The Trinity algorithm: local gyrokinetics + global transport = predictive model of core plasma dynamics

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Overview

- Motivation
- Theoretical framework
- Numerical approach
- Trinity simulation results
- Conclusions

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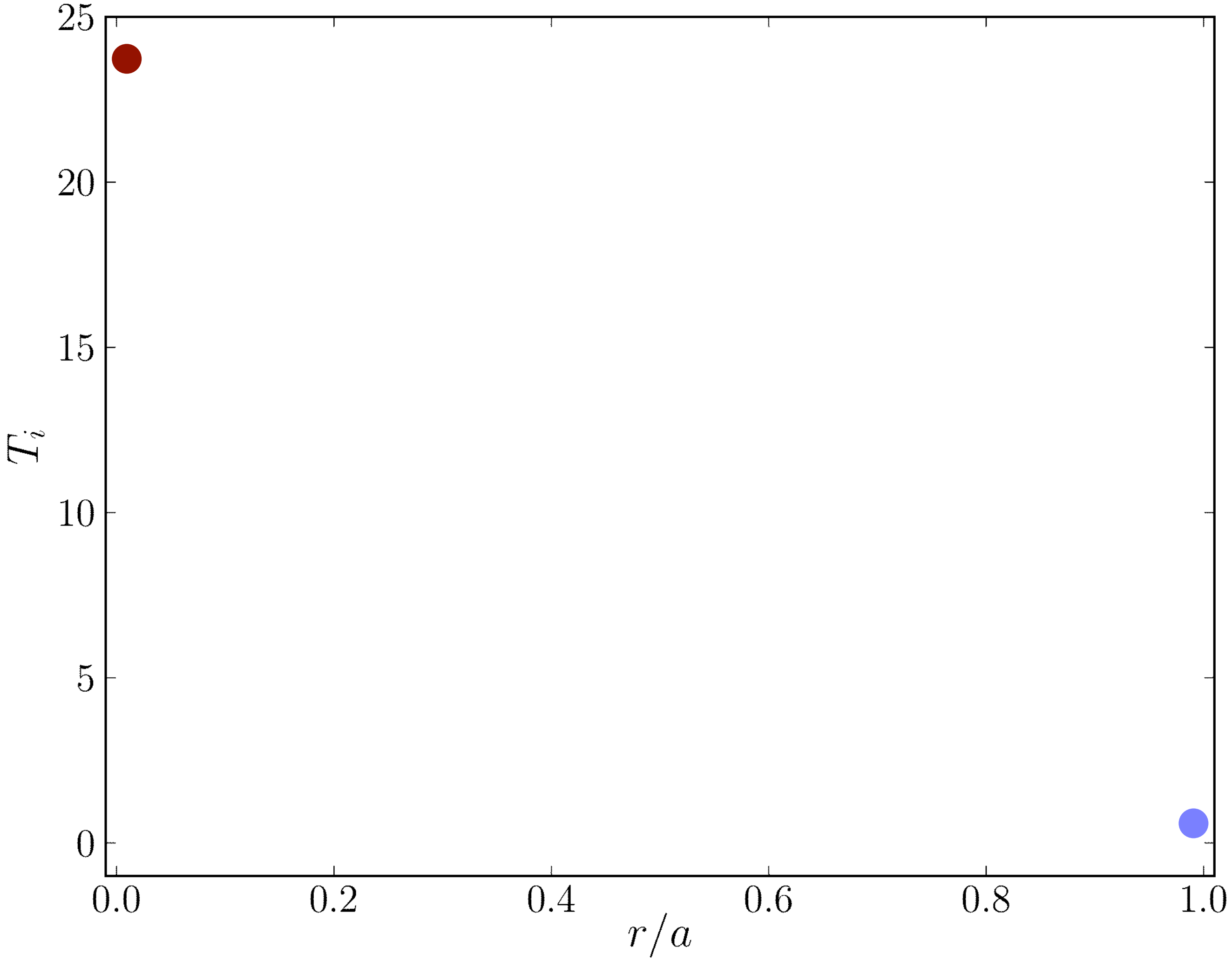
Objective



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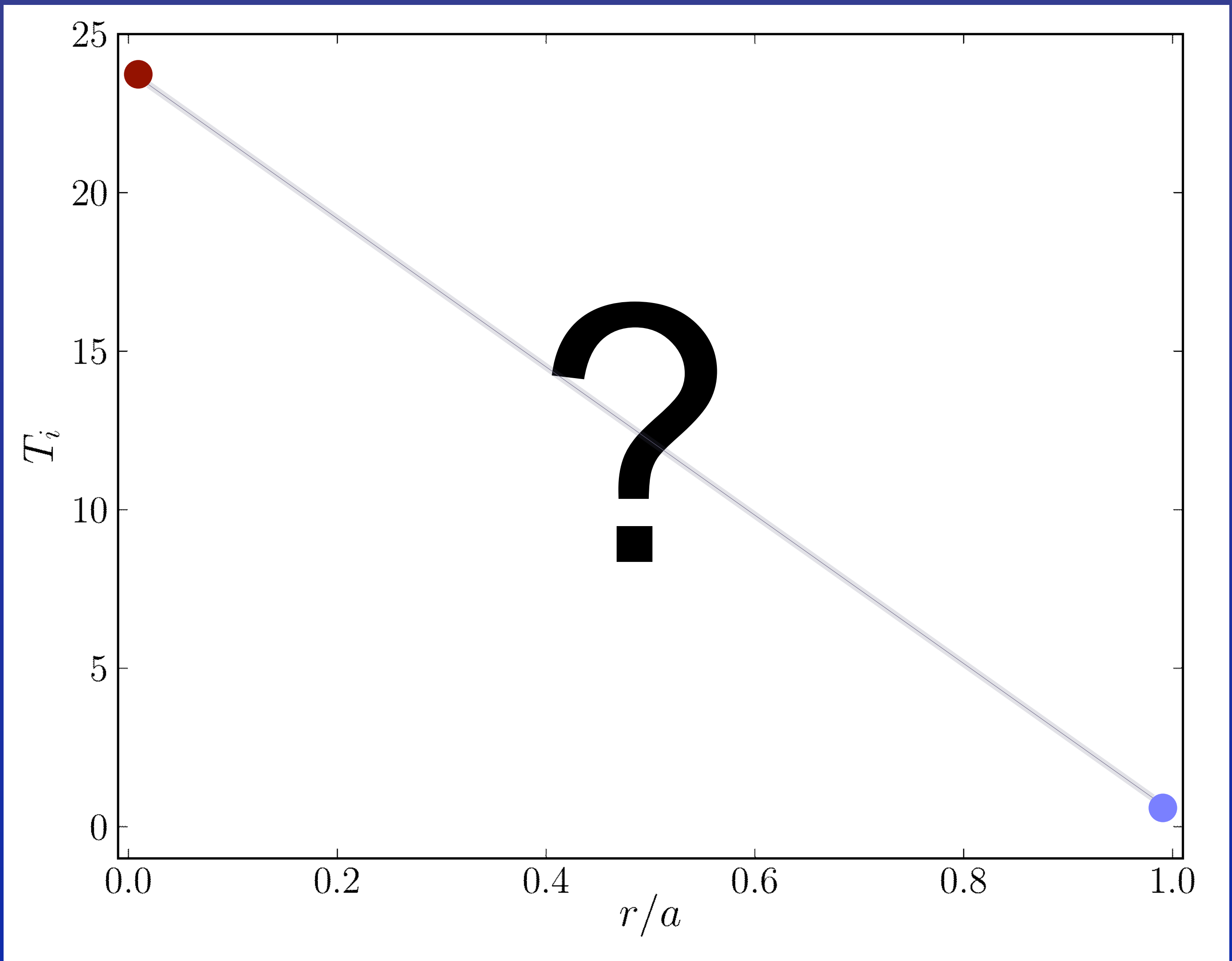

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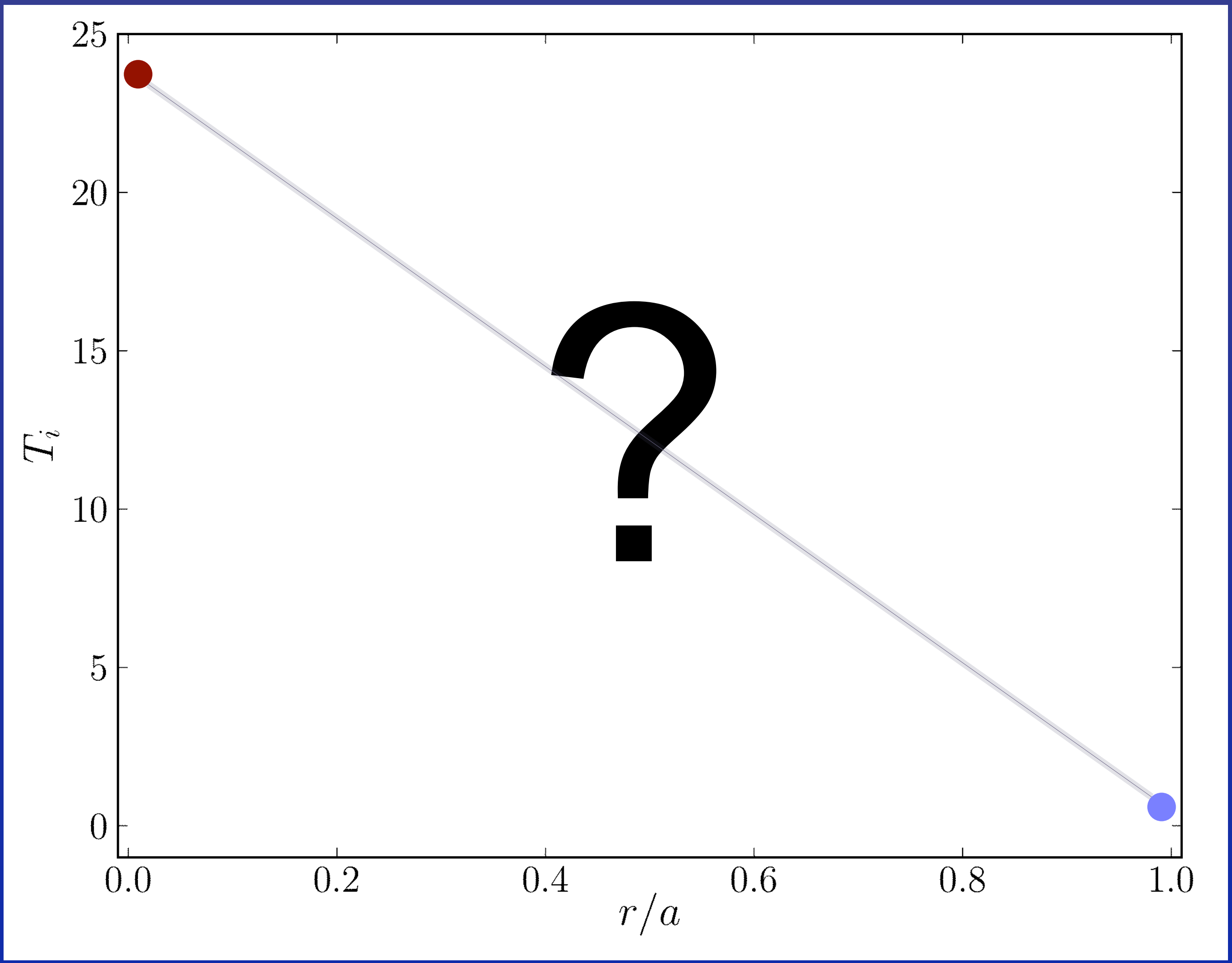

Core:
multi-physics,
multi-scale

Edge:
multi-physics,
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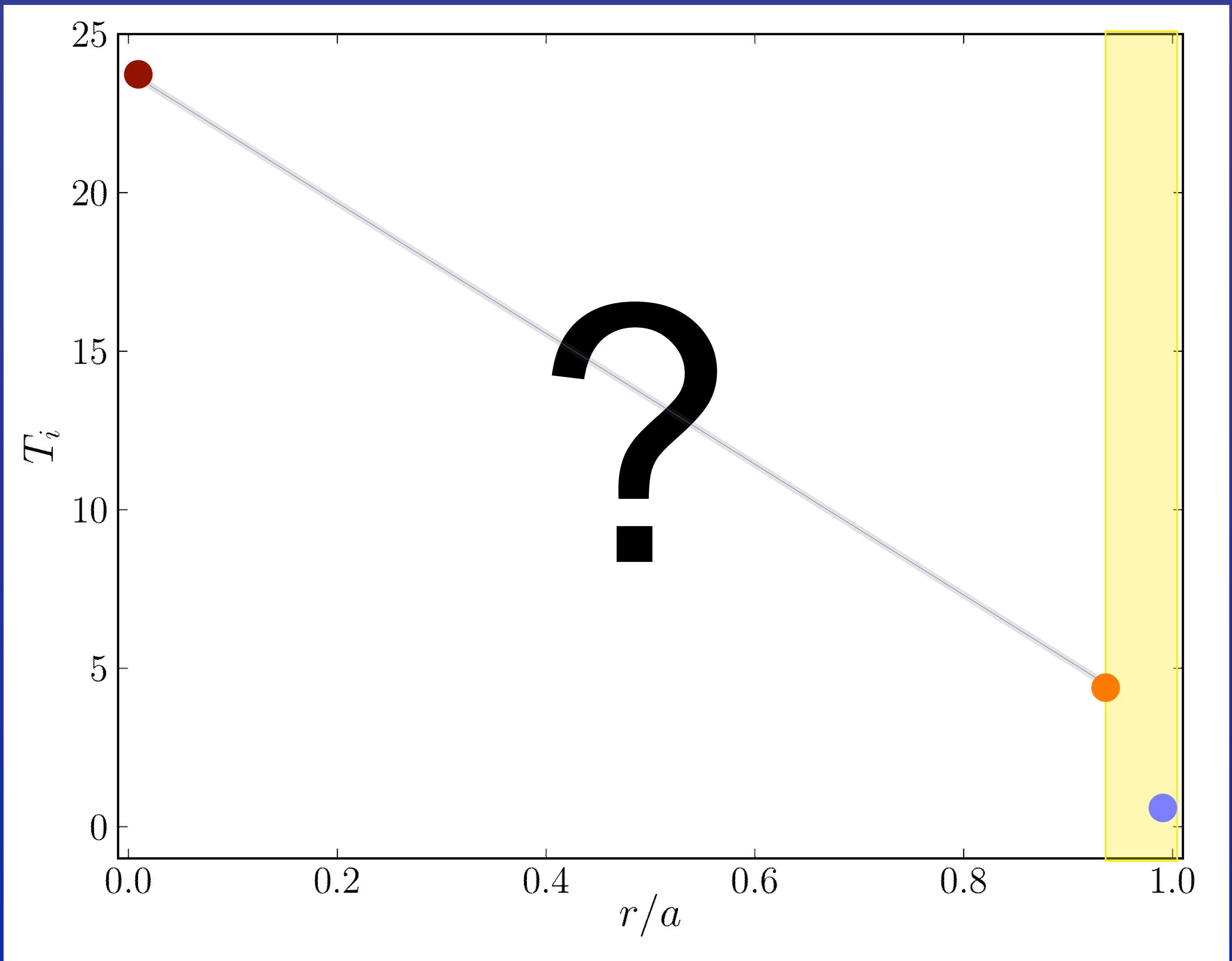

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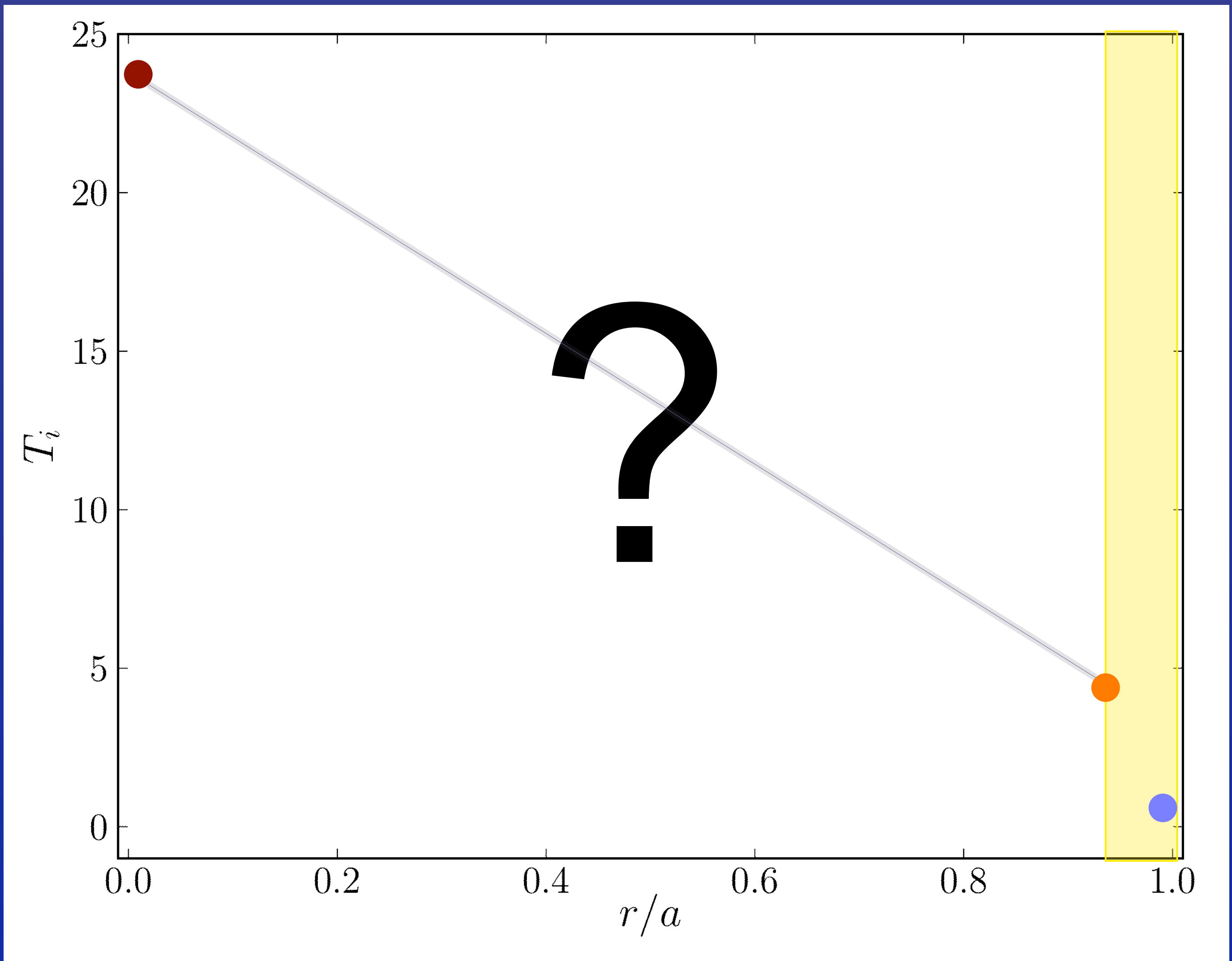

Core:
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- kinetic turbulence
- neoclassical
- sources
- magnetic equilibrium
- MHD

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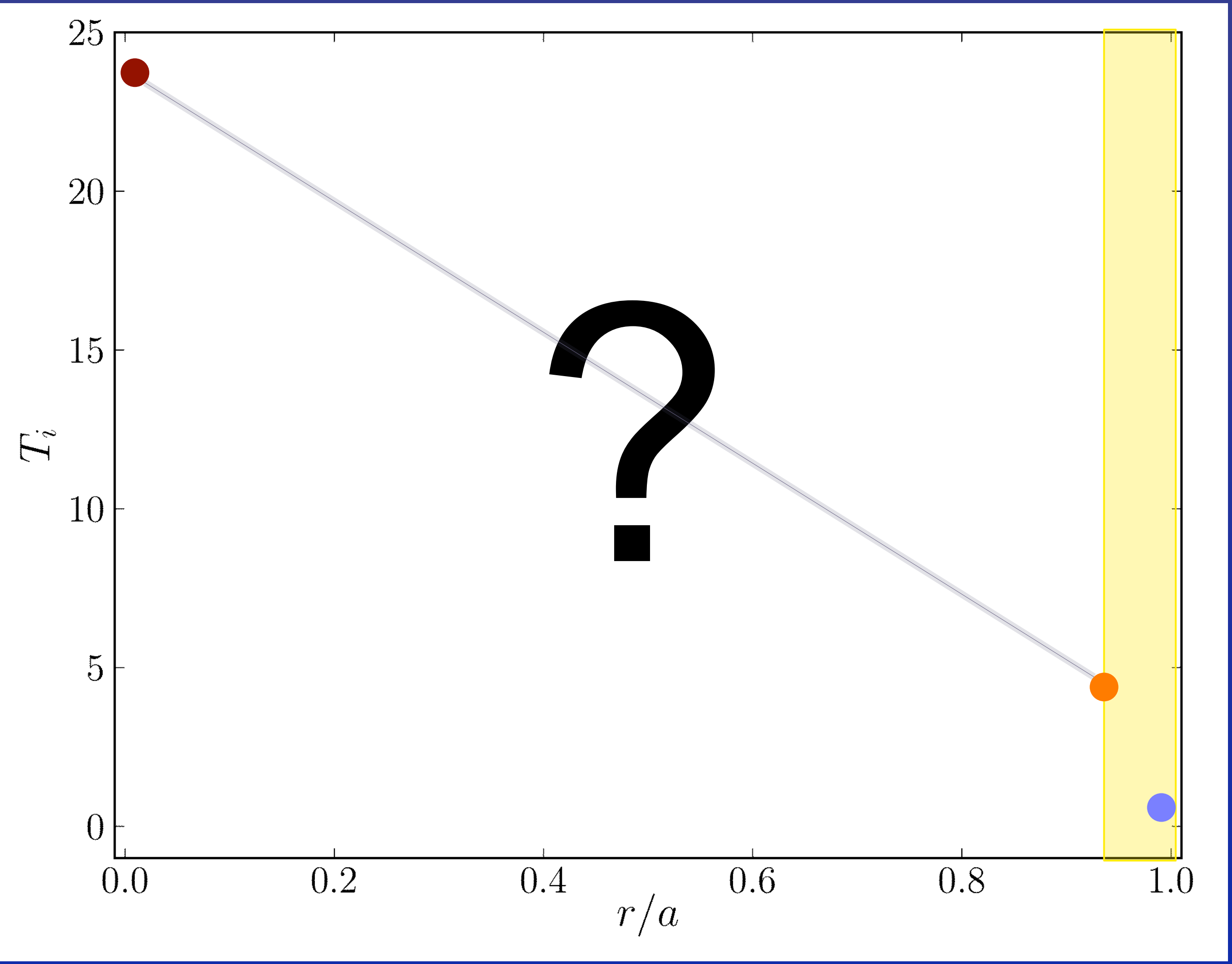

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- **kinetic turbulence**
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Scale separation in ITER

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

Physics	Perpendicular spatial scale	Temporal scale
Turbulence from ETG modes	$k_\perp^{-1}$ ~ 0.001 - 0.1 cm	ω_* ~ 0.5 - 5.0 MHz
Turbulence from ITG modes	$k_\perp^{-1}$ ~ 0.1 - 8.0 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

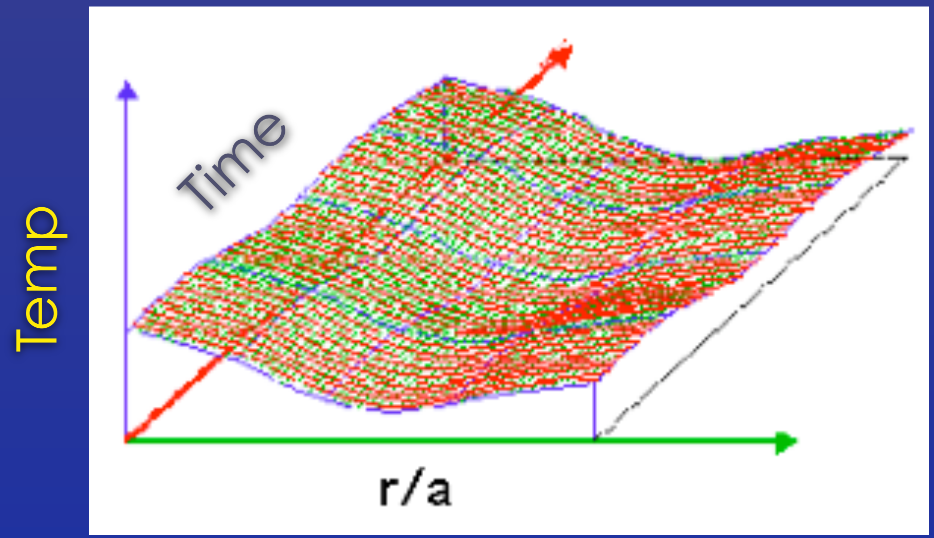
Direct simulation cost

- 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^{10} 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
- Statistical periodicity in poloidal direction takes advantage of $k_{\perp}^{-1} \ll L_{\theta}$: savings of ~100
- Total saving of ~10^5
- Factor of ~10^5 more than largest fluid turbulence calculations
- Simulation still not possible; need multiscale approach

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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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- Turbulent fluctuations are low amplitude:

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

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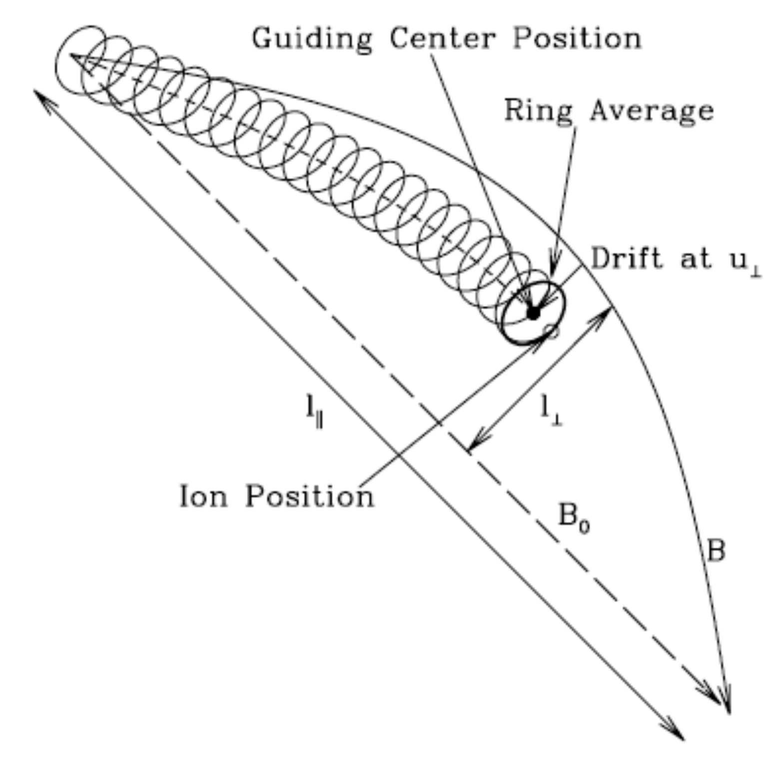
$$\frac{\partial_t \delta f}{\delta f} \sim \omega \sim \epsilon \Omega$$



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- Separation of space scales:

$$\nabla F \sim F/L, \;\; \nabla_{\|} \delta f \sim \delta f/L, \;\; \nabla_{\perp} \delta f \sim \delta f/\rho$$

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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

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

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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:

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

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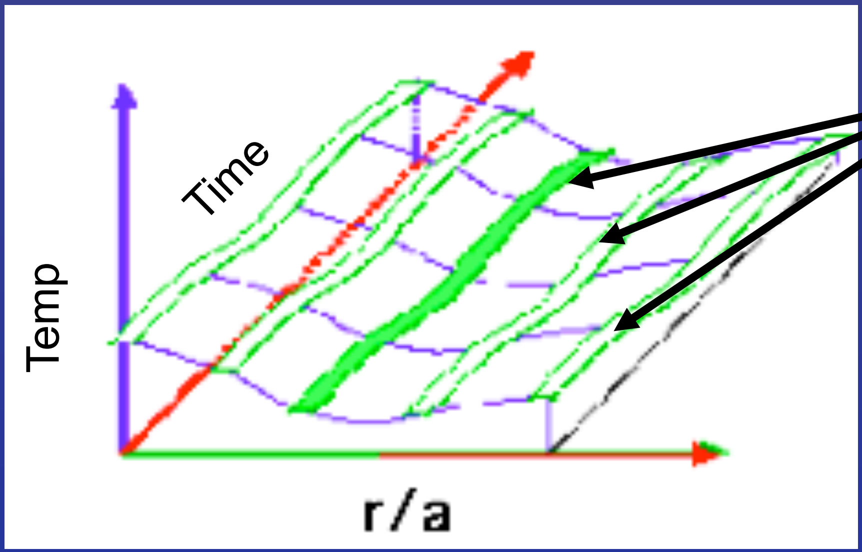
Multiscale grid

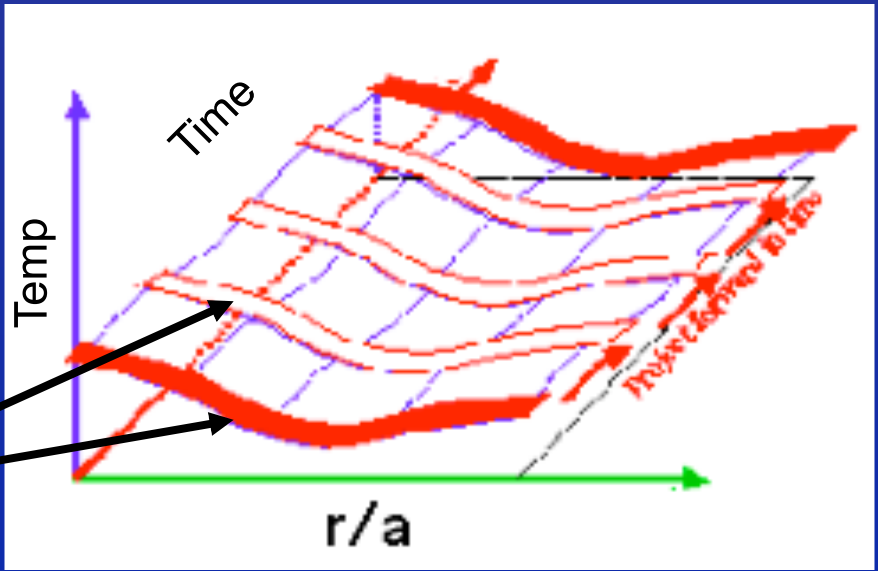


Flux tube spatial simulation domain for microturbulence

- Small regions of fine grid (for turbulence) embedded in "coarse" radial grid (for equilibrium)
- Turbulent fluxes and heating in small regions calculated using flux tubes (equivalent to flux surfaces)
- Flux tubes = radial grid points in large-scale transport equations

- Small regions of fine grid (for turbulence) embedded in "coarse" time grid (for equilibrium)
- Steady-state (time-averaged) turbulent fluxes and heating in this volume simulated using flux tubes
- Flux tube sim = time grid point in long-time transport equations

Flux tube temporal simulation domain for microturbulence



Flux tubes minimize flux surface grid points

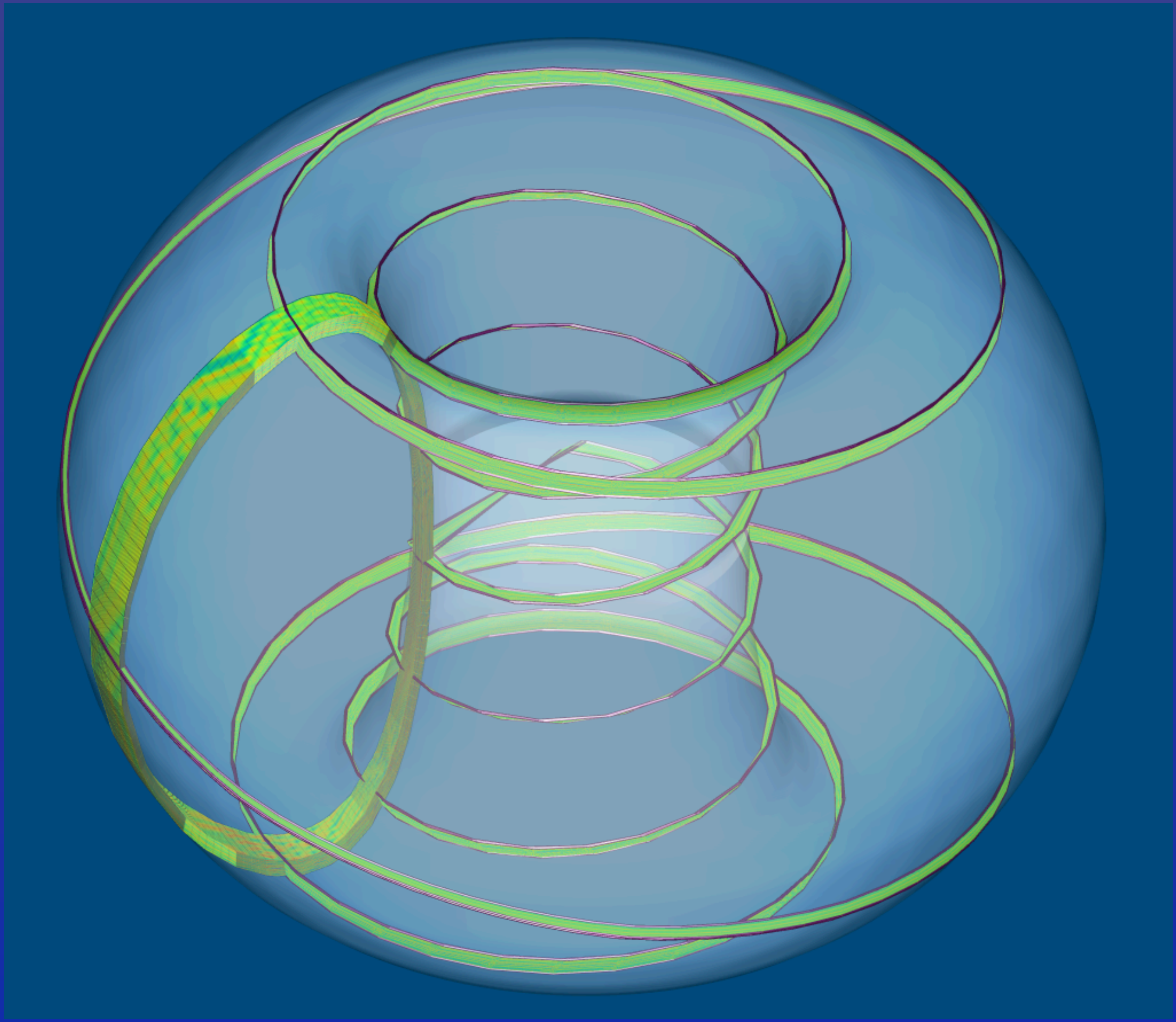
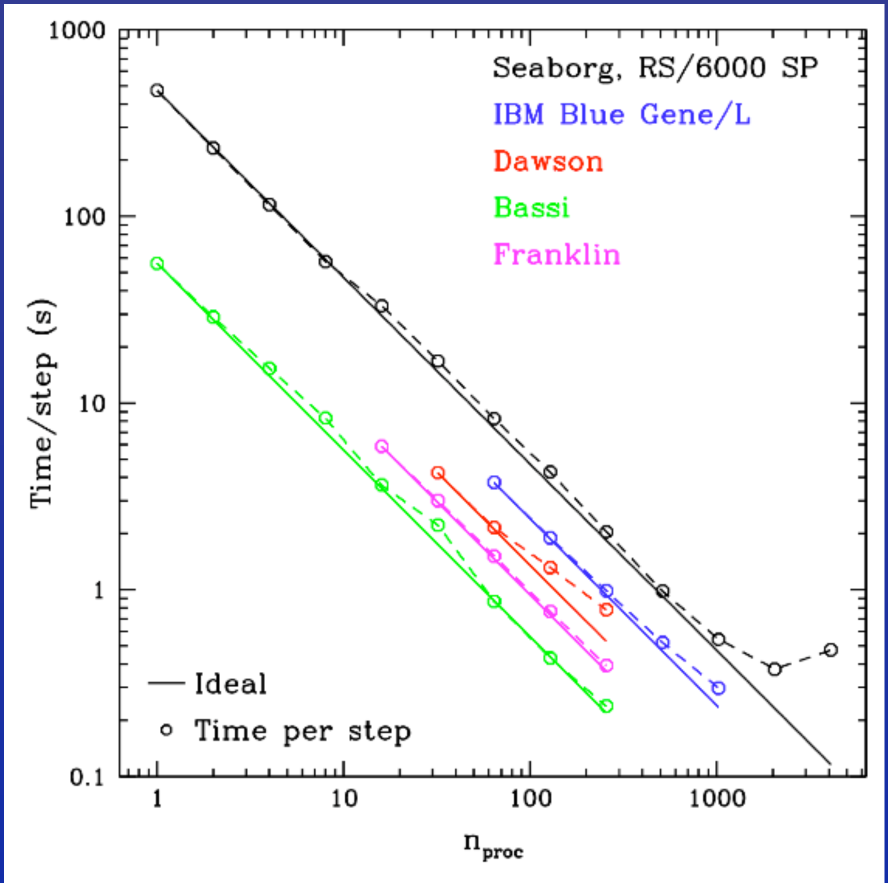


Image of MAST simulation courtesty of G. Stantchev

More flux tube savings

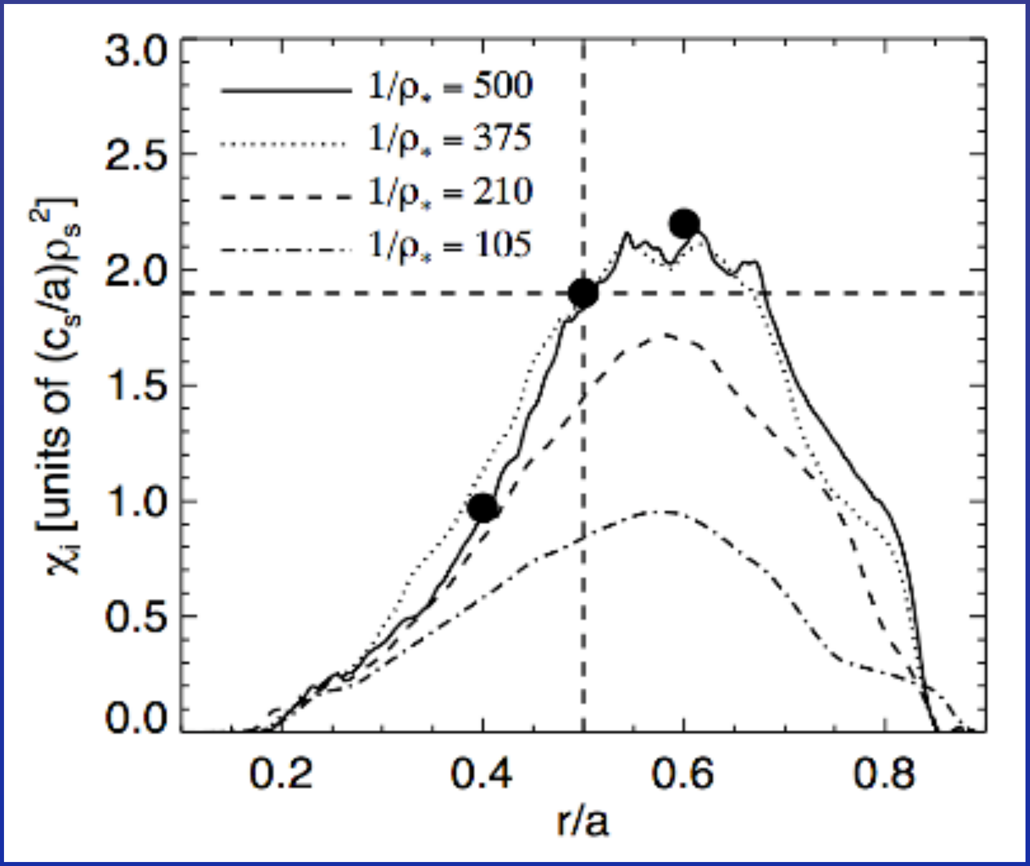
- (Near) perfect parallelization:
  - Only communication between flux tubes occurs when solving transport equations, which is infrequent
  - Flux tube calculations are independent



Strong scaling of a single flux tube simulation (GS2)

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.

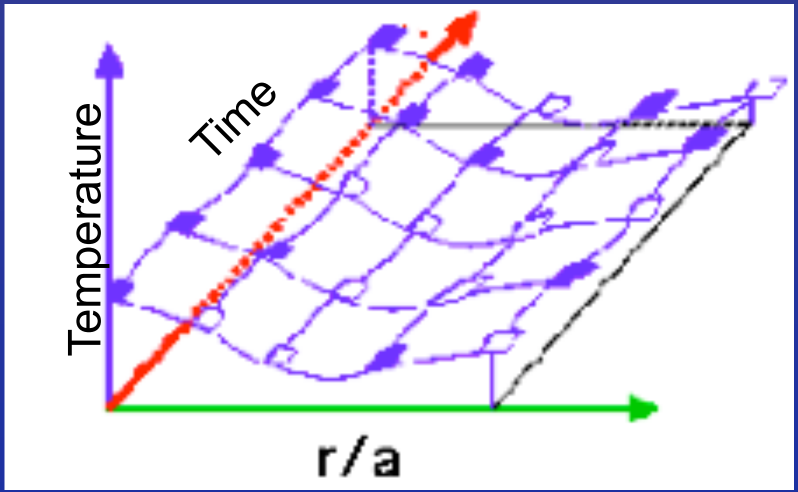
Multiscale simulation cost

- Grid spacings in radius and velocity (2D) roughly unchanged
- Savings in time domain:

Turbulence: $\Delta t \sim 10^{-7}\ s, \quad L_t \sim 10^{-4}\ s$

Transport: $\Delta\tau \sim 10^{-2} s, \quad L_\tau \sim 1s$

Coarse space-time grid



- Savings due to radial parallelization:

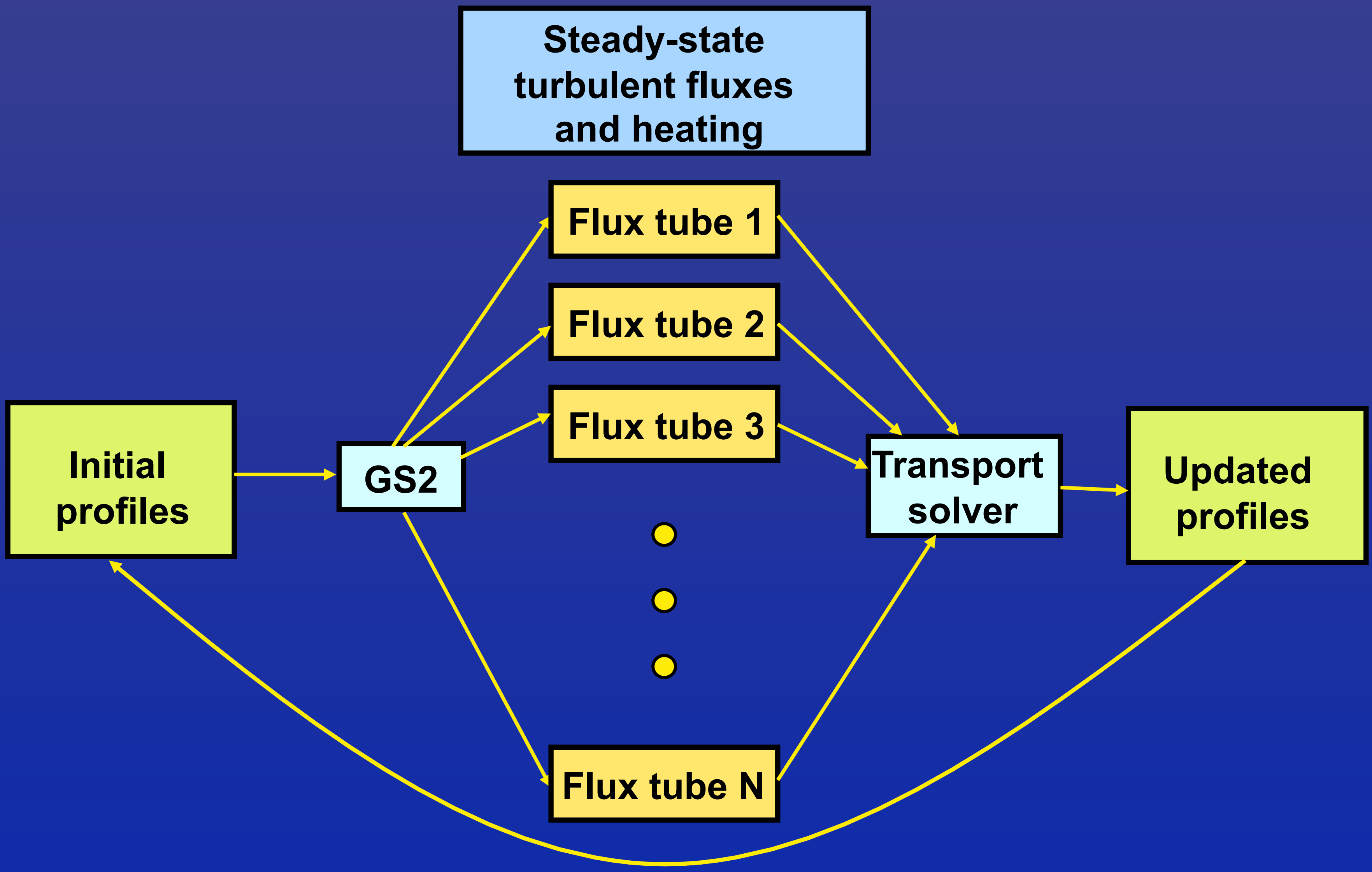
$$L_r \sim (100/nr)\ cm, \quad n_r \sim 10$$

- Required number of grid points:

$$(L_r/\Delta r) \times (L_\theta/\Delta\theta) \times (L_\phi/\Delta\phi) \times (L_v/\Delta v)^2 \times (L_t/\Delta t) \times (L_\tau/\Delta\tau) \sim 10^{17}$$

- Savings of ~10^3 over conventional numerical simulation

Trinity schematic



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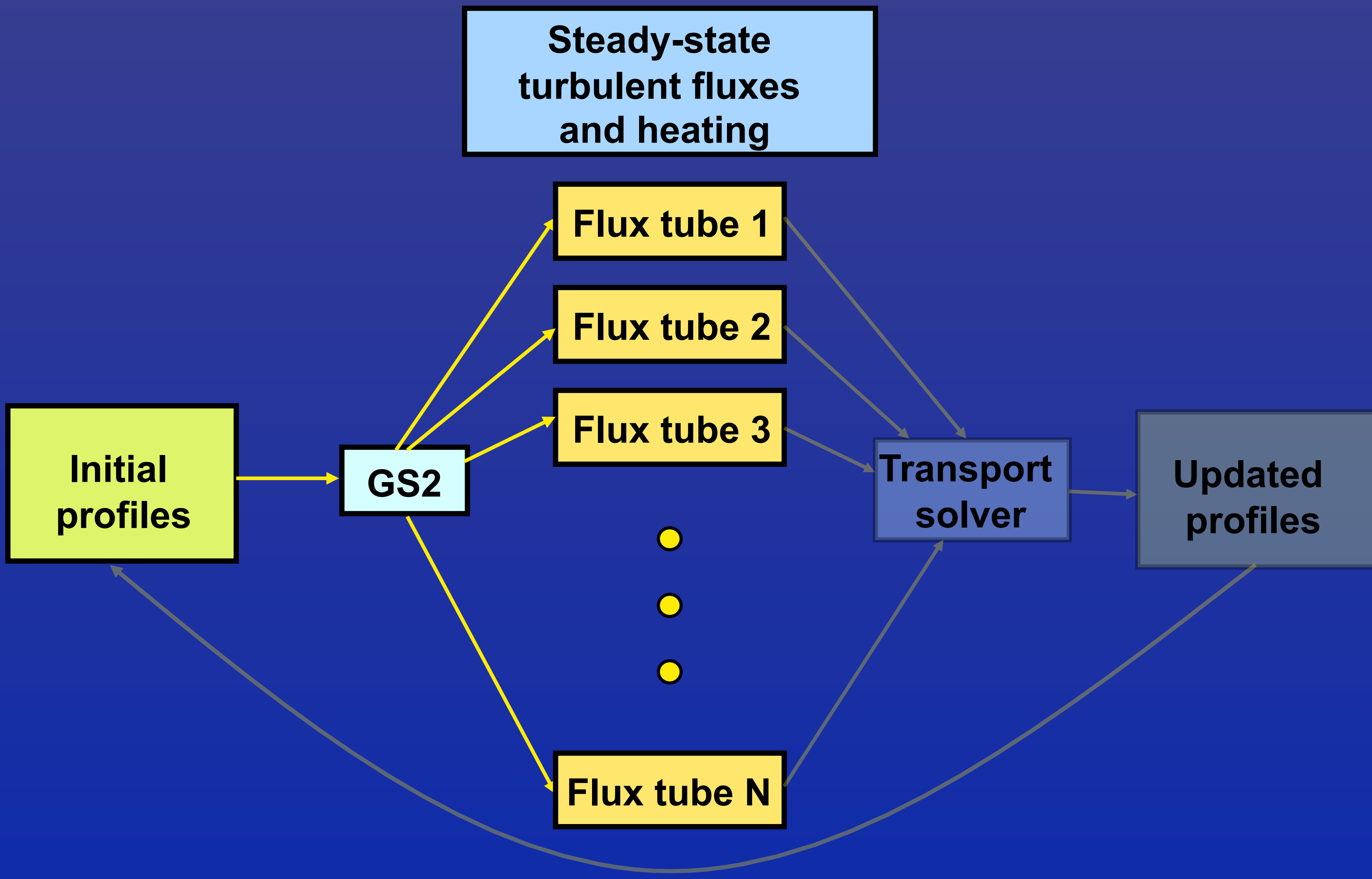
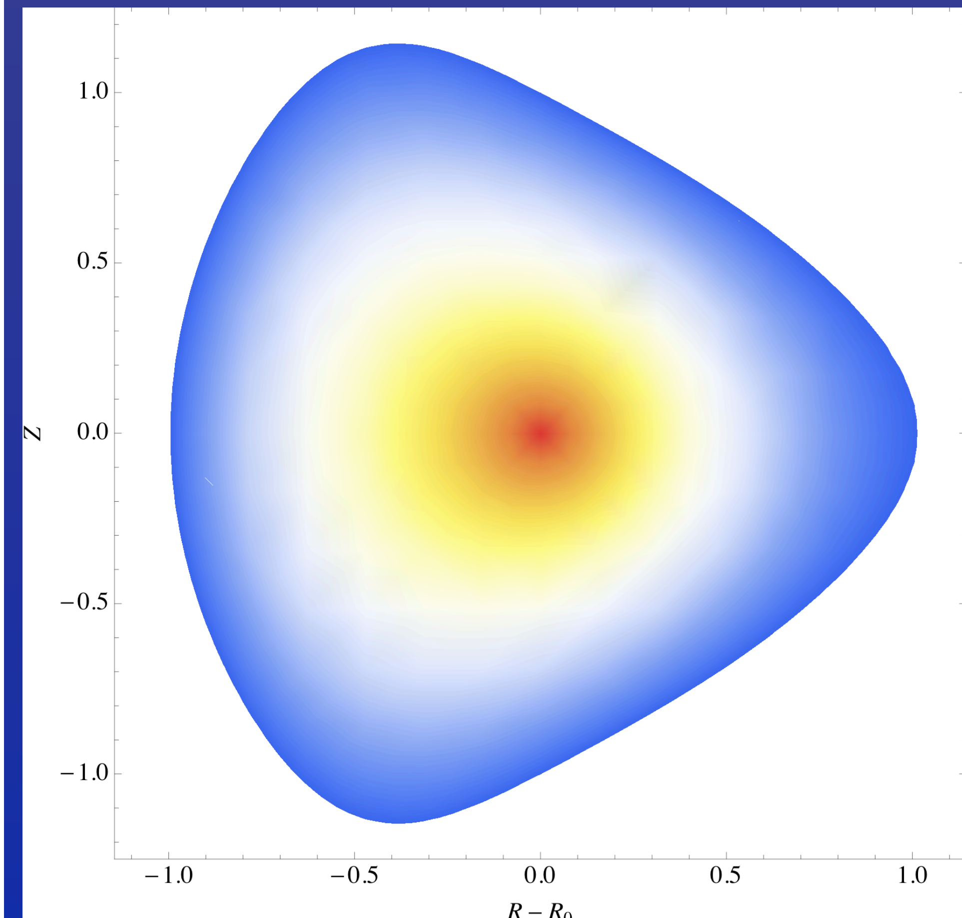
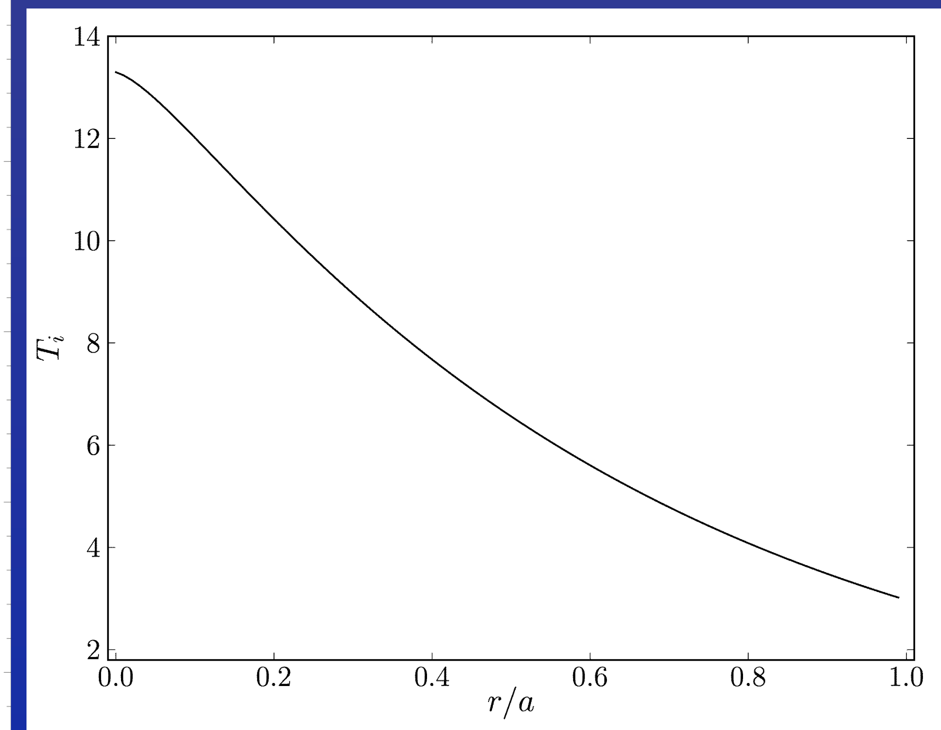


Sampling profile with flux tubes





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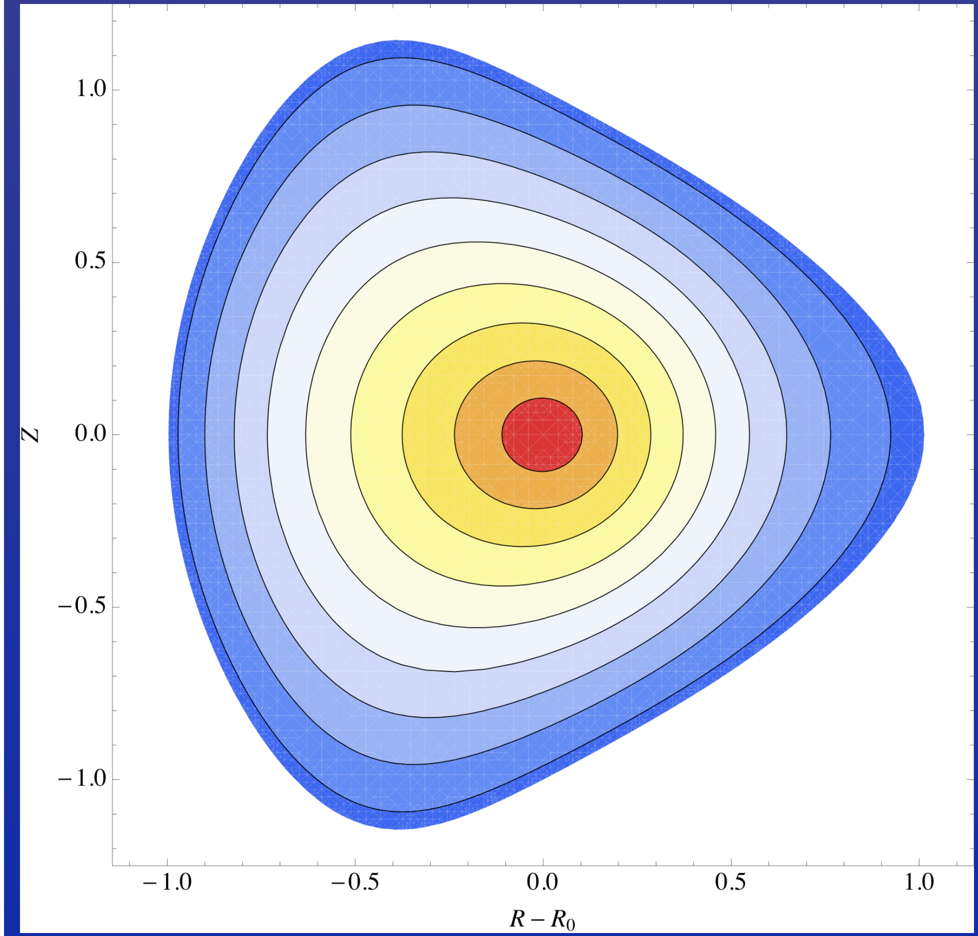

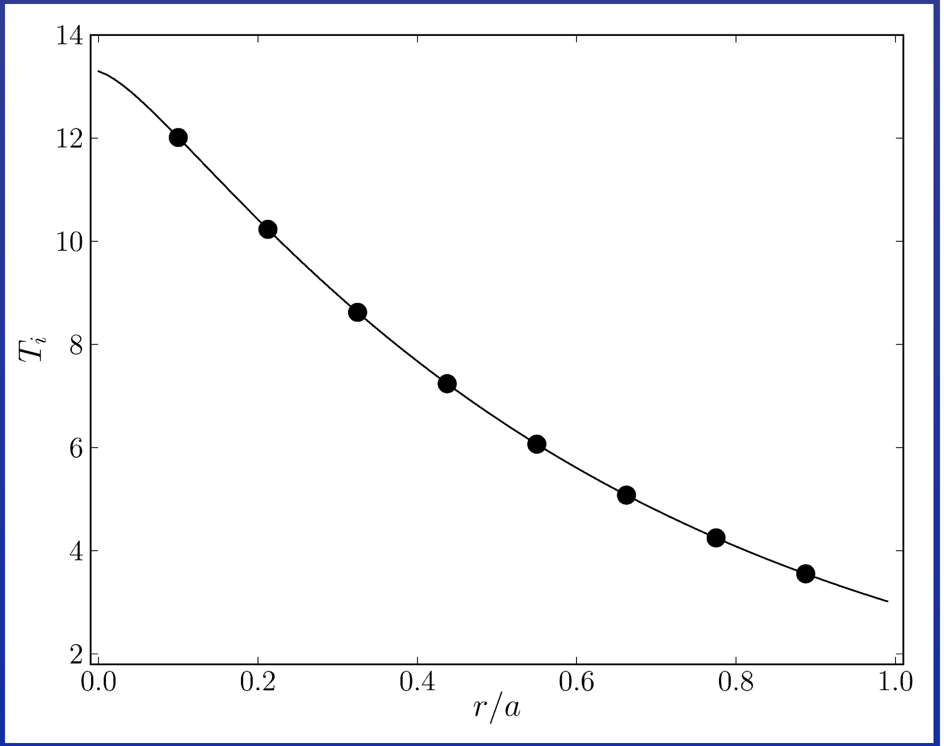

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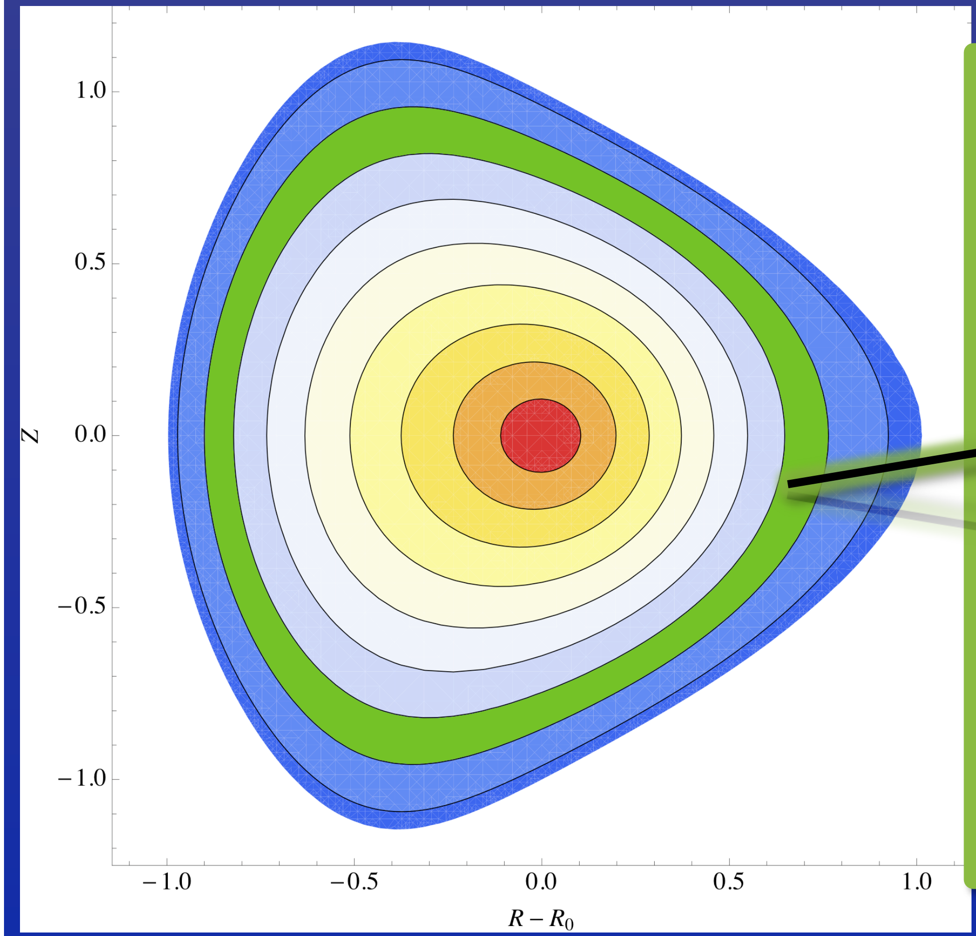

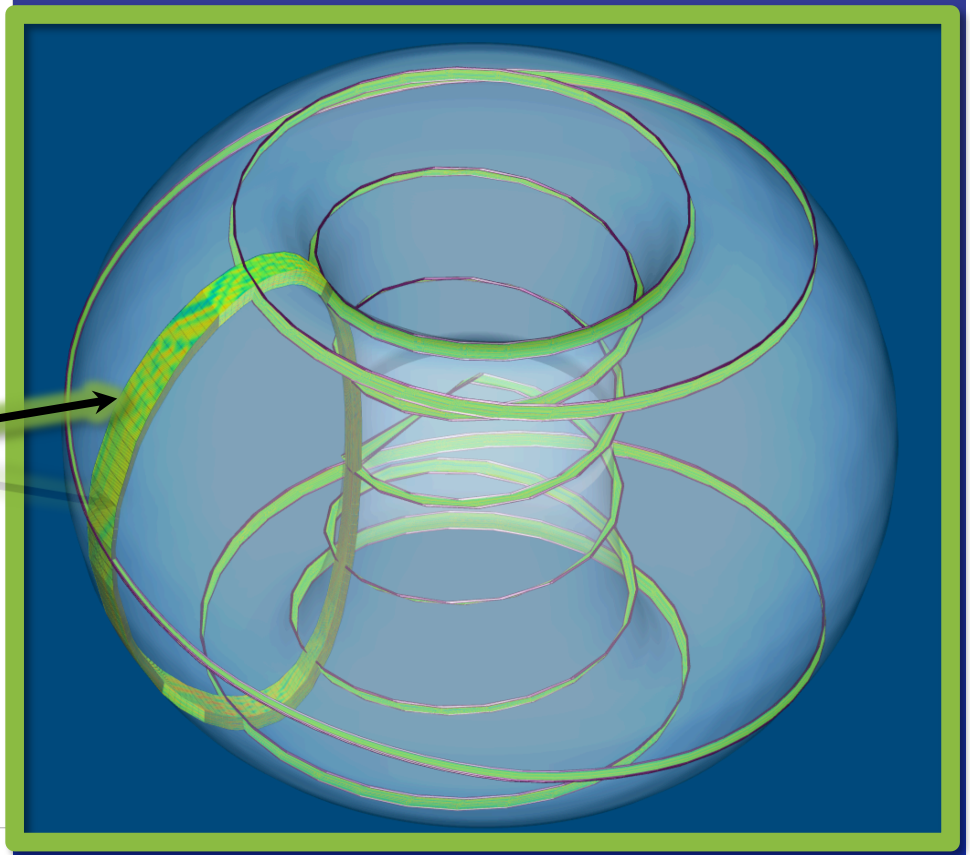

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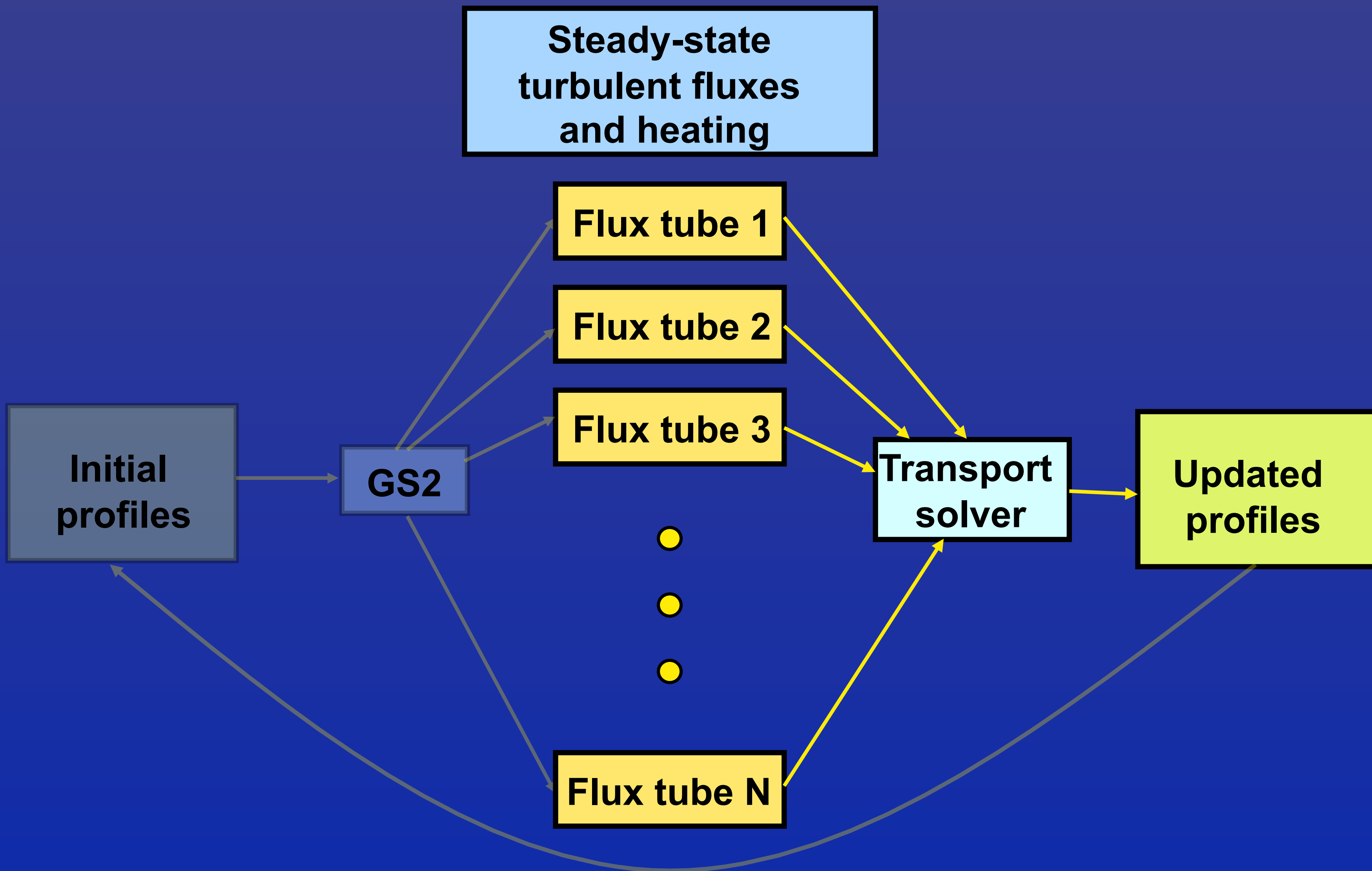

Trinity transport solver

- Transport equations are stiff, nonlinear PDEs:

$$\frac{\partial n}{\partial t} = H(r)\frac{\partial G[\Gamma, n, T, r]}{\partial r} \qquad \Gamma \rightarrow \frac{\Gamma}{n v_{th}}$$

- General (single-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):

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

*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

- Treat nonlinear terms implicitly with (single-iteration) Newton's Method

$$G_j^{m+1} \approx G_j^m + (\mathbf{y} - \mathbf{y}^m) \left. \frac{\partial G_j}{\partial \mathbf{y}} \right|_{\mathbf{y}^m}$$

$$\mathbf{y} = \left[\{n_k\}, \{p_{i_k}\}, \{p_{e_k}\}\right]^T$$

- Simplifying assumption: normalized fluxes depend primarily on gradient scale lengths

$$\Gamma_j \approx \Gamma[(R/L_n)_j, (R/L_{p_i})_j, (R/L_{p_e})_j]$$

$$\Rightarrow \frac{\partial \Gamma_j}{\partial n_k} \approx \frac{\partial \Gamma_j}{\partial (R/L_n)_j} \frac{\partial (R/L_n)_j}{\partial n_k} \qquad \left(\frac{R}{L_n}\right)_{\pm} \approx \mp \frac{R}{\Delta r} \frac{n_{\pm} - n_j}{n_{\pm}}$$

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:

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

- Example calculation with 10 radial grid points:
  - evolve density and electron/ion pressures
  - simultaneously calculate fluxes for equilibrium profile and for 3 separate profiles (one for each perturbed gradient scale length)
  - total of 40 flux tube simulations running simultaneously
  - ~2000-4000 processors per flux tube => scaling to over 100,000 processors with >80% efficiency

Trinity transport solver

- Nonlinear turbulence simulation runs until fluxes converged
  - convergence criterion:

$$\epsilon \equiv \sqrt{\frac{1}{m-j}\sum_{i=j}^{m-1}\left(\overline{\Gamma}_m^2 - \overline{\Gamma}_i^2\right)} < \epsilon_0 \qquad \overline{\Gamma}_m = \frac{1}{t_m}\sum_{i=1}^{m}\Gamma_i\,(\Delta t)_i$$

  - turbulence for new transport time step initialized to saturated state from previous transport time step -- faster convergence

- Sources and initial profiles are analytically specified. In process of adding capability to read in experimental profiles for these quantities
- Option to use model fluxes (IFS-PPPL, offset linear, quasilinear, etc.)
- Boundary conditions:
  - fixed n and T at outer edge of simulation domain
  - zero flux boundary condition at magnetic axis

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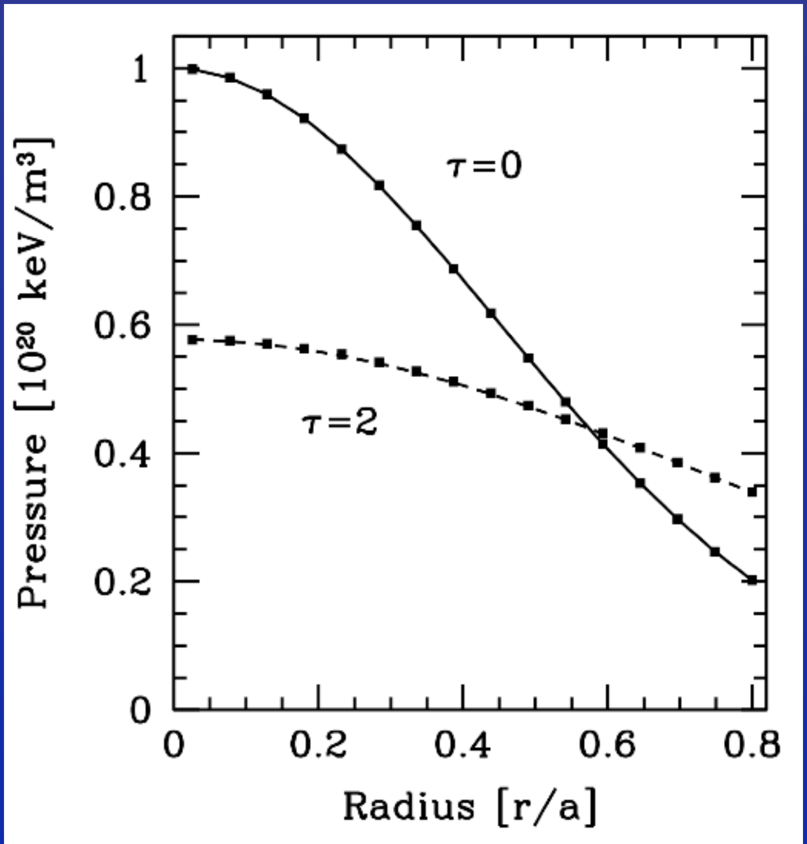
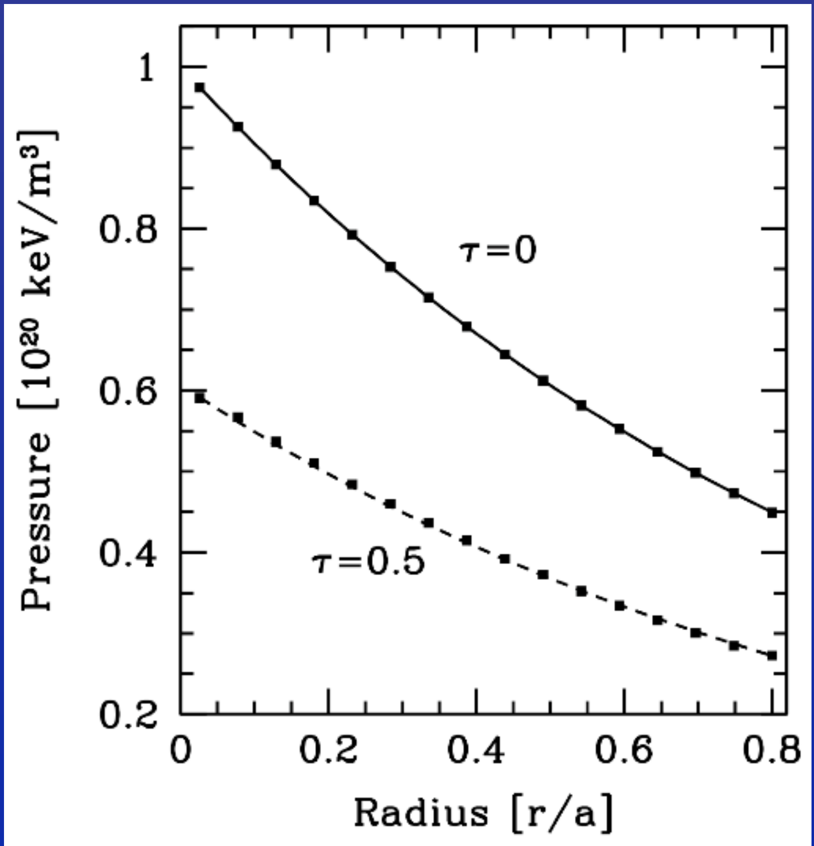
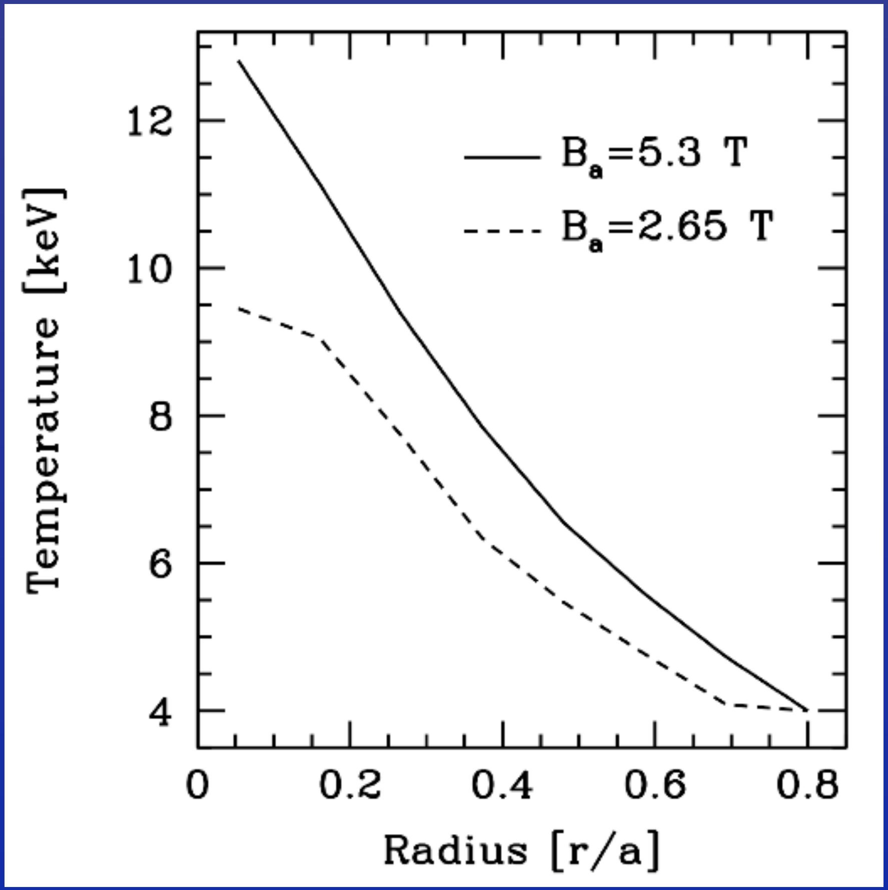
Preliminary tests for Trinity

- Test 1: choose fluxes so that heat transport equations reduce to diffusion equation
- Test 2: choose fluxes so that heat transport equations reduce to advection equation





Preliminary results from Trinity



- Single ion species
- Adiabatic electrons
- Electrostatic
- 60 MW external heat source into ions
- Local equilibrium model with circular flux surfaces
- 8 radial grid points (flux tubes)
- Temperature at r=0.8a fixed at 4 keV
- Only ion temperature evolved
- Takes ~20 minutes on ~2000 processors

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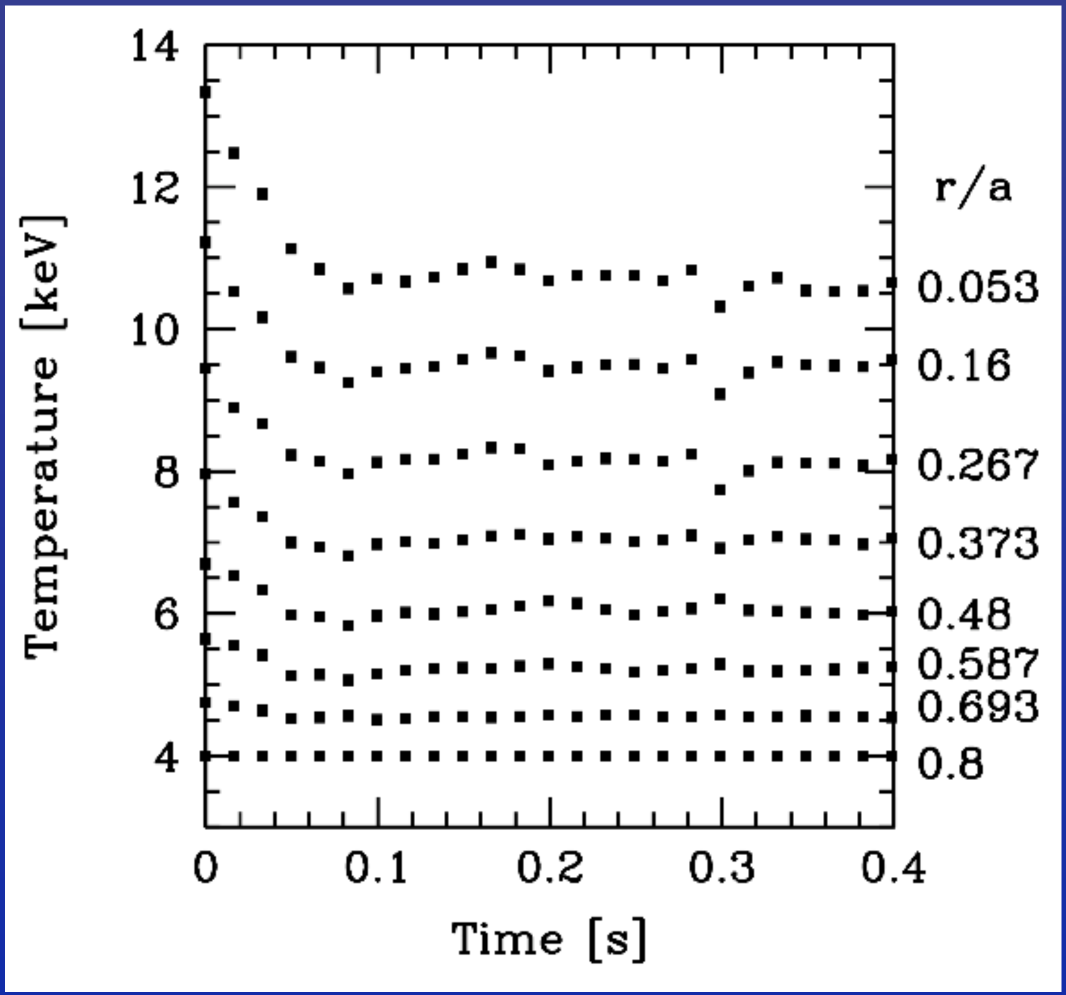

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- Multiscale nature of turbulent transport can be exploited to provide significant savings in time domain
- Highly parallelized -- should scale to over 10^5 processors
- Trinity (interfaced with GS2 and soon GENE) is capable of running with multiple species, electromagnetic effects, realistic geometry, physical collisional effects (such as heating), etc.
- Still in development: higher order implicit scheme (BDF3), higher order finite differences, model for momentum transport, etc.
- Turbulent transport/heating code like Trinity necessary and feasible part of full numerical tokamak simulations