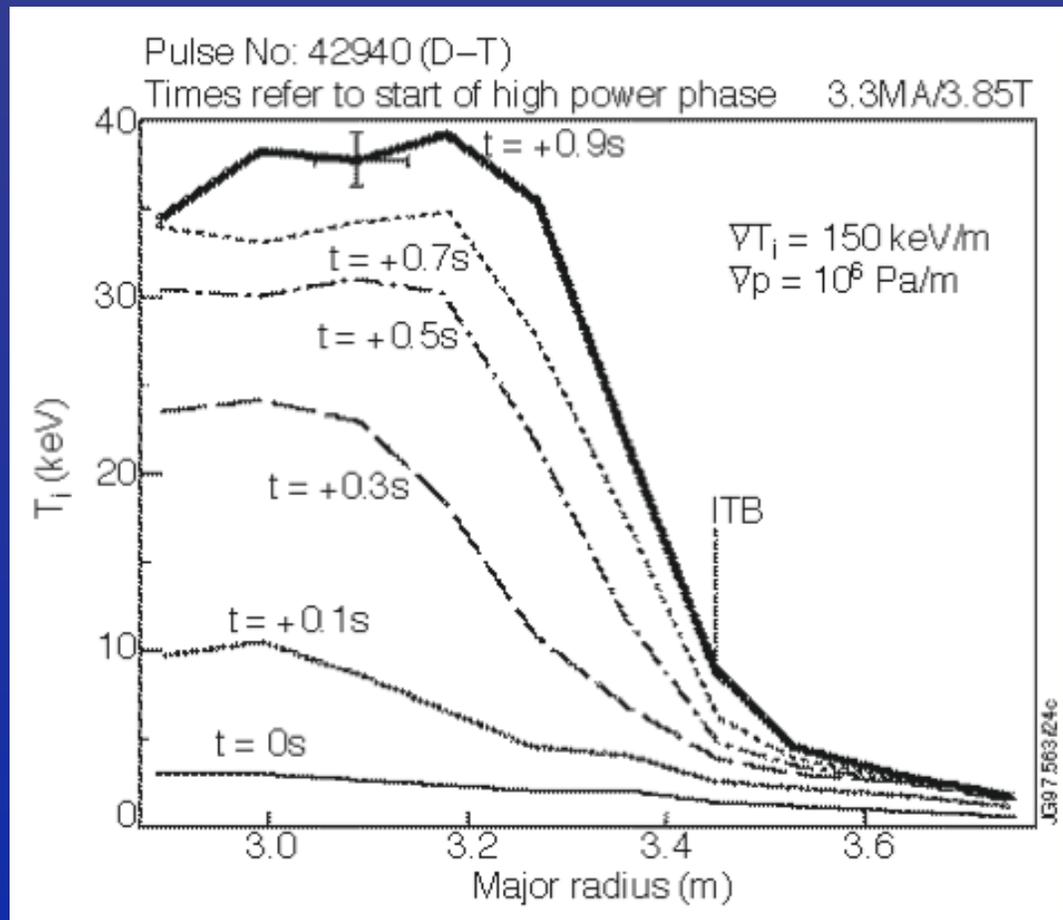
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# Overview

- Motivation
- Theoretical framework
- Numerical approach
- Trinity simulation results
- Future work

# Objective

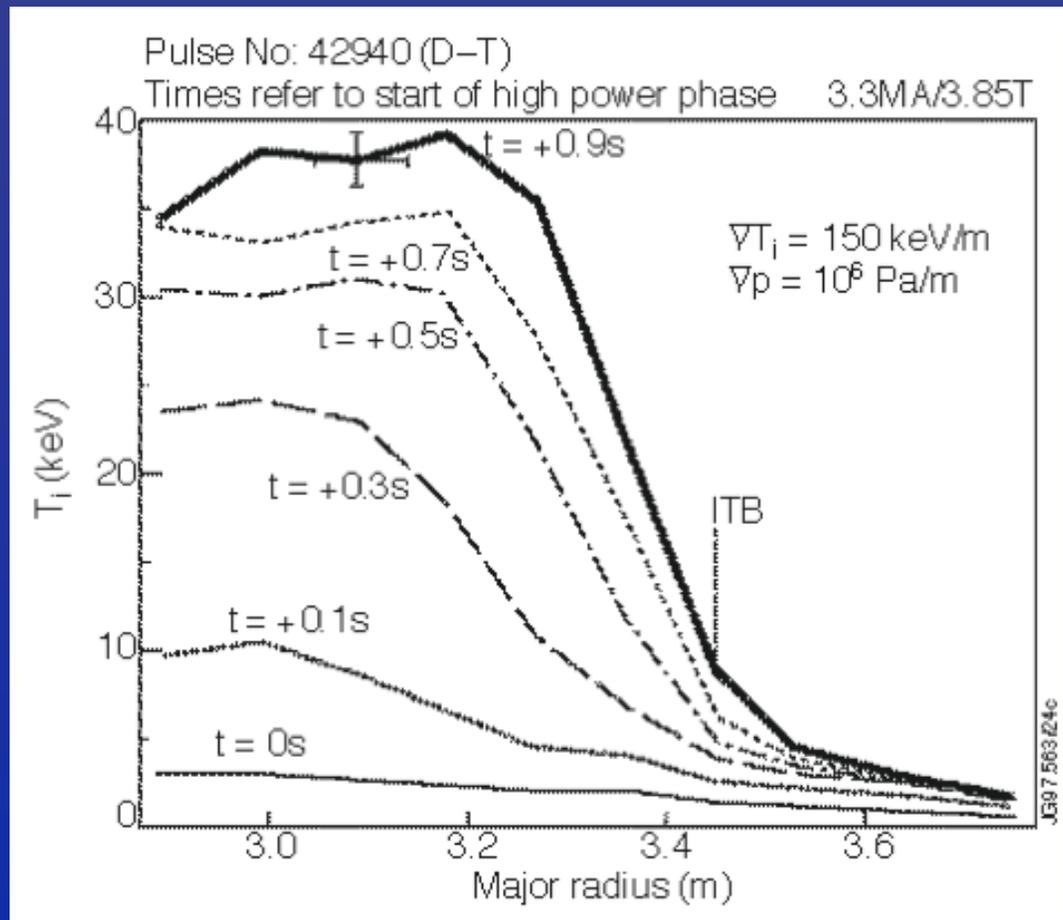


Core:  
multi-physics,  
multi-scale

Edge:  
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multi-scale

Connor et al. (2004)

# Objective



Core:  
multi-physics,  
multi-scale

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

Connor et al. (2004)

# Multiple scale problem

$$\frac{df}{dt} = C[f] \quad + \quad \frac{\omega}{\Omega_i} \sim \frac{\rho}{L} \ll 1$$

Physics	Perpendicular spatial scale	Temporal scale
Turbulence from ETG modes	$k_{\perp}^{-1} \sim 0.001 - 0.1 \text{ cm}$	$\omega_* \sim 0.5 - 5.0 \text{ MHz}$
Turbulence from ITG modes	$k_{\perp}^{-1} \sim 0.1 - 8.0 \text{ cm}$	$\omega_* \sim 10 - 100 \text{ kHz}$
Transport barriers	Measurements suggest width $\sim 1 - 10 \text{ cm}$	100 ms or more in core?
Discharge evolution	Profile scales $\sim 100 \text{ cm}$	Energy confinement time $\sim 2 - 4 \text{ s}$

# Full-f simulation cost

- Grid spacings in space (3D), velocity (2D) and time:

$$\Delta_{\perp} \sim 0.001 \text{ cm}, \quad L_{\perp} \sim 100 \text{ cm}$$

$$\Delta_{\parallel} \sim 10 \text{ cm}, \quad L_{\parallel} \sim 10 \text{ m}$$

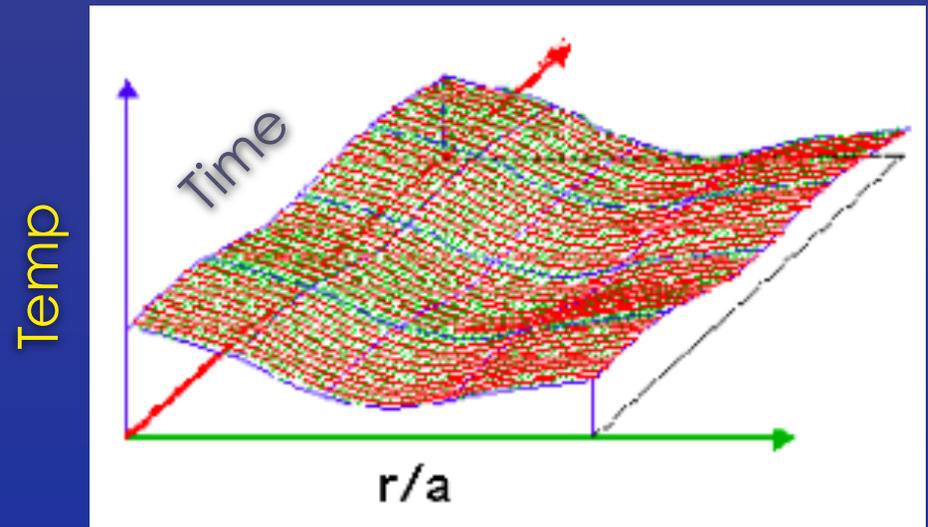
$$\Delta v \sim 0.1 v_{th}, \quad L_v \sim v_{th}$$

$$\Delta t \sim 10^{-7} \text{ s}, \quad L_t \sim 1 \text{ s}$$

- Grid points required:

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

- Factor of  $\sim 10^6$  more than largest fluid turbulence calculations
- Direct simulation not possible; need physics guidance



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# Gyrokinetic multiscale assumptions

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \frac{\partial f}{\partial \mathbf{R}} + \frac{d\mu}{dt} \frac{\partial f}{\partial \mu} + \frac{dE}{dt} \frac{\partial f}{\partial E} + \frac{d\vartheta}{dt} \frac{\partial f}{\partial \vartheta} = C[f]$$

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$$f = F + \delta f \quad \delta f \sim \epsilon f$$

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- Separation of time scales:

$$\frac{\partial_t \delta f}{\delta f} \sim \omega \sim \epsilon \Omega \quad \frac{\partial_t F}{F} \sim \tau^{-1} \sim \epsilon^2 \omega$$

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- Separation of space scales:

$$\nabla F \sim F/L, \quad \nabla_{\parallel} \delta f \sim \delta f/L, \quad \nabla_{\perp} \delta f \sim \delta f/\rho$$

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$$\frac{\partial f}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \frac{\partial f}{\partial \mathbf{R}} + \frac{d\mu}{dt} \frac{\partial f}{\partial \mu} + \frac{dE}{dt} \frac{\partial f}{\partial E} + \frac{dv}{dt} \frac{\partial f}{\partial v} = C[f]$$

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- Separation of space scales:

$$\nabla F \sim F/L, \quad \nabla_{\parallel} \delta f \sim \delta f/L, \quad \nabla_{\perp} \delta f \sim \delta f/\rho$$

- “Smooth” velocity space:

$$\epsilon \lesssim \nu/\omega \lesssim 1 \Rightarrow \sqrt{\epsilon} \lesssim \delta v/v_{th} \lesssim 1$$

# Key results: turbulence and transport

$$f = F_0 + h + \dots \quad F_0 = F_M(\mathbf{R}) \exp\left(-\frac{q\Phi}{T}\right)$$

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Gyrokinetic equation for turbulence:

$$\partial h / \partial t + v_{\parallel} \hat{\mathbf{b}} \cdot \nabla h + \langle \mathbf{v}_{\chi} \rangle_{\mathbf{R}} \cdot \nabla (F_0 + h) + \mathbf{v}_{\mathbf{B}} \cdot \nabla h = \frac{qF_0}{T_0} \frac{\partial \langle \chi \rangle_{\mathbf{R}}}{\partial t} + \langle C[h] \rangle_{\mathbf{R}}$$

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Moment equations for equilibrium evolution:

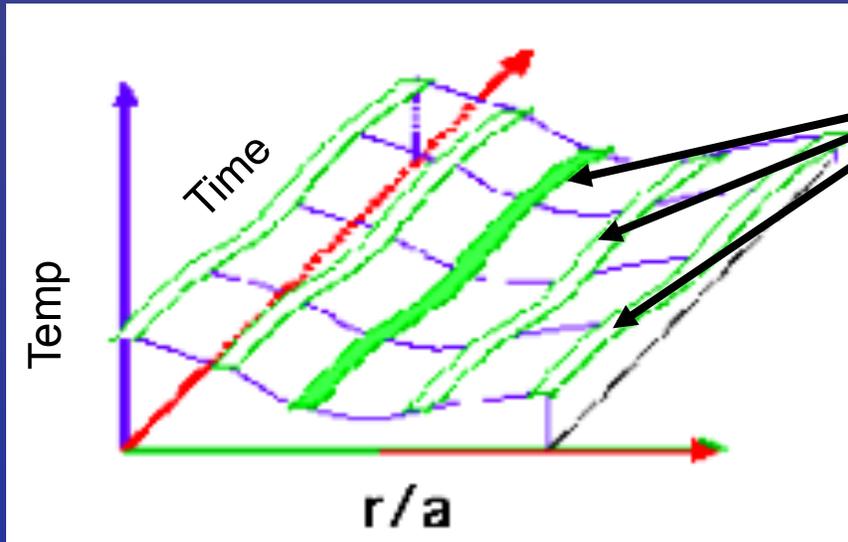
$$\begin{aligned} \frac{\partial n_s}{\partial t} &= -\frac{1}{V'} \frac{\partial}{\partial \psi} (V' \langle \mathbf{\Gamma}_s \cdot \nabla \psi \rangle) + S_n \\ \frac{3}{2} \frac{\partial n_s T_s}{\partial t} &= -\frac{1}{V'} \frac{\partial}{\partial \psi} (V' \langle \mathbf{Q}_s \cdot \nabla \psi \rangle) \\ &+ T_s \left( \frac{\partial \ln n_s}{\partial \psi} - \frac{3}{2} \frac{\partial \ln T_s}{\partial \psi} \right) \langle \mathbf{\Gamma}_s \cdot \nabla \psi \rangle + \frac{\partial \ln T_s}{\partial \psi} \langle \mathbf{Q}_s \cdot \nabla \psi \rangle \\ &- \left\langle \int d^3 v \frac{h_s T_s}{F_{0s}} \langle C[h_s] \rangle_{\mathbf{R}} \right\rangle + n_s \nu_{\epsilon}^{su} (T_u - T_s) + S_p \end{aligned}$$

All terms in each equation same order

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# Multiscale grid

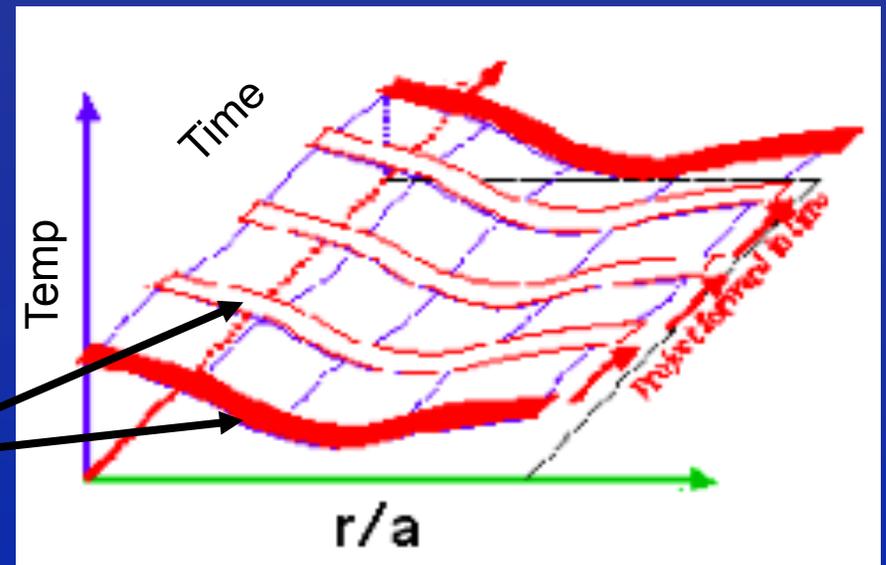


## Flux tube simulation domain

- Turbulent fluxes calculated in small regions of fine grid embedded in "coarse" radial grid (for equilibrium)

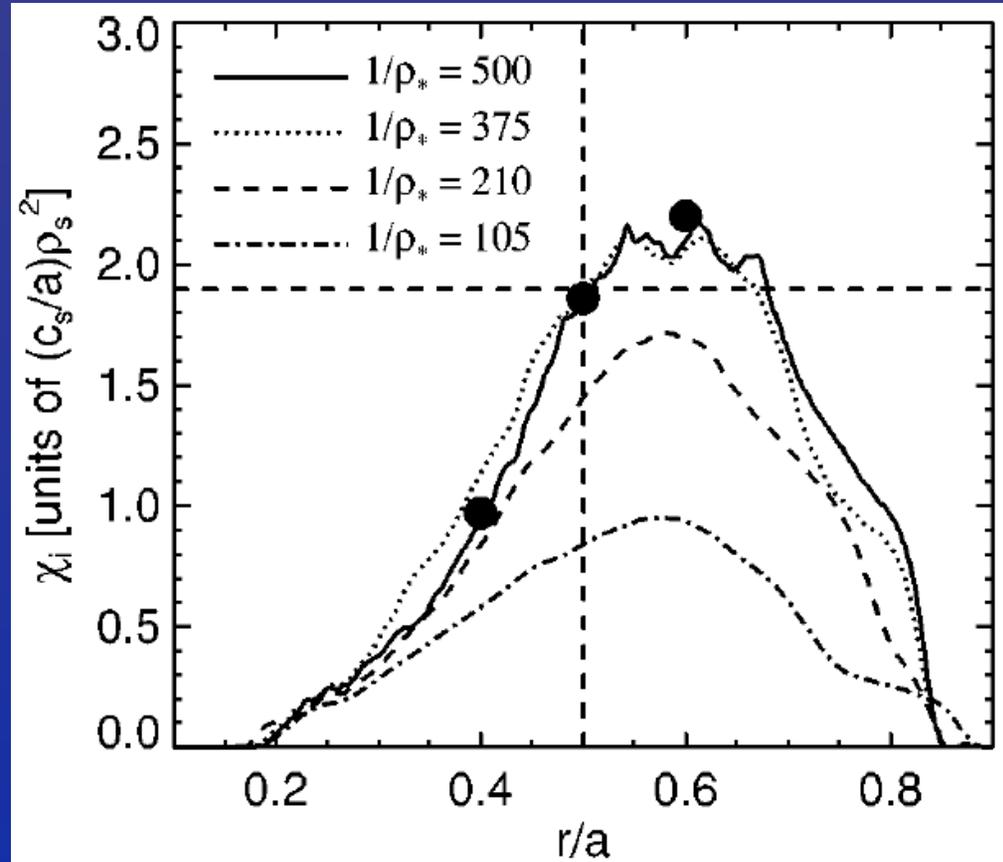
- Steady-state (time-averaged) turbulent fluxes calculated in small regions of fine grid embedded in "coarse" time grid (for equilibrium)

## Flux tube simulation domain



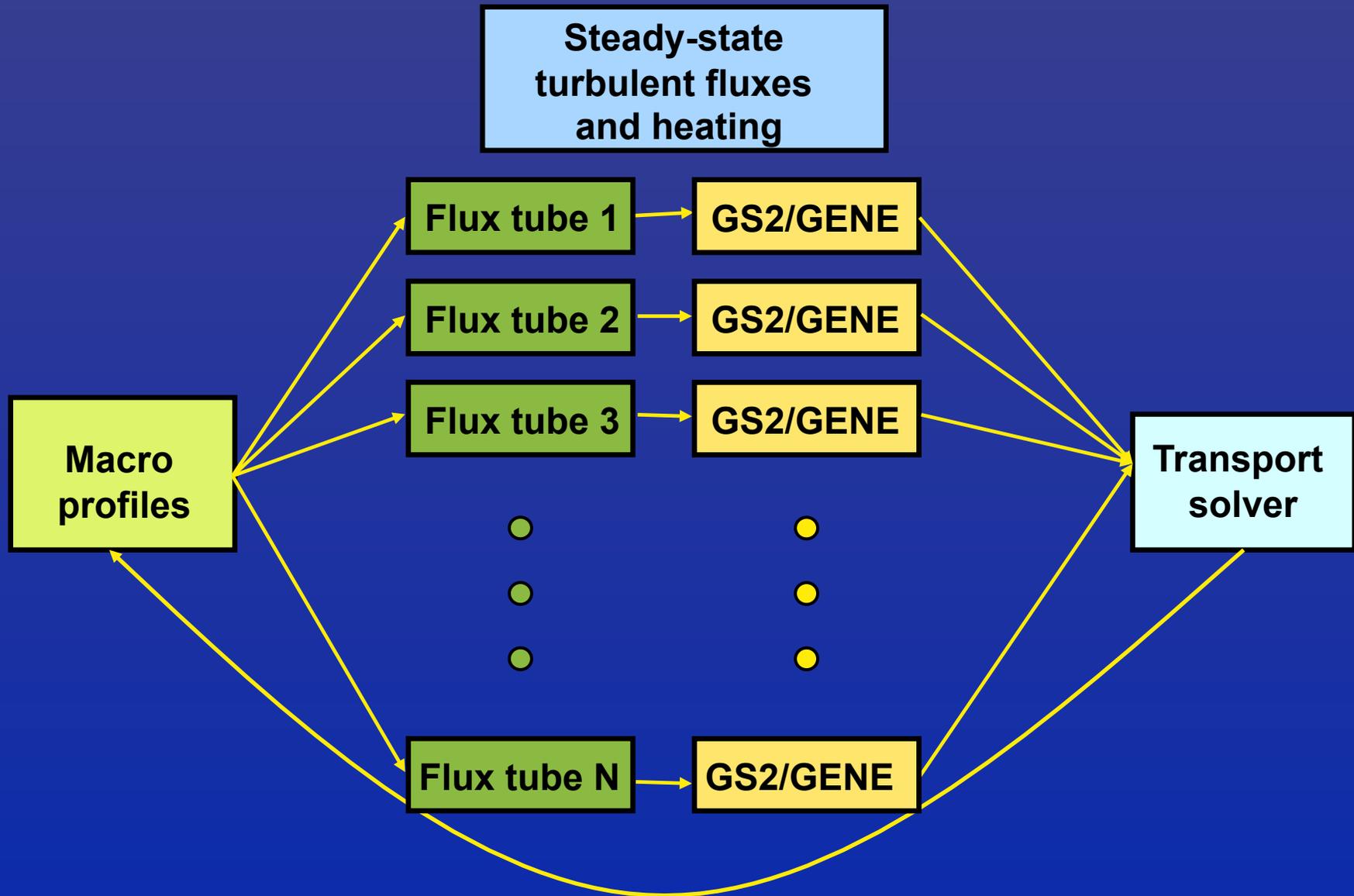
# Validity of flux tube approximation

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

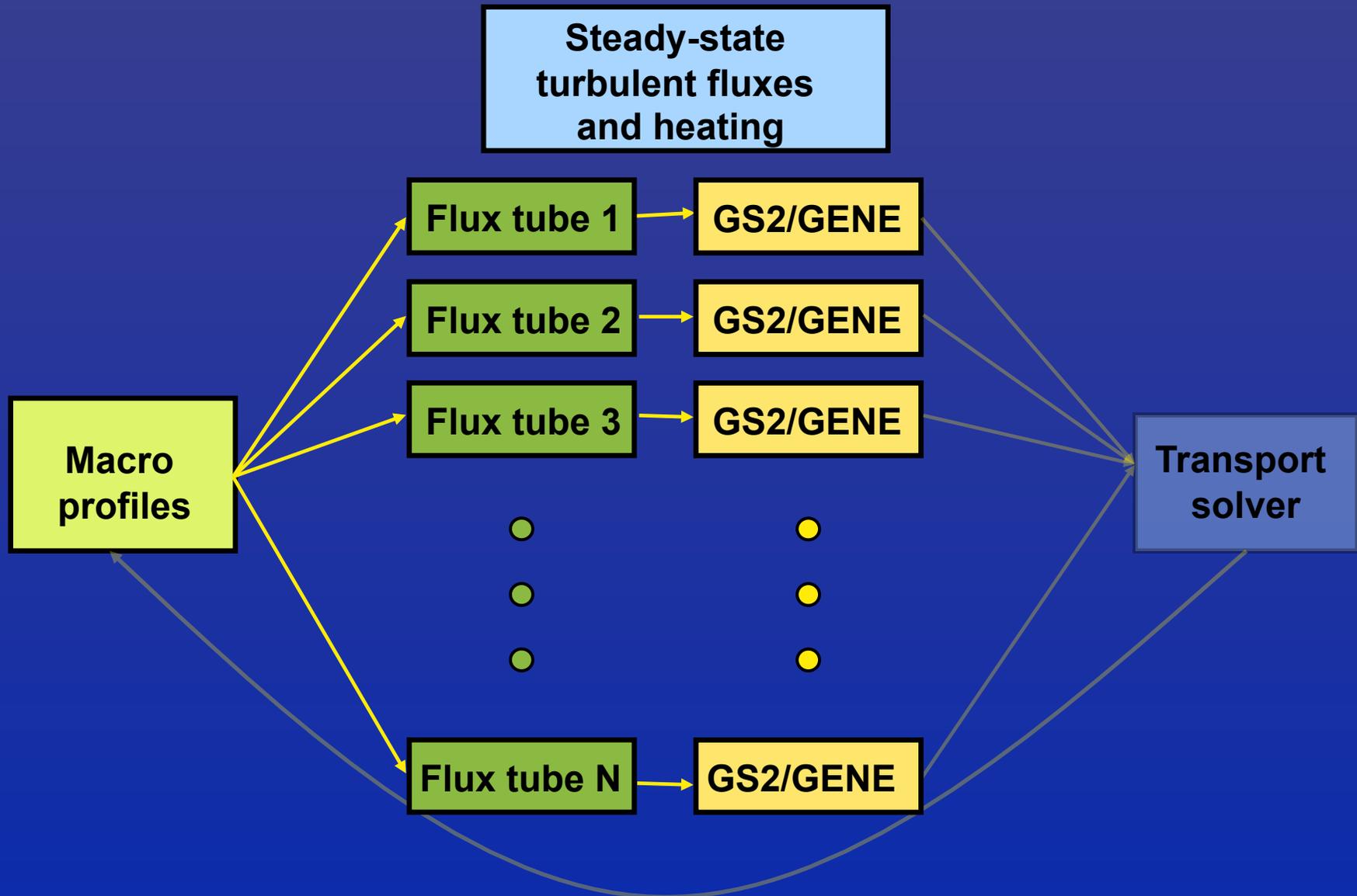


Candy et al (2004)

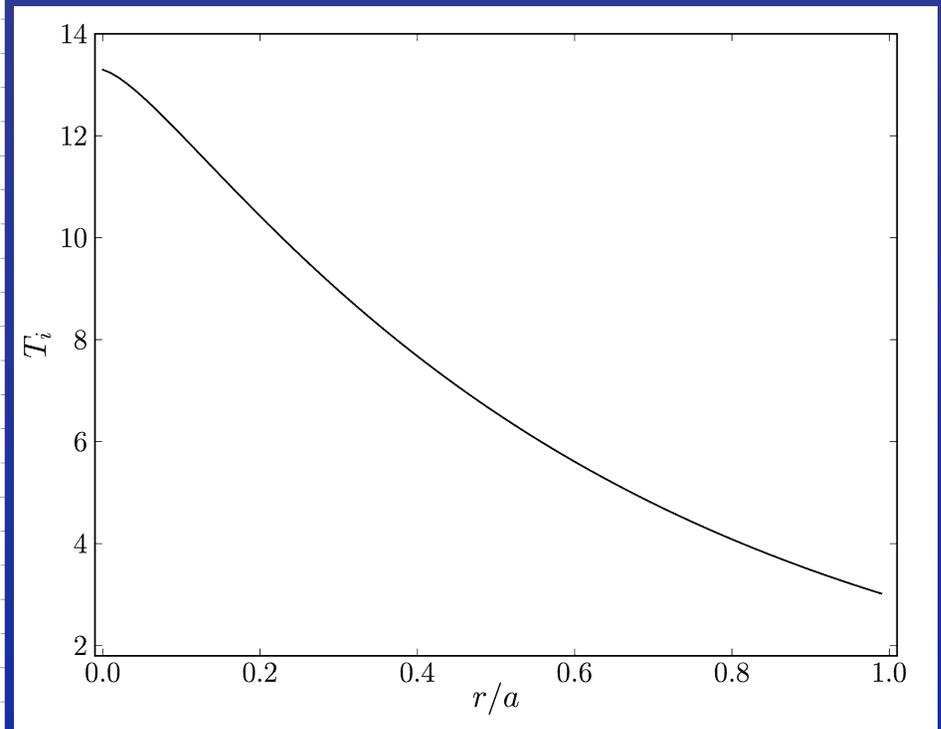
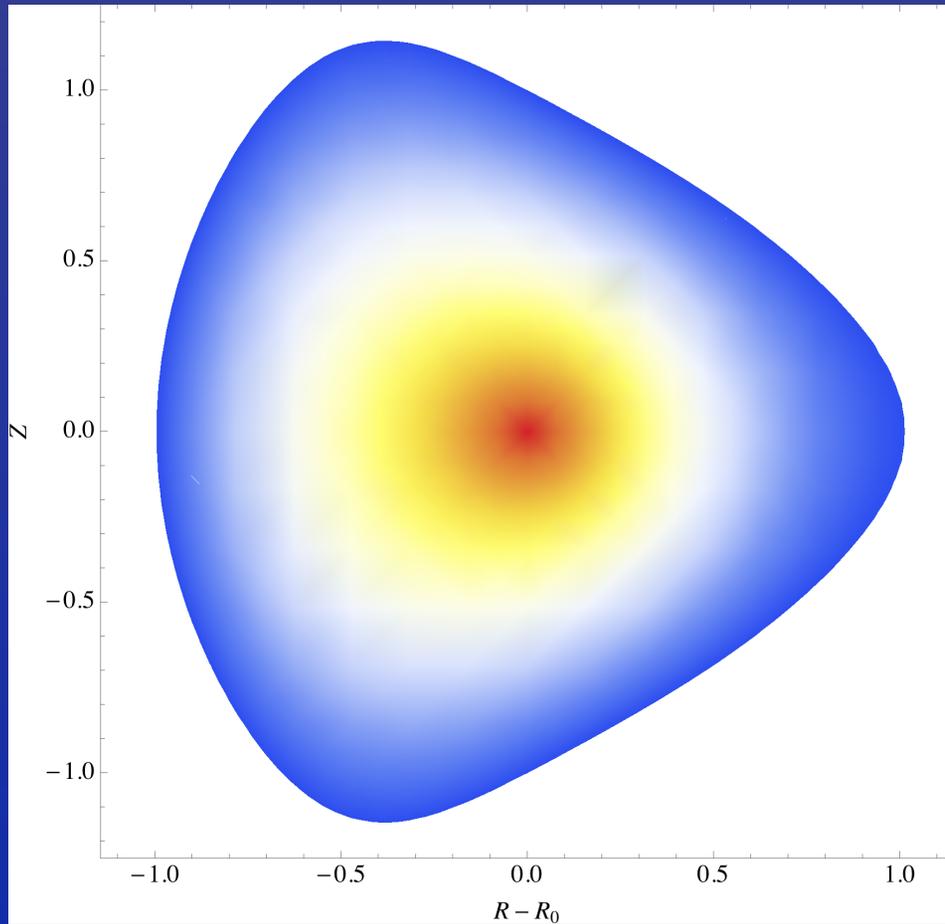
# Trinity schematic



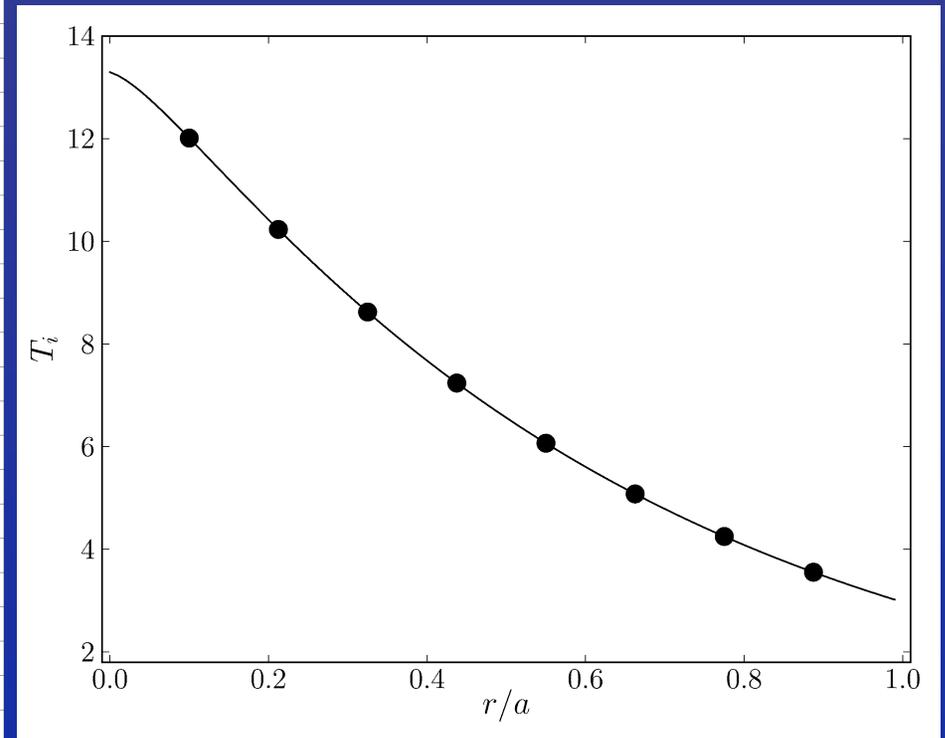
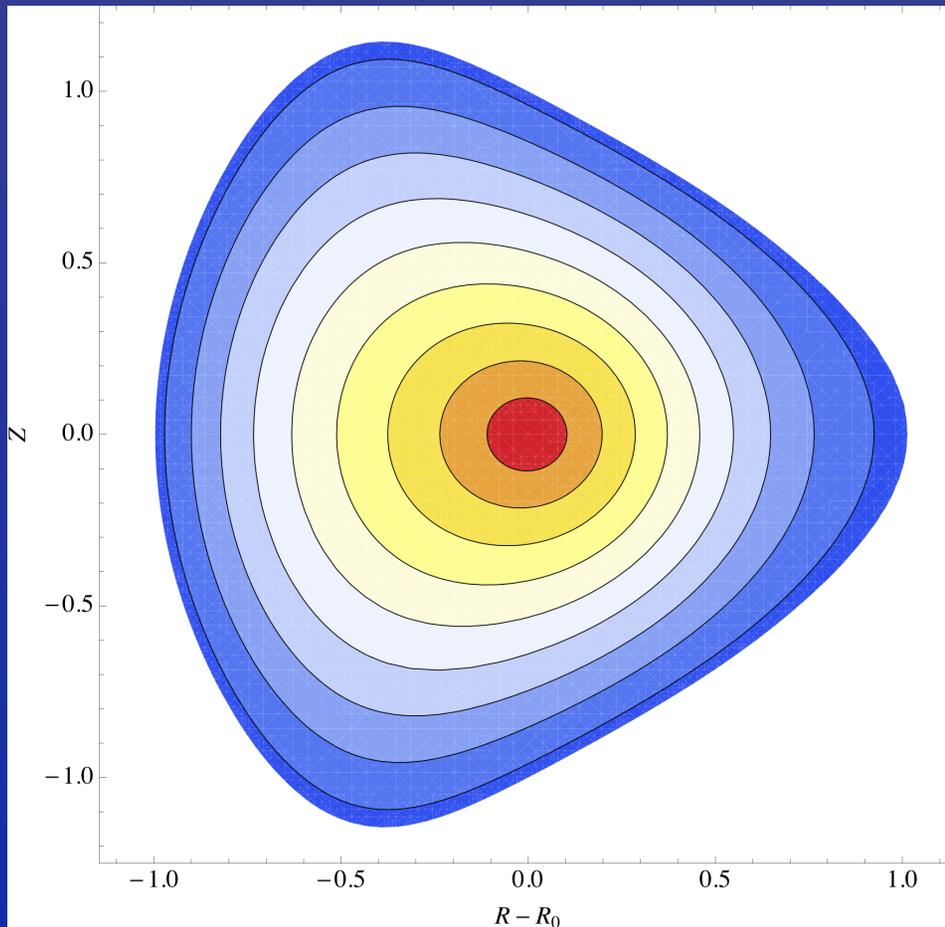
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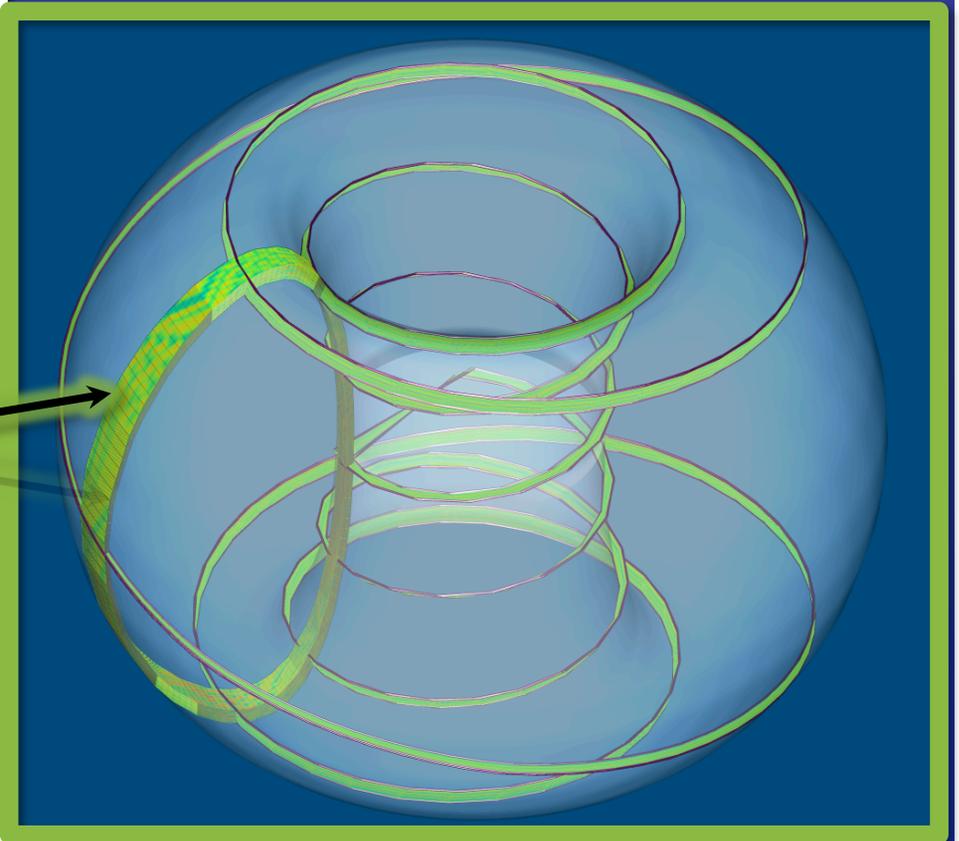
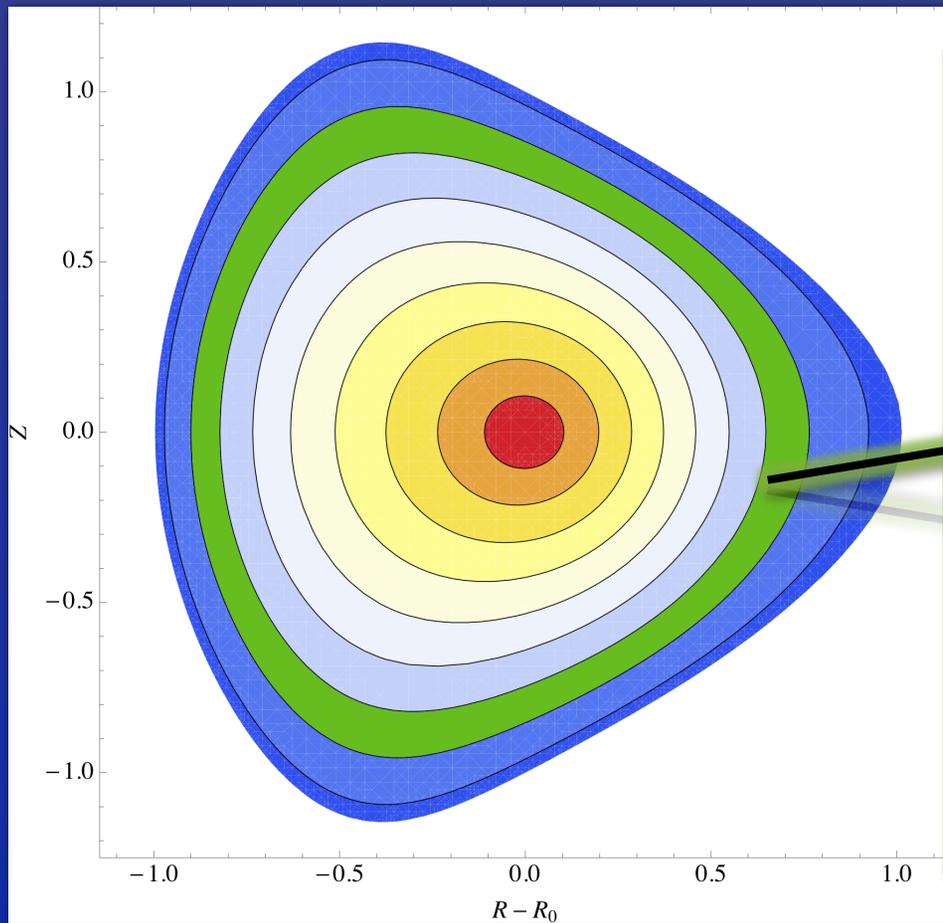
# Sampling profile with flux tubes



# Sampling profile with flux tubes

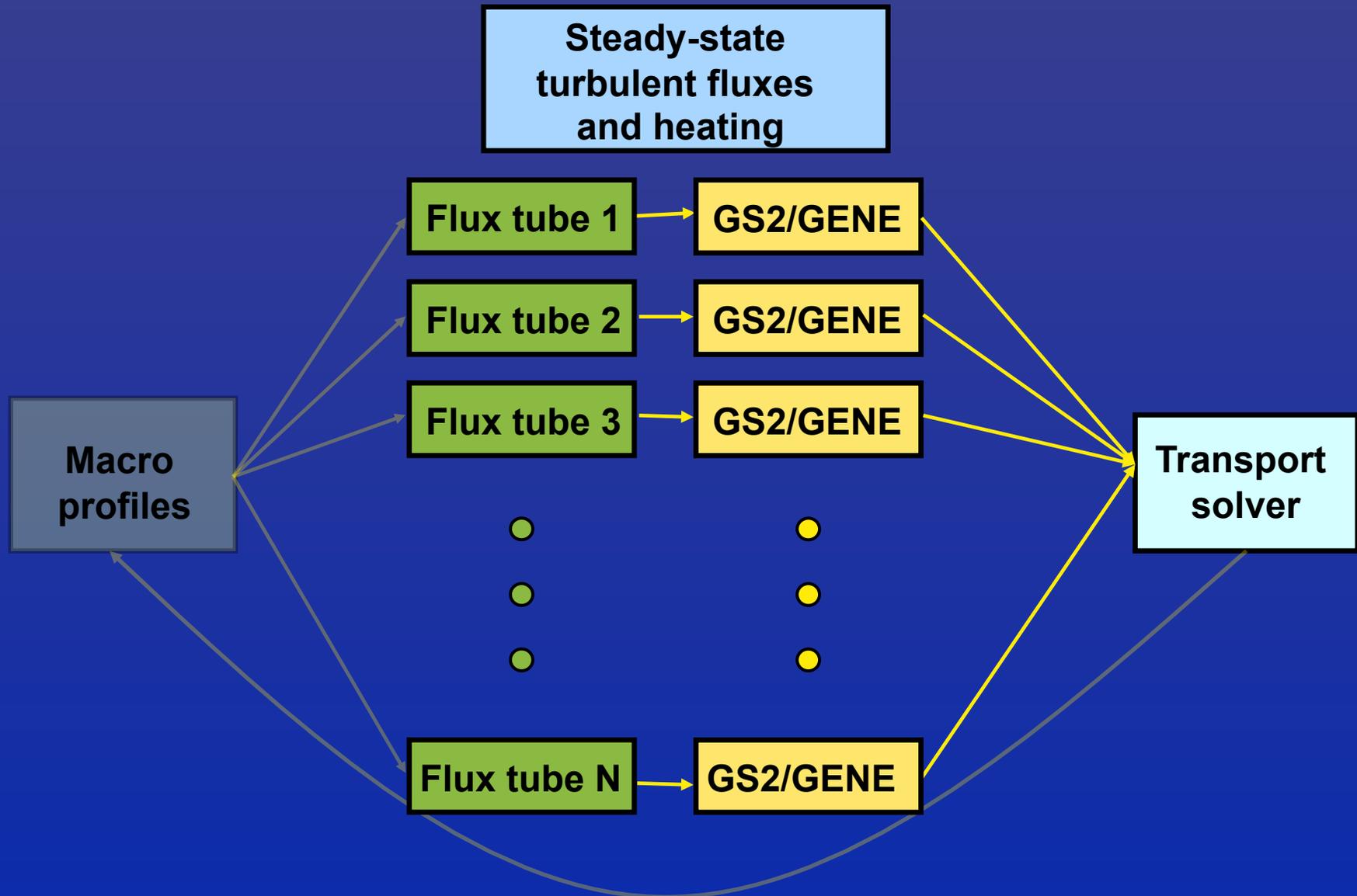


# Sampling profile with flux tubes



Simulation volume reduced  
by factor of  $\sim 100$

# Trinity schematic



# Trinity transport solver

- Transport equations are stiff, nonlinear PDEs. Implicit treatment via Newton's Method (multi-iteration, adaptive time step) allows for time steps  $\sim 0.1$  seconds (vs. turbulence sim time  $\sim 0.001$  seconds)

$$\frac{\partial n}{\partial t} + \frac{\partial G(n, T, \Gamma)}{\partial r} = S_n \quad \Gamma = \Gamma_{phys} / n v_t$$

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

- Challenge: requires computation of quantities like

$$\frac{\partial \Gamma_j}{\partial n_k} = \frac{\partial \Gamma_j}{\partial n_j} + \frac{\partial \Gamma_j}{\partial (R/L_n)_j} \frac{\partial (R/L_n)_j}{\partial n_k}$$

- 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
  - Possible because flux tubes independent (do not communicate during calculation)
  - Perfect parallelization
  - use 2-point finite differences:

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

# Trinity transport solver

- 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 >80% efficiency

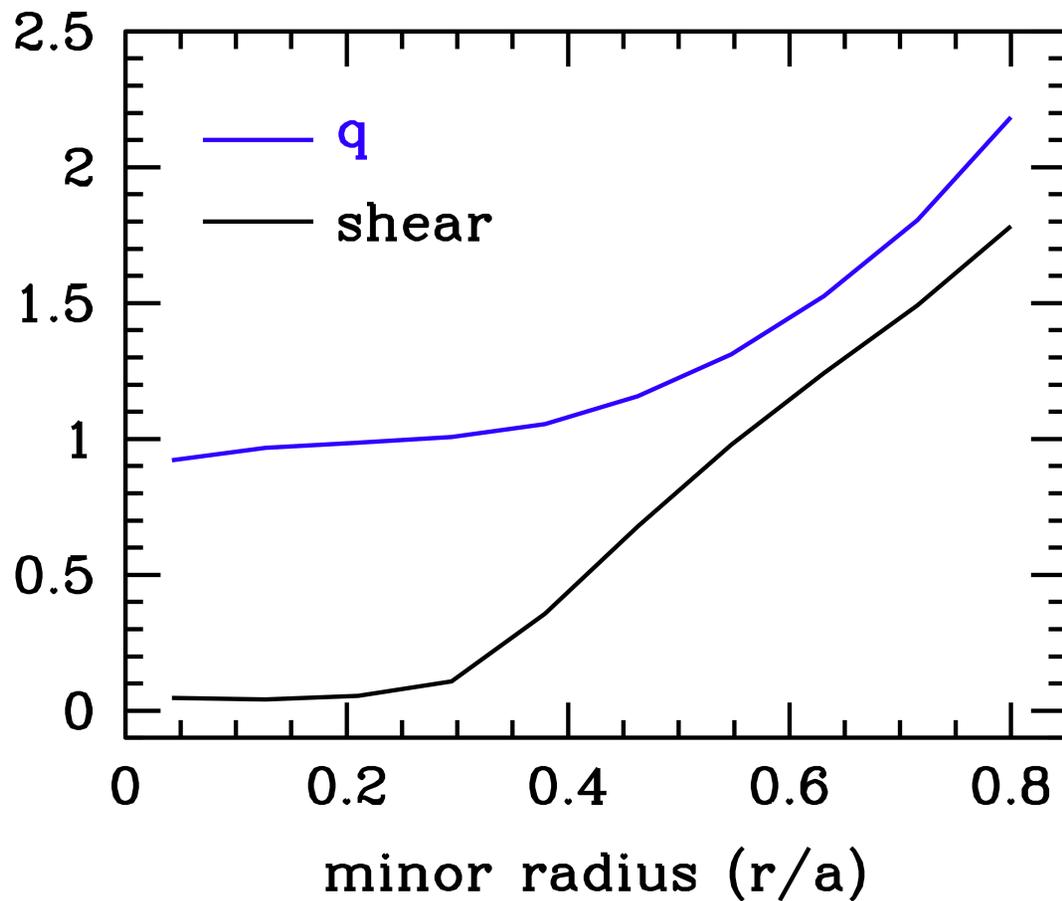
# Improved simulation cost

- Statistical periodicity in poloidal direction takes advantage of  $k_{\perp}^{-1} \ll L_{\theta}$  : savings factor of  $\sim 100$
- Exploitation of scale separation between turbulence and equilibrium evolution: savings factor of  $\sim 100$
- Extreme parallelizability: savings factor of  $\sim 10$
- Total saving of  $\sim 10^5$ : simulation possible on current machines
- In addition to savings from not having to resolve  $f_0, f_1, f_2$  at the same time

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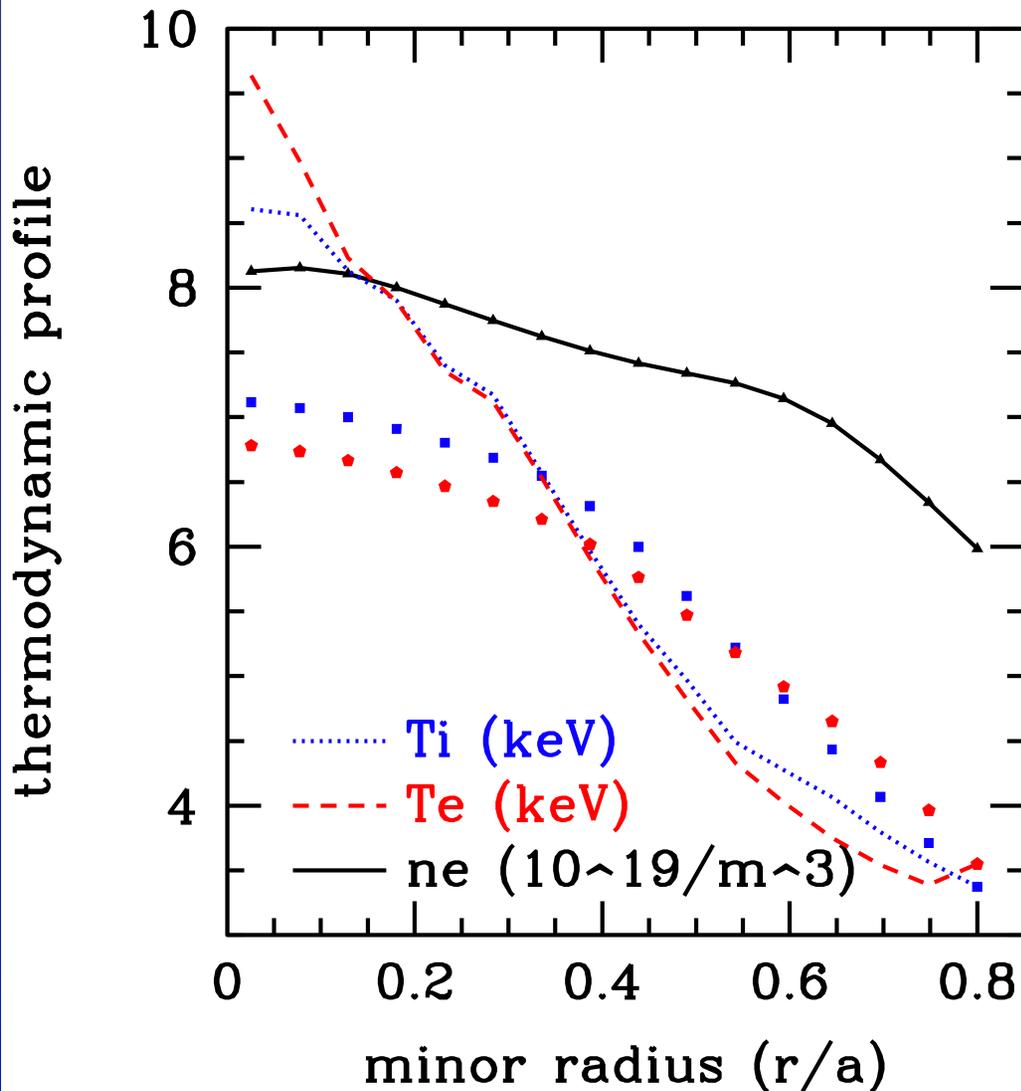
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# JET shot #42982



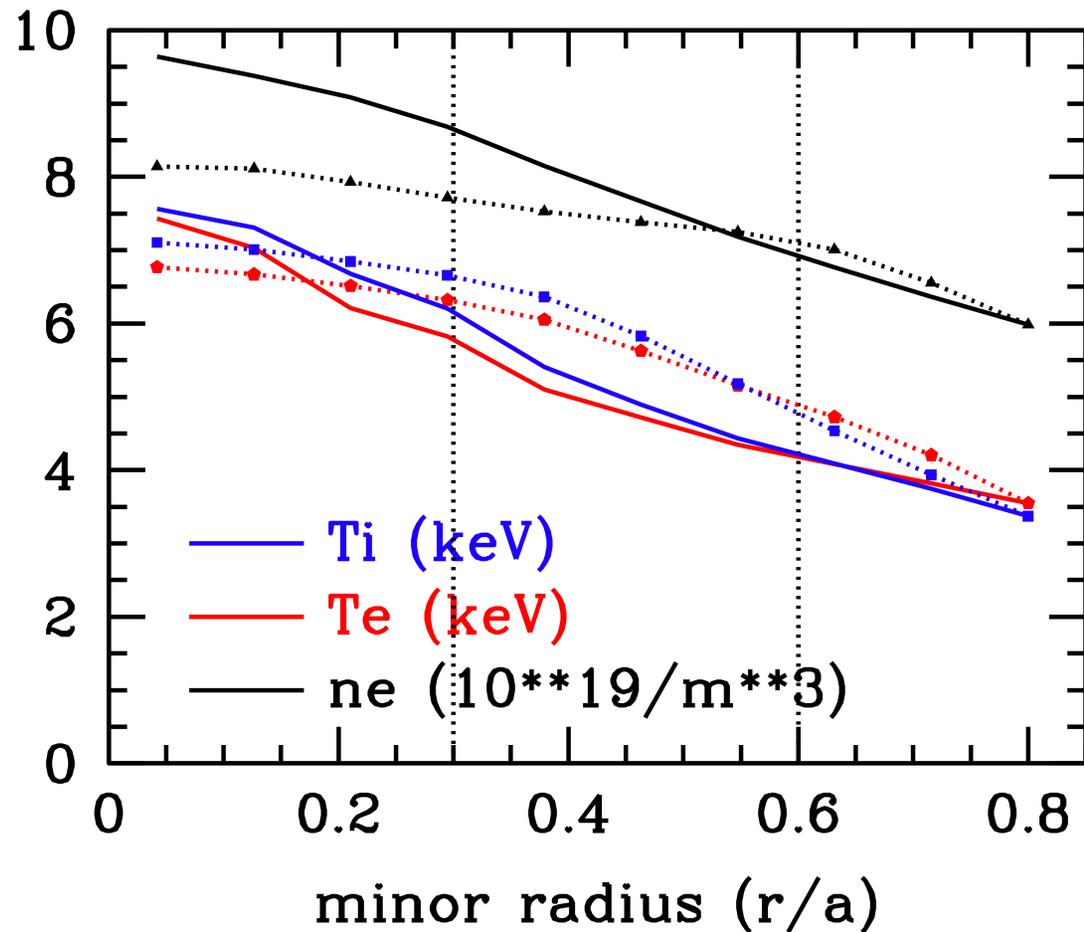
- ITER demo discharge
- H-mode D-T plasma, record fusion energy yield
- Miller local equilibrium model:  $q$ , shear, shaping, shift
- Low triangularity, elongation  $\sim 1.4$ ,
- $B = 3.9$  T on axis
- TRANSP fits to experimental data taken from ITER profile database

# Profile comparison



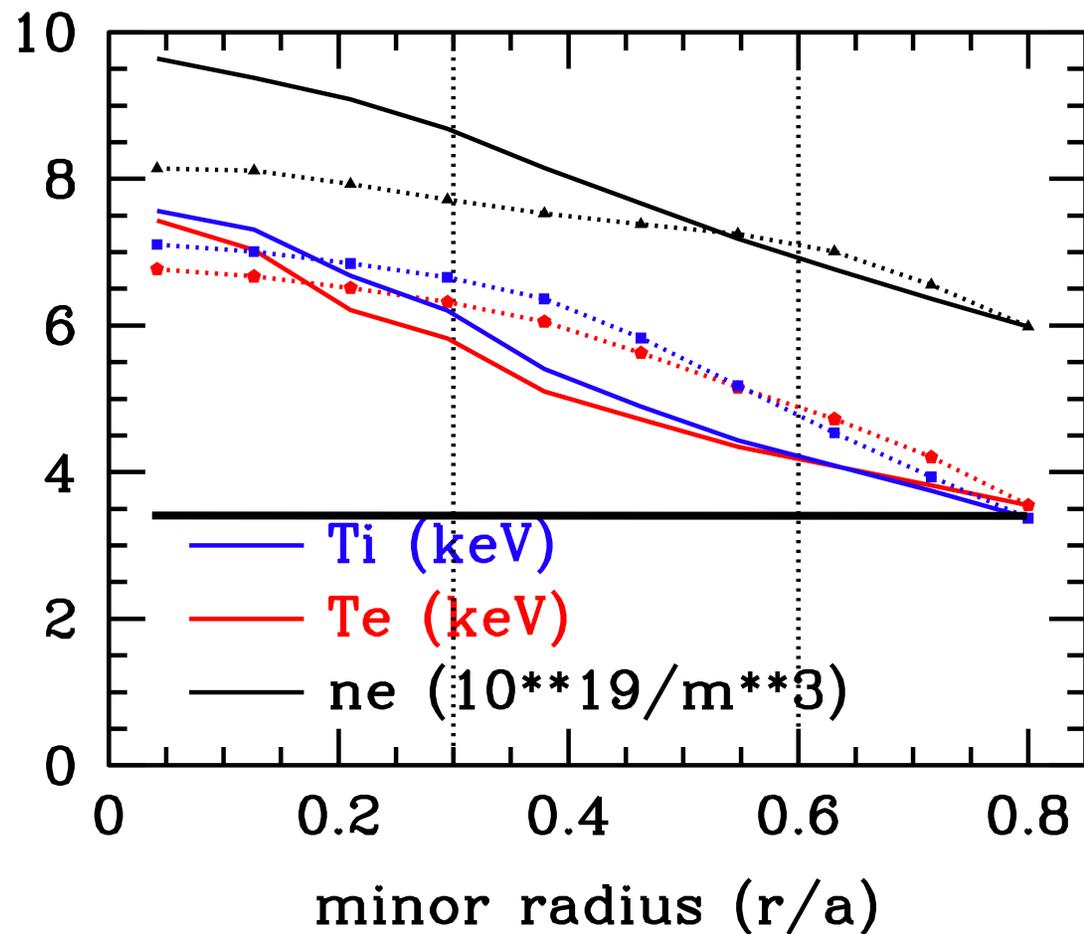
- Relatively low gs2 resolution: 9 ky's, 31 kx's, 24 field line points, 20 pitch angles, 12 energies
- ITG physics
- Electrostatic, collisionless
- 16 radial grid points
- Costs ~90k CPU hrs (<10 clock hrs)
- Fixed density profile
- Qualitative agreement, but dip in Te near edge...

# Evolving density profile



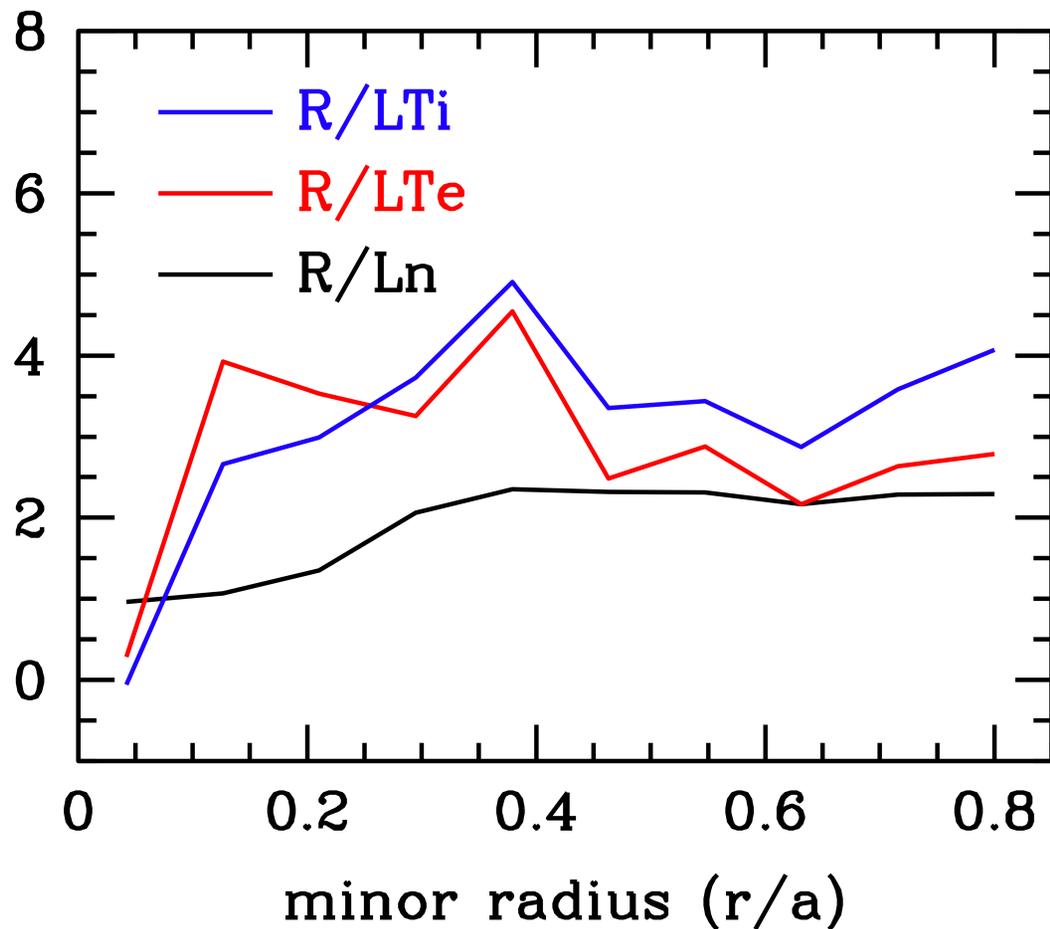
- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%
- Sources of discrepancy:
  - Large error bars
  - Low res fluxes
  - Flow shear absent

# Evolving density profile



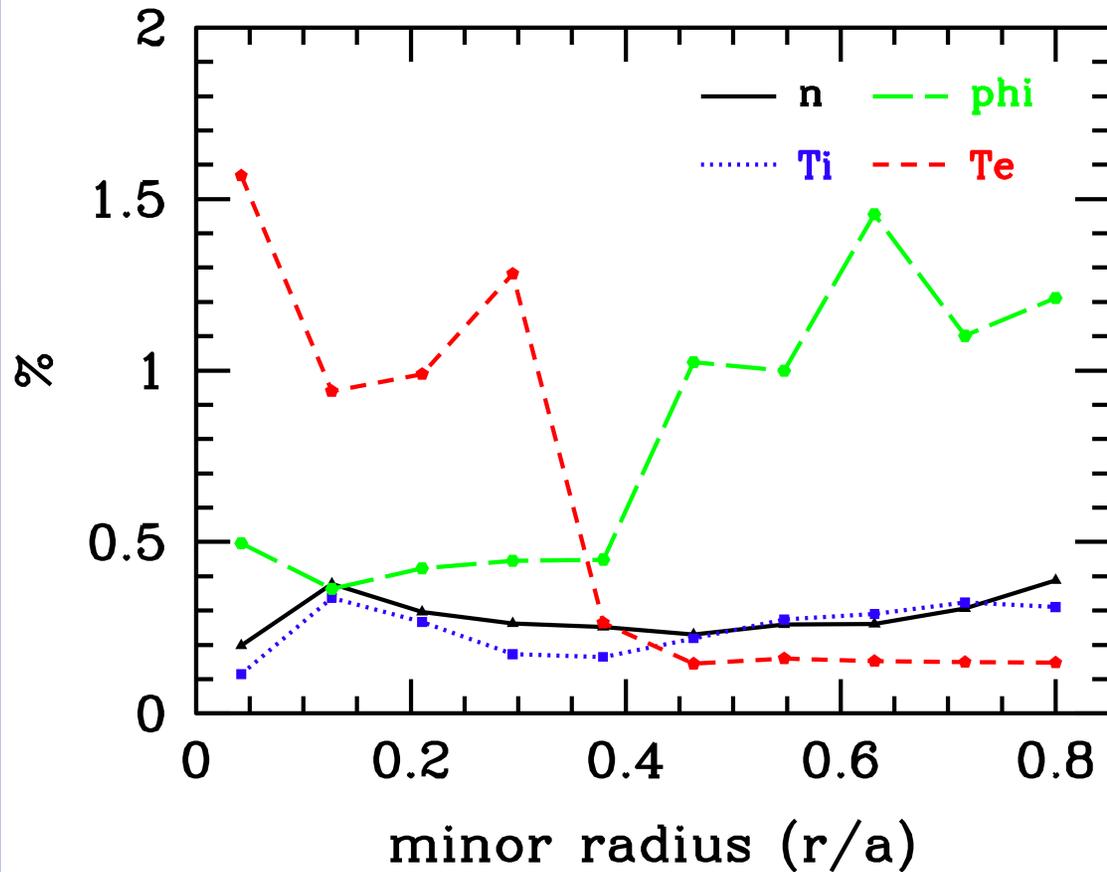
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# Profile stiffness



- Illustrates challenging aspect of solving for profiles (instead of gradients)
- Perhaps useful to employ smoothing?
- $\sim$  flat grad scale lengths indicative of stiffness (near critical gradient across most of minor radius)

# Fluctuations



- Steady-state fluctuation levels (time-averaged) calculated in gs2
- Fluctuations small (in agreement with experiment), so  $\delta f/f \ll 1$  valid

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# Conclusions and future work

- Scale separation + theory provides significant savings in time and space domains
- First-principles simulations of self-consistent interaction between turbulence and equilibrium possible
- Still to do:
  - Momentum transport equations
  - Magnetic equilibrium evolution
  - MHD stability
  - Further comparisons with experimental measurements