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

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Overview

- Motivation
- Theoretical framework
- Numerical approach
- Example simulation results
- Future directions

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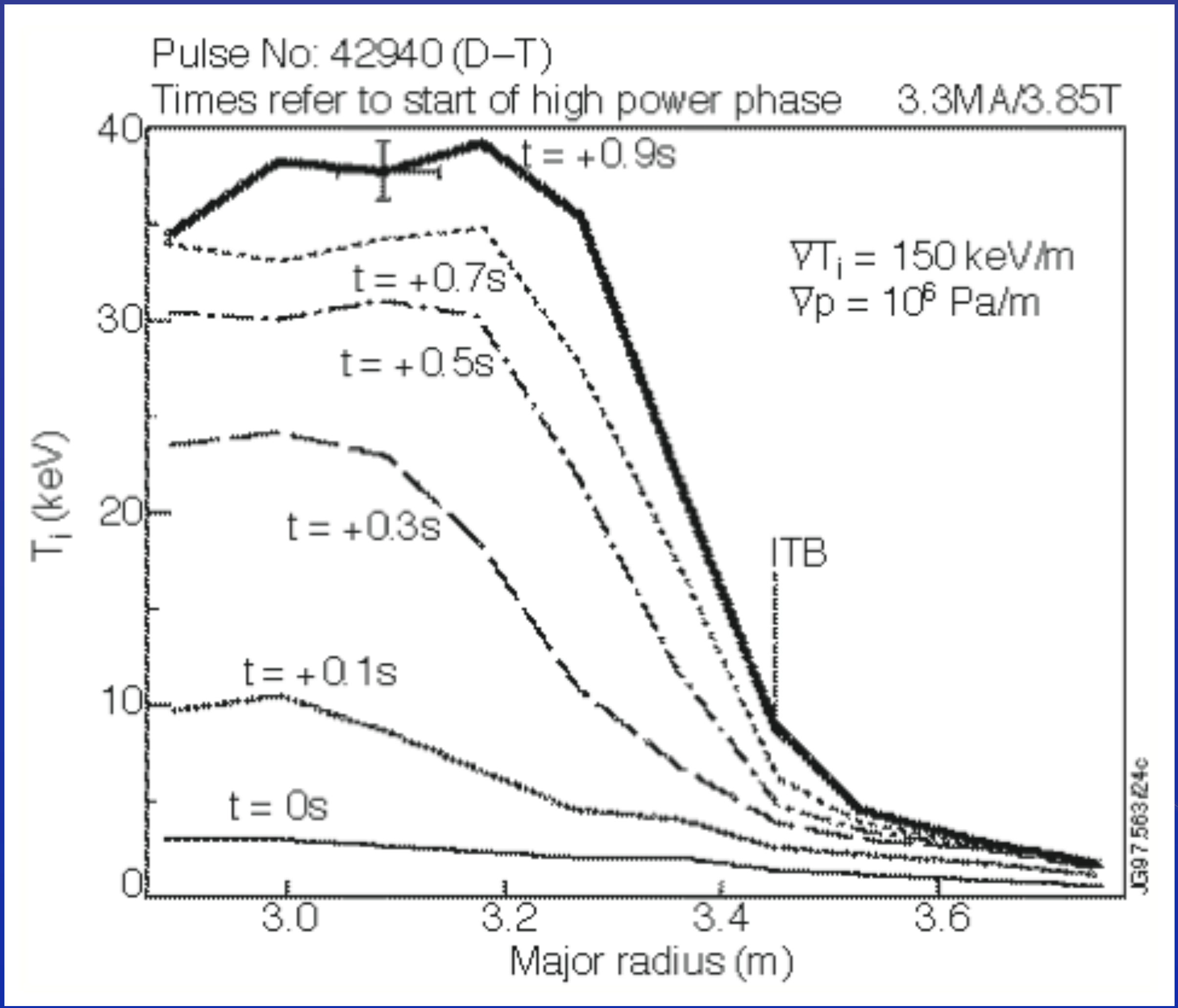
Objective



Connor et al. (2004)

Core:
multi-physics,
multi-scale

Edge:
multi-physics,
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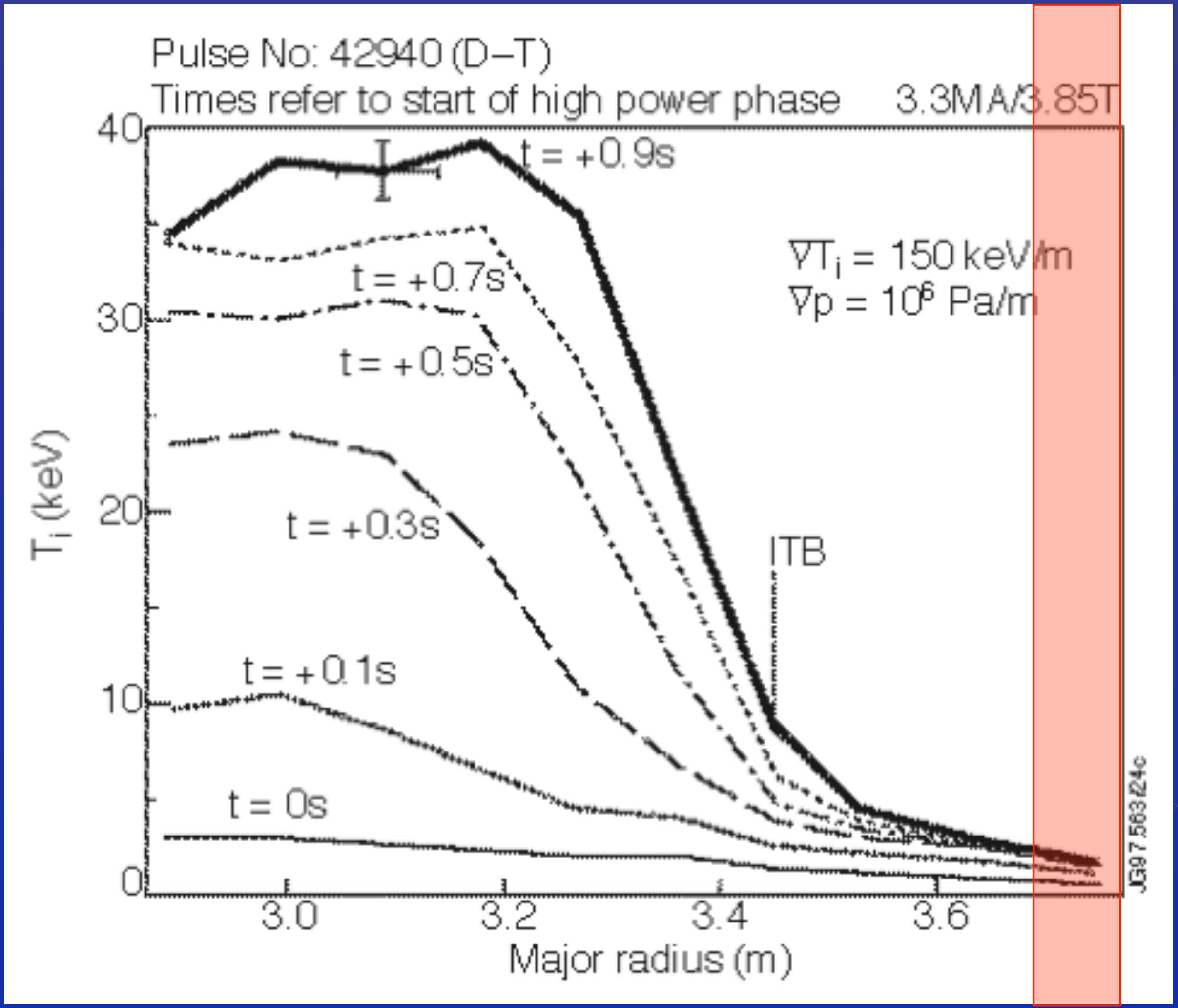


Connor et al. (2004)

Core:
multi-physics,
multi-scale

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

Scale separation in ITER

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{\Gamma} = S_n \qquad \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{Q} + ... = S_p$$

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 ~ 100 cm	Energy confinement time ~ 2 - 4 s

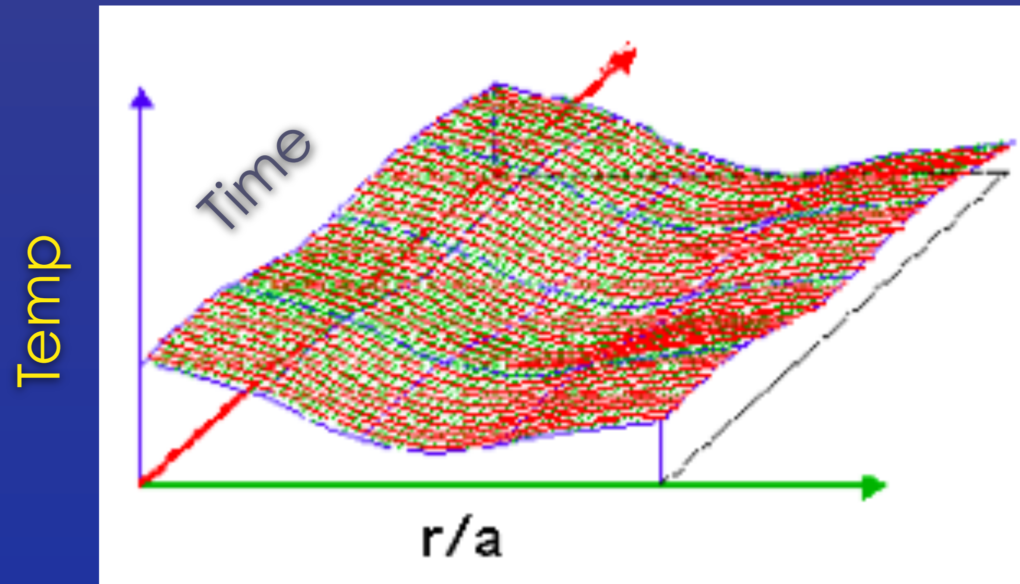
Direct simulation cost

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

$$\Delta x \sim 0.001\ cm, \quad L_x \sim 100\ cm$$

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

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



- Grid points required:

$$(L_x/\Delta x)^3 \times (L_v/\Delta v)^3 \times (L_t/\Delta t) \sim 10^{25}$$

- Factor of ~10^9 more than largest fluid turbulence calculations
- Direct simulation not possible; need physics guidance

Improved simulation cost

- Field-aligned coordinates take advantage of $k_{||} \ll k_{\perp}$: savings of ~1000
- Eliminate gyro-angle variable: savings of ~10
- Total saving of ~10^4
- Factor of ~10^5 more than largest fluid turbulence calculations
- Simulation still not possible; need multiscale approach

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. $\omega_{pe}/\Omega_{ci} \sim m_i/m_e$ — $\times 10^3$
  - ion polarization eliminates ρ_e & Debye scales $(\rho_i/\rho_e)^3$ — $\times 10^5$
  - average over fast ion gyration, $\Omega_{ci} / \omega_* \sim 1/\rho_*$ — $\times 10^3$
- Continuum or δf PIC, reduces noise, $(f_0/\delta f)^2 \sim 1/\rho_*^2$ — $\times 10^6$
- Field-aligned coordinates (nonlinear extension of ballooning coord.)

$$\Delta_{||} / (\Delta_\perp q R / a) \sim a / (q R \rho_*) \qquad \times 70$$

- Flux-tube / Toroidal annulus wedge, ↓ simulation volume
  - $k_\theta \rho_i = 0, 0.05, 0.1, \ldots, 1.0$
    $n = 0, \; 15, \; 30, \ldots, \; 300$ (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, $2^5 \times 2$ — x64
- Implicit electrons — x5-50
- Total combined speedup of all algorithms — $\times 10^{23}$
- Massively parallel computers (Moore's law 1982-2007) — $\times 10^5$

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

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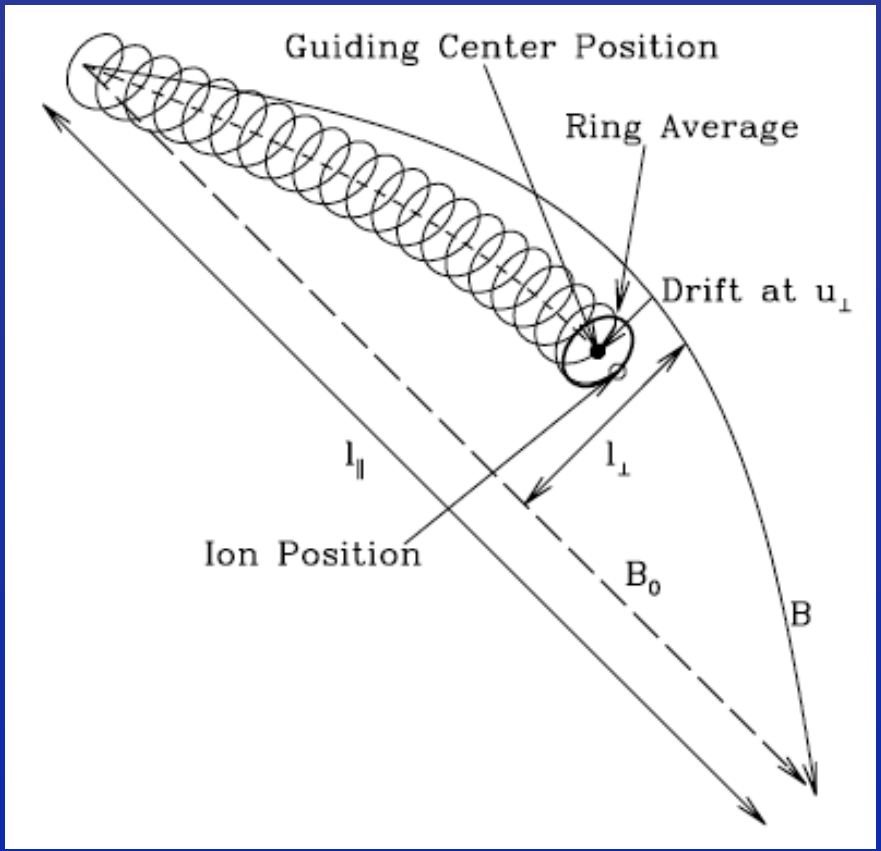

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- "Smooth" velocity space:

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

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- Sub-sonic drifts: $v_D \sim \epsilon v_{th}$

Key results: turbulence and transport

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

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Gyrokinetic equation for turbulence:

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

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Moment equations for equilibrium evolution:

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

Sugama (1997)

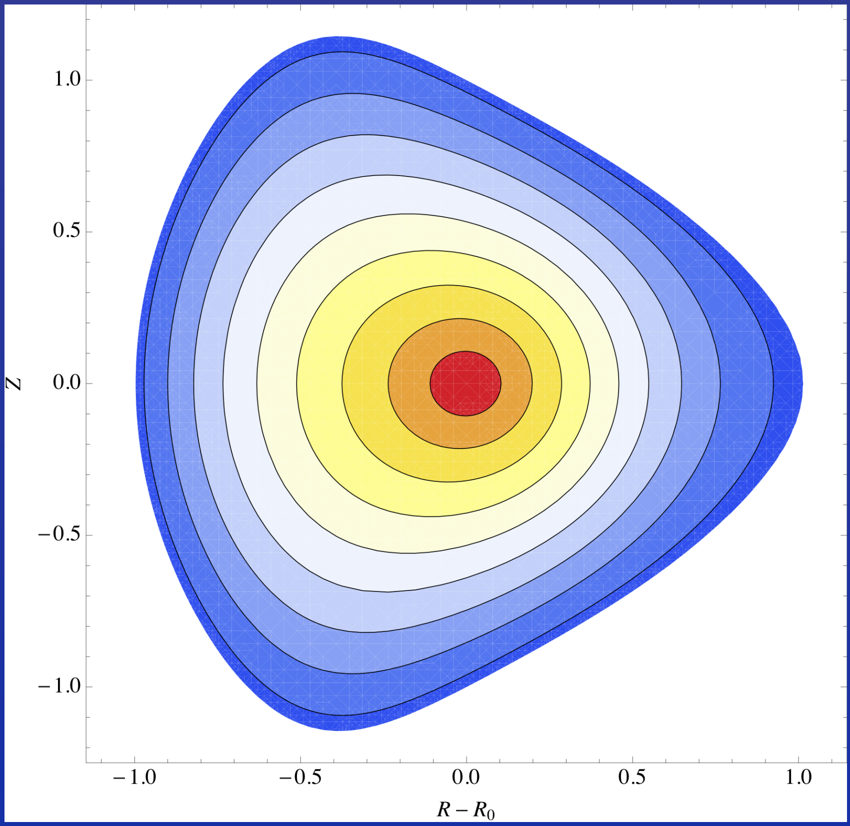
Space-time averages

- Flux surface average
- Intermediate space average:

$$\rho \ll \Delta_\psi \ll L$$

- Intermediate time average:

$$\tau_t \ll \Delta_\tau \ll \tau_E$$



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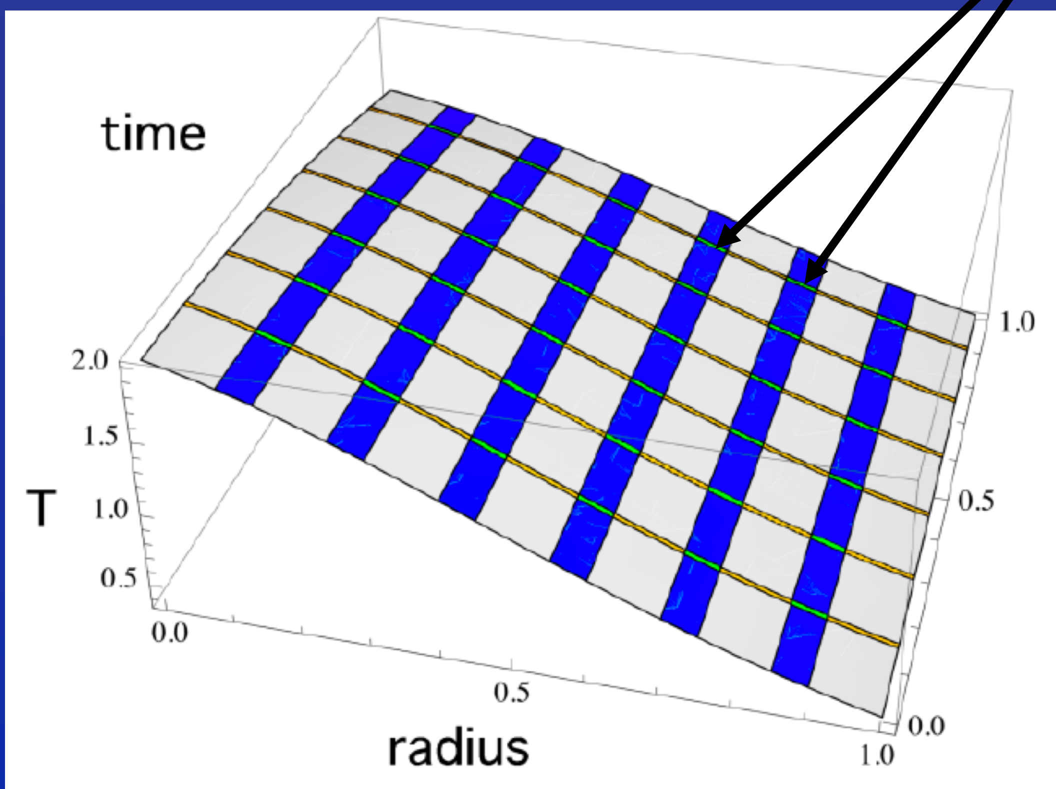
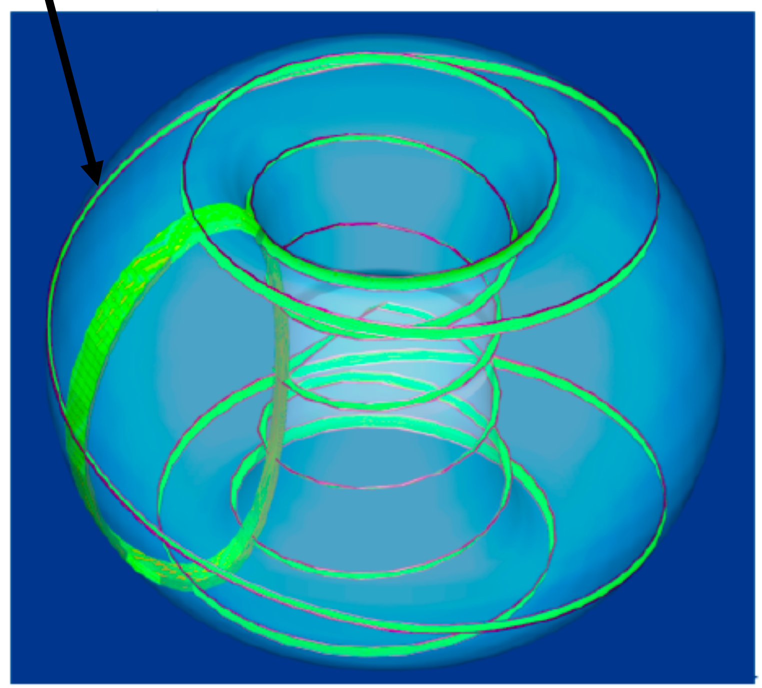
Multiscale grid

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

Flux tube simulation domain





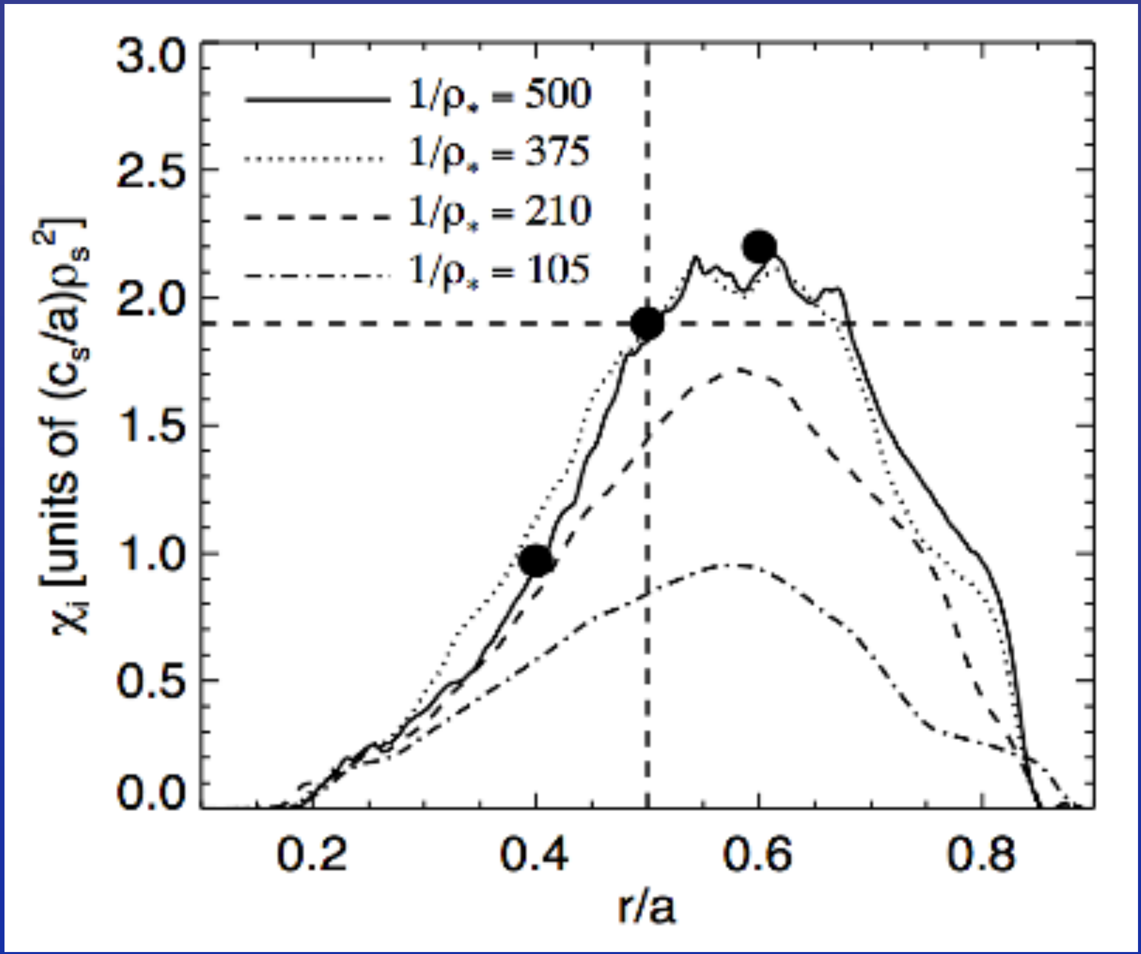
Flux tube assumptions

- Macroscopic quantities (density, flow, temperature, etc. constant across simulation domain)
- Gradient scale lengths of macroscopic quantities constant across simulation domain
  - Total gradient NOT constant (corrugations possible due to fluctuation + equilibrium gradients)
- In addition to delta-f assumption that equilibrium quantities constant in time over simulation
- => No important meso-scale physics

Validity of flux tube approximation

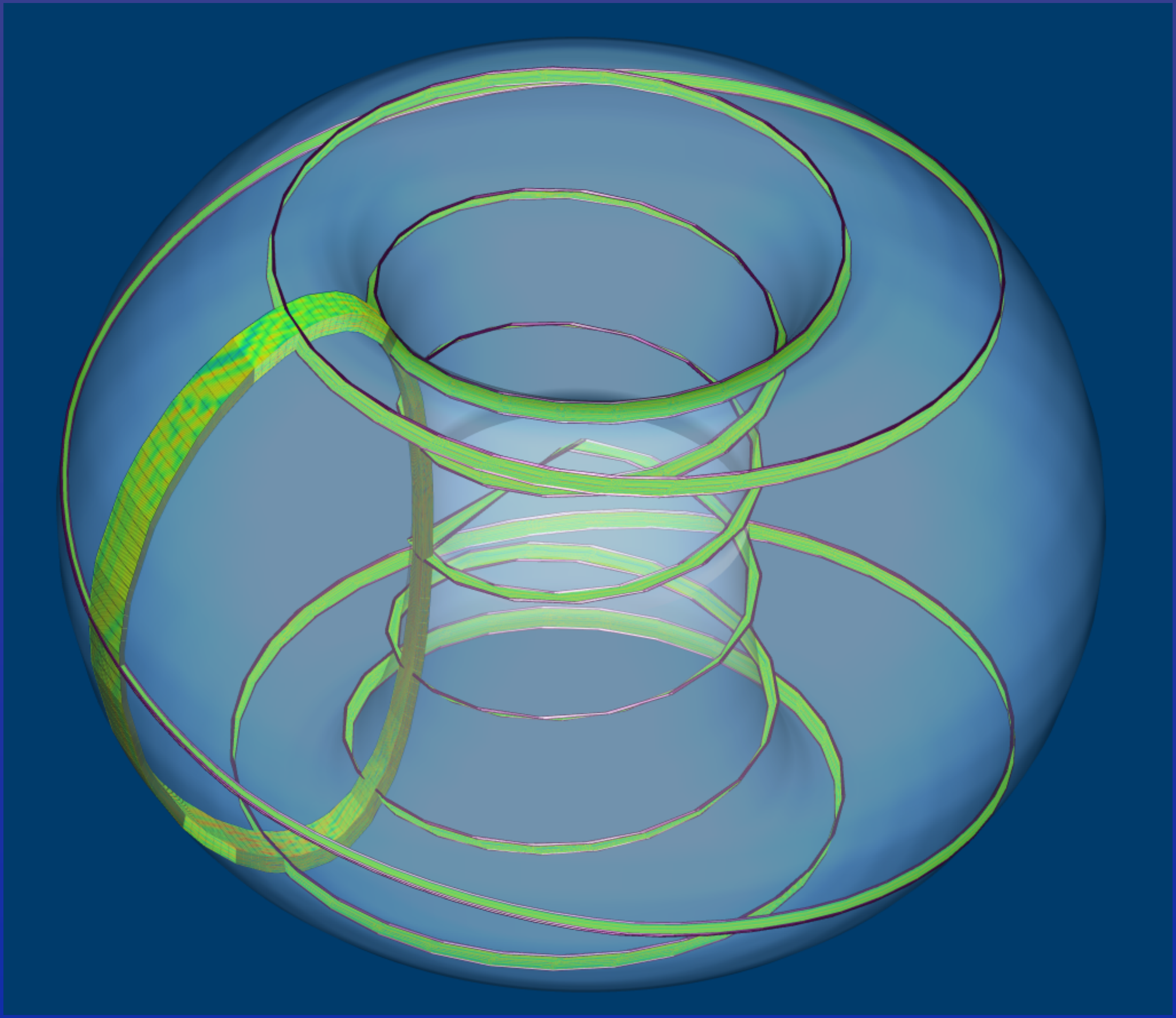
- Lines represent global simulations from GYRO
- Dots represent local (flux tube) simulations from GS2
- Excellent agreement for

$$\rho_* \ll 1$$



*J. Candy, R.E. Waltz and W. Dorland, The local limit of global gyrokinetic simulations, Phys. Plasmas **11** (2004) L25.

Flux tubes minimize flux surface grid points



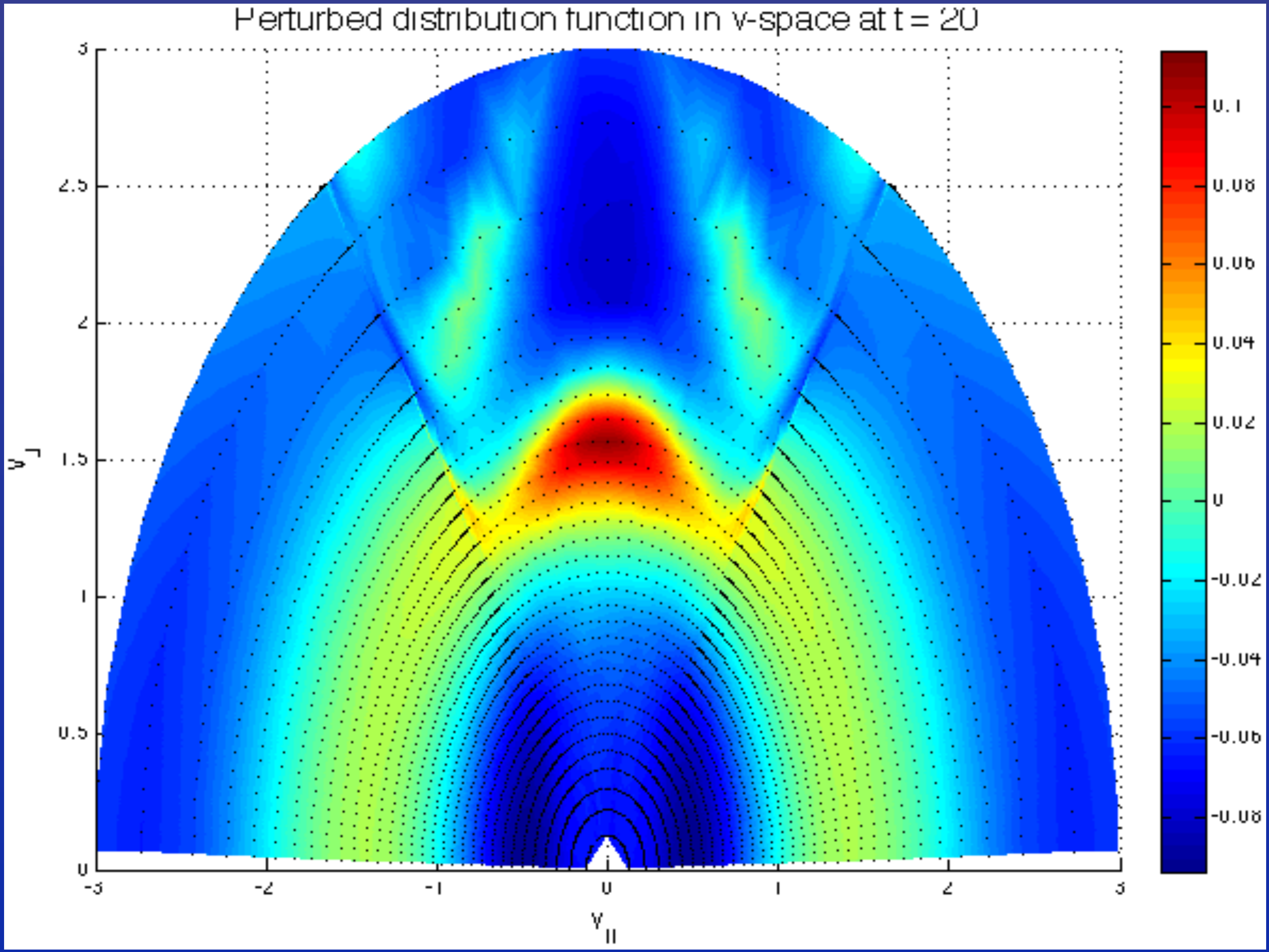
Simulation volume reduced by factor of ~10s

GS2 features

- V-space variables: energy and magnetic moment
- Realistic magnetic geometry
  - Numerical equilibrium from experiment
  - Miller local equilibrium
  - S-alpha model
- Multiple kinetic species
- Model Fokker-Planck collision operator
- Implicit treatment of linear physics
- Includes background flow shear

GS2 v-space

$$\frac{\langle \delta f \rangle_{\mathbf{R}}}{F_M}$$



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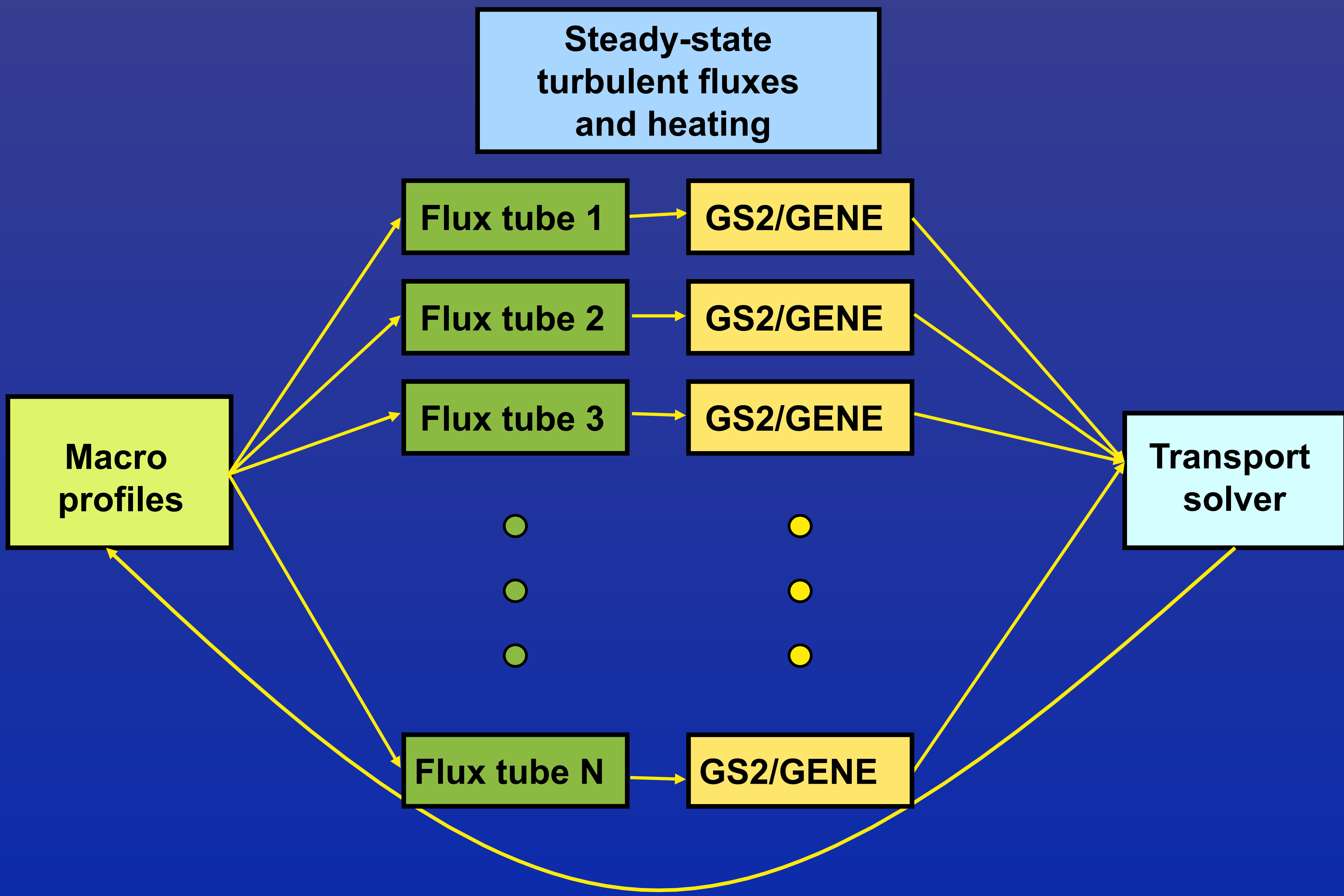
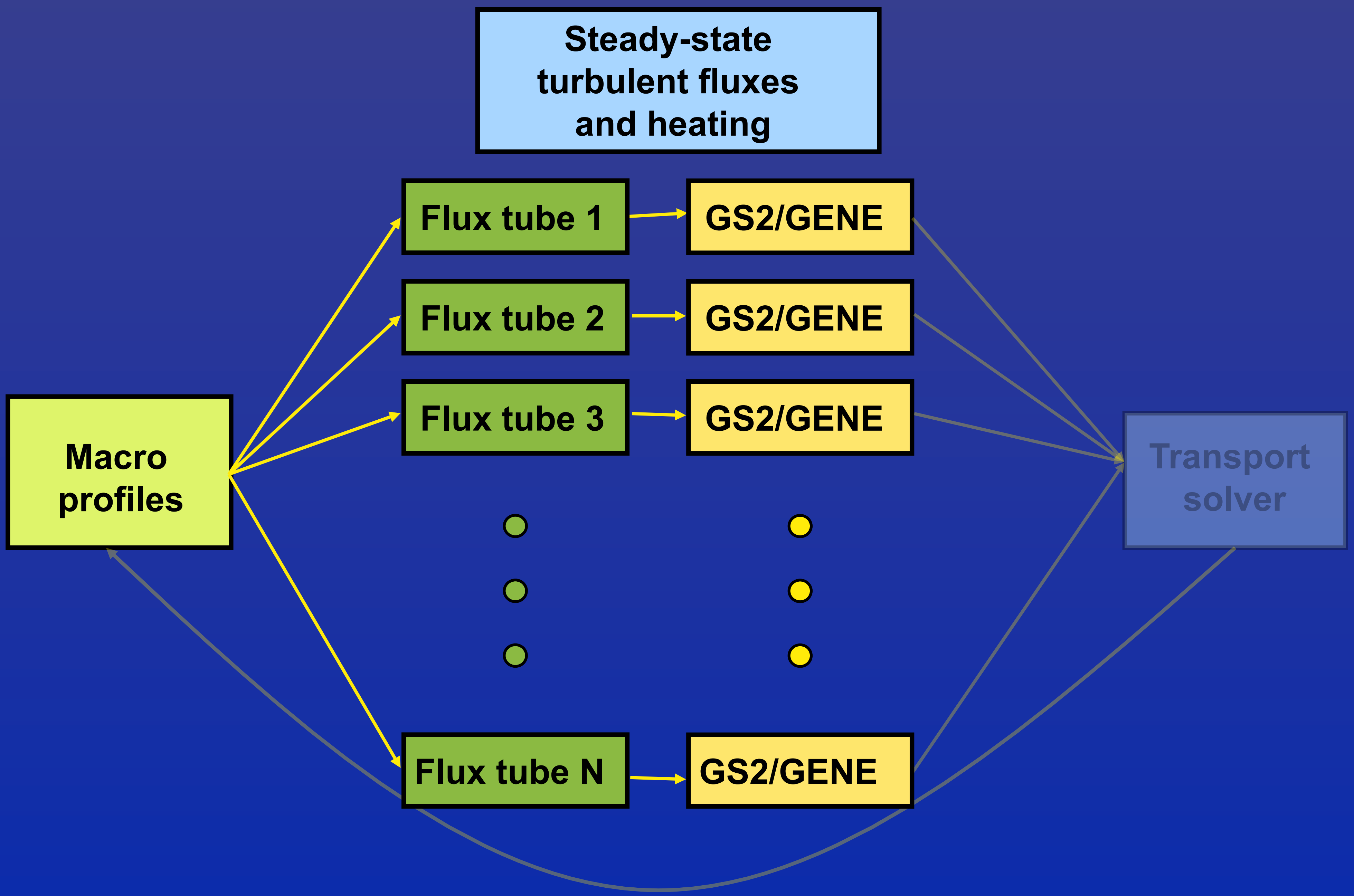
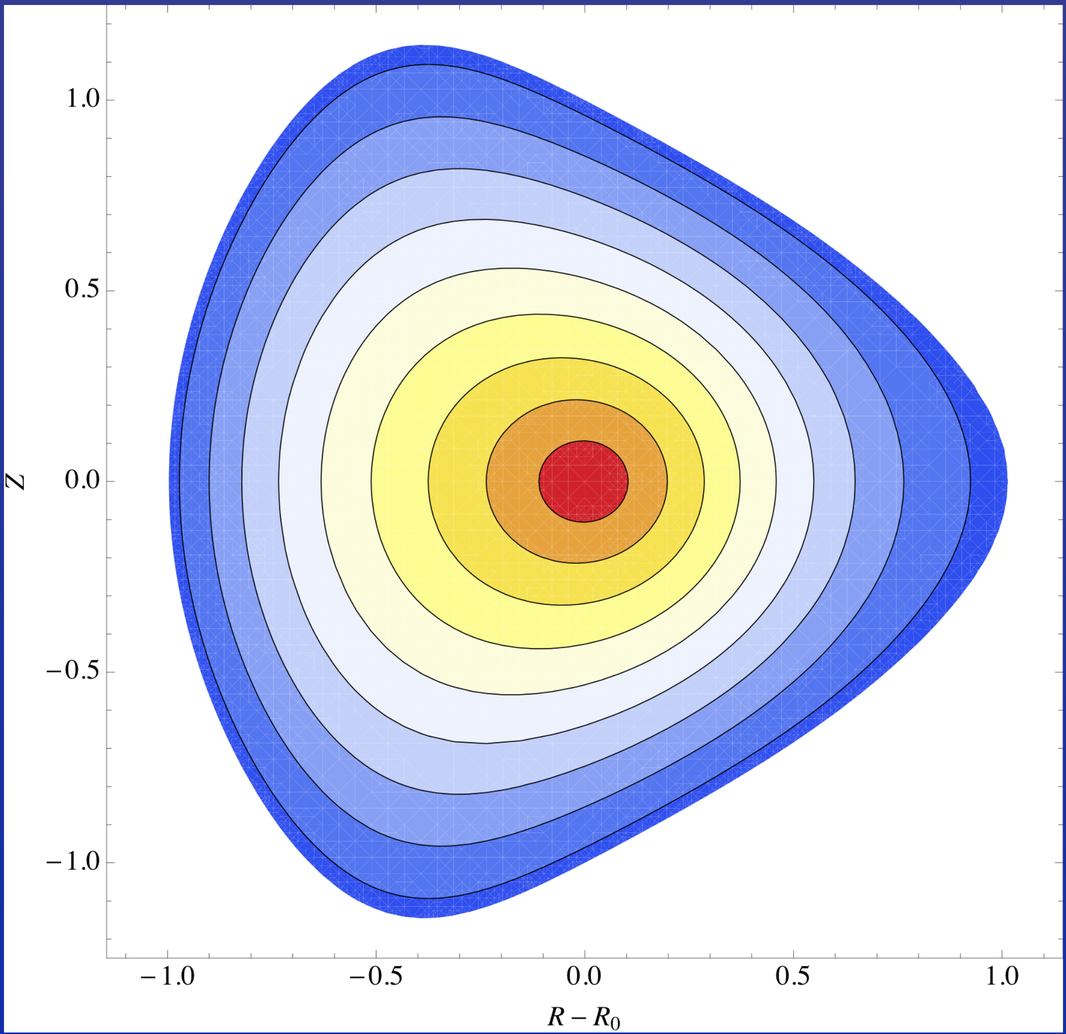
Trinity schematic

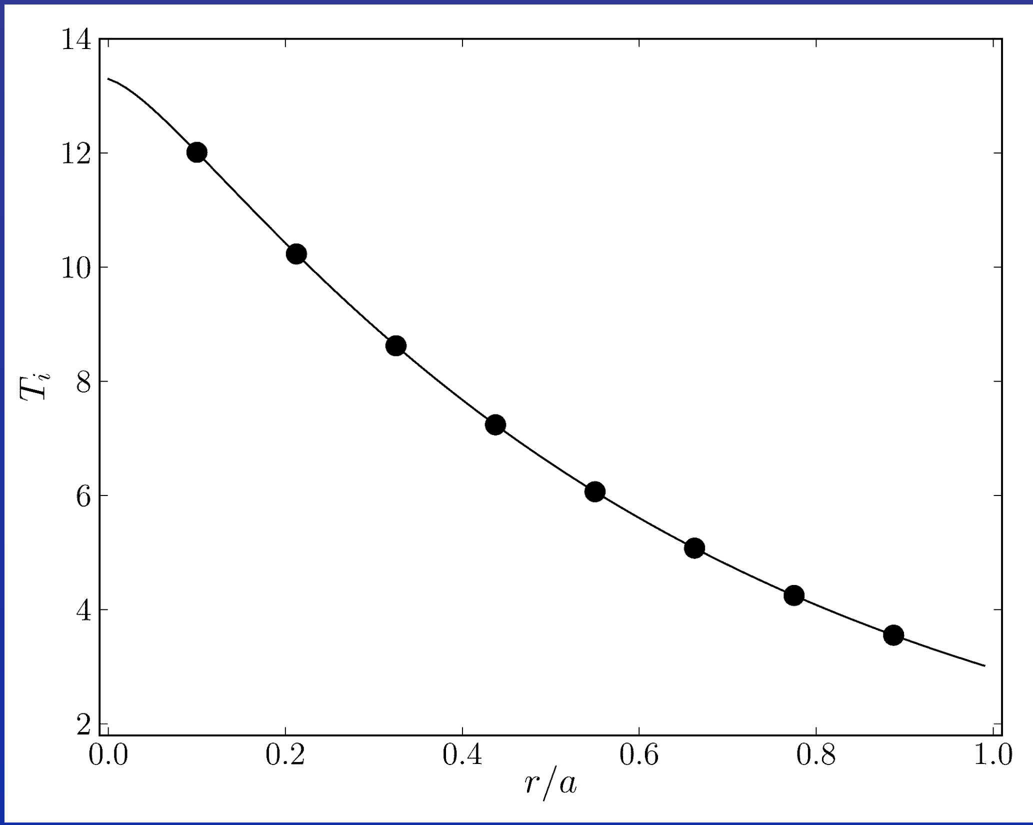


Trinity schematic



Sampling profile with flux tubes





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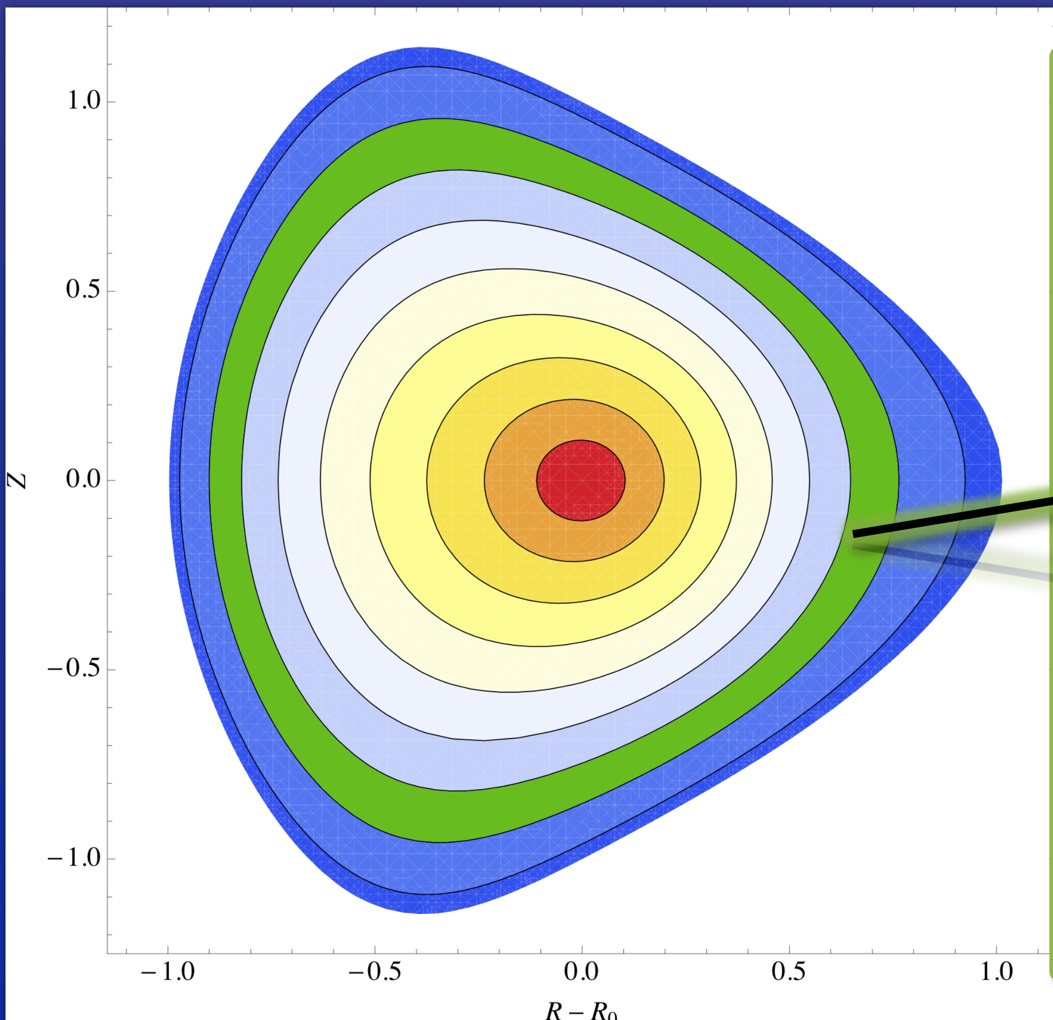

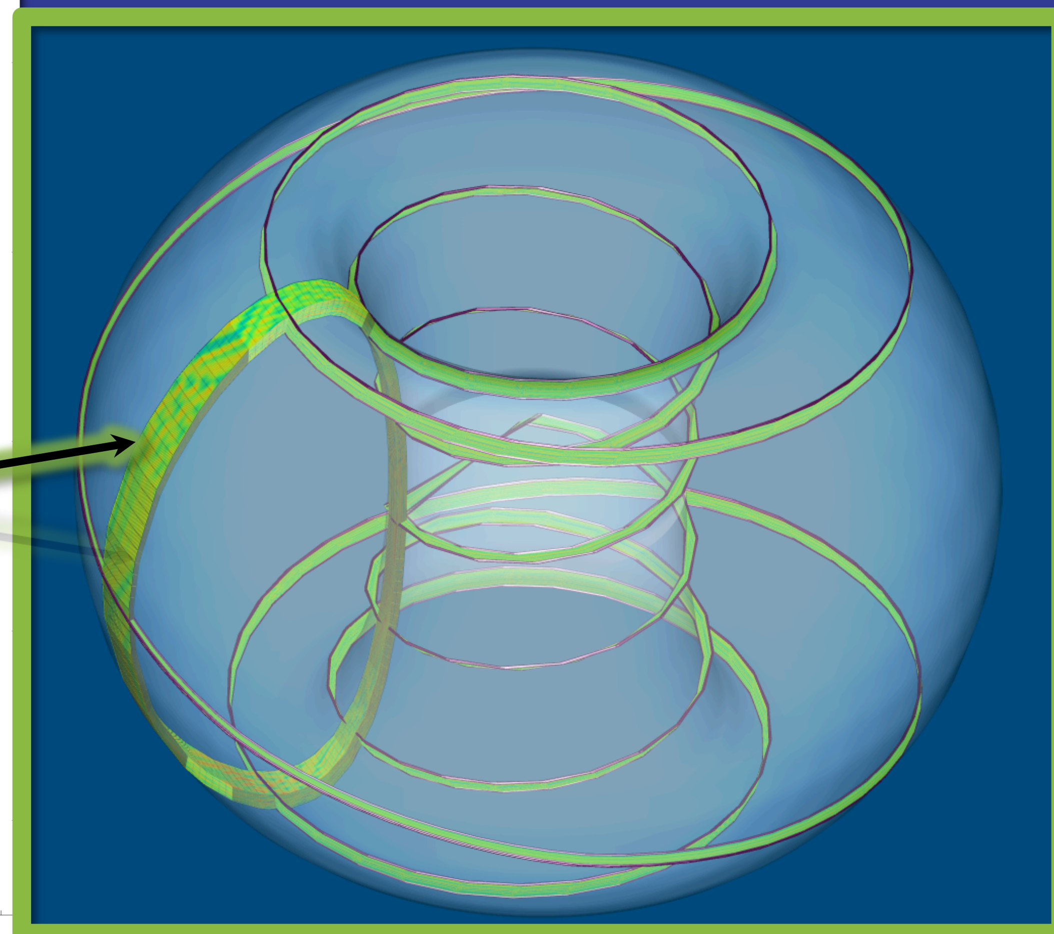

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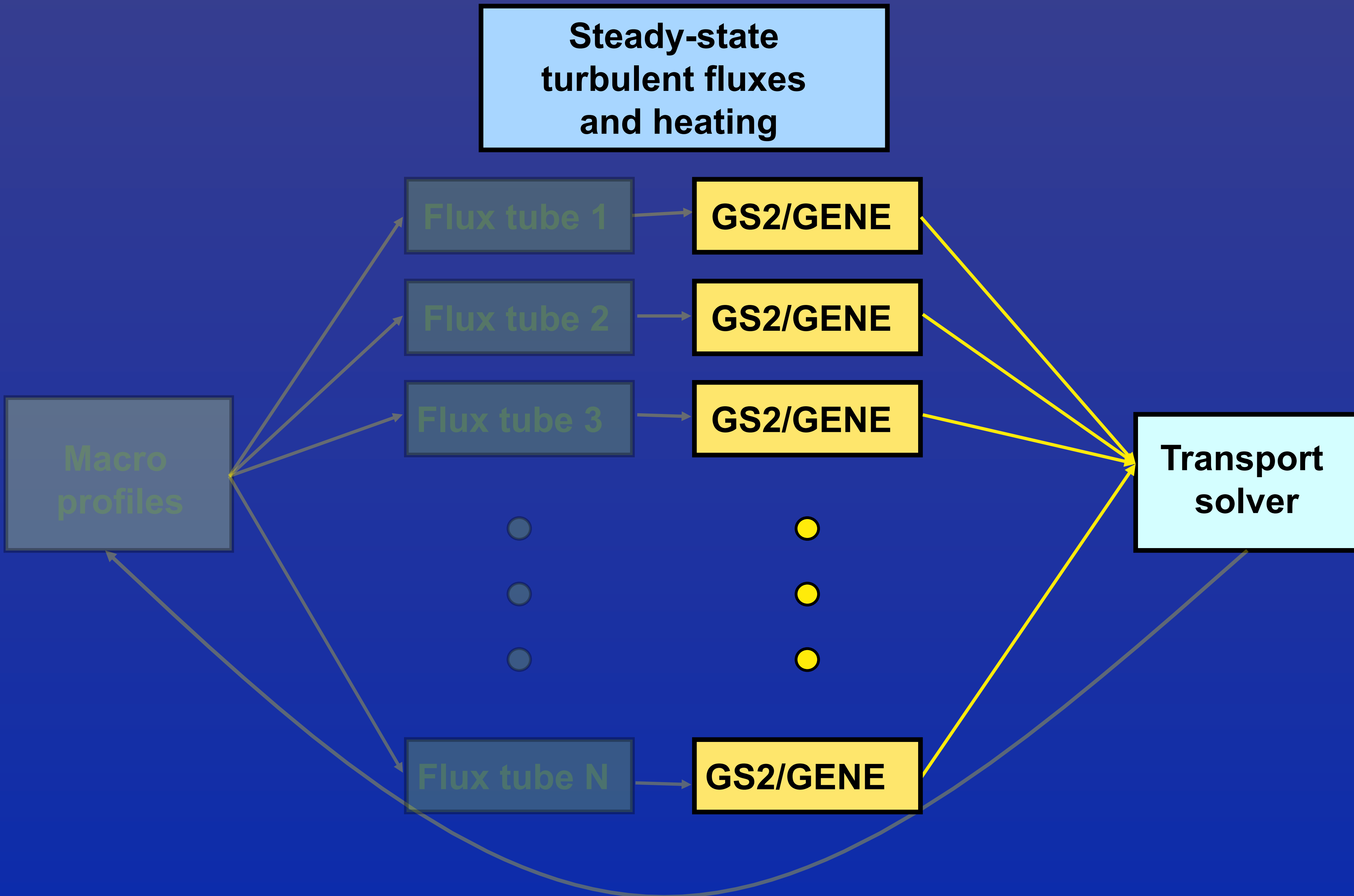

Transport equations in GK

Moment equations for evolution of mean quantities:

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

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

...depend on fluctuations

Sugama (1997)

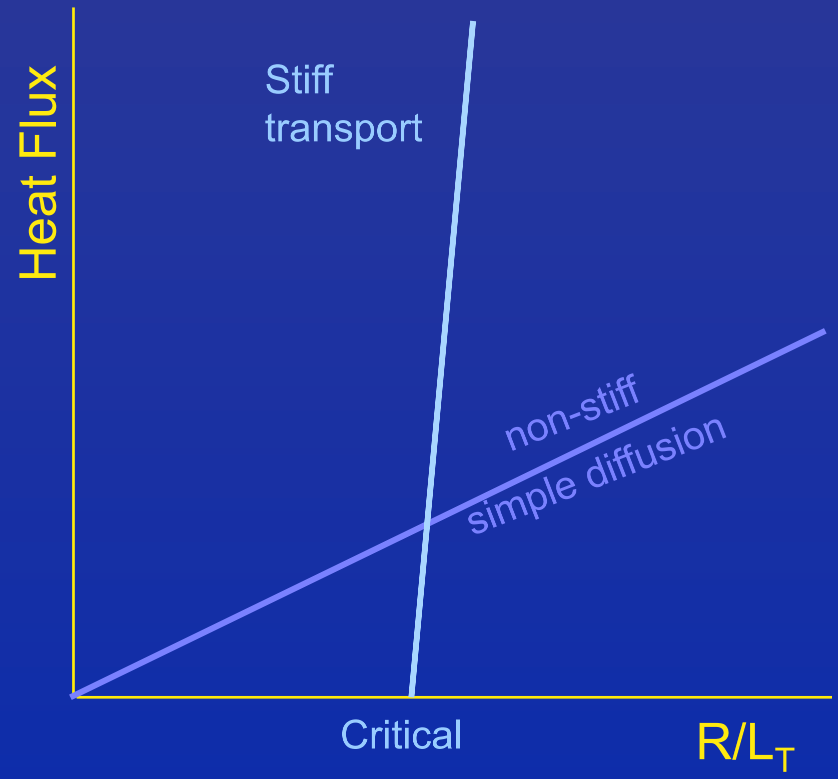
Trinity transport solver

- Transport equations are stiff, nonlinear PDEs:

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

$$\mathbf{Q}_s = \mathbf{Q}_s(n(\psi,t), T(\psi,t); \psi, t)$$

Implicit treatment needed for stiffness



Trinity transport solver

$$\frac{\partial n}{\partial t} = H(r)\frac{\partial}{\partial r}G[n(r,t),T(r,t);r,t]$$

- General (single-step or multi-step) time discretization:

$$\frac{n^{m+1}-n^{m}}{\Delta\tau} = \alpha\left[H\frac{\partial G}{\partial r}\right]^{m+1} + (1-\alpha)\left[H\frac{\partial G}{\partial r}\right]^{m}$$

- 2nd order centered difference in radial coordinate (equally spaced grid):

$$\frac{\partial G}{\partial r} = \frac{G_{j+1/2}-G_{j-1/2}}{\Delta r}$$

Trinity transport solver

- Implicit treatment via Newton's Method) 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

*S.C. Jardin, G. Bateman, G.W. Hammett, and L.P. Ku, On 1D diffusion problems with a gradient-dependent diffusion coefficient, J. Comp. Phys. **227**, 8769 (2008).

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)

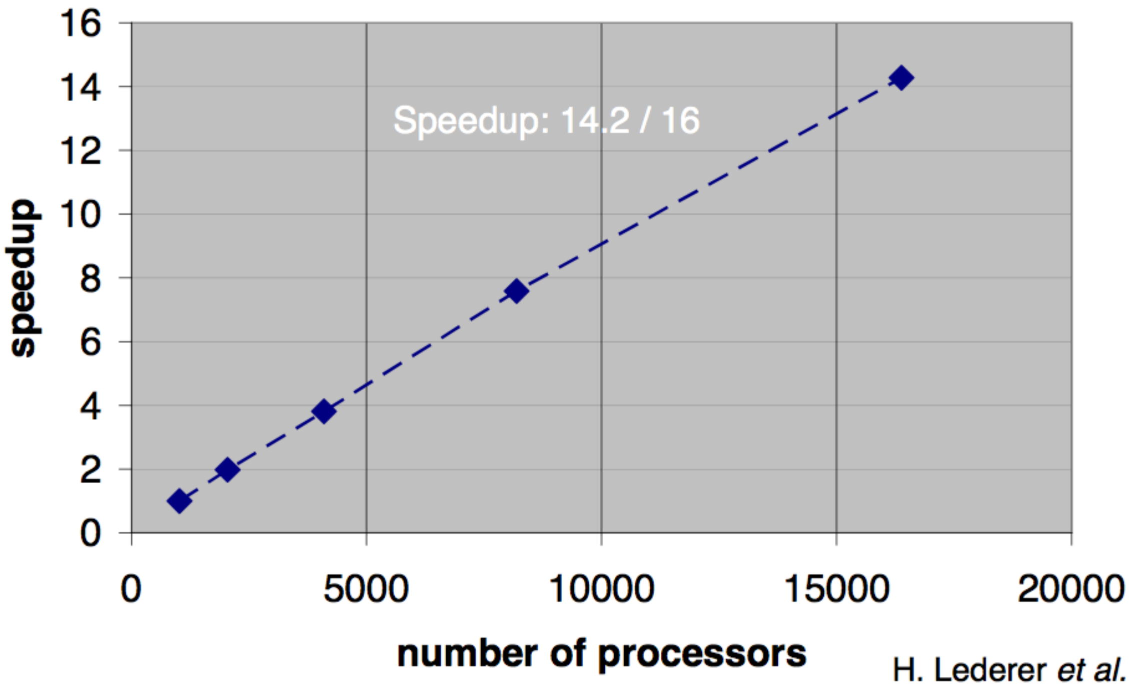
Trinity transport solver

- Nonlinear turbulence simulation runs until fluxes converged
- Turbulence for new transport time step initialized to saturated state from previous transport time step – faster convergence
- Option to use model fluxes (IFS-PPPL, quasilinear, etc.)
- Sources specified analytically or taken from experiment

Trinity scaling

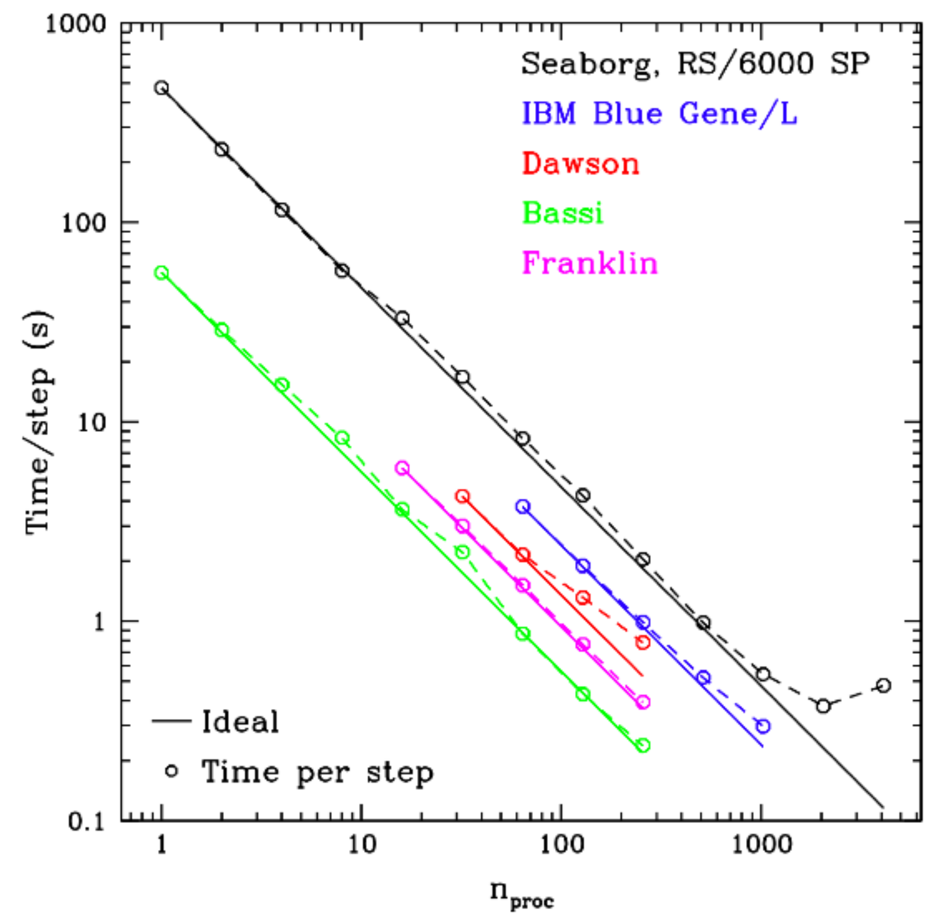
- Example calculation with 10 radial grid points:
  - evolve density, toroidal angular momentum, and electron/ion pressures
  - simultaneously calculate fluxes for equilibrium profile and for 4 separate profiles (one for each perturbed gradient scale length)
  - total of 50 flux tube simulations running 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

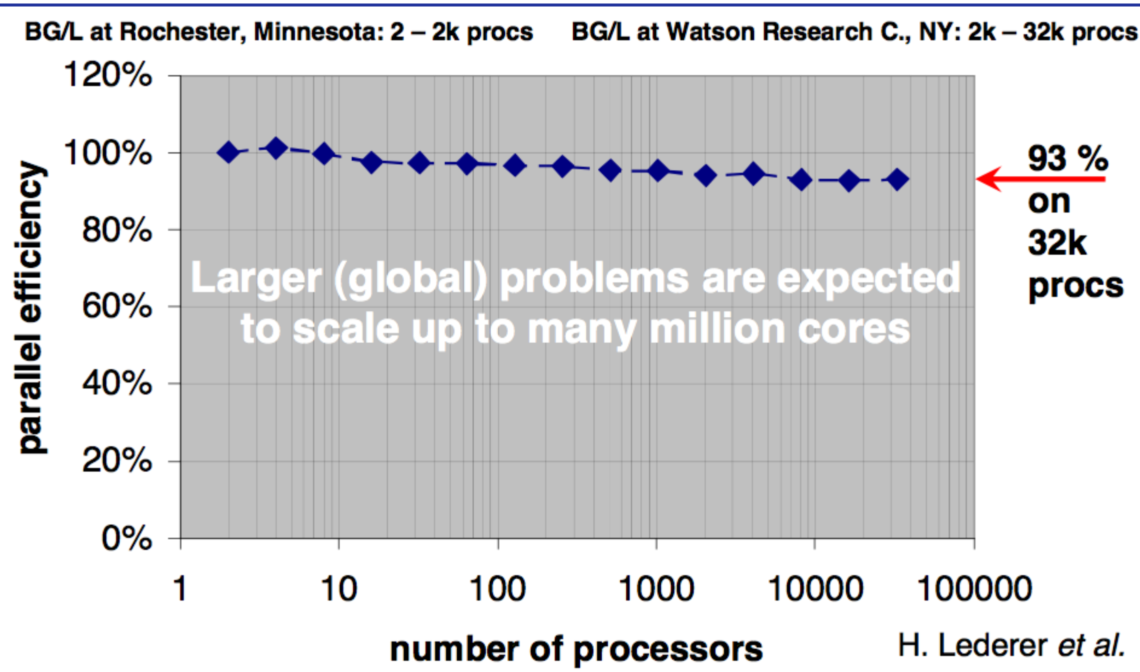
Flux tube scaling



GENE strong scaling

GS2 strong scaling





GENE weak scaling

Boundary conditions

- Various initialization options:
  - Analytic specification
  - Experimental profiles
  - Numerical profiles (from IFS-PPPL, etc.)
- Fix density and temperature at outer edge of simulation domain
  - Predict performance as a function of pedestal height
- Vanishing fluxes at magnetic axis:

$$\psi \rightarrow 0 : \quad V'Q = V'\Gamma = 0$$

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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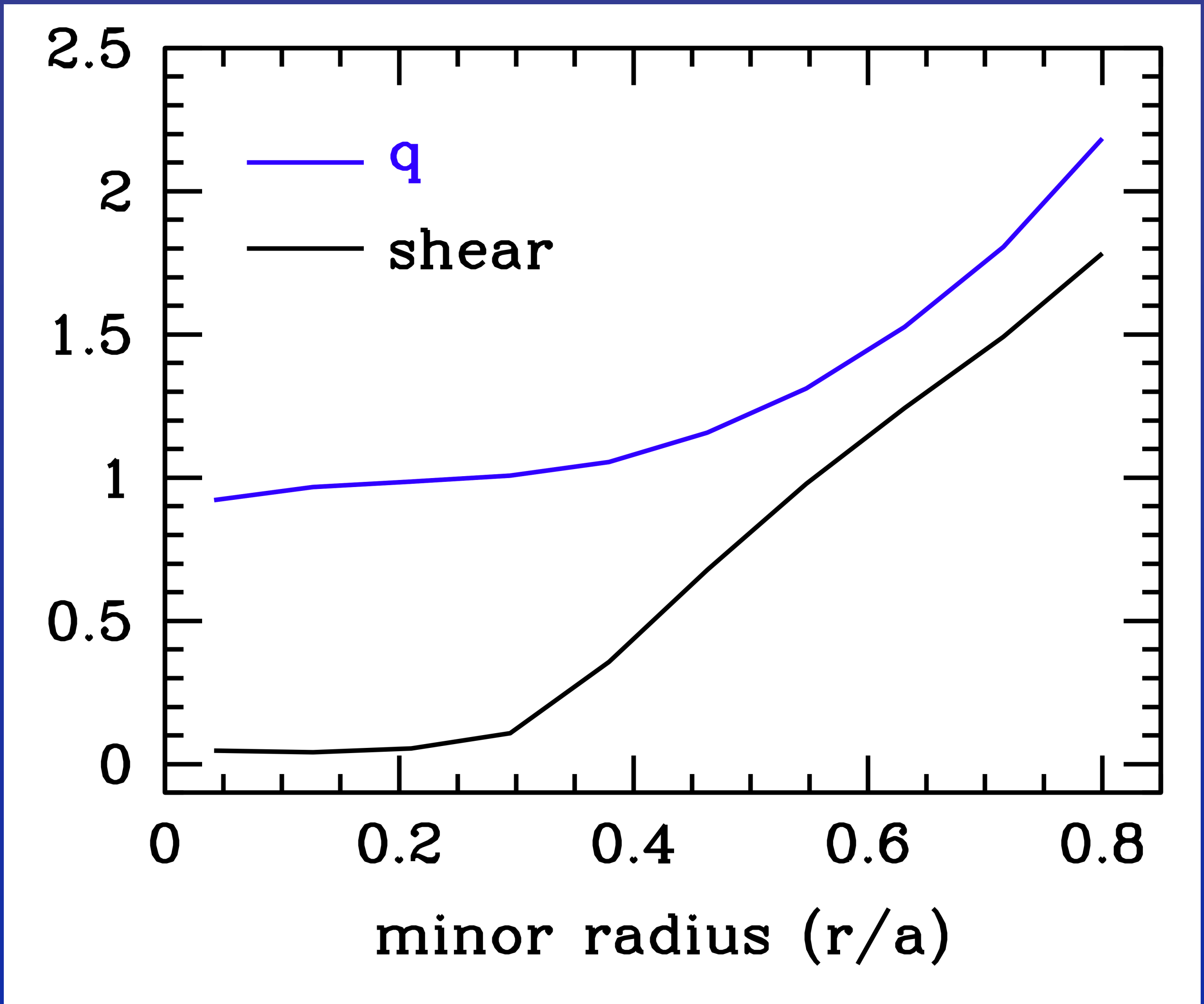
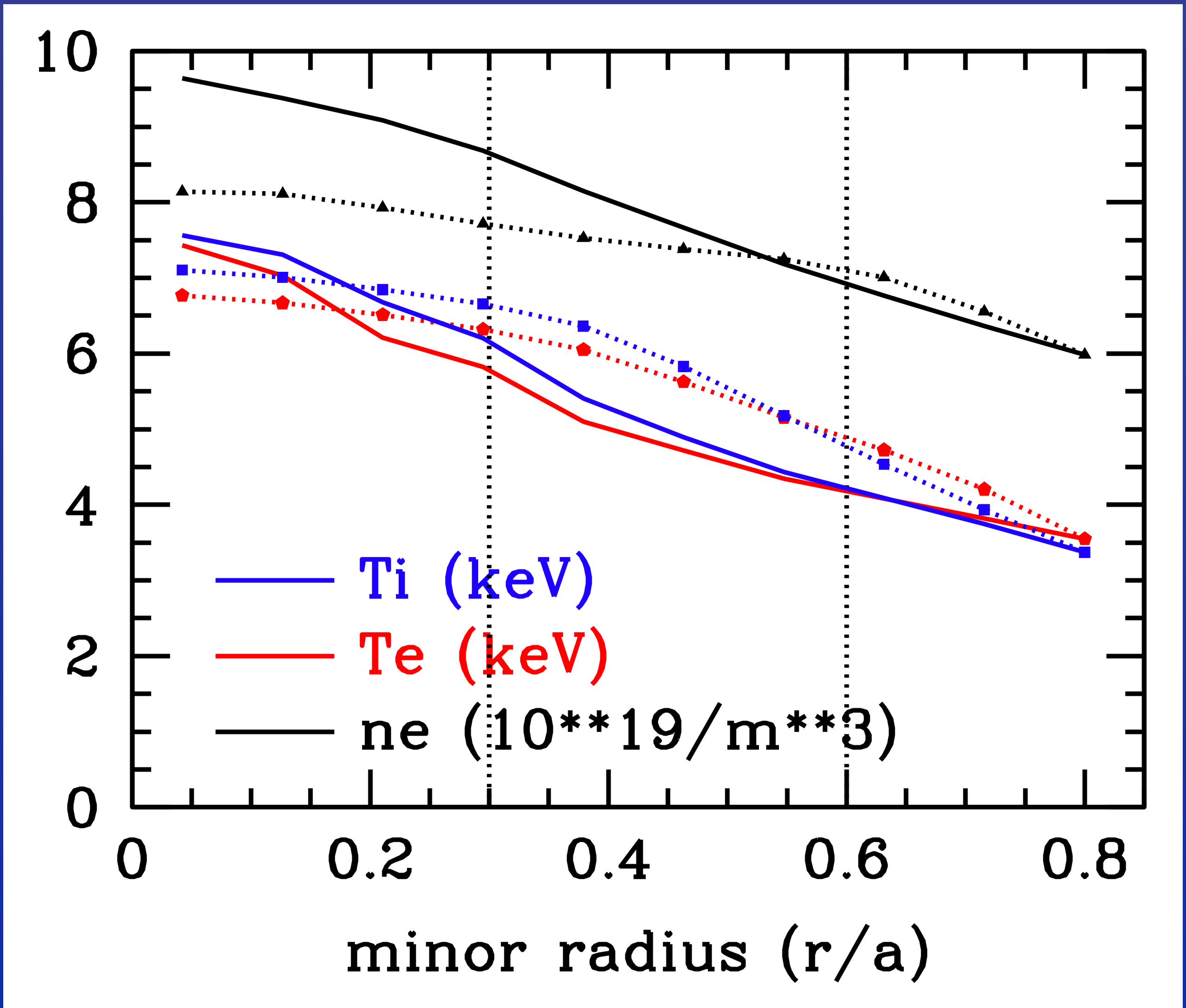
JET shot #42982



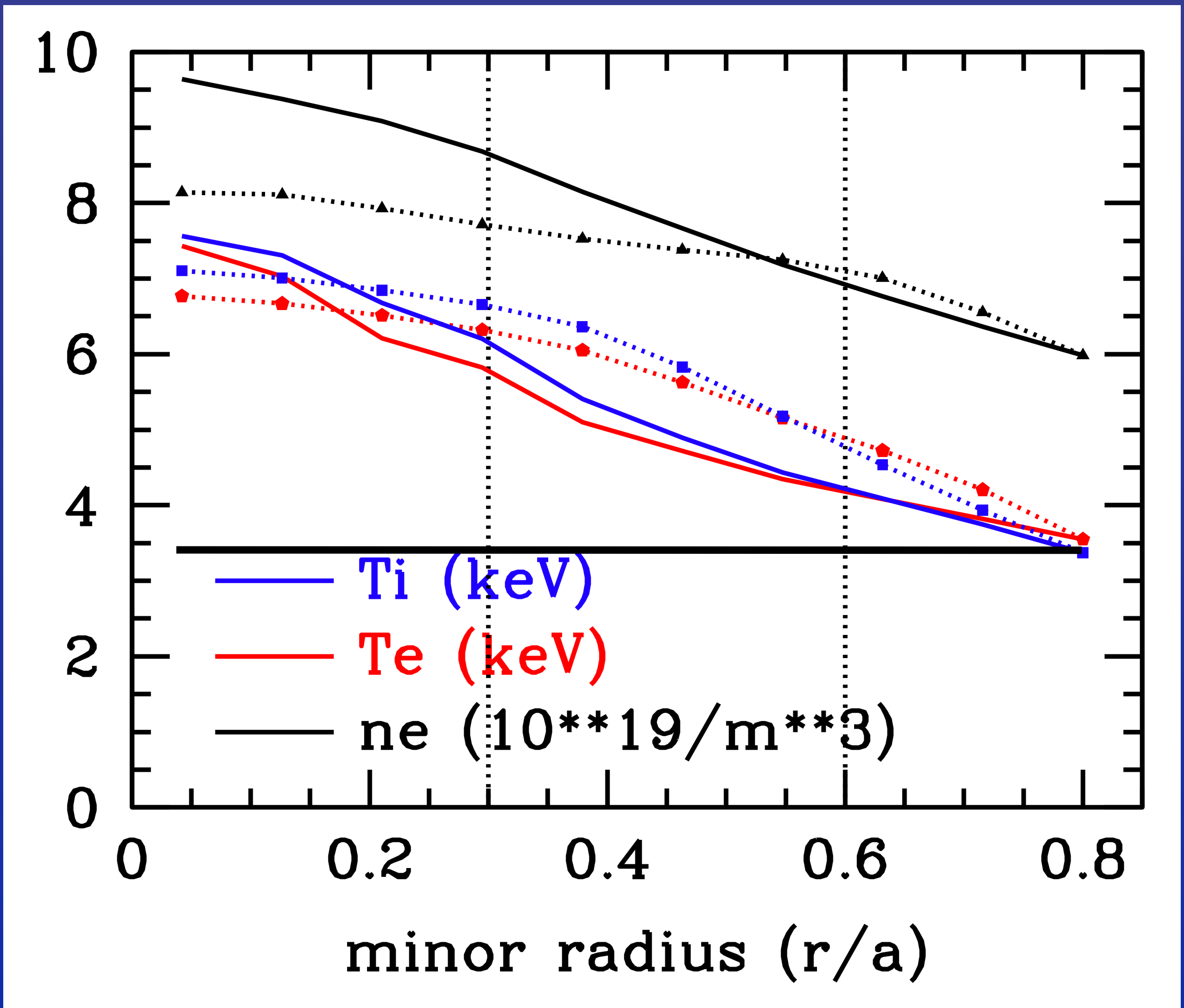
- ITER demo discharge
- H-mode D-T plasma, record fusion energy yield
- Miller local equilibrium model: q, shear, shaping
- B = 3.9 T on axis
- TRANSP fits to experimental data taken from ITER profile database

Evolving density profile



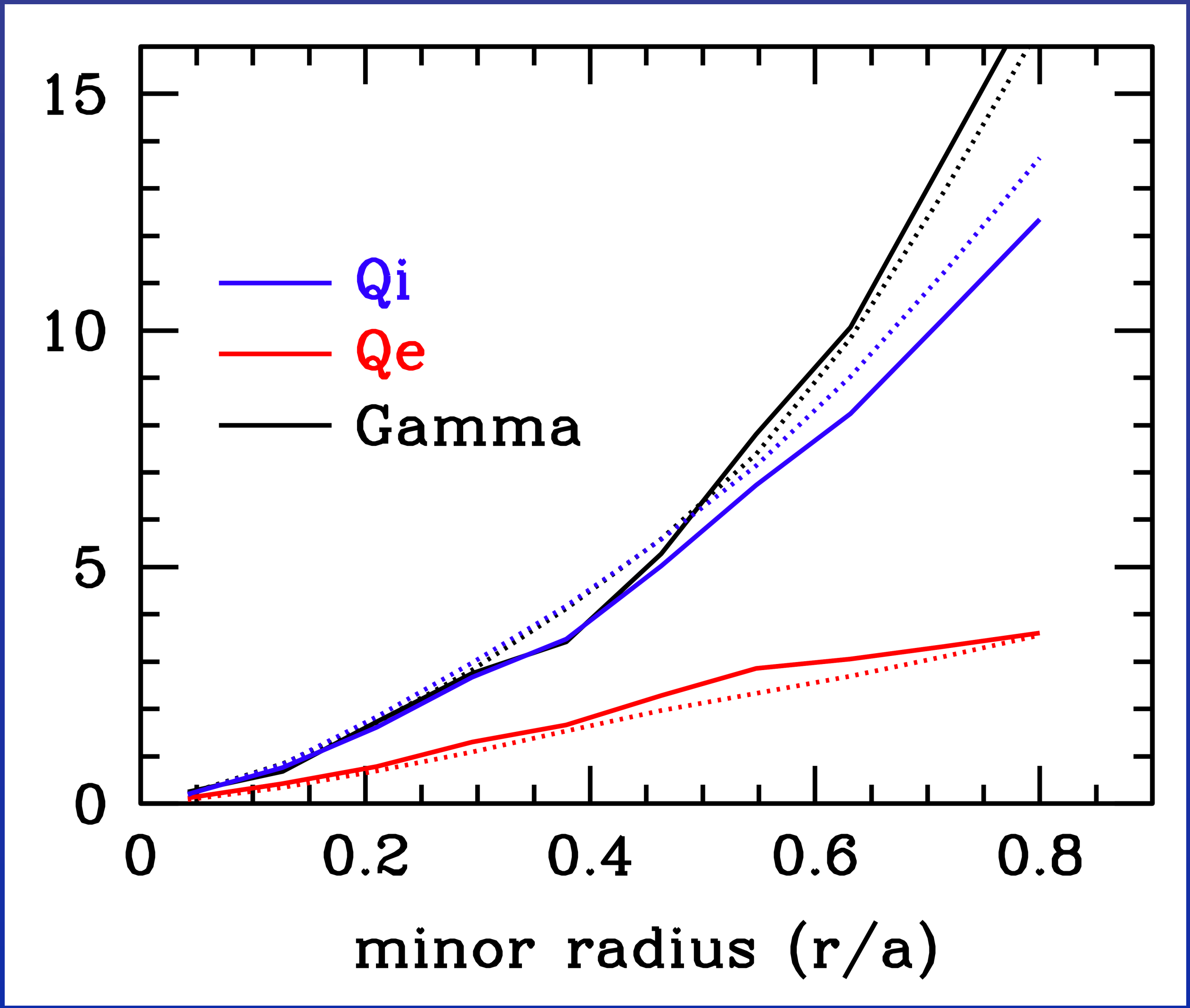
- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%
- Sources of discrepancy:
  - Large error bars
  - Flow shear absent

Evolving density profile



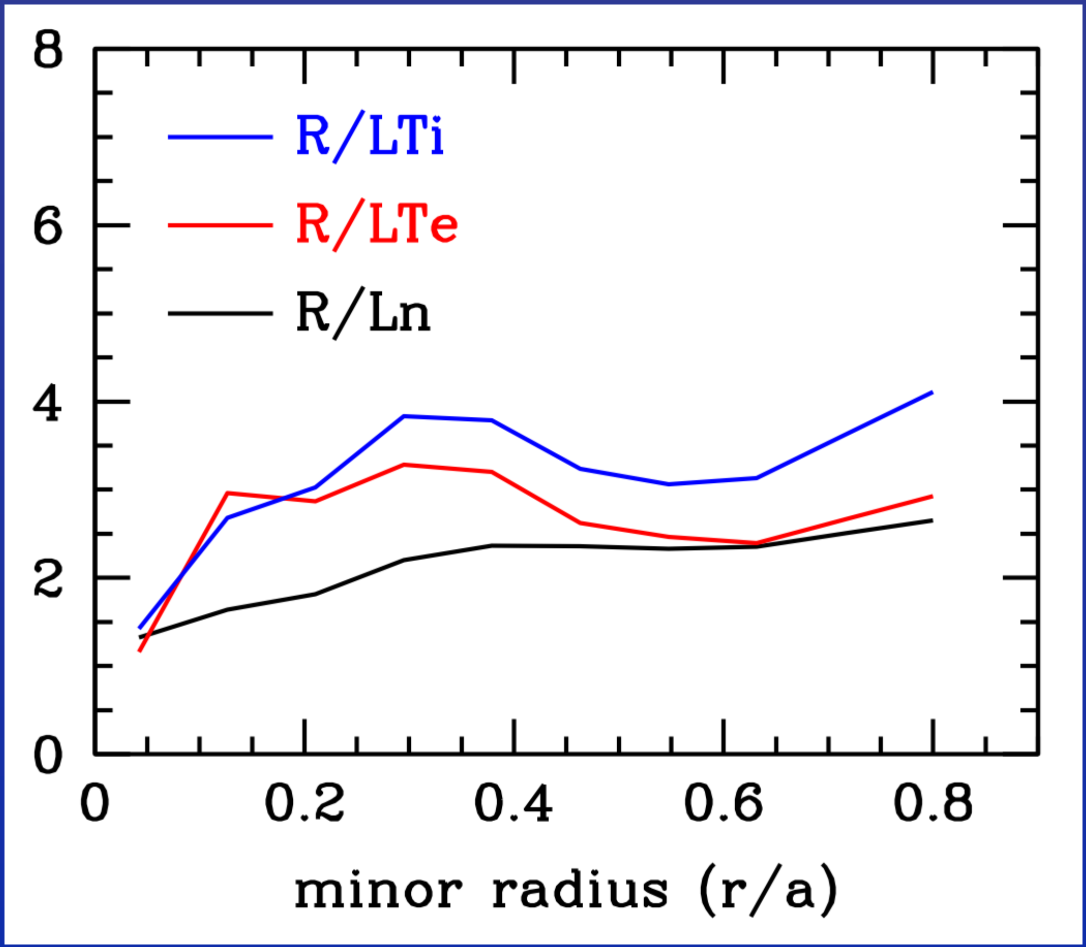
- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%
- Sources of discrepancy:
  - Large error bars
  - Flow shear absent

Power balance

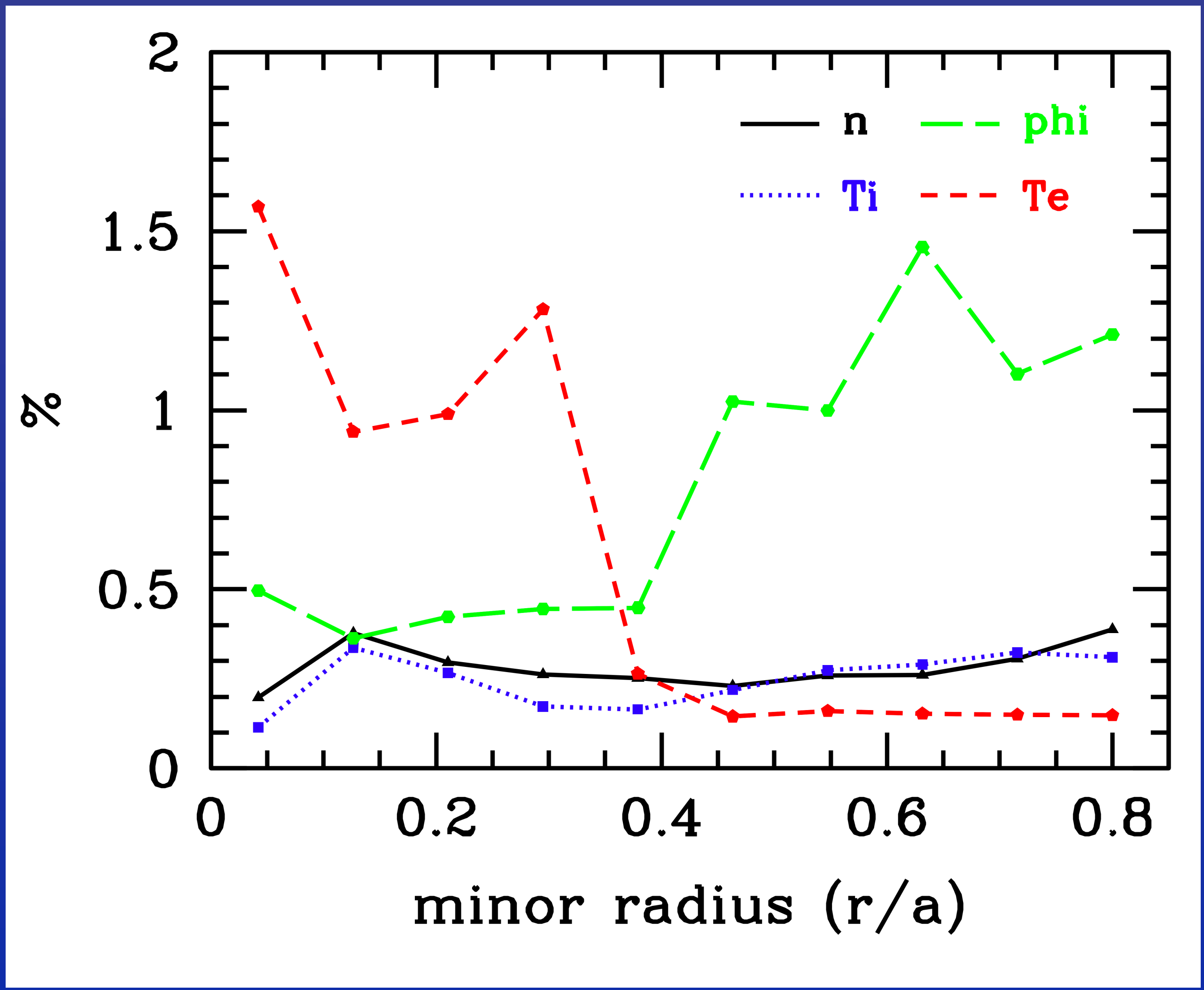


Profile stiffness

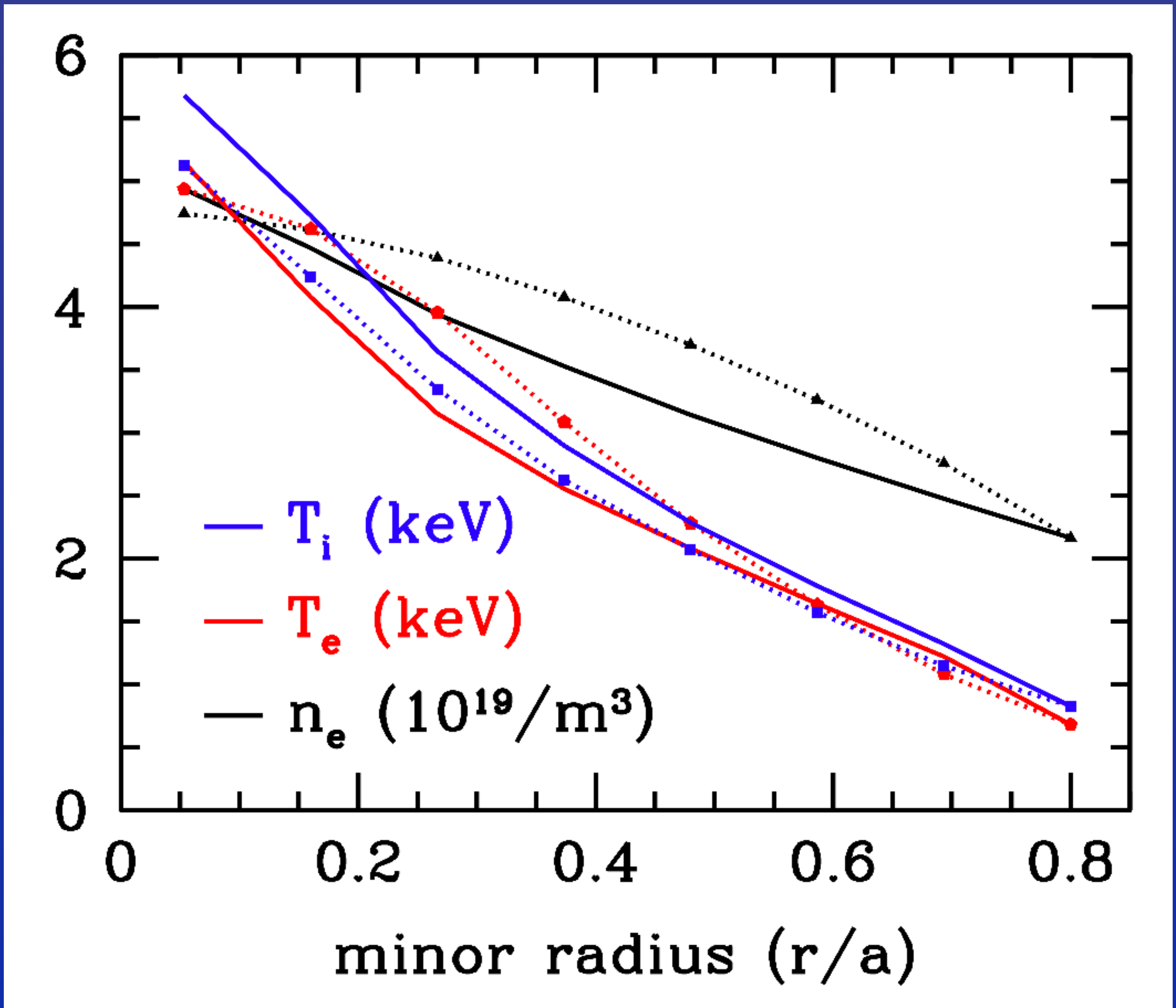
- ~ flat grad scale lengths indicative of stiffness (near critical gradient across most of minor radius)



Fluctuations

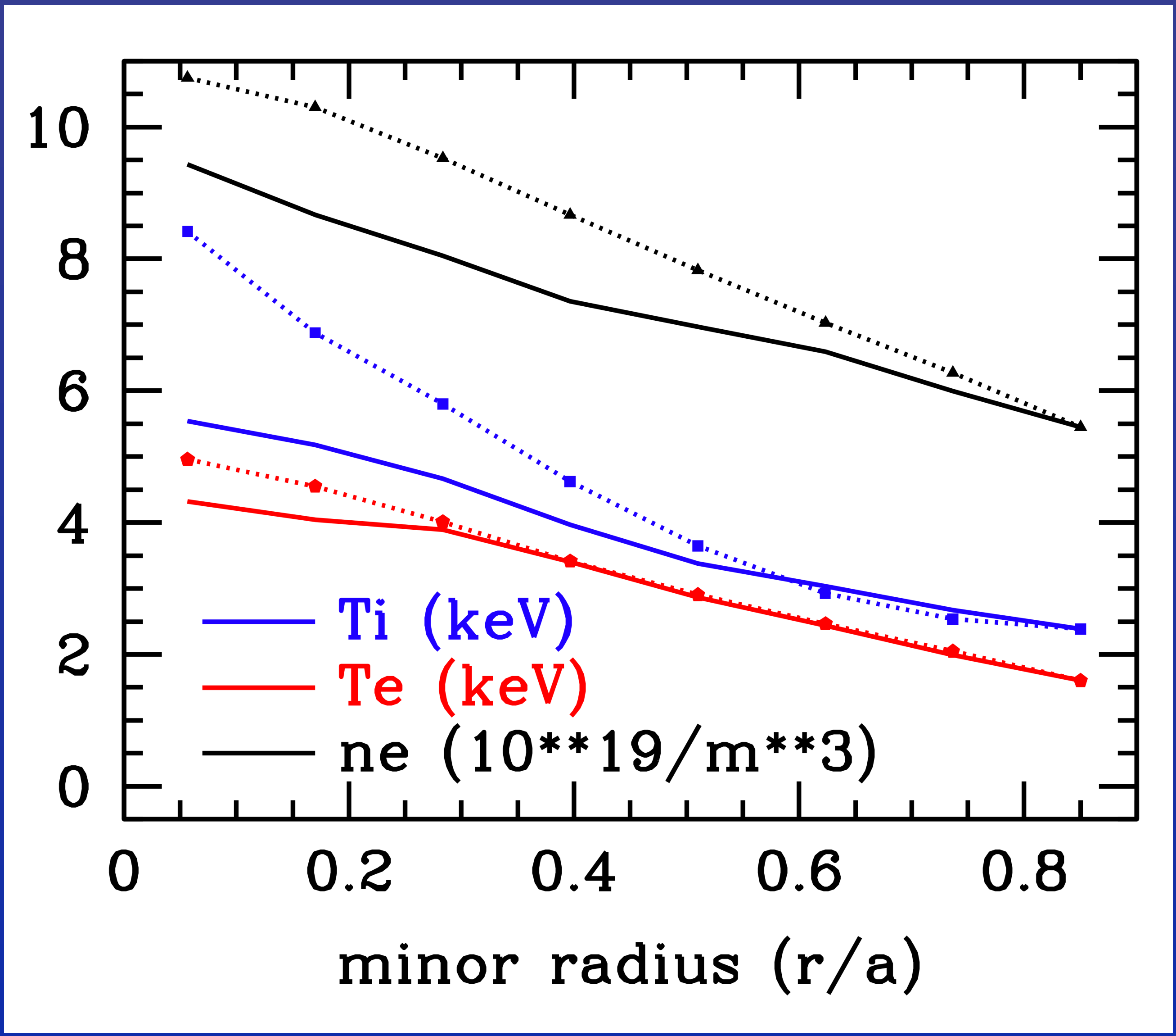


JET shot #19649



- L-mode discharge
- 8 radial grid points
- Costs ~25k CPU hrs (4 clock hrs)
- Flow shear absent

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

Overview

- Motivation
- Theoretical framework
- Numerical approach
- Example simulation results
- Future directions

Future directions

- Summary: multi-scale approach saves factor of 10^3-10^4 and highly parallelizable
- Capture more physics
  - Magnetic equilibrium evolution
  - MHD stability
  - Momentum transport
  - Improved neoclassical model
- 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