Global gyrokinetic simulation of ITER plasmas using coupled flux tubes

M. Barnes[1], W. Dorland[1], and G. W. Hammett[2]

[1]University of Maryland

[2]Princeton Plasma Physics Lab

Center for Multiscale Plasma Dynamics

In collaboration with:

I. G. Abel, A. A. Schekochihin, S. C. Cowley

D. Ernst, G. Plunk, P. Ricci, B. Rogers, T. Tatsuno, E. Wang

Abstract

To faithfully simulate ITER and other modern fusion devices, we must resolve electron and ion fluctuation scales in a five-dimensional phase space and time. Simultaneously, we must account for the interaction of this turbulence with the slow evolution of the large-scale plasma profiles. Because of the enormous range of scales involved and the high dimensionality of the problem, resolved first-principles global simulations are very challenging using conventional (brute force) techniques. We have developed a new approach in which turbulence calculation from multiple gyrokinetic flux tube simulations from GS2 are coupled together using transport equations to obtain self-consistent, steady-state background profiles and corresponding turbulent fluxes. The resulting code (TRINITY) has been used to simulate the core of an ITER-like plasma. We present preliminary results.

Wide range of scales

- Turbulent transport in ITER and other fusion plasmas involves interaction of phenomena spanning a wide range of time and space scales:

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

Direct simulation cost

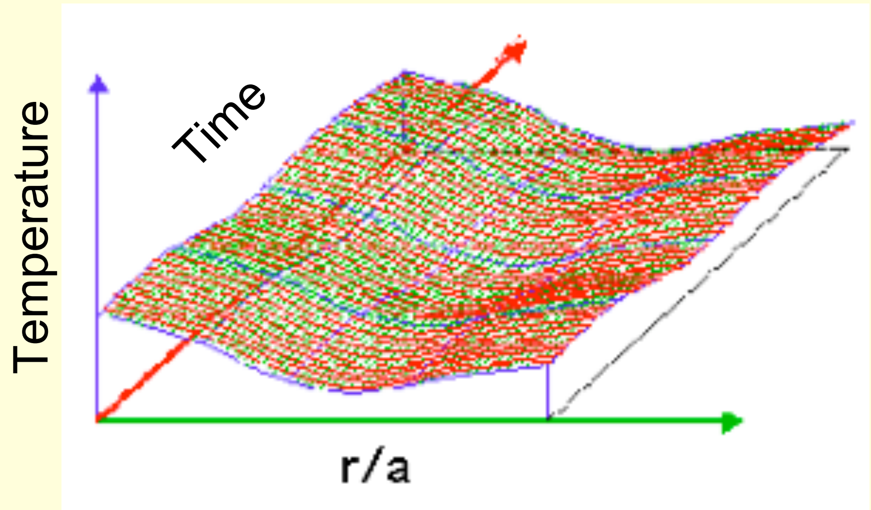
- Grid spacings in space (3D), velocity (2D), and time:

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

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

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

Fine space-time grid



- Required number of grid points:

$$(L_x/\Delta x)^3 \times (L_v/\Delta v)^2 \times (L_t/\Delta t) \sim 10^{24}$$

- Current largest fluid turbulence calculations ~ 10^{14} grid points
- Direct simulation not possible. Need simplification. Seek guidance from theory.

Gyrokinetic multiscale assumptions

- Fluctuation amplitude small compared with equilibrium:

$$f = F_0 + \delta f, \quad \delta f / F_0 \sim \epsilon \equiv \rho / L$$

- Separation of turbulence and equilibrium spatial scales:

$$\nabla F_0 \sim F_0 / L, \quad \nabla_{\|} \delta f \sim \delta f / L, \quad \nabla_{\perp} \delta f \sim \delta f / \rho$$

- Separation of turbulence and equilibrium time scales:

$$\partial_t F_0 \sim \tau^{-1} F_0, \quad \partial_t \delta f \sim \omega \delta f \sim \nu \delta f$$

$$\tau^{-1} \sim \epsilon^2 \omega \sim \epsilon^3 \Omega$$

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

- Reasonably smooth velocity space: $\partial_v f \sim f / v_{th}$

Key results*

$$f = F_M(1 - q\Phi/T_0) + h + \delta f_2$$

- Equilbrium Maxwellian, no gyrophase dependence:

$$F_0 \sim F_M, \quad \partial F_0/\partial\vartheta = 0$$

- Non-Boltzmann part of delta f (h) independent of gyrophase at fixed guiding center position R:

$$(\partial h/\partial\vartheta)_{\mathbf{R}} = 0$$

- Gyrokinetic equation describes evolution of turbulence:

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

*S. C. Cowley, G. Plunk, and E. Wang, Manuscript in preparation.

Key results (continued)

$$
\begin{aligned}
\frac{\partial n_s}{\partial t} &= -\frac{\partial \psi}{\partial V}\frac{\partial}{\partial \psi}\left[\frac{\partial V}{\partial \psi}\left\langle \mathbf{\Gamma}_s \cdot \nabla\psi\right\rangle\right] \\
\frac{3}{2}\frac{\partial\left(n_s T_s\right)}{\partial t} &= -\frac{\partial \psi}{\partial V}\frac{\partial}{\partial \psi}\left[\frac{\partial V}{\partial \psi}\left\langle \mathbf{Q}_s \cdot \nabla\psi\right\rangle\right] \\
&+ T_s\left(\frac{\partial \ln n_s}{\partial \psi} - \frac{3}{2}\frac{\partial \ln T_s}{\partial \psi}\right)\left\langle \mathbf{\Gamma}_s \cdot \nabla\psi\right\rangle + \frac{\partial \ln T_s}{\partial \psi}\left\langle \mathbf{Q}_s \cdot \nabla\psi\right\rangle \\
&- \left\langle \int d^3\mathbf{v}\,\frac{h_s T_s}{F_{0,s}}\left\langle C(h_s)\right\rangle_{\mathbf{R}}\right\rangle + n_s \nu_{\mathcal{E}}^{su}\left(T_u - T_s\right)
\end{aligned}
$$

particle transport

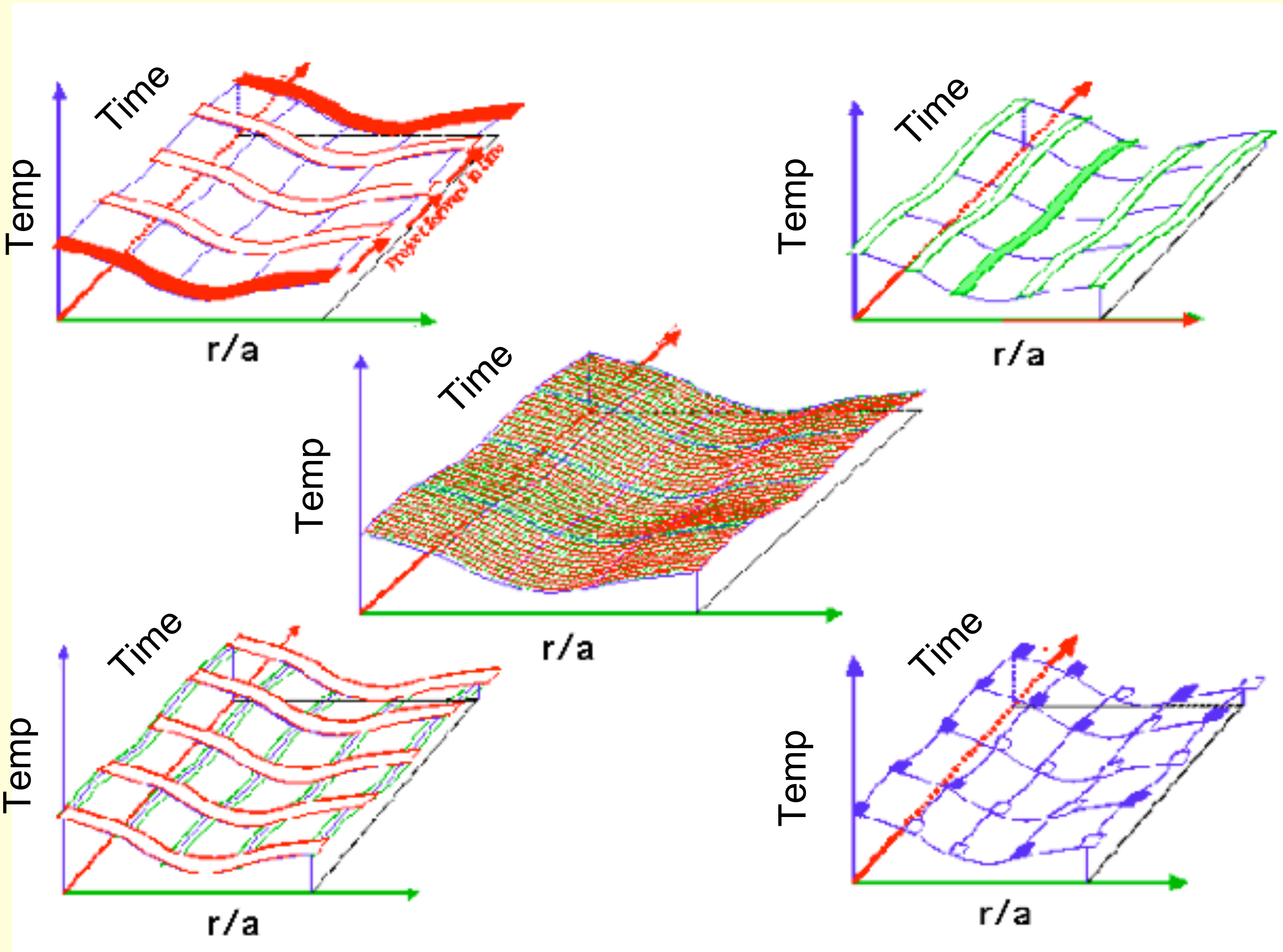
energy transport

energy injected into turbulence by background inhomogeneity

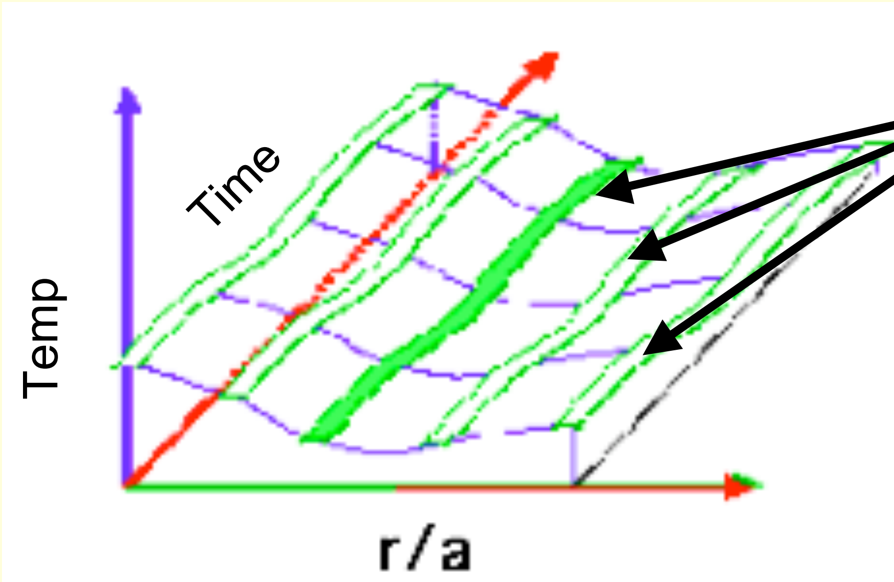
turbulent collisional heating

collisional temperature equilibration

Multiscale grid



Multiscale grid (continued)

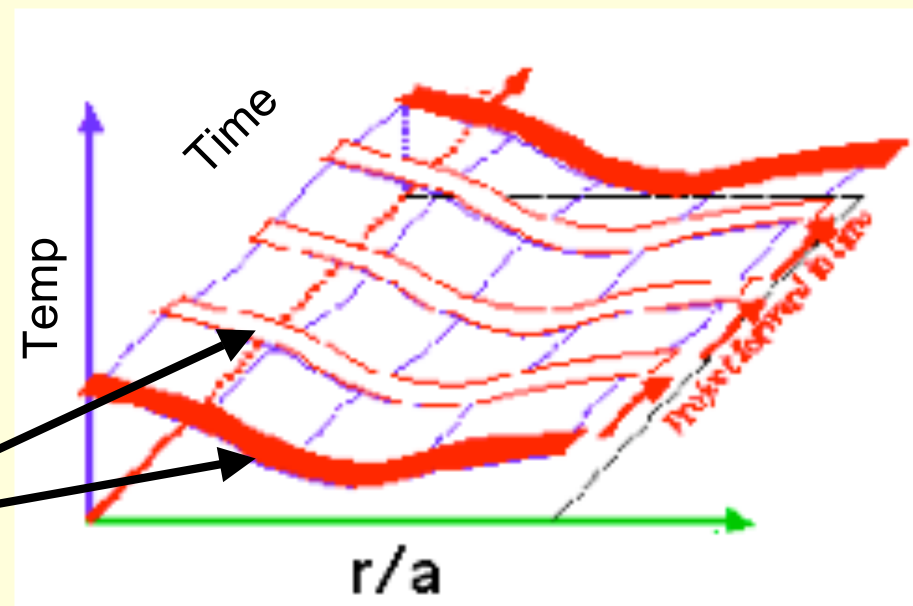


Flux tube spatial simulation domain for microturbulence

- 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)
- Effective 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
- Effective time grid points in long-time transport equations

Flux tube temporal simulation domain for microturbulence



Flux tubes minimize volume

- Single flux tube maps out an entire flux surface (simulation domain in green, along with constructed flux surface at poloidal cut)

- Savings estimate:

$$L_\perp \sim L_\theta / n_\phi q$$

$$n_\phi q \sim k_\perp a \sim 100$$

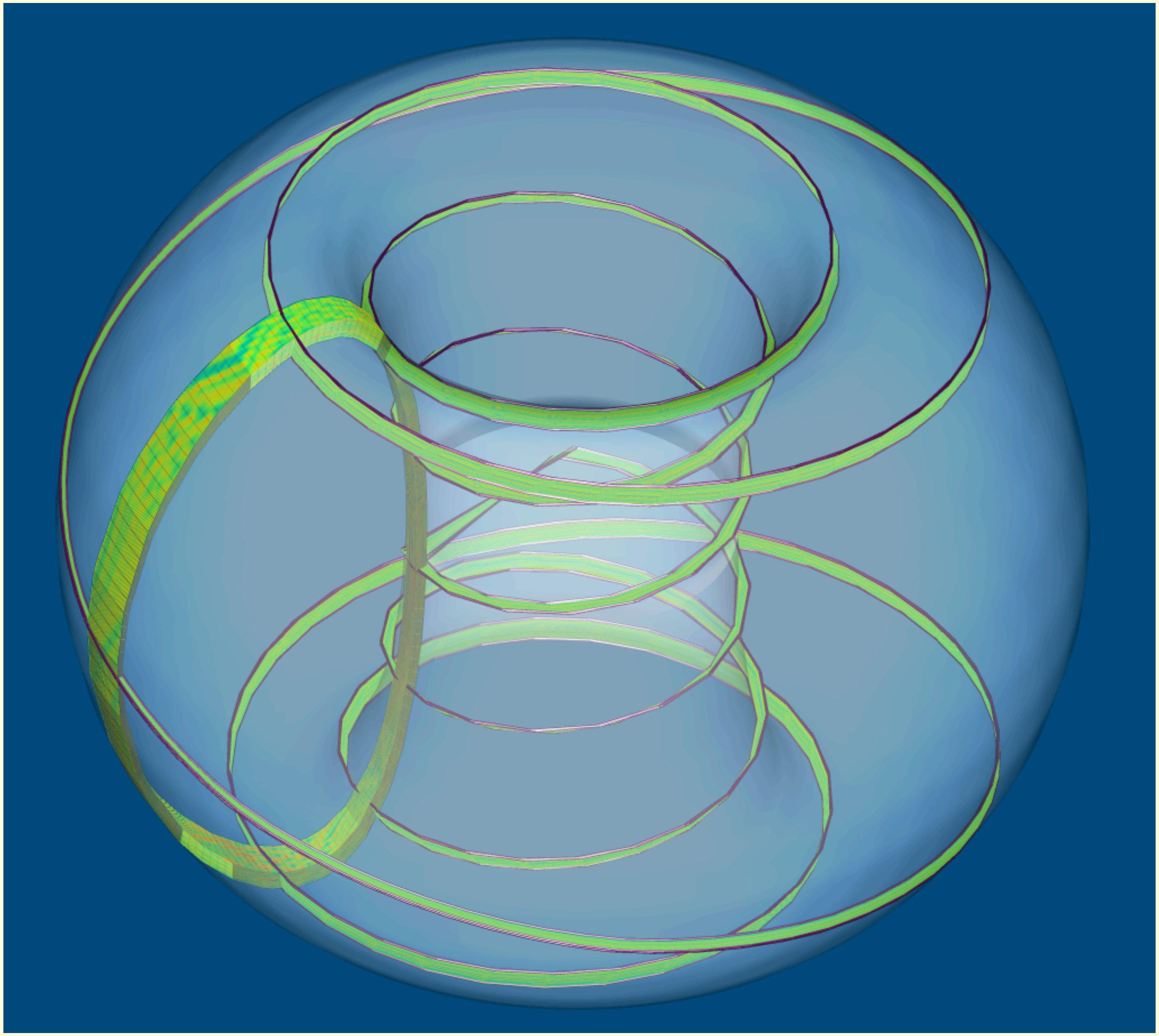


Image of MAST simulation courtesty of G. Stantchev

Optimizes grid resolution

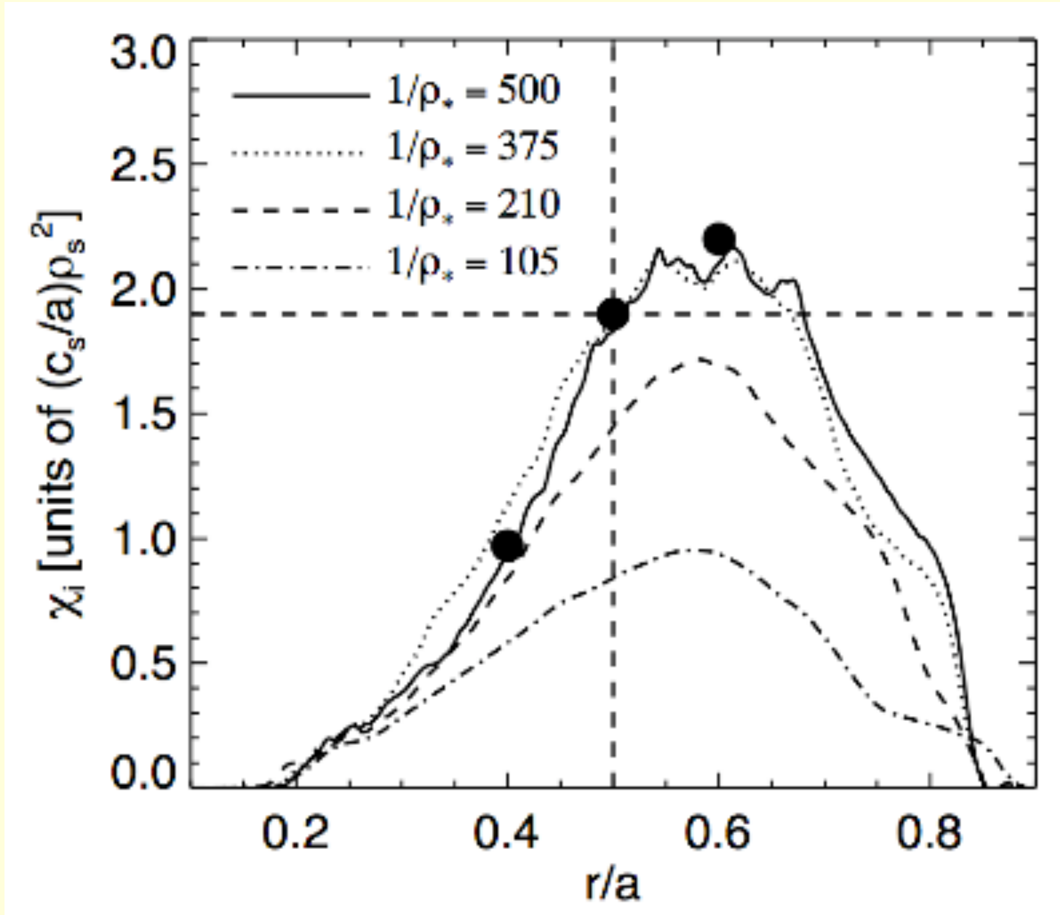
- Standard global simulations use fixed $k_\perp$ range across minor radius
- Each flux tube calculation is independent, allowing for different $k_\perp$ ranges at each radial position

i.e. $\alpha < k_\perp < \beta$ vs. $\tilde{\alpha} < k_\perp \rho(\psi) < \tilde{\beta}$

- Results in factor of $\sqrt{T_C/T_E}$ savings in required $k_\perp$ range ($T_C \equiv$ core temp, $T_E \equiv$ edge temp)

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.

Minimizes number of time steps

- Transport and turbulence time scales widely separated in gyrokinetic ordering:

$$t \sim \epsilon^2 \tau, \;\; \tau \equiv \text{ transport time scale}$$

$$\epsilon \sim \rho_*, \;\; t \equiv \text{ turbulence time scale}$$

- Multiscale hierarchy exploits intrinsic scale separation by:
  - taking small turbulence time steps to get steady-state fluxes (with stationary background profiles)
  - taking large transport time steps to evolve background profiles (factor of ϵ^{-2} bigger than turbulent time steps)

Multiscale simulation cost

- Grid spacings in radius and velocity (2D) roughly unchanged
- In poloidal direction:

$$\Delta\theta \sim 0.001\ cm, \quad L_\theta \sim 1\ cm$$

- Along the field line:

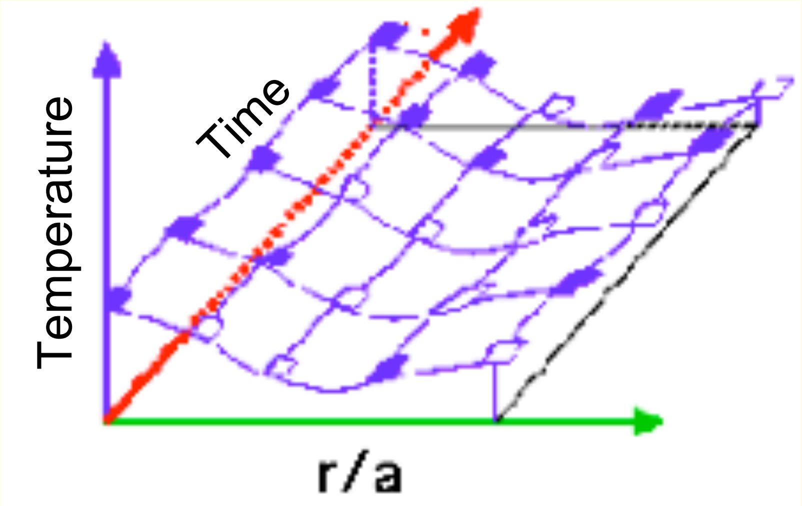
$$\Delta\phi \sim 1\ m, \quad L_\phi \sim 10\ m$$

- In time:

Turbulence: $\Delta t \sim 10^{-7}\ s, \quad L_t \sim 10^{-5}\ s$

Transport: $\Delta\tau \sim 0.1\ s, \quad L_\tau \sim 1\ s$

Coarse space-time grid

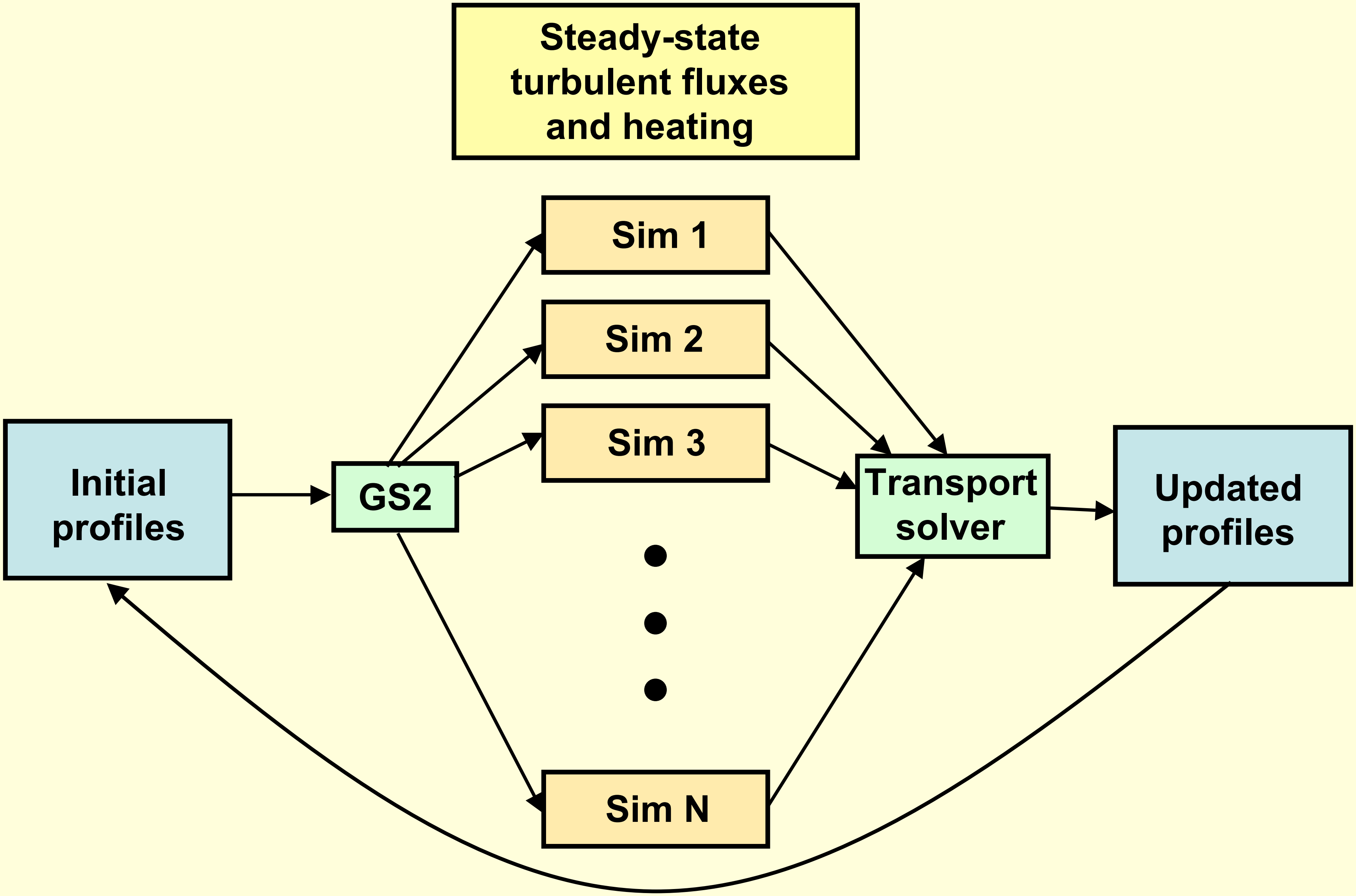


- Required number of grid points:

$$(L_r/\Delta r) \times (L_\theta/\Delta\theta) \times (L_\phi/\Delta\phi) \times (L_v/\Delta v)^2 \times (L_t/\Delta t) \times (L_\tau/\Delta\tau) \sim 10^{14}$$

- Savings of order ~10^{10} over direct numerical simulation

Schematic of multiscale scheme in TRINITY



Transport solver algorithm

- Implicit treatment of nonlinear transport equations (single-iteration Newton's method)*
- Example treatment of heat flux (linearization):

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

$$\mathbf{y} = (\{n_j\}, \{p_{i_j}\}, \{p_{e_j}\})$$

$$j \equiv \text{spatial index}, \quad m \equiv \text{temporal index}$$

- We assume turbulent fluxes and heating depend predominantly on gradient scale lengths:

$$\frac{\partial Q}{\partial \mathbf{y}} \approx \frac{\partial Q}{\partial (R/L_n)} \frac{\partial (R/L_n)}{\partial n} + \frac{\partial Q}{\partial (R/L_{p_i})} \frac{\partial (R/L_{p_i})}{\partial p_i} + \frac{\partial Q}{\partial (R/L_{p_e})} \frac{\partial (R/L_{p_e})}{\partial p_e}$$

*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).

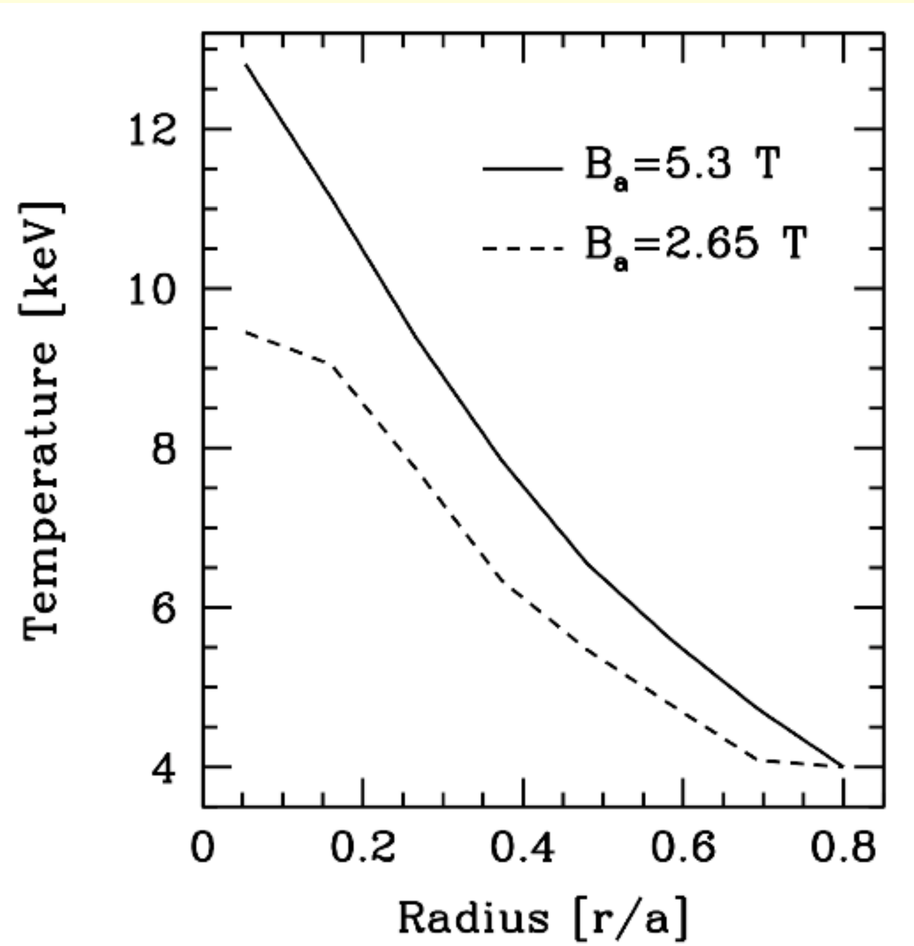
Transport solver algorithm (continued)

- Derivatives of fluxes with respect to gradient scale lengths approximated by perturbing gradients associated with each evolved profile, calculating associated fluxes, and using 2-point finite differences:

$$\frac{\partial Q}{\partial (R/L_{p_i})} \approx \frac{Q[(R/L_{p_i})_0] - Q[(R/L_{p_i})_0 + \delta]}{\delta}$$

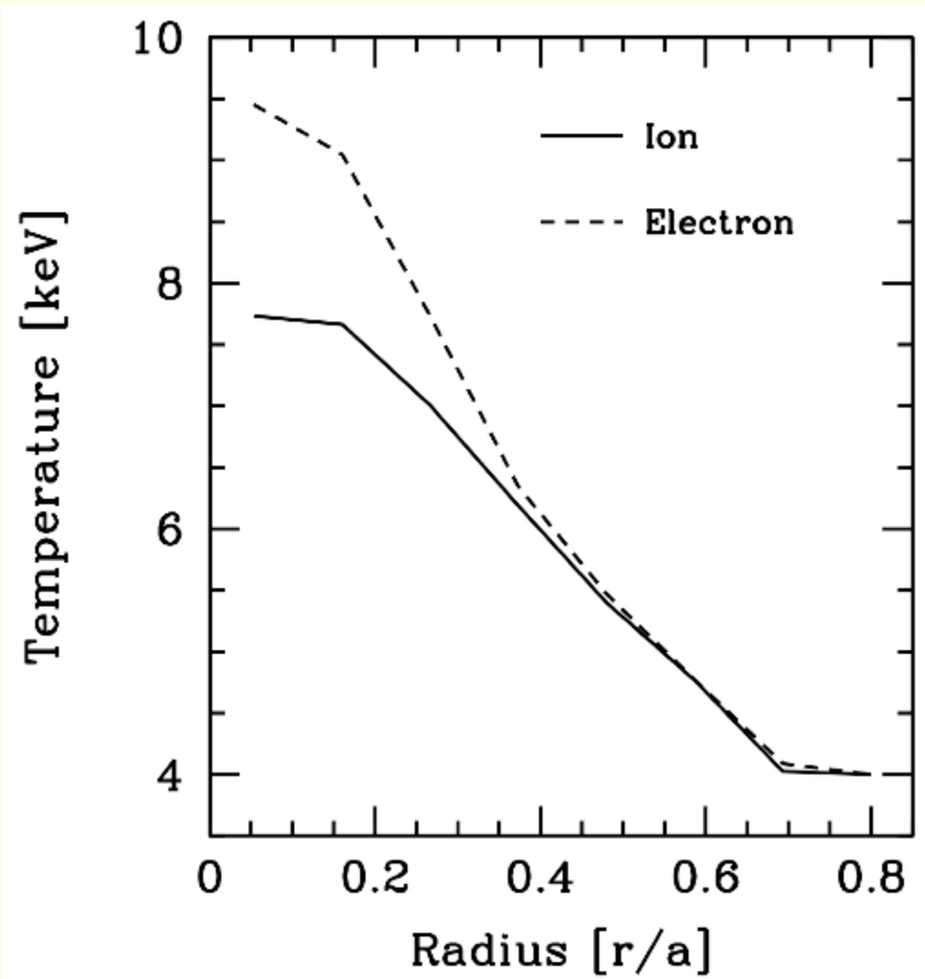
- All flux tubes, including those with perturbed gradients can be run independently; perfectly parallelizable
- Turbulence calculations dominate runtime. Added expense of implicit transport solver easily offset by ability to take larger time steps
- Radial derivatives currently calculated with centered (2-point) differences
  - could widen stencil with virtually no additional cost; would only lead to denser transport matrix to invert, which is cheap compared to turbulence calculation
  - size of transport matrix remains unchanged -- # equations x # radial grid points (# equations fixed at 3 currently)

Preliminary nonlinear results



- 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

Preliminary nonlinear results

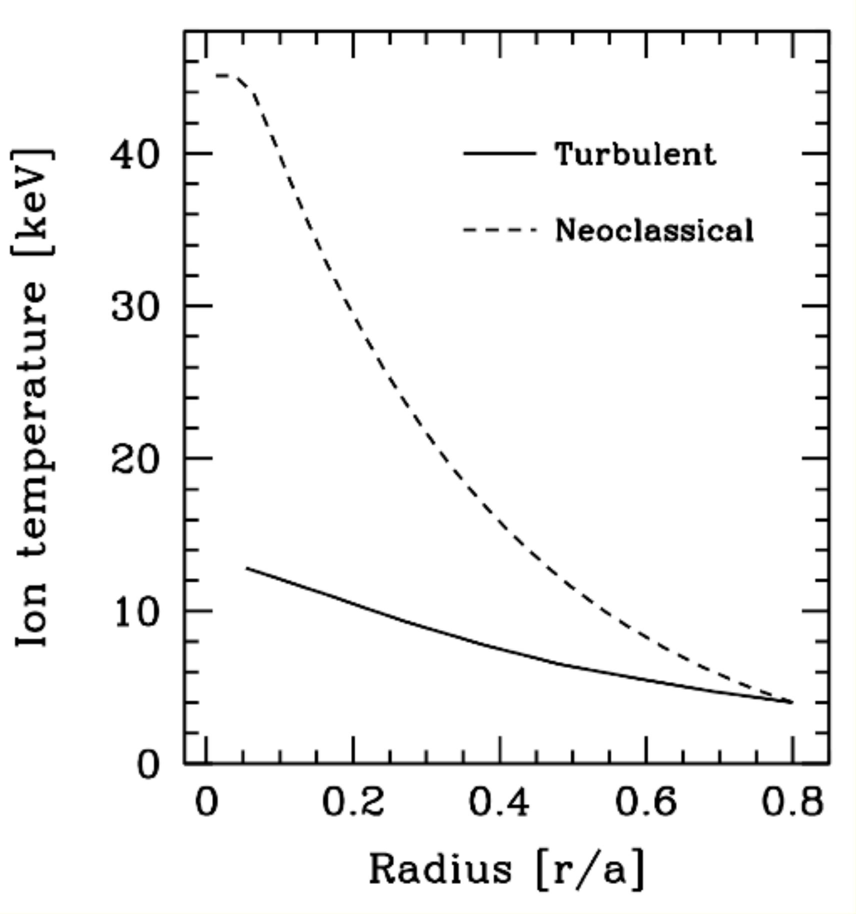


- Single ion species
- Kinetic electrons
- Electrostatic
- 120 MW external heat source (split evenly between species)
- Local equilibrium model with circular flux surfaces
- 8 radial grid points (flux tubes)
- Temperature at r=0.8a fixed at 4 keV
- Electron and ion temperature evolved
- Takes ~60 minutes on ~4000 processors

Comparison with neoclassical transport

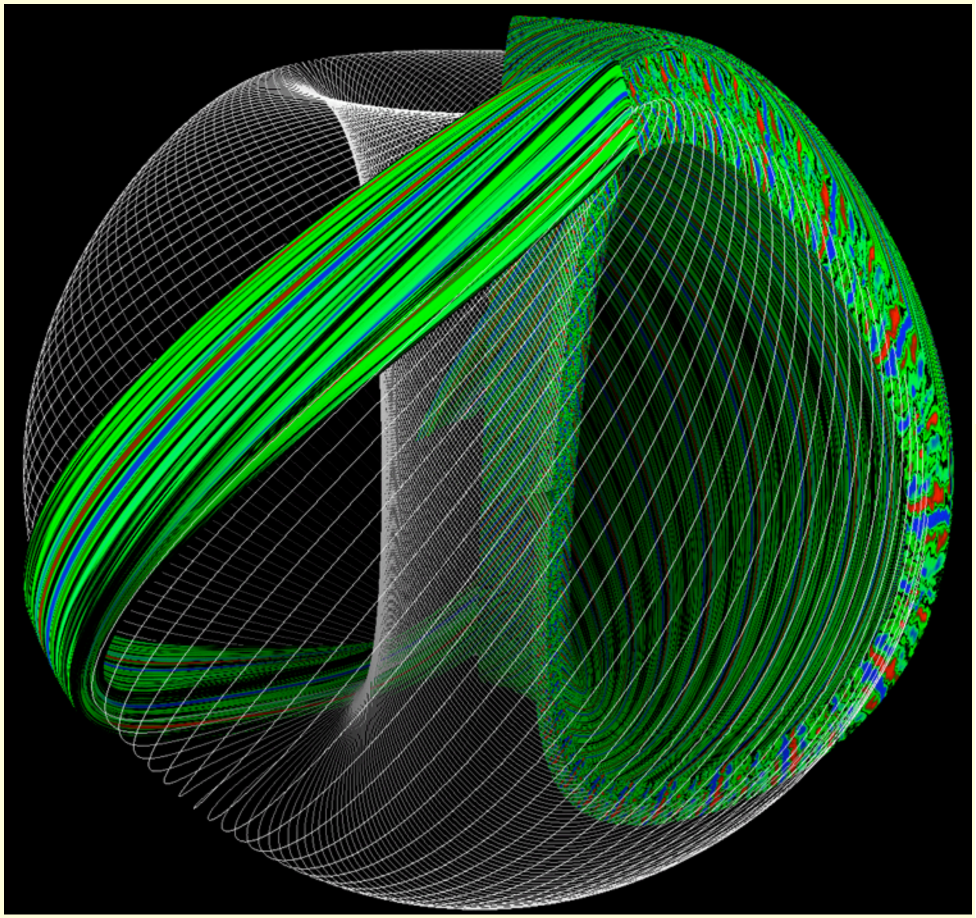
- Neoclassical run evolves only ions
- Neoclassical ion heat flux calculated using analytic result of Chang and Hinton*
- Profile calculated with turbulent + neoclassical fluxes is taken from single species (adiabatic electron) run described earlier

Illustration of dominance of turbulent transport in ITER-like plasma

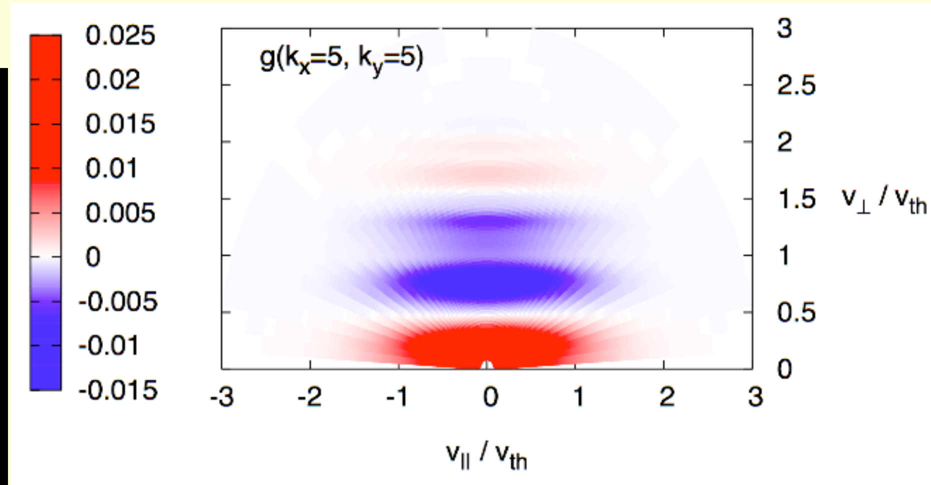


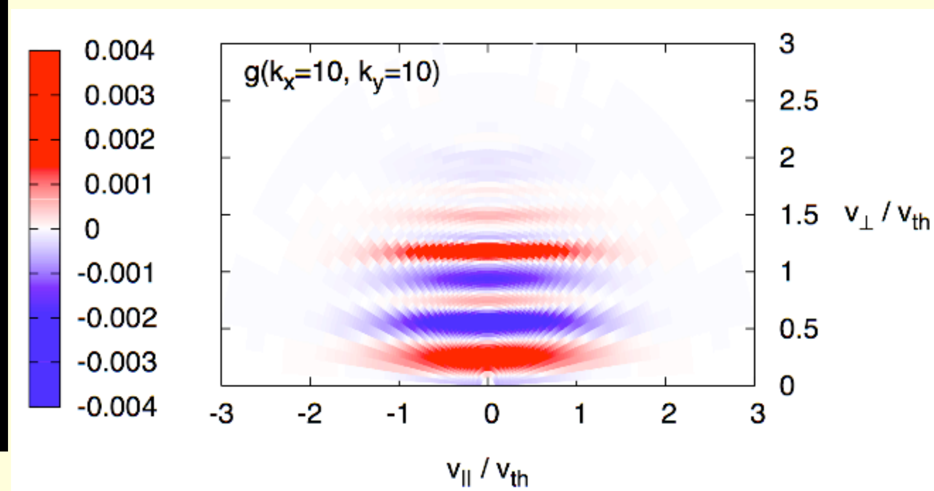
*C. S. Chang and F. L. Hinton, Phys. Fluids, **25**, 1493 (1982).

Resolving kinetic turbulence



Electrostatic potential from GS2 spherical tokamak simulation (courtesy W. Dorland)

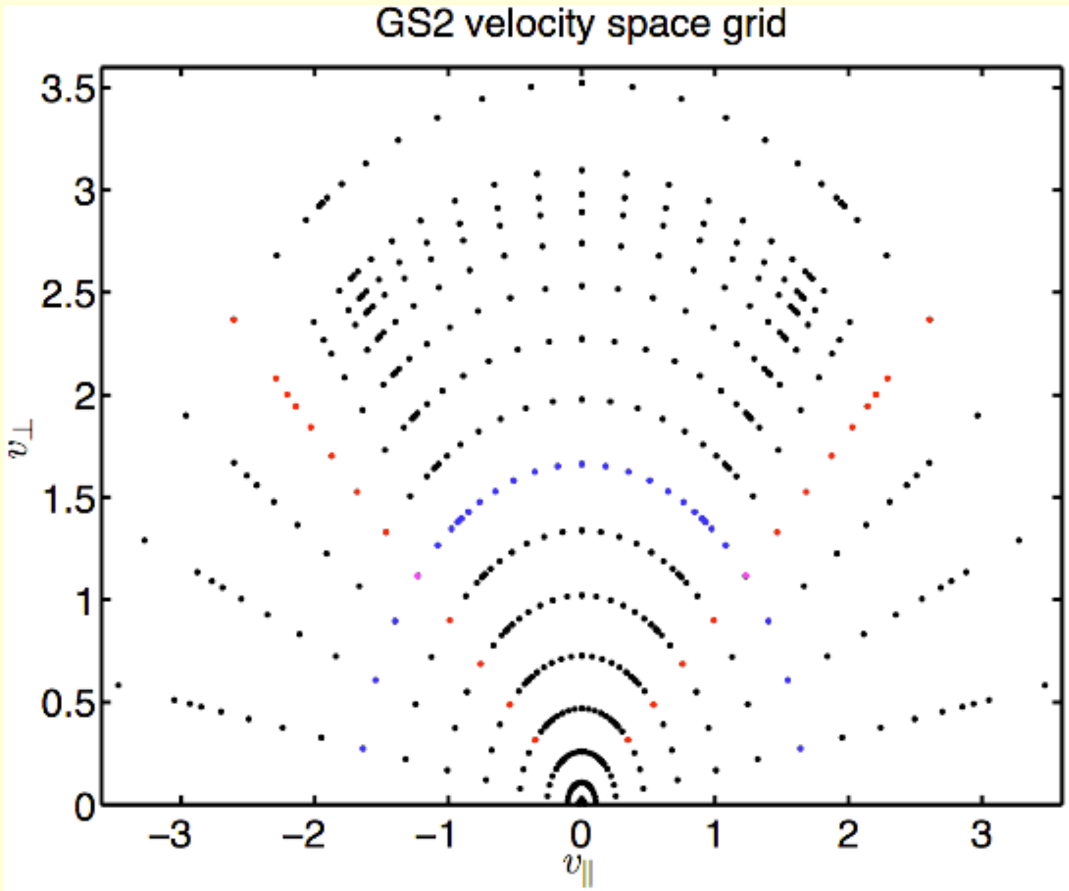




Velocity space structure in gyroaveraged distribution function (courtesy T. Tatsuno)

- Can monitor v-space resolution by estimating error in numerical evaluation of field integrals:
  - Only nontrivial v-space operation in collisionless GK eqn. is integration to get fields
  - Estimate error in field integrals by comparing with integrals performed after dropping grid points in v-space

- Drop all points with same pitch-angle (red points on right) to get error estimate for pitch-angle integration and repeat for each pitch-angle
- Same process for energy (blue points on right)



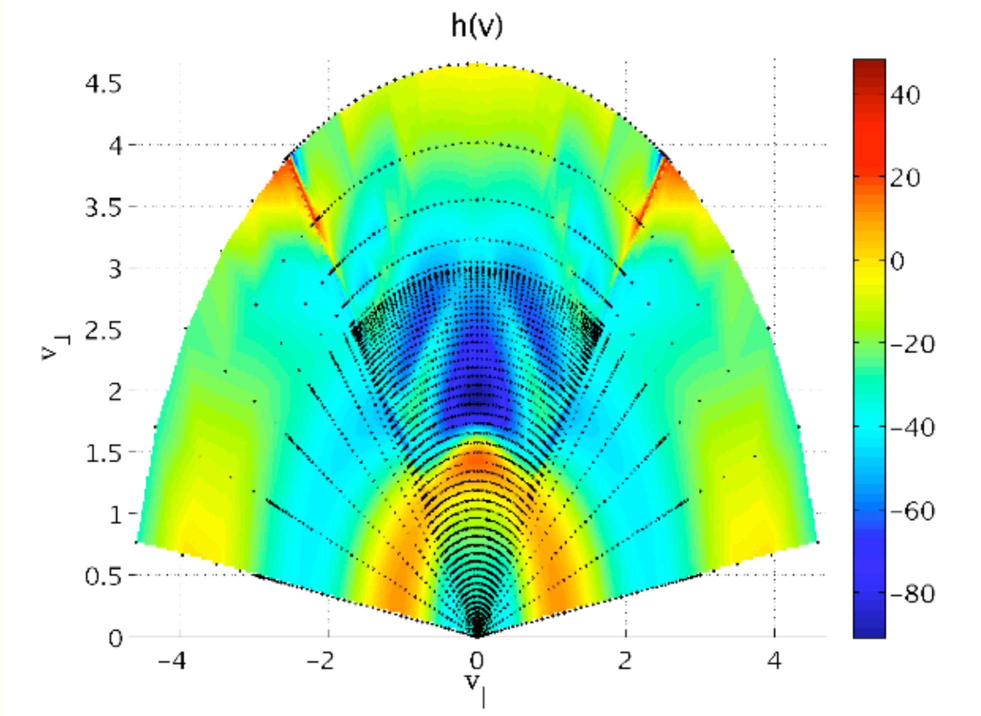
- Can also monitor v-space resolution by calculating relative amplitude of coefficients in distribution function expansion:

$$h(x) \approx \sum_{i=1}^{N} c_i P_i(x) \Rightarrow c_i \sim \int dx\ P_i(x) h(x)$$

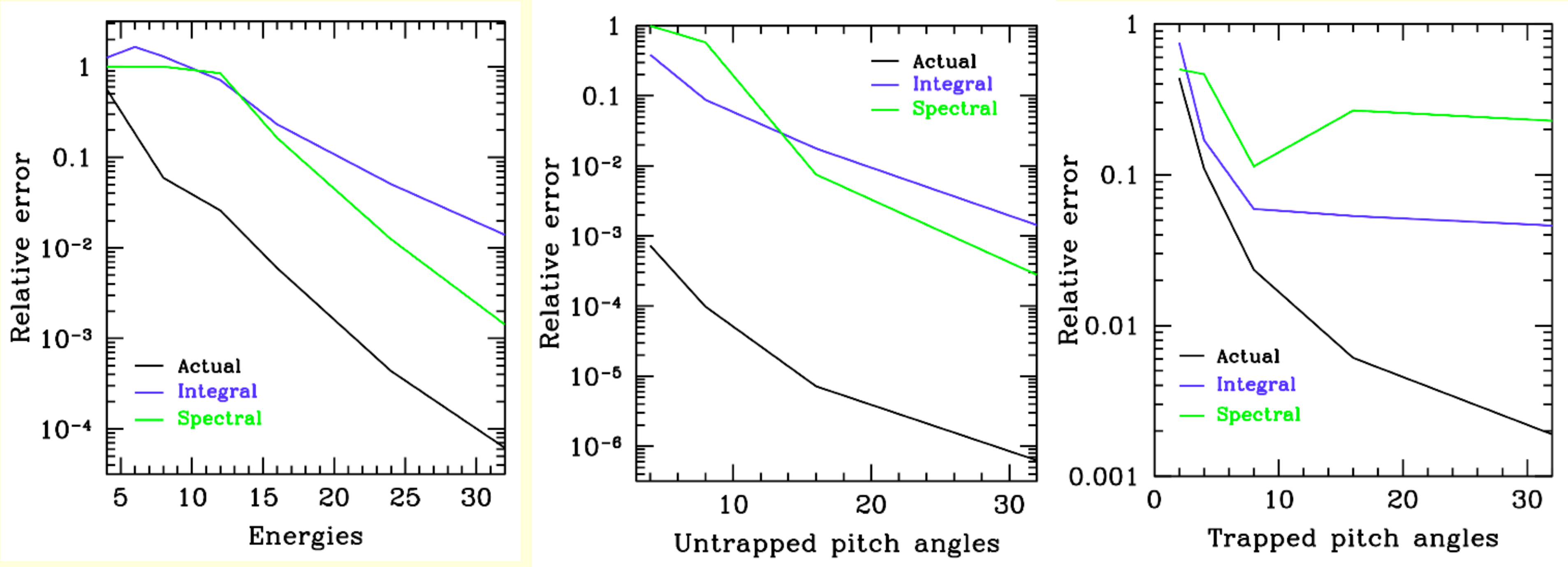
$$\text{Error estimate} \equiv \max_{i=N-2}^{N} c_i / \max_{i=1}^{N} c_i$$

- Error estimate for each scheme is conservative
  - for integral scheme, this is due to use of Gaussian quadrature rules (dropping grid point changes order of accuracy from 2N-1 to N-2)
  - for spectral scheme, this is due to fact that we can only accurately calculate c_i for $i < N$ (because it's a numerical integral over the product of two polynomials)

Linear, toroidal ITG mode

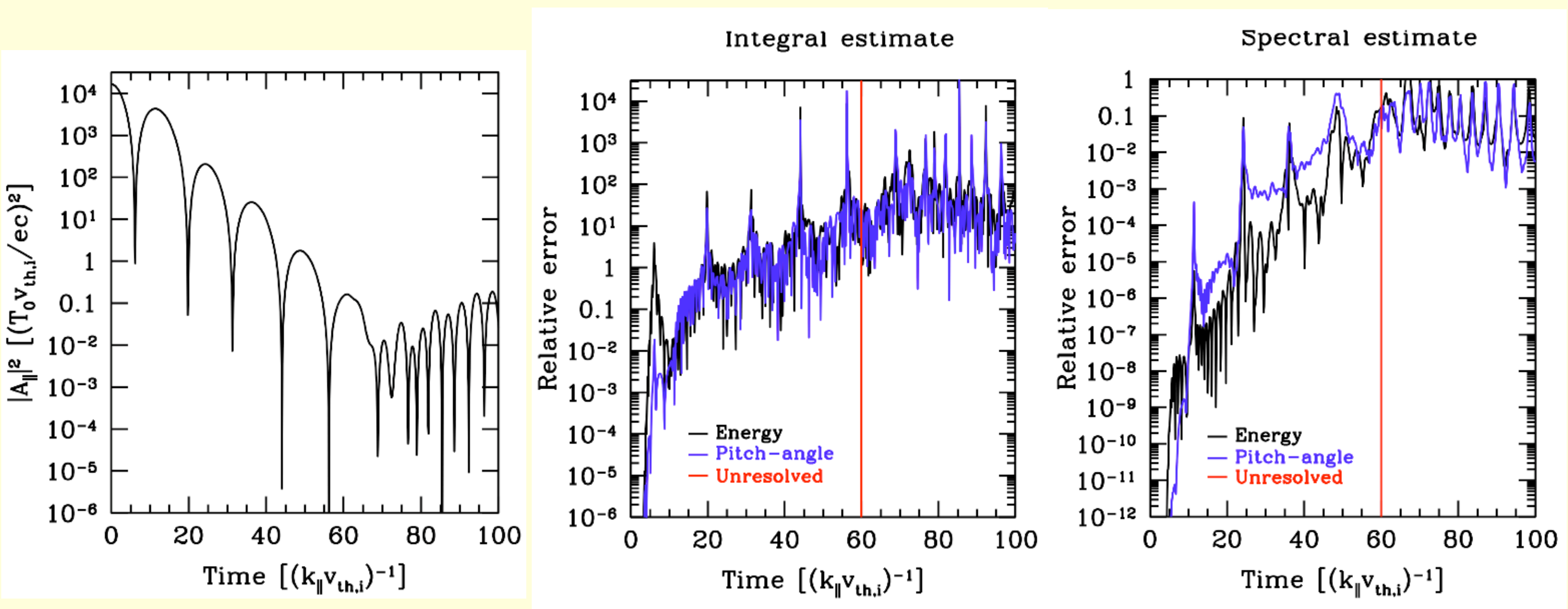


Error estimates conservative, require empirical scaling



Collisionless damping of kinetic Alfven wave

- Unable to resolve damping indefinitely with finite grid spacing in absence of dissipation



Model collision operator for gyrokinetics

- New collision operator* in GS2

$$C_{GK}[h_k] = L[h_k] + D[h_k] + U_L[h_k] + U_D[h_k] + E[h_k]$$

$$L[h_k] = \frac{\nu_D}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial h_k}{\partial \xi} - \frac{k_\perp^2 v^2}{4\Omega_0^2}\nu_D\left(1+\xi^2\right)h_k$$

$$D[h_k] = \frac{1}{2v^2}\frac{\partial}{\partial v}\left(\nu_\parallel v^4 F_0 \frac{\partial}{\partial v}\frac{h_k}{F_0}\right) - \frac{k_\perp^2 v^2}{4\Omega_0^2}\nu_\parallel\left(1-\xi^2\right)h_k$$

$$U_L[h_k] = \nu_D F_0\left(J_0 v_\parallel \frac{\int d^3v\ \nu_D v_\parallel J_0 h_k}{\int d^3v\ \nu_D v_\parallel^2 F_0} + J_1 v_\perp \frac{\int d^3v\ \nu_D v_\perp J_1 h_k}{\int d^3v\ \nu_D v_\parallel^2 F_0}\right)$$

$$U_D[h_k] = -\Delta\nu F_0\left(J_0 v_\parallel \frac{\int d^3v\ \Delta\nu v_\parallel J_0 h_k}{\int d^3v\ \Delta\nu v_\parallel^2 F_0} + J_1 v_\perp \frac{\int d^3v\ \Delta\nu v_\perp J_1 h_k}{\int d^3v\ \Delta\nu v_\parallel^2 F_0}\right)$$

$$E[h_k] = \nu_E v^2 J_0 F_0 \frac{\int d^3v\ \nu_E v^2 J_0 h_k}{\int d^3v\ \nu_E v^4 F_0}$$

*Abel et al., Phys. Plasmas, accepted (2008), arXiv: 0806.1069.
Barnes et al., Phys. Plasmas, submitted (2008), arXiv: 0809.3945.

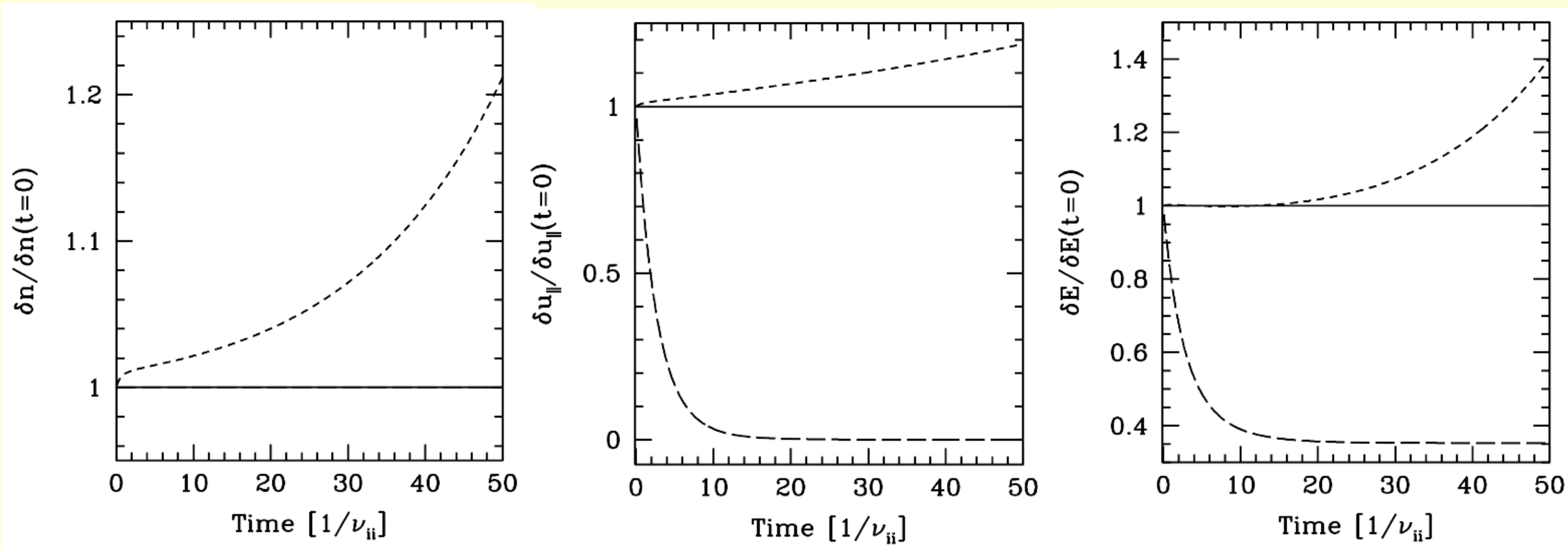
Numerical properties

- Fully implicit
  - Pitch-angle scattering and energy diffusion treated separately through Godunov splitting
  - Finite difference scheme first order accurate and satisfies discrete versions of Fundamental Theorem of Calculus and integration by parts (upon double application). Leads to tridiagonal matrices
  - Conserving terms incorporated at little additional cost using repeated application of Sherman-Morrison formula:

If $M\mathbf{x} = \mathbf{b}$ and $M = A + \mathbf{u} \otimes \mathbf{v}$, then $\mathbf{x} = \mathbf{y} - \dfrac{\mathbf{v} \cdot \mathbf{y}}{1 + \mathbf{v} \cdot \mathbf{z}}\mathbf{z}$,

where: $\mathbf{y} = A^{-1}\mathbf{b}$ and $\mathbf{z} = A^{-1}\mathbf{u}$

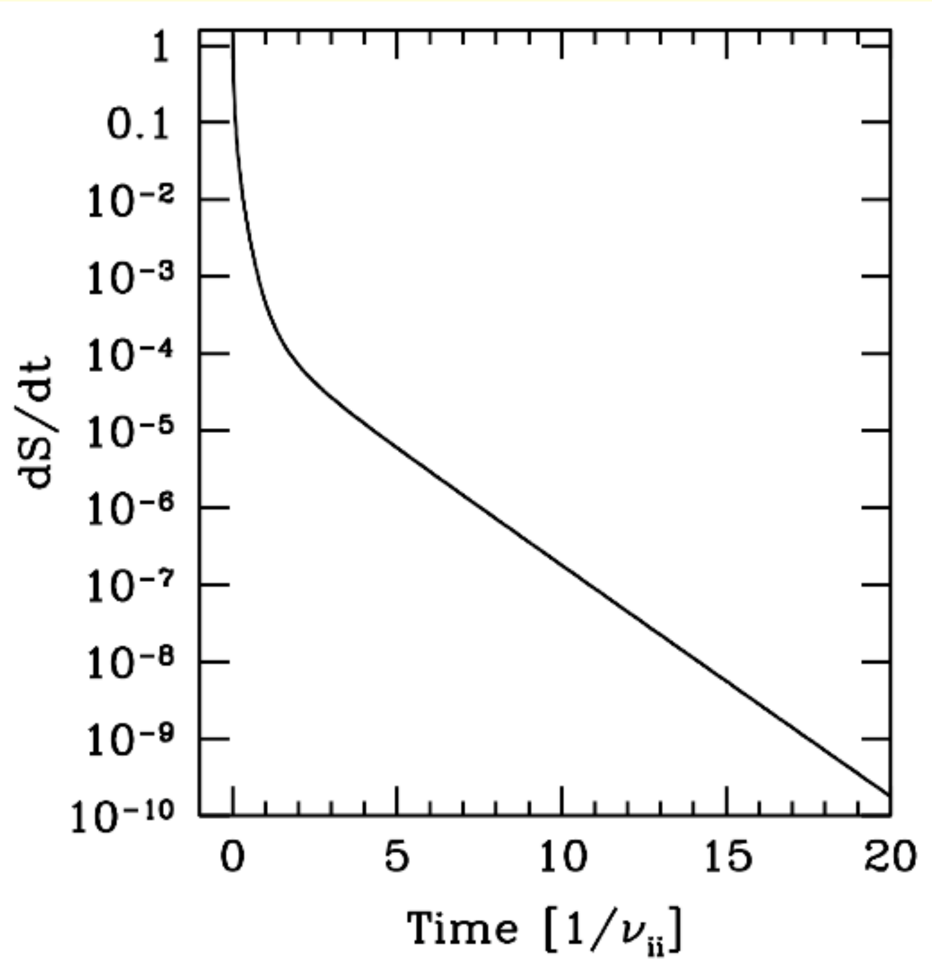
Exact local conservation of particle number, momentum, and energy



Solid lines: conservative discretization used in GS2
Short dashed lines: non-conservative discretization
Long dashed lines: model operator without conserving terms.

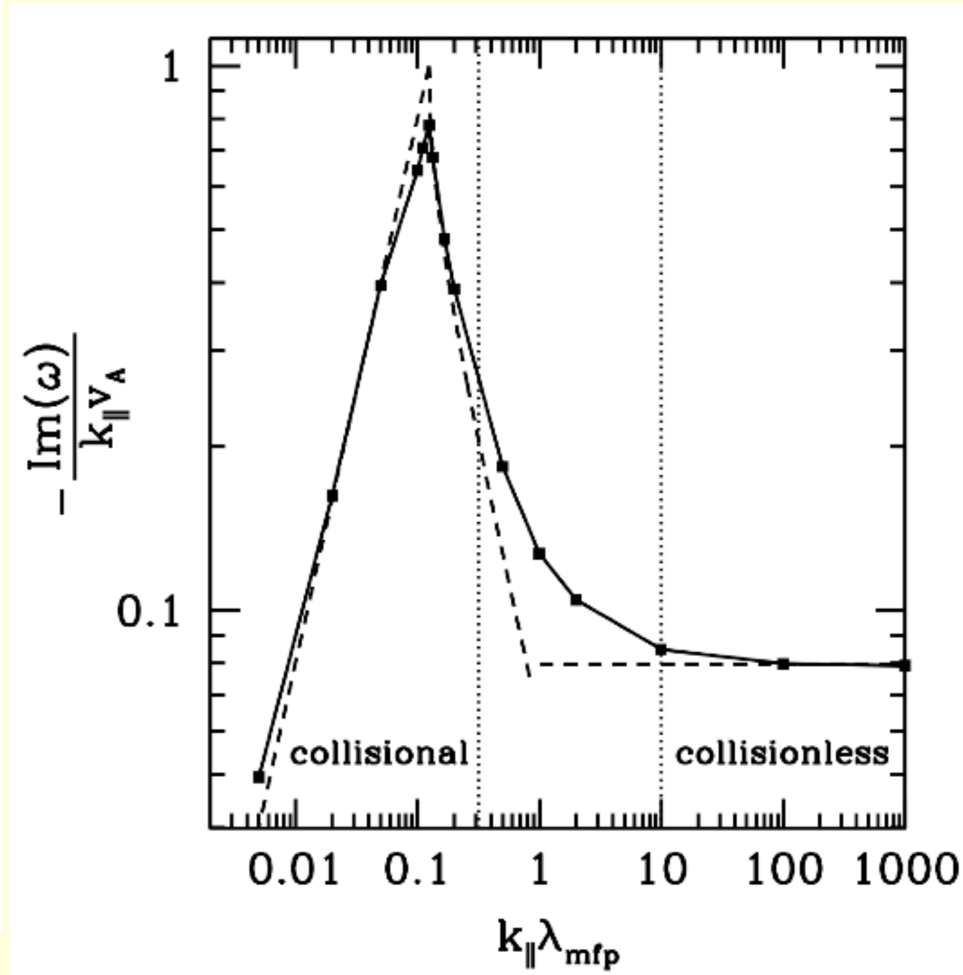
Satisfies H-Theorem

$$\left(\frac{dS}{dt} \geq 0\right)$$



homogeneous slab initialized with noise in v-space

Correct viscous, collisional, and collisionless damping

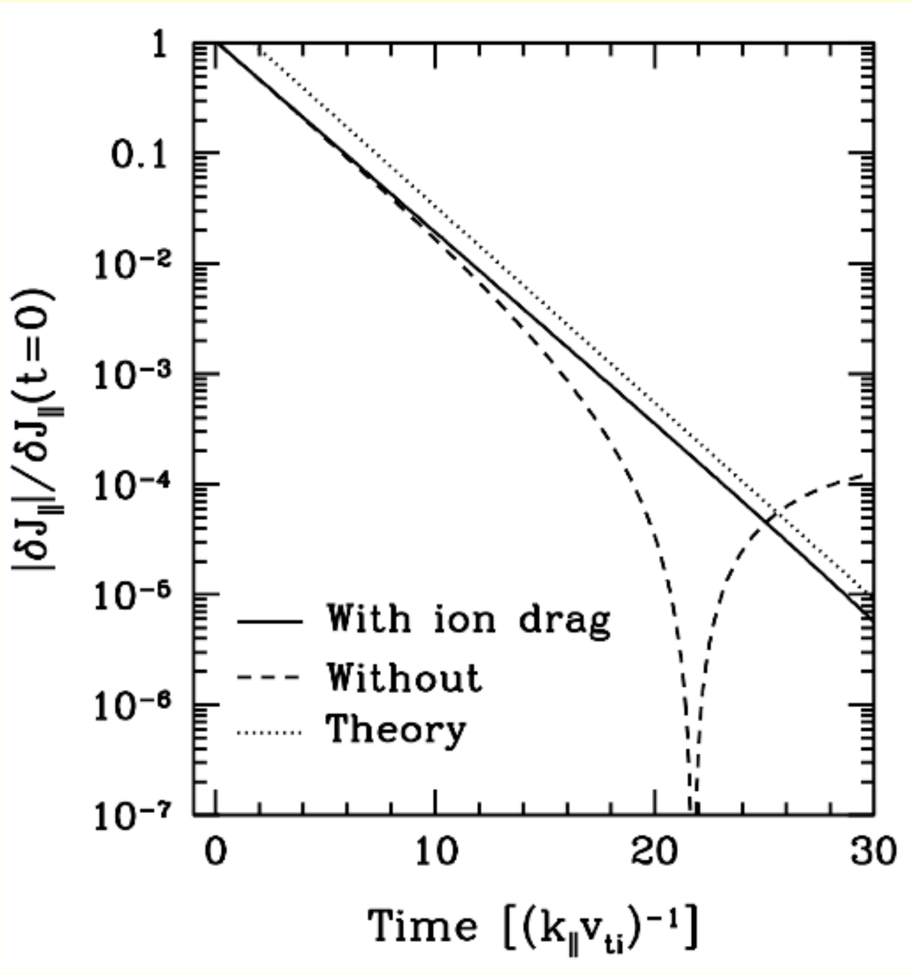


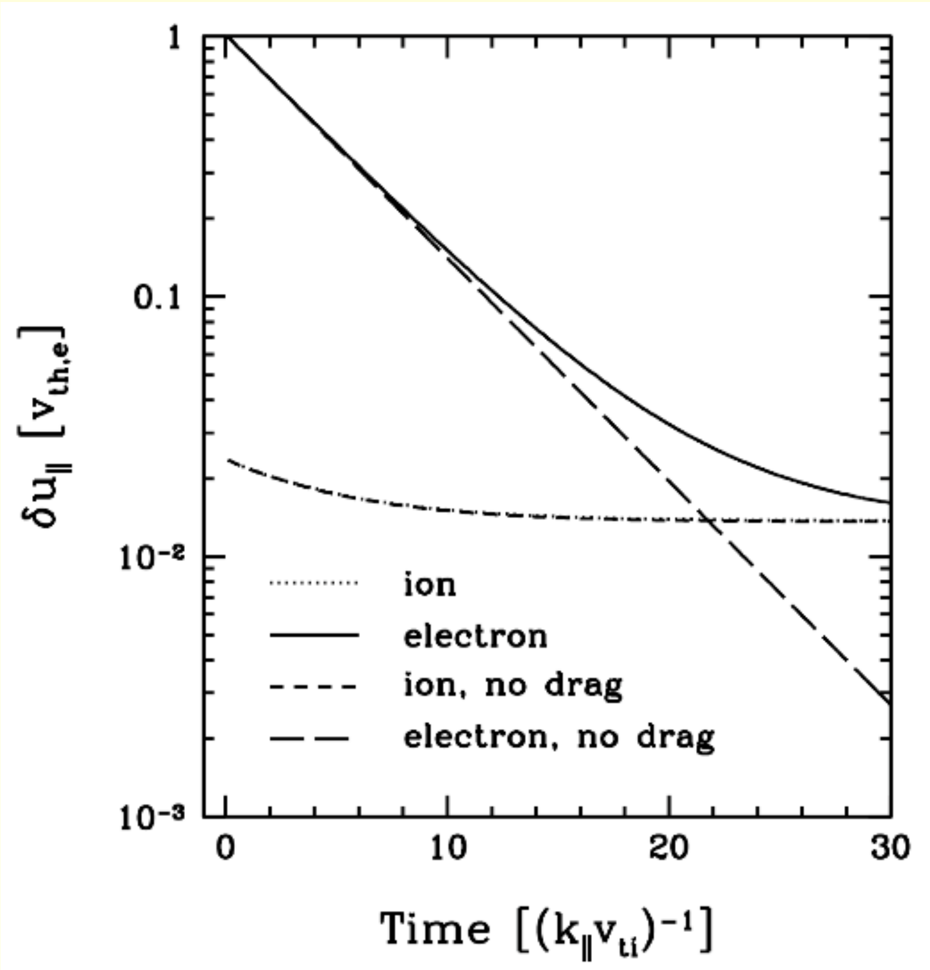
high-β slow mode

Correctly captures resistivity

For electrons:

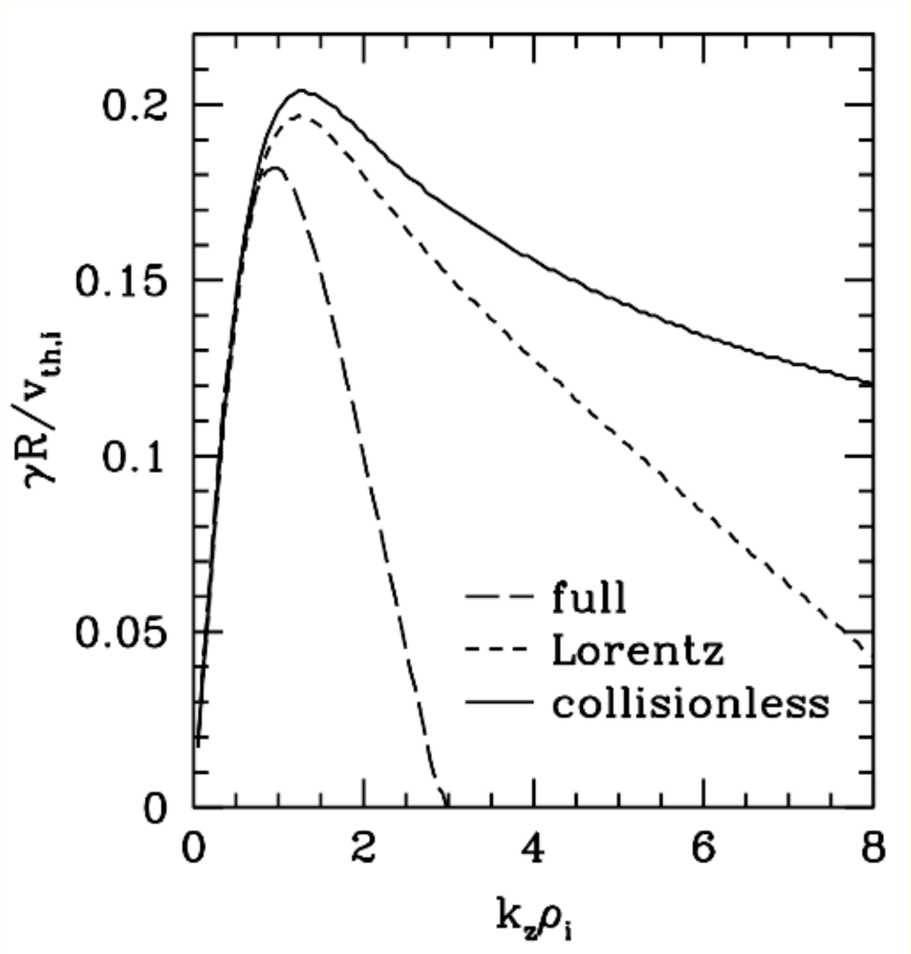
$$C_{GK}^{e}[h_e] = C_{GK}^{ee}[h_e] + \frac{\nu_D^{ei}}{2}\frac{\partial}{\partial \xi}\left(1-\xi^2\right)\frac{\partial h_e}{\partial \xi} - \frac{k_\perp^2 v^2}{4\Omega_0^2}\nu_D^{ei}\left(1+\xi^2\right)h_e + \nu_D^{ei}\frac{2v_\parallel u_{\parallel,i}}{v_{th,e}^2}J_0F_0$$

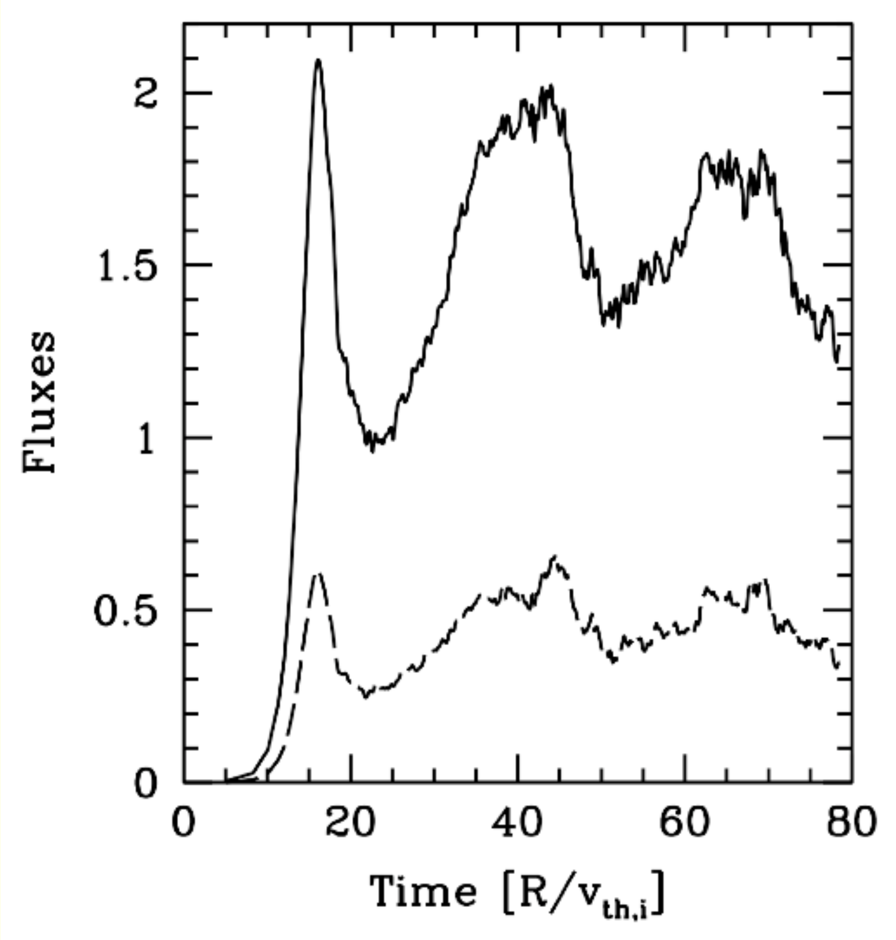




Efficient small-scale cutoff in phase space

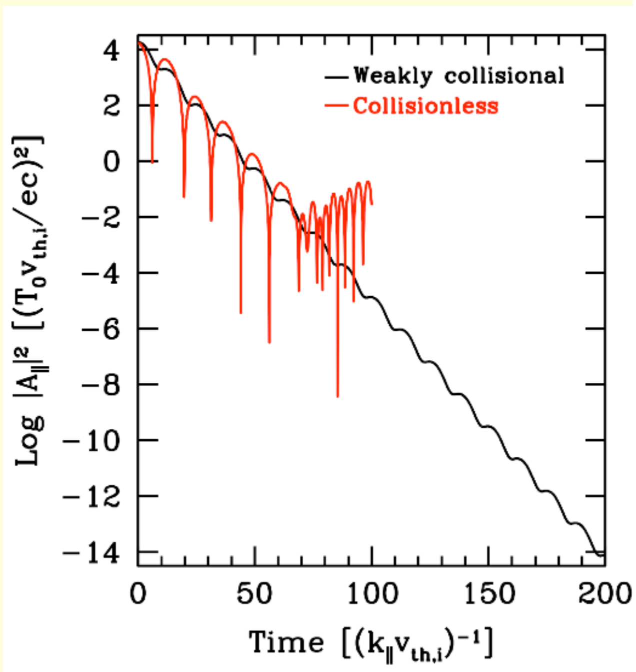
- Weakly collisional, electrostatic turbulence in Z-pinch. No artificial dissipation necessary to obtain steady-state fluxes

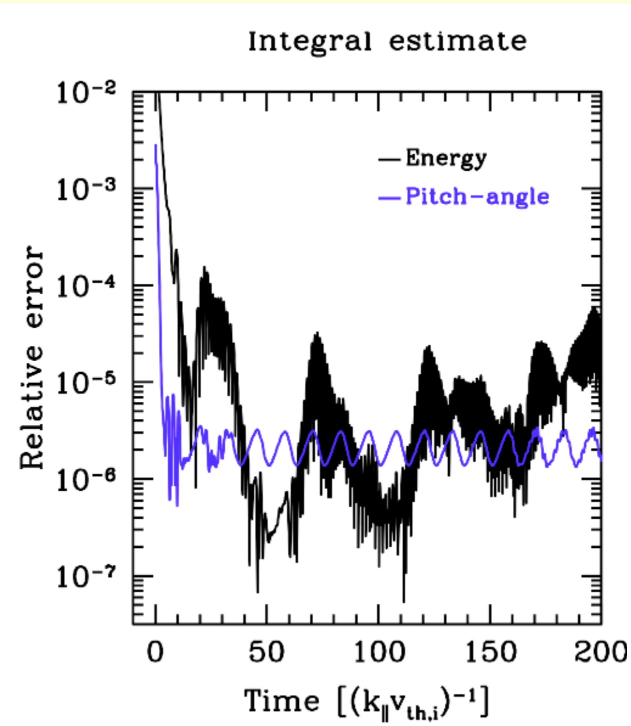


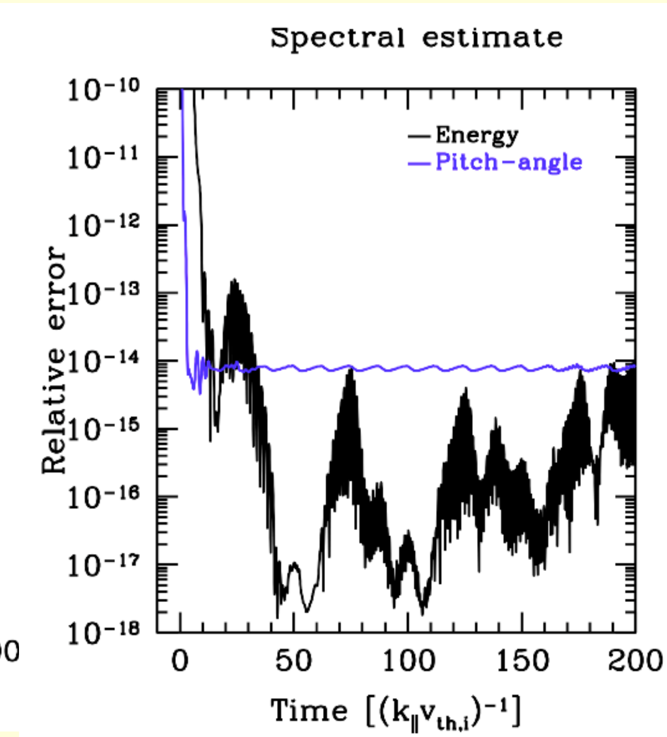


Weakly collisional damping of kinetic Alfven wave

- Small collisionality leads to well-resolved long-time simulation and recovery of collisionless damping rate

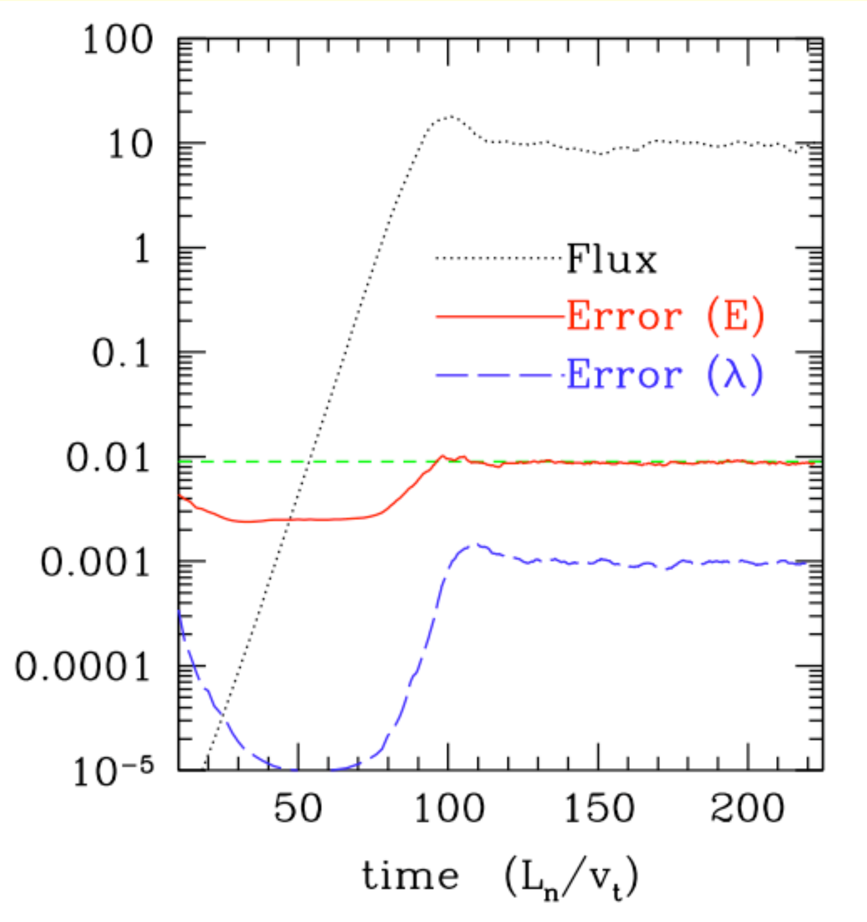


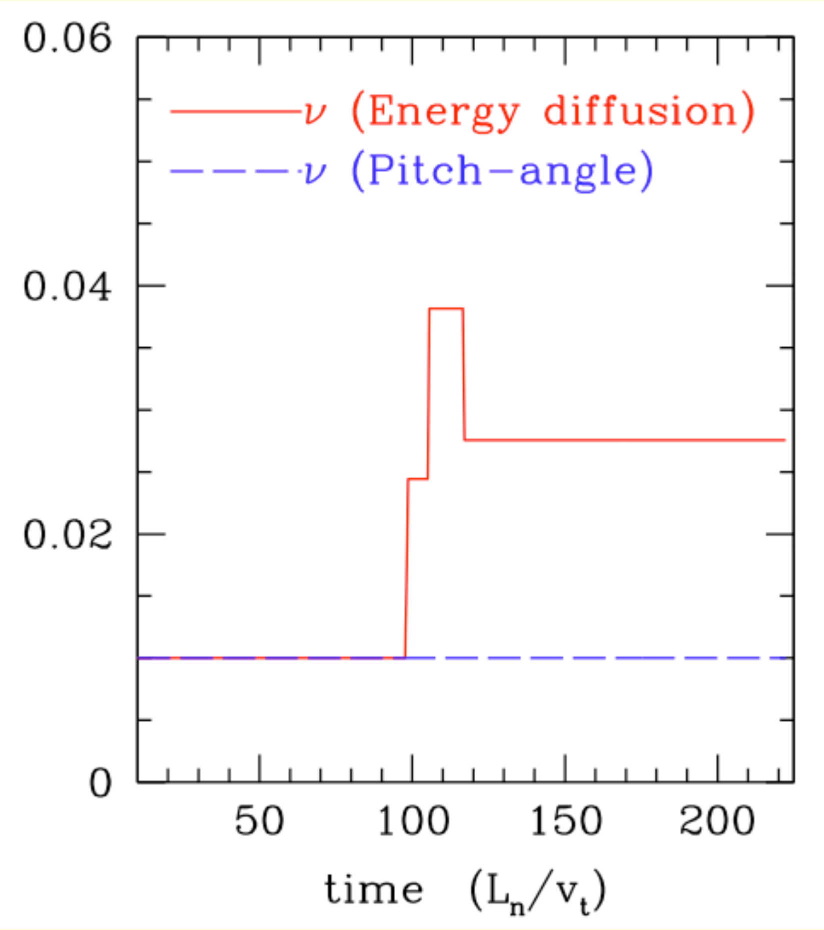




Adaptive collisionality

- Specify v-space error tolerance and calculate v-space error estimate
- Adaptively change collisionality to ensure error not too large
- Provides approximate minimal collisionality necessary for resolution





slab ETG

Summary

- Developed a working code (TRINITY) for efficiently simulating the self-consistent interaction between turbulence and transport/heating
- TRINITY is capable of running with multiple species, electromagnetic effects, realistic geometry (numerical equilibria, etc.), physical collisional effects (such as heating), etc.
- Resolution in GS2 velocity space monitored and adaptively improved through the use of new diagnostics
- Future work includes:
  - addition of radial electric field and momentum transport equation
  - evolution of flux surfaces (equations already derived)