A Framework for First-Principles Simulations of Coupled Turbulent Transport

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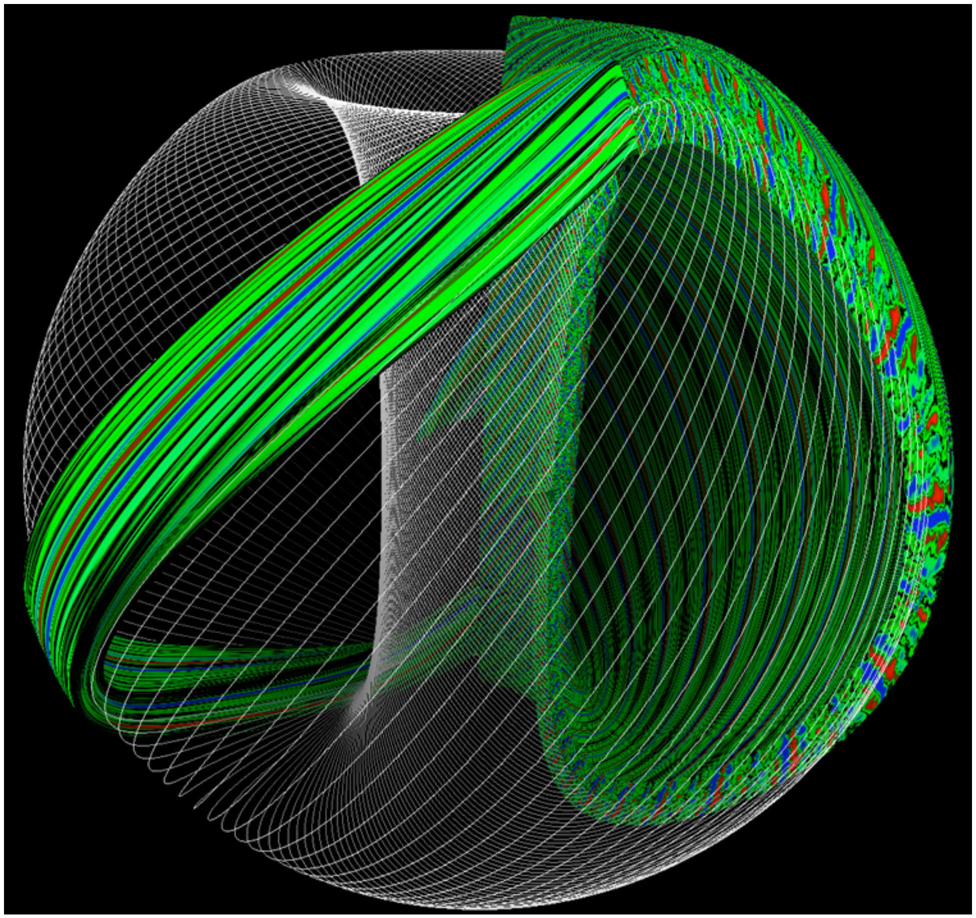
Challenges

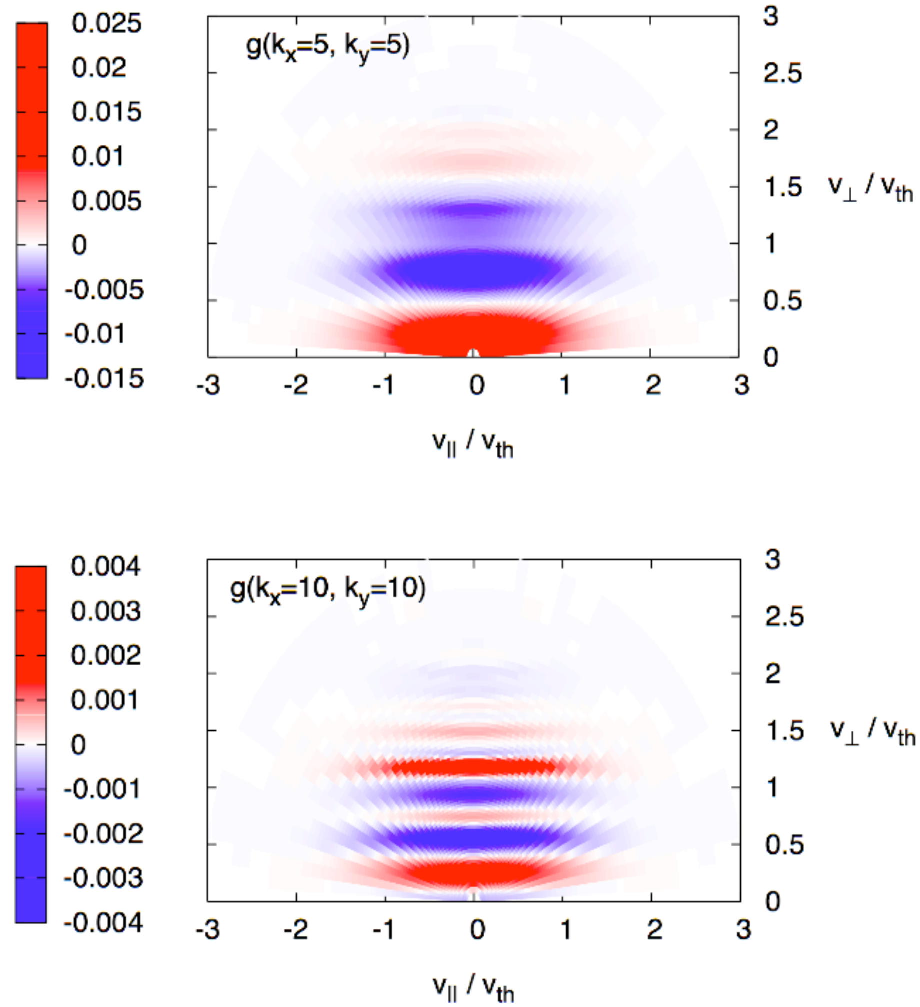
- Turbulent transport in ITER and other fusion plasmas involves interaction of phenomena spanning a wide range of time and space scales:

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

- Turbulence driving transport is kinetic (requires 5D description):



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



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

Resolving kinetic turbulence

- Fine scales possible in velocity space:

$$\frac{\partial h}{\partial t} + \left(\mathbf{v}_\parallel + \overline{\mathbf{v}}_\chi + \mathbf{v}_d\right) \cdot \nabla h = -\overline{\mathbf{v}}_\chi \cdot \nabla F_0 + \frac{q}{T_0}\frac{\partial \overline{\chi}}{\partial t} F_0 + \overline{C}[h]$$

$$\frac{\partial h_s}{\partial t} \sim \overline{C}[h_s] \sim \nu_s v_{th}^2 \frac{\partial^2 h_s}{\partial v^2} \Rightarrow \left(\frac{\delta v}{v_{th}}\right)_s \sim \sqrt{\frac{\nu_s}{\omega}}$$

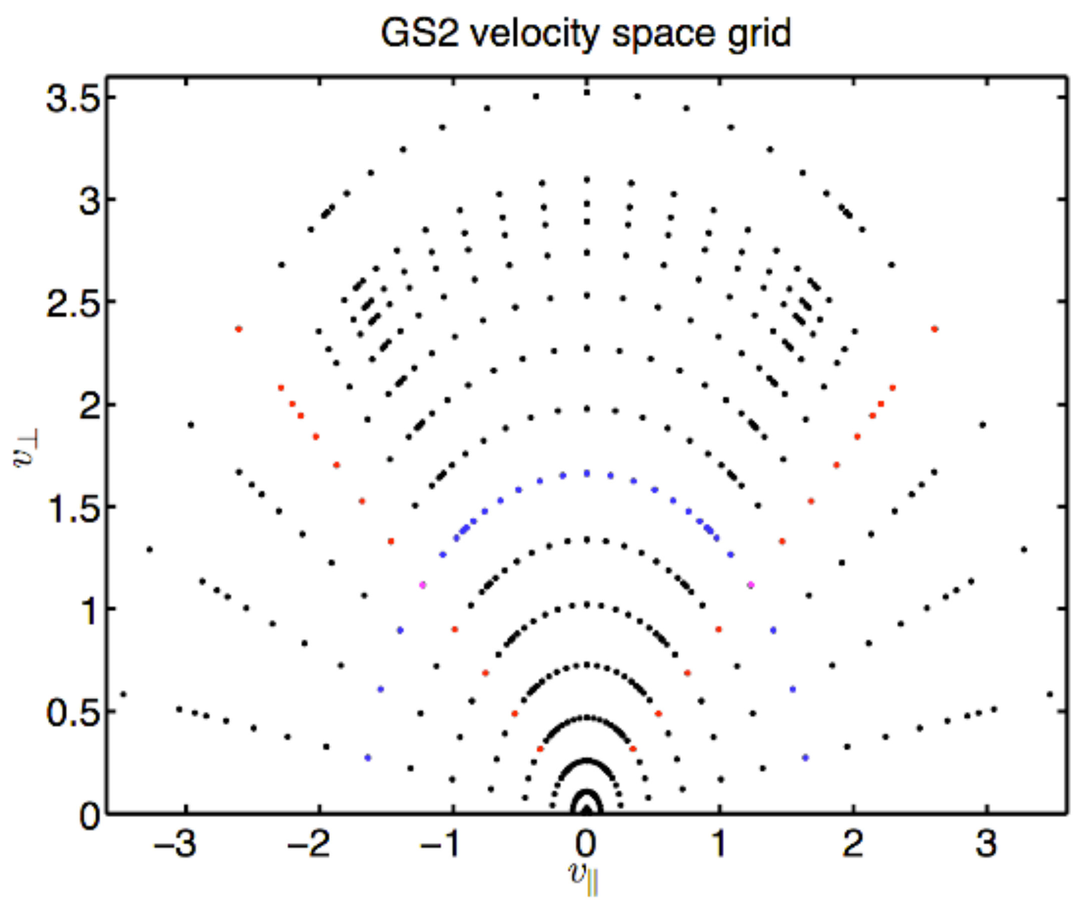
For ITER:

$$\omega \sim \omega_* \sim 10^4\ Hz, \quad \nu_i \sim 10^2\ Hz$$

$$\Rightarrow \frac{\delta v}{v_{th}} \sim 0.1$$

- 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:

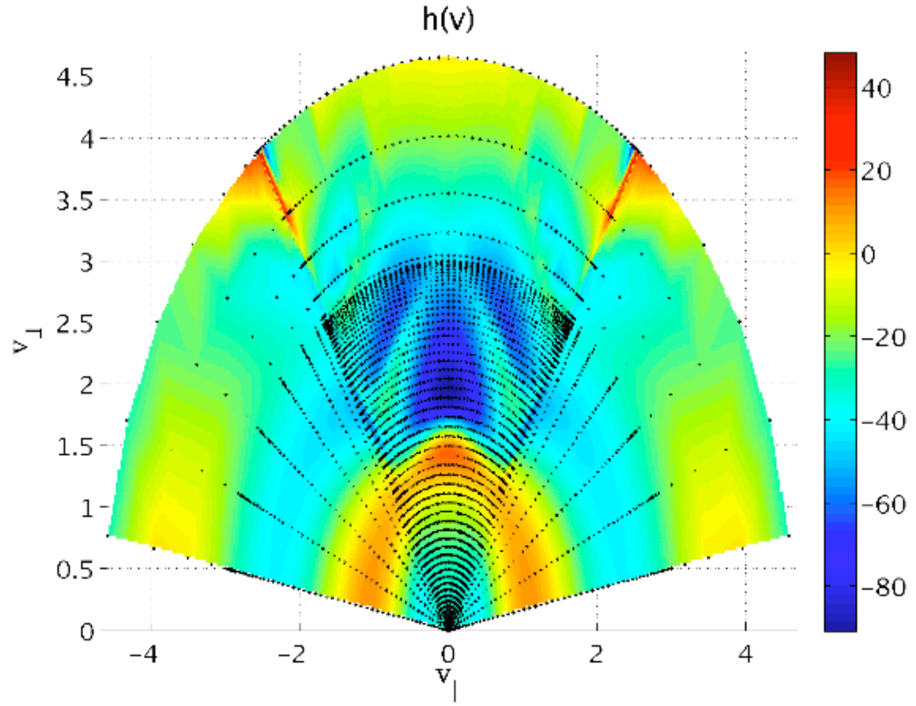
$$h(x) \approx \sum_{i=1}^{N} c_i P_i(x) \Rightarrow c_i \sim \int dx \; P_i(x) h(x)$$

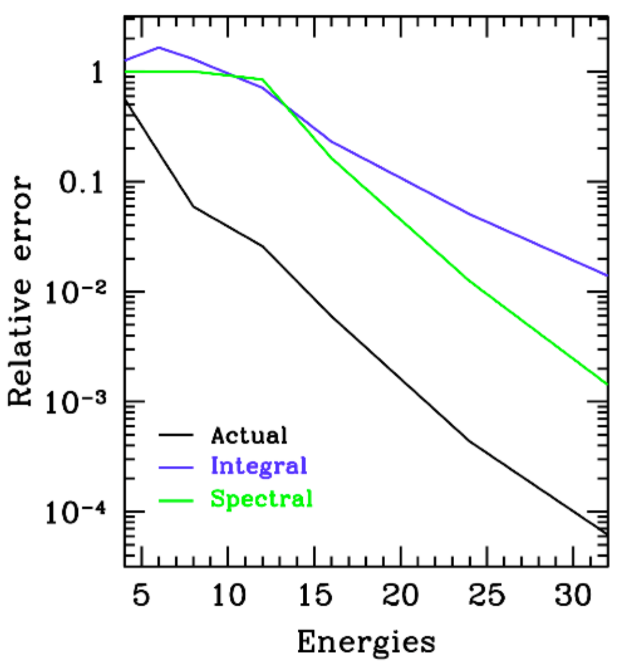
$$\text{Error estimate} \equiv \max_{i=N-2}^{N} c_i / \max_{i=1}^{N} c_i$$

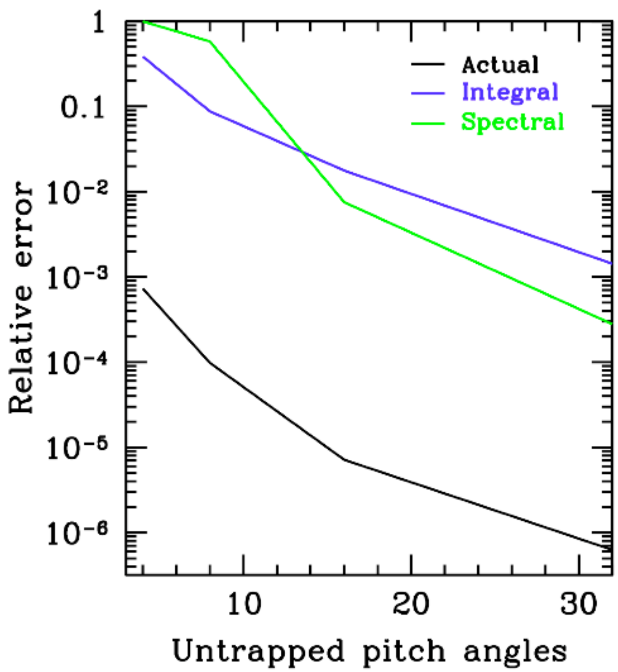
- Error estimate for each scheme is conservative
  - for integral scheme, this is due to use of Gaussian quadrature rules (dropping grid point changes order of accuracy from 2N-1 to N-2)
  - for spectral scheme, this is due to fact that we can only accurately calculate c_i for $i < N$ (because it's a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

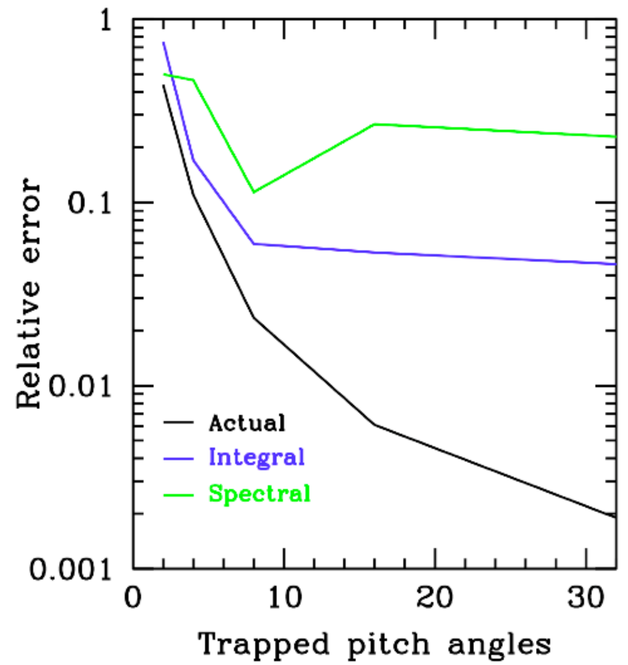
Linear, toroidal ITG mode

Error estimates conservative, require empirical scaling



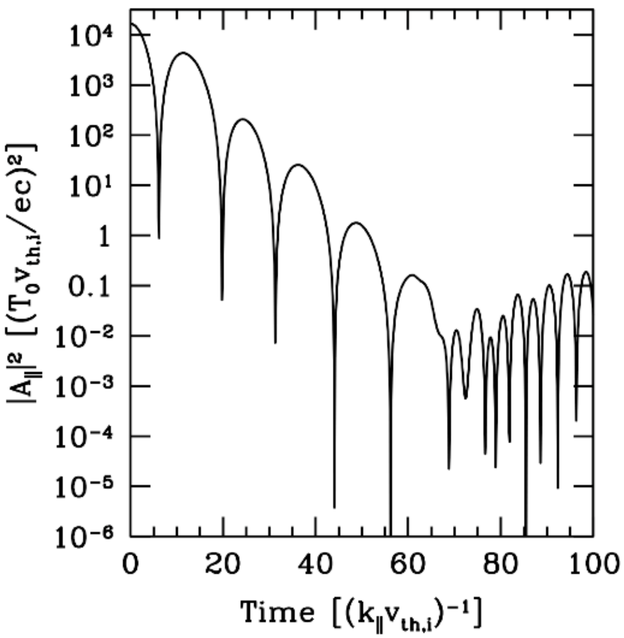


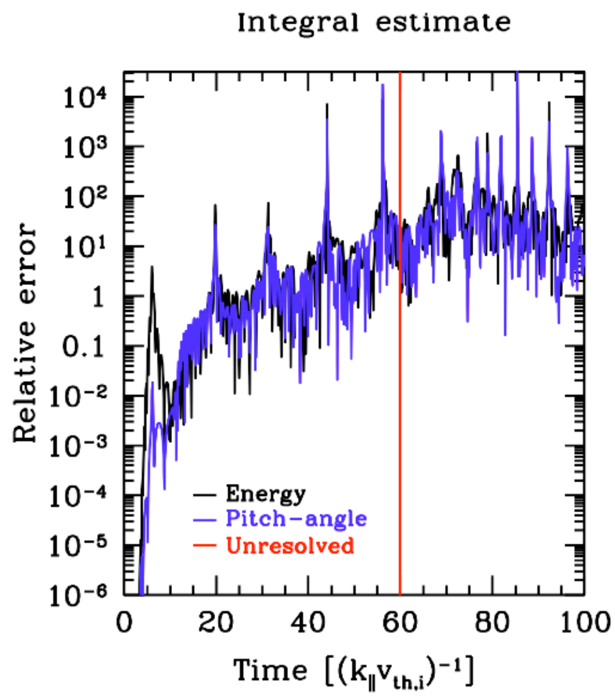


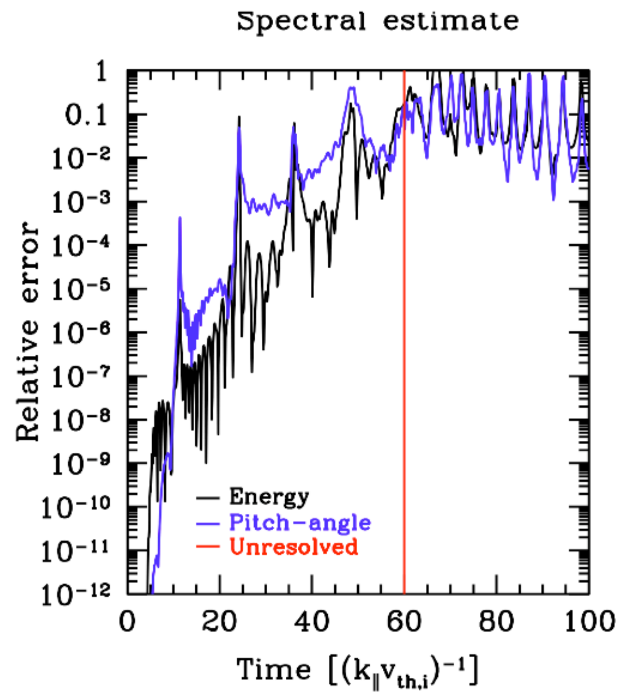


Collisionless damping of kinetic Alfven wave

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







Model collision operator for gyrokinetics

- Implemented new collision operator in GS2

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

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

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

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

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

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

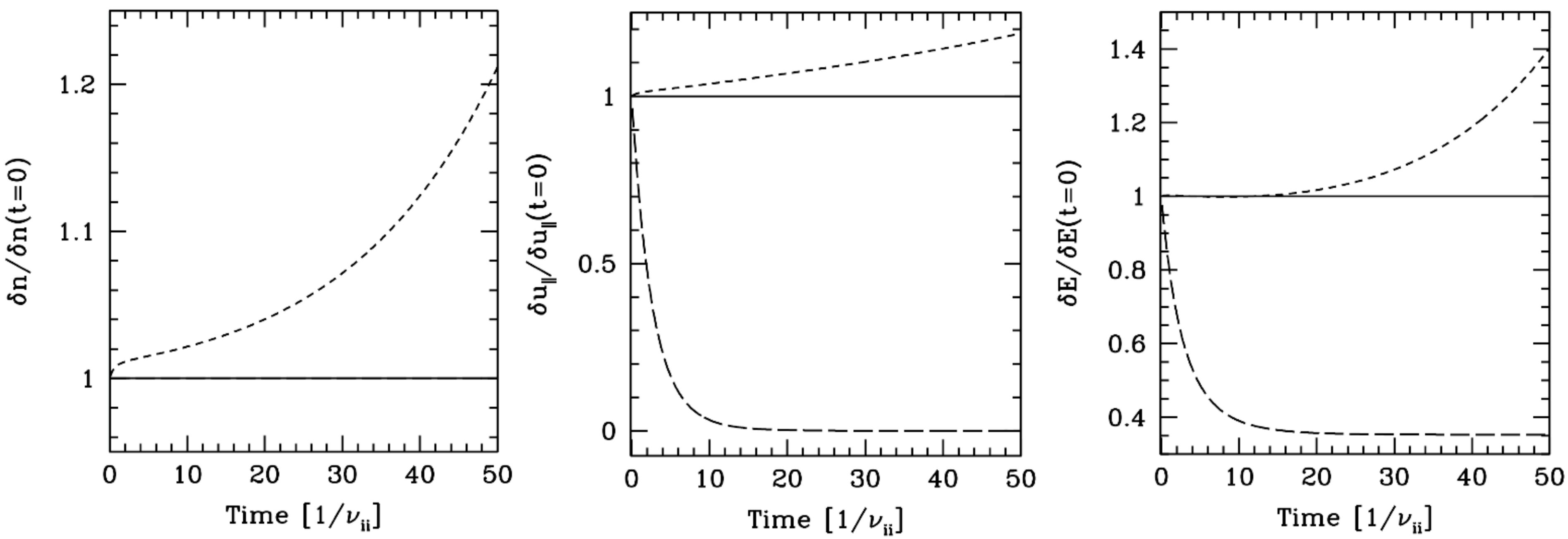
Numerical properties

- 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 $\mathbf{z} = A^{-1}\mathbf{u}$

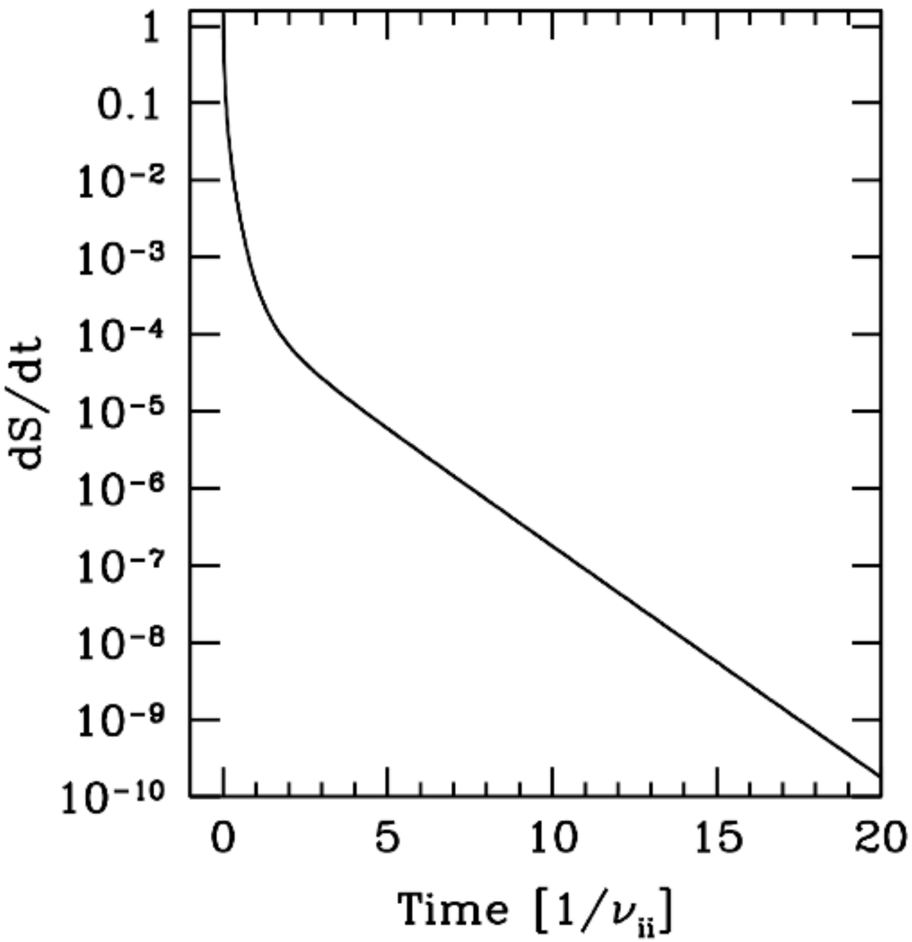
Exact local conservation of particle number, momentum, and energy



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

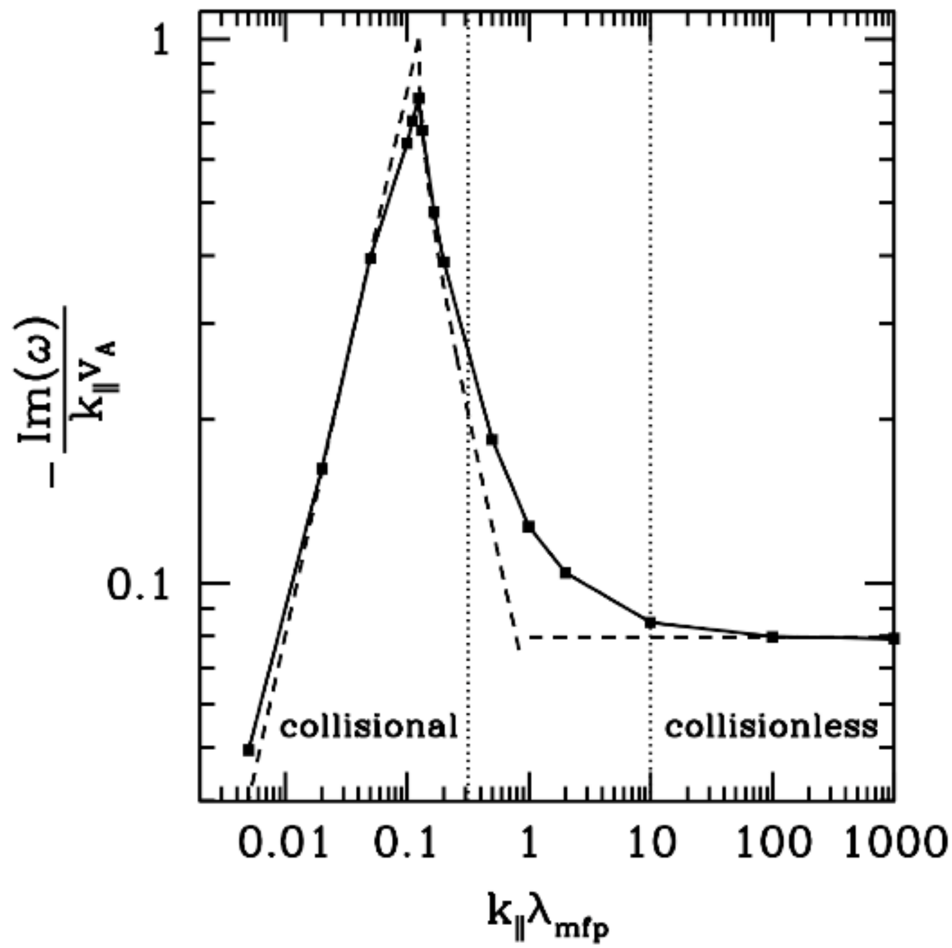
Satisfies H-Theorem

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



homogeneous slab initialized with noise in v-space

Correct viscous, collisional, and collisionless damping

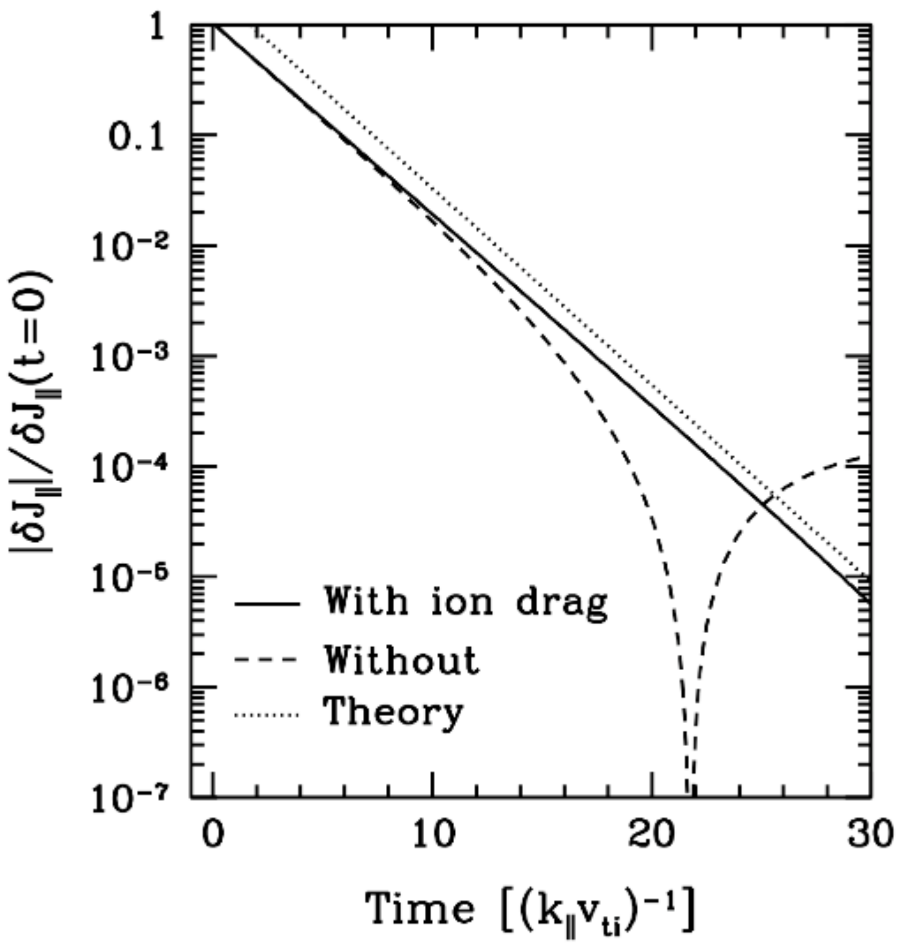


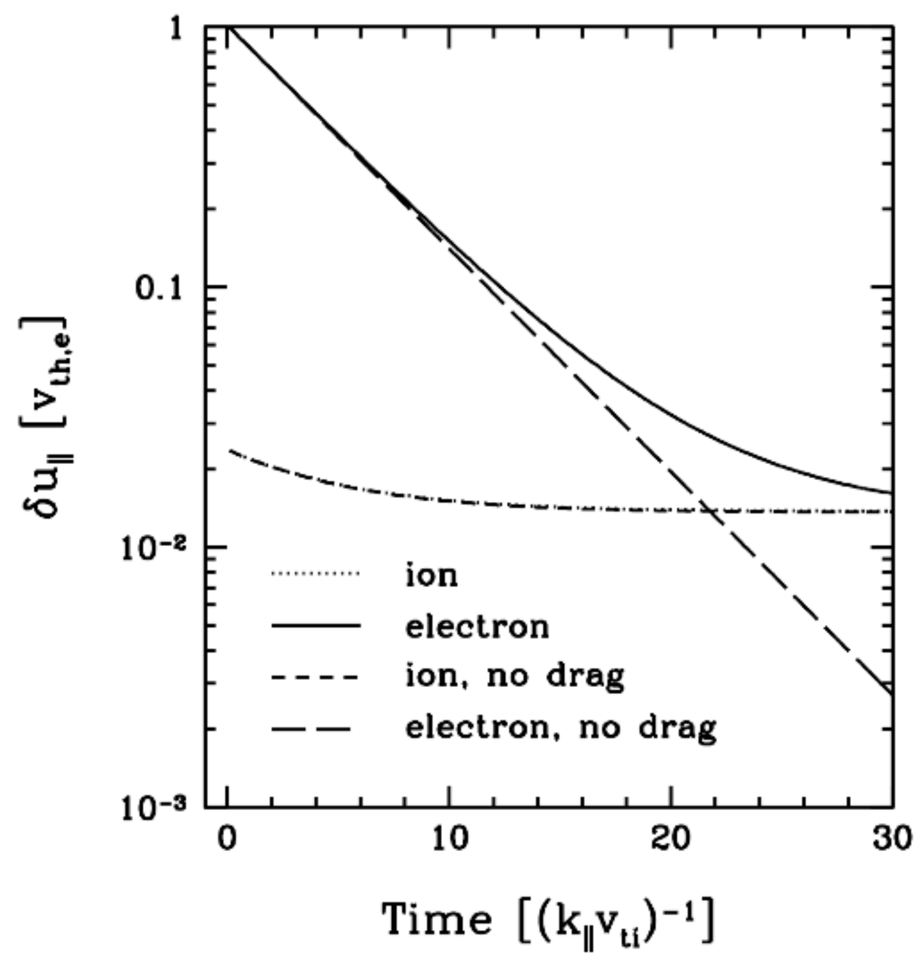
high-β slow mode

Correctly captures resistivity

For electrons:

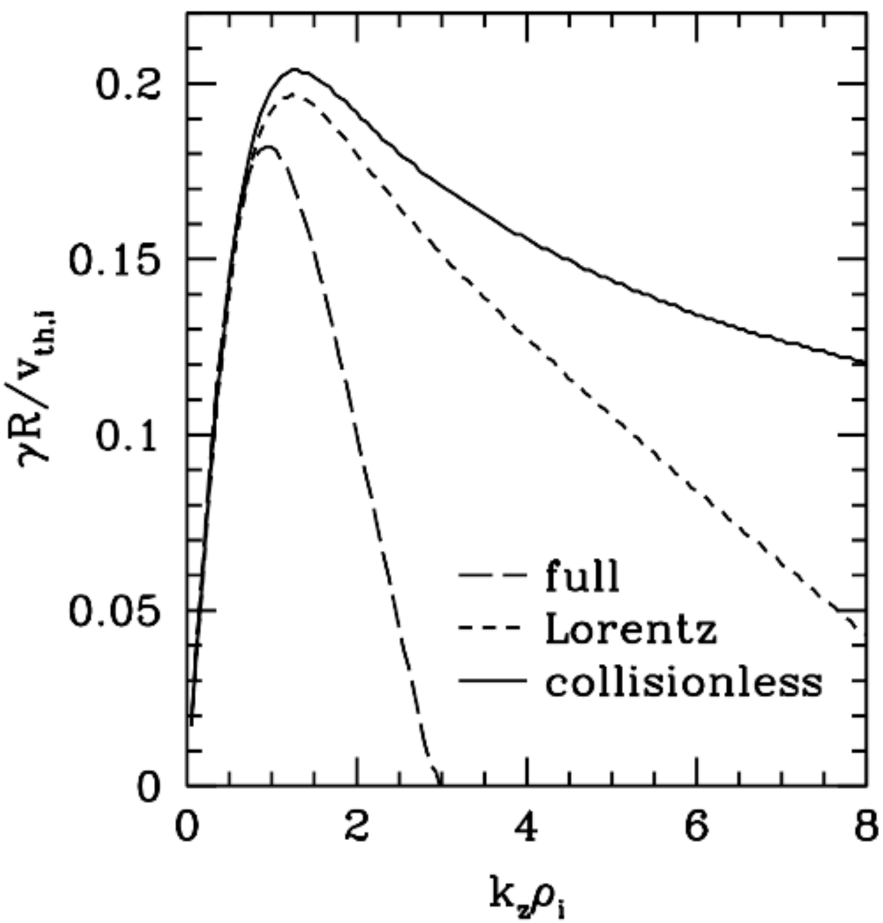
$$C_{GK}^{e}[h_e] = C_{GK}^{ee}[h_e] + \frac{\nu_D^{ei}}{2}\frac{\partial}{\partial\xi}\left(1-\xi^2\right)\frac{\partial h_e}{\partial\xi} - \frac{k_\perp^2 v^2}{4\Omega_0^2}\nu_D^{ei}\left(1+\xi^2\right)h_e + \nu_D^{ei}\frac{2v_\parallel u_{\parallel,i}}{v_{th,e}^2}J_0 F_0$$

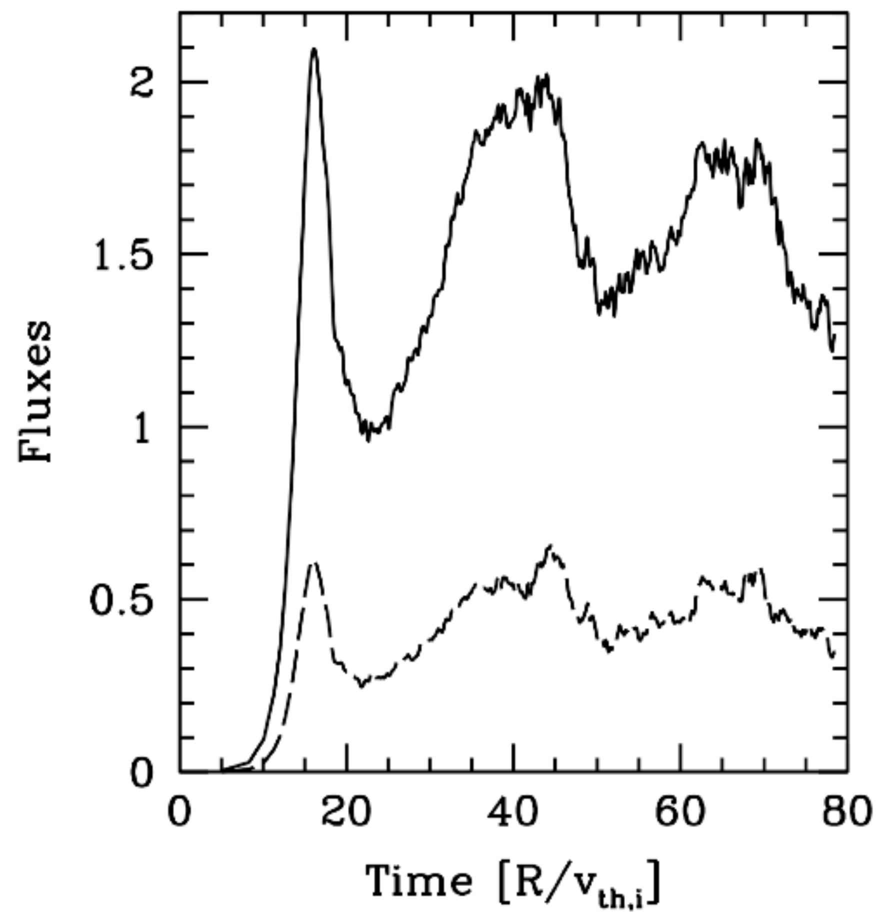




Efficient small-scale cutoff in phase space

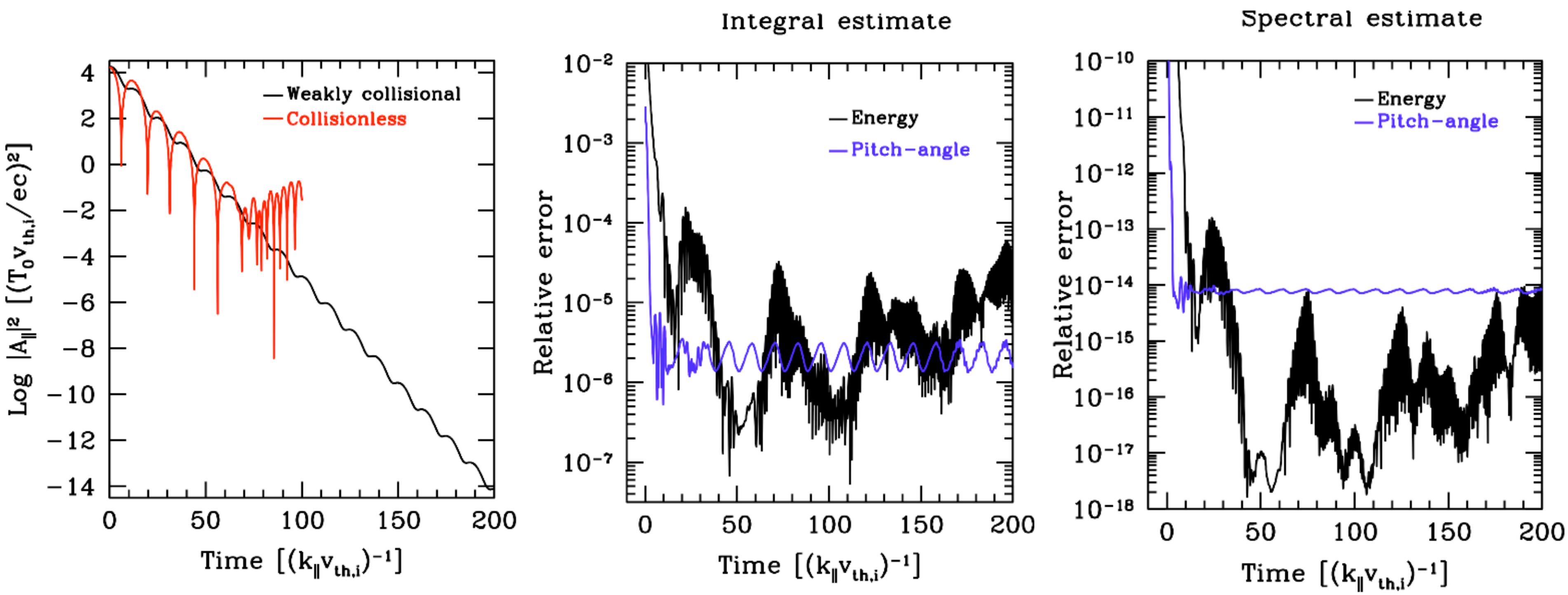
- Weakly collisional, electrostatic turbulence in Z-pinch. No artificial dissipation necessary to obtain steady-state fluxes





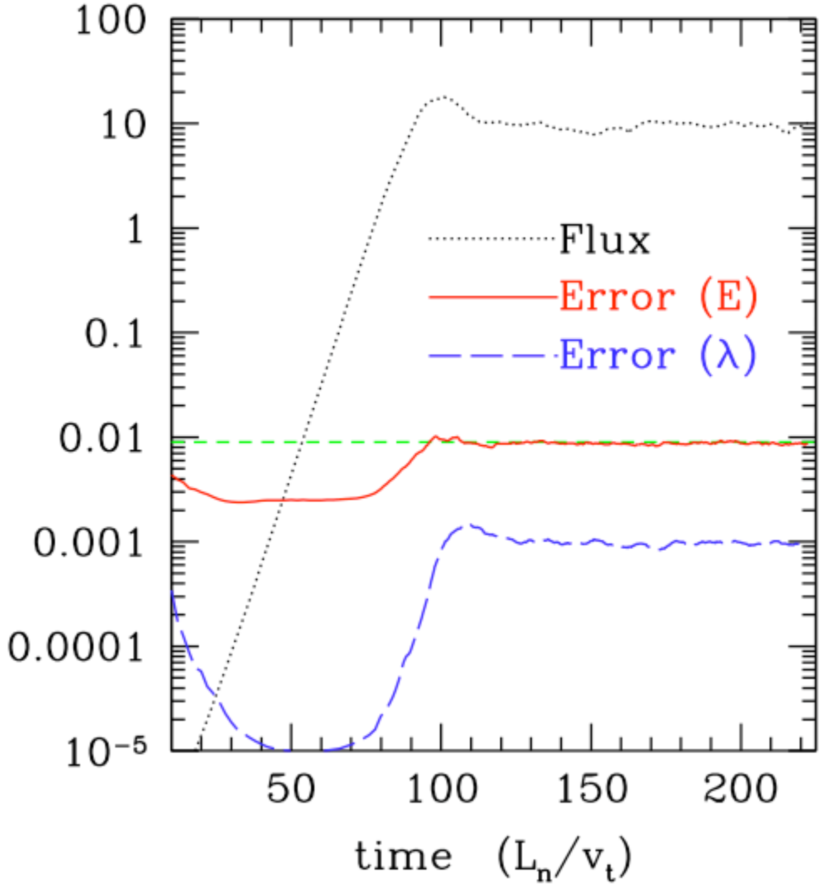
Weakly collisional damping of kinetic Alfven wave

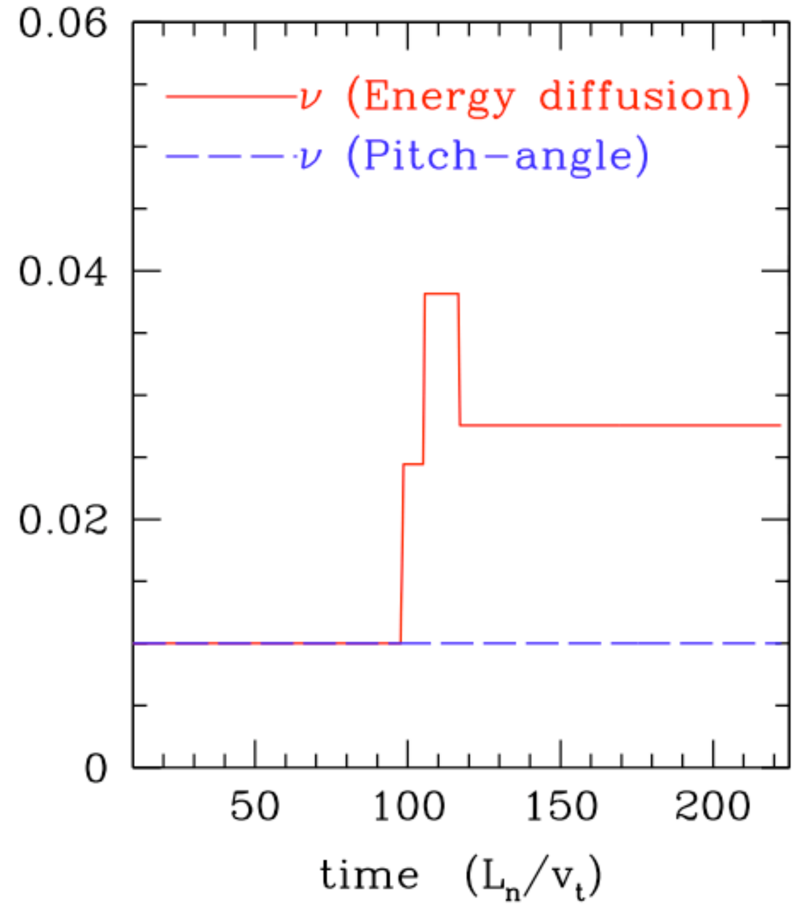
- Small collisionality leads to well-resolved long-time simulation and recovery of collisionless damping rate



Adaptive collisionality

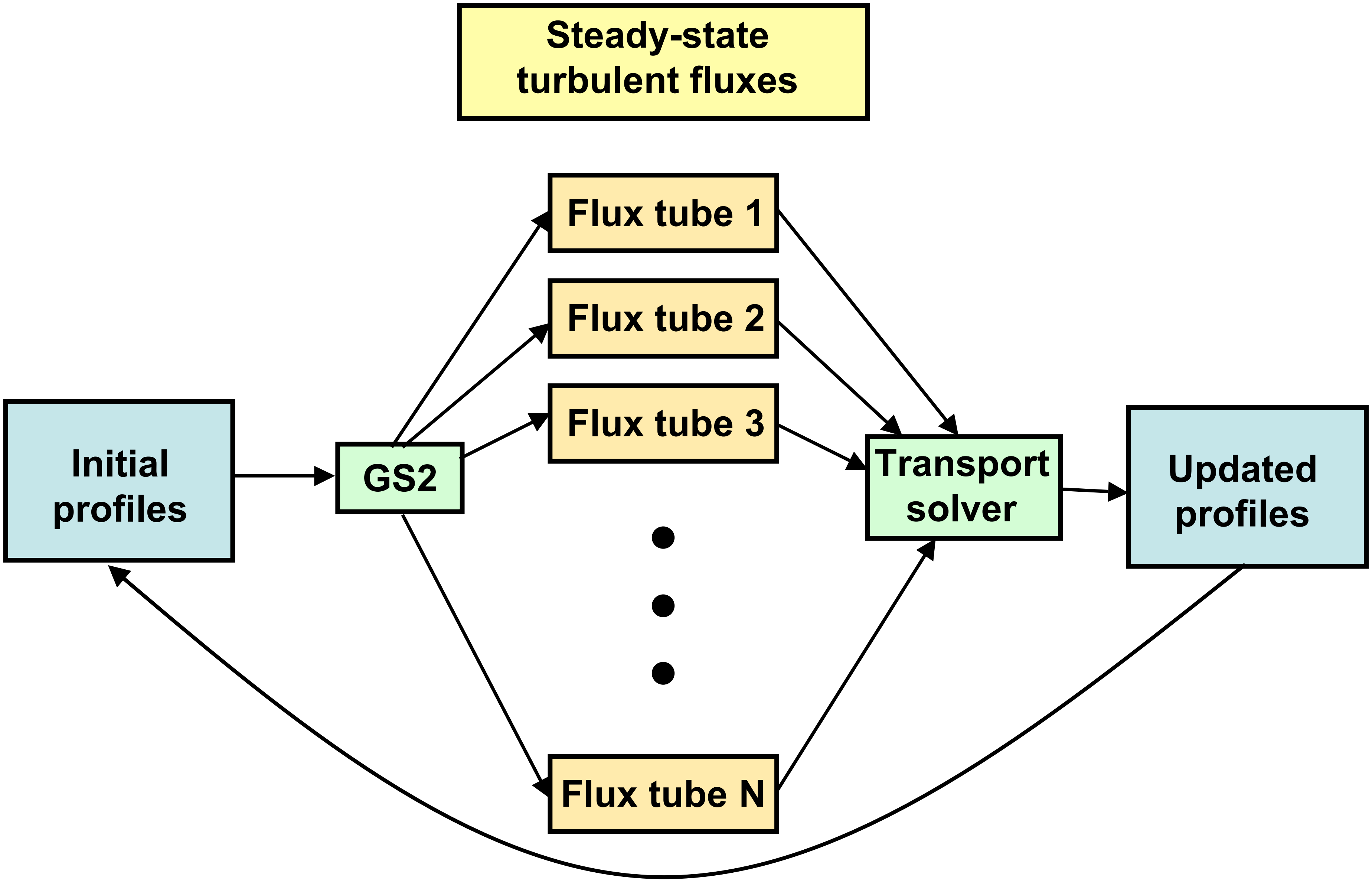
- Specify v-space error tolerance and calculate v-space error estimate
- Adaptively change collisionality to ensure error not too large
- Provides approximate minimal collisionality necessary for resolution





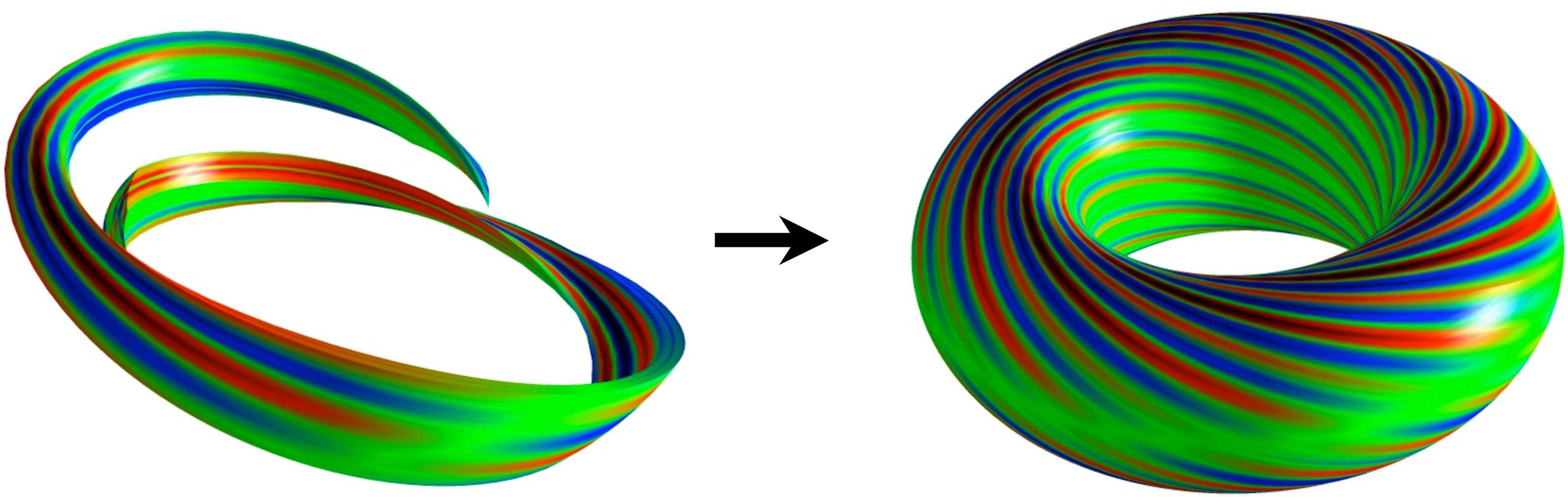
slab ETG

Coupling turbulence and transport



Minimizes simulation volume

- Flux tube simulations take advantage of statistical periodicity along field lines, giving factor of n_ϕ savings in volume compared to global simulations ($n_\phi \equiv$ toroidal mode #)



Tokamak simulation from GS2
(D. Applegate)

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)

Minimizes number of time steps

- Transport and turbulence time scales 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 scheme 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)

Example: ITER simulation savings

- Relevant n_ϕ ~ 100 --> factor of ~100 savings in simulation volume
- T_C/T_E ~ 7 --> factor of ~3 savings in $k_\perp$ resolution
- ρ_* ~ 10^{-5} --> factor of ~10^6 savings in number of time steps
- Overall factor of ~10^8 savings over standard global simulation!
- Translates to hours of gigaflop computations instead of weeks of petaflop computations

Transport model

$$\frac{\partial n_s}{\partial t} = -\frac{\partial \psi}{\partial V}\frac{\partial}{\partial \psi}\left[\frac{\partial V}{\partial \psi}\langle \mathbf{\Gamma}_s \cdot \nabla\psi\rangle\right]$$

← particle transport

$$\frac{3}{2}\frac{\partial\left(n_s T_s\right)}{\partial t} = -\frac{\partial \psi}{\partial V}\frac{\partial}{\partial \psi}\left[\frac{\partial V}{\partial \psi}\langle \mathbf{Q}_s \cdot \nabla\psi\rangle\right]$$

← energy transport

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

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

energy injected into turbulence by background inhomogeneity

turbulent collisional heating

collisional temperature equilibration

Comments on multiscale scheme

- Turbulent flux calculations are orders of magnitude more expensive than advancing transport equations
- Calculation of turbulent fluxes in each flux tube is completely independent of other flux tubes
- Consequently, coupling of multiple flux tubes is almost perfectly parallelizable
- Critical for computational feasibility:
  - optimized nonlinear flux calculations in GS2
  - minimized number of sets of nonlinear flux calculations required for background profiles to reach steady-state

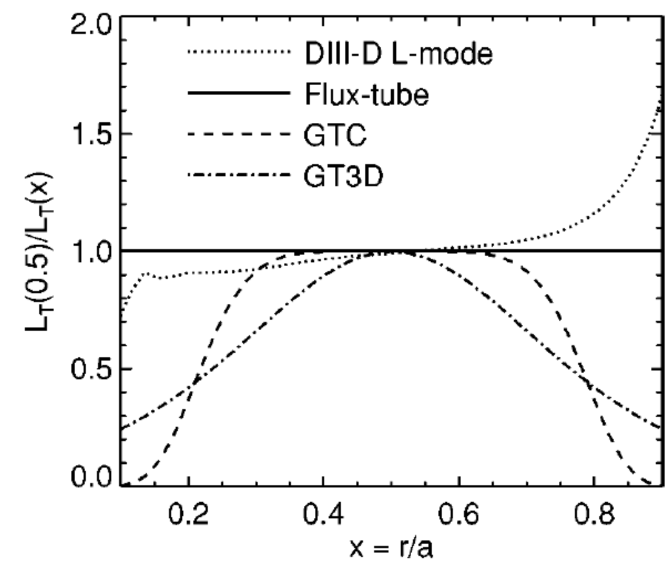
Transport solver algorithm

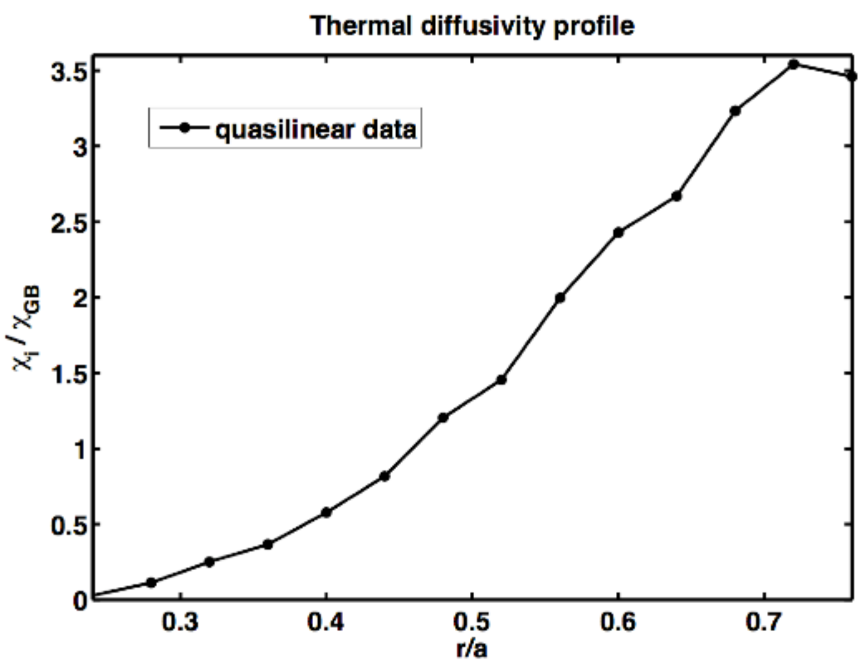
- Currently using 4th-order compact differencing in space with optional artificial dissipation for smoothing
- Time advanced at present with explicit predictor-corrector for fluxes and implicit Crank-Nicholson for all other terms
- Full nonlinearly implicit scheme (Newton solver) being implemented
  - based on algorithm developed by Jardin et. al*
  - algorithm implemented in existing production tokamak transport codes and shown to improve stability of standard Crank-Nicholson scheme

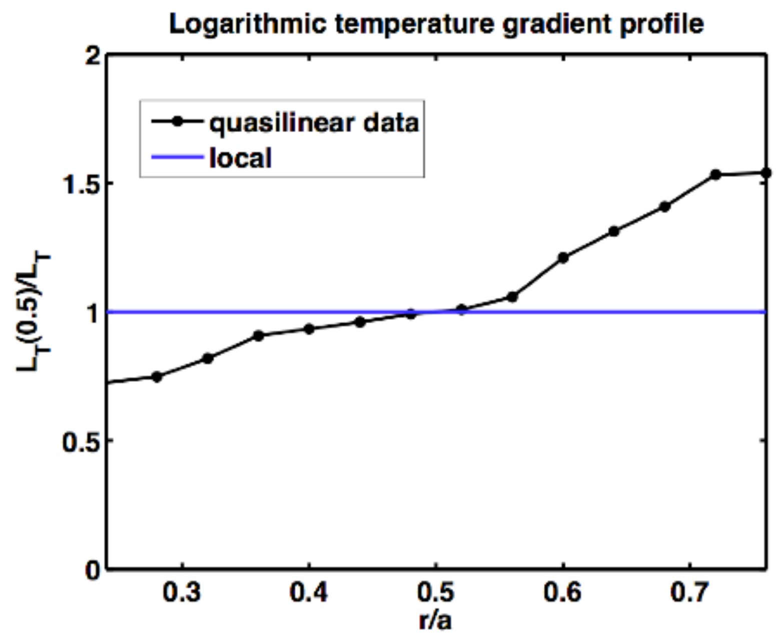
*S.C. Jardin, G. Bateman, G.W. Hammett, and L.P. Ku, On 1D diffusion problems with a gradient-dependent diffusion coefficient, J. Comp. Phys.

Preliminary results

- Collisionless, adiabatic electrons, single transport channel, quasilinear estimate for heat flux, Cyclone geometry
- Qualitatively correct behavior for and fluxes and profiles:





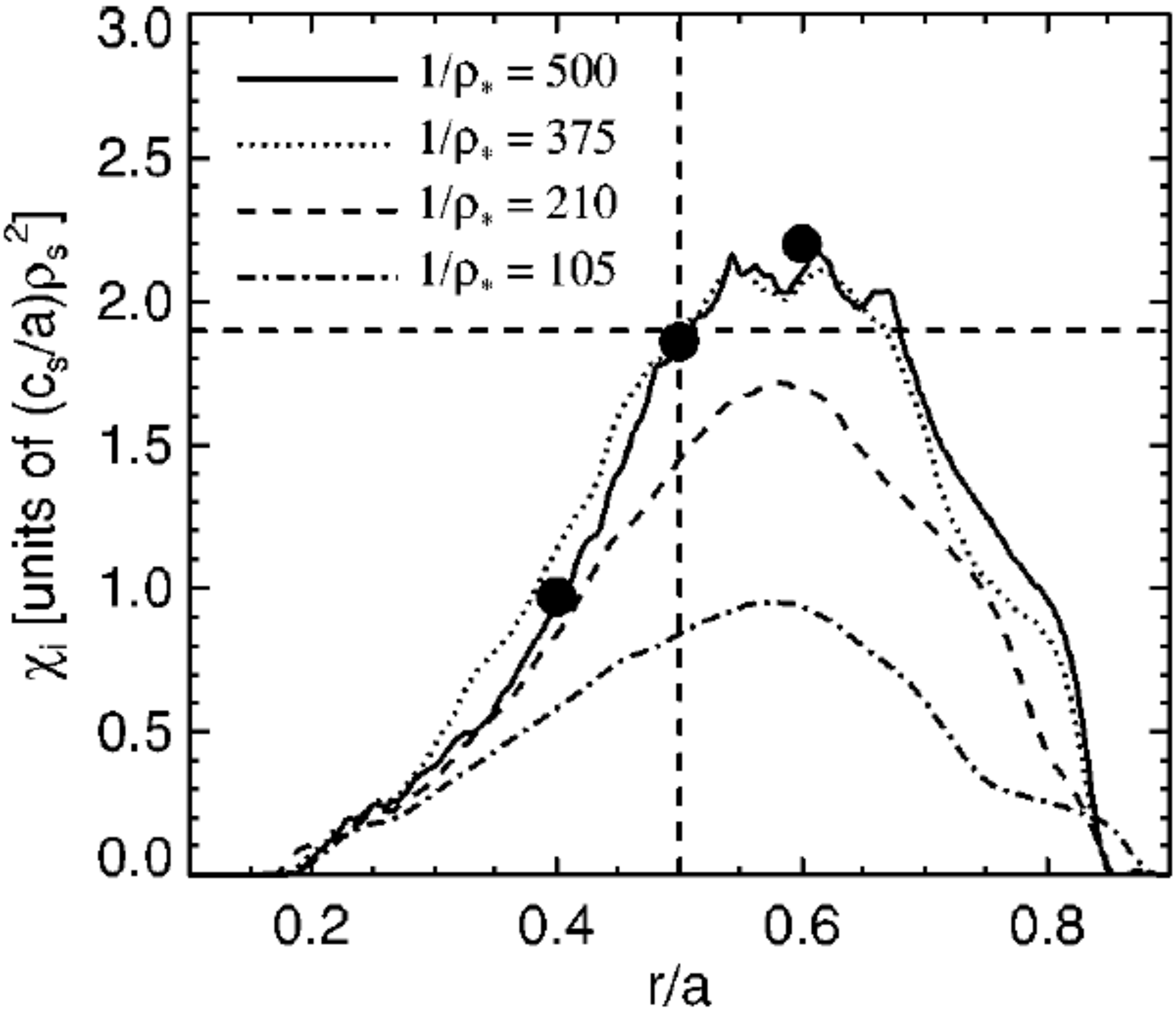


Top figure: J. Candy, R.E. Waltz and W. Dorland, The local limit of global gyrokinetic simulations, Phys. Plasmas **11** (2004) L25.

Future work

- Finish implementation of Newton solver
- Implement more sophisticated quasilinear model as pre-conditioner for nonlinear simulations
- Include neoclassical transport and evolving background magnetic field (via Grad-Shafronov)
- Include sheared radial electric field profile
- Include equations for parallel and toroidal angular momentum transport
- Apply algorithm to nonlinear simulations of multiple species, electromagnetic turbulent transport

Validity of local approximation*



- lines represent global simulations from GYRO
- dots represent local simulations from GS2
- good 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.

Transport model (2)

- Definitions:

$$\langle \mathcal{F} \rangle \equiv \text{flux surface average of } \mathcal{F}$$

$$V \equiv \text{infinitesimal volume between flux surfaces}$$

$$\mathbf{\Gamma}_s = \int d^3v \; \mathbf{v}_\chi h_s, \; \mathbf{Q}_s = \int d^3v \frac{m_s v^2}{2} \mathbf{v}_\chi h_s$$

$$\mathbf{v}_\chi = \frac{c}{B_0^2}\left(\hat{\mathbf{b}} \times \nabla\chi\right), \; \chi = \Phi - \frac{\mathbf{v}}{c} \cdot \mathbf{A} \qquad h_s = \delta f_s + \frac{q_s \Phi}{T_s}$$

- Derivation of equations describing momentum transport is work in progress
- However, recent studies suggest that inclusion of momentum transport is negligible effect

Efficiency of GS2 flux calculations

- Simulation length at new transport time step decreased by initializing with parameters from end of previous transport time step (bypasses linear phase of flux evolution)