General Parallel Closures for Plasma Fluid Simulations [1]

E.D. Held

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Abstract

The rapid thermal motion of electrons along magnetic field lines represents a dominant process in astrophysical and terrestrial plasmas. The purpose of this talk is to describe the incorporation of this dominant physics in plasma fluid models.

In the first part of this talk, we discuss a closure scheme that incorporates the kinetic effects of free-streaming, time-dependence, pitch-angle scattering and trapped electrons in the parallel components of the heat flow and viscous stress tensor [**?**]. In the nearly collisionless limit, these closures map onto previous collisionless expressions for the parallel heat flow and viscous stress [**?**]. It is emphasized that the physics of both the fluid and adiabatic limits is incorporated in a unified formalism involving integrals along characteristics of the perturbed, non-Maxwellian part of the distribution function.

In the second part of this talk, we discuss the implementation of the closure scheme in the plasma fluid code NIMROD [**?**]. Over the course of a one-second simulation of a toroidal fusion experiment, electrons traveling at 1/7 the speed of light travel millions of meters along the magnetic field. Capturing the essential physics of this motion entails integrating kilometers along magnetic field lines at a sufficient number of locations in the computational domain to resolve the parallel closure dynamics. Modest estimates of the number of integrations needed at each time step exceed 10,000. Results show that a massively parallel computational approach that has hundreds of processors independently calculating the integral closure relations can be completed in a time comparable to that needed for the advance of the fluid equations. A further numerical complication involves the stiffness that results when the parallel closures are inserted into the fluid equations. In particular, a semi-implicit time advance for the electron temperature equation is discussed. The semi-implicit operator incorporates the anisotropic heat diffusion operator in the left side of the time-discretized equation to provide numerical stability.

In the final part of this talk, the application of the closure scheme to studies of transport in the vicinity of helical magnetic islands in tori of arbitrary aspect ratio and shaping is discussed. Calculations show the importance of trapped particle effects which reduce parallel heat transport by an order of magnitude in moderate-aspect-ratio ($A \sim 3$) tori. This reduction in parallel heat flow can significantly alter electron temperature flattening across magnetic islands and hence the development of neoclassical tearing modes, especially in low-aspect-ratio devices. The application of the closure scheme to studies of heat transport along chaotic magnetic fields in reversed field pinches (RFPs) is also discussed. Results show that the reduction due to particle trapping is essential to accurate estimates of electron heat confinement times in RFPs.

Outline

- **Motivation: Numerically simulate magnetized plasmas confined by slowly evolving magnetic fields.**

- **Derive closed system of equations with general treatment of parallel dynamics.**

  Parallel closures in homogeneous magnetic geometry.

  Parallel closures in inhomogeneous magnetic geometry.

- **Heat flow calculation for steady state magnetic field**

  in vicinity of helical magnetic island

  along chaotic magnetic field

- **Implementation of electron temperature equation in NIMROD.**

  implementation of field line integrations for closure calculation

  implementation of semi-implicit operator to numerically stabilize advance of temperature equation

- **Conclusion**

Two-fluid plasma codes evolve particle, momentum and energy conservation equations

- **Evolution equations for density, n, flow, $\vec{V}$, and temperature, T are:**

$$\begin{aligned}
\frac{\partial n}{\partial t} + \vec{\nabla} \cdot n\vec{V} &= 0, \\
mn\left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \vec{\nabla}\vec{V}\right) &= qn\left(\vec{E} + \vec{V} \times \vec{B}\right) - \vec{\nabla}P - \vec{R} - \underline{\vec{\nabla} \cdot \Pi}, \\
\frac{3}{2}n\left(\frac{\partial T}{\partial t} + \vec{V} \cdot \vec{\nabla}T\right) &= -P\vec{\nabla} \cdot \vec{V} + Q - \underline{\Pi : \vec{\nabla}\vec{V} - \vec{\nabla} \cdot \vec{q}},
\end{aligned}$$

where expressions for ion and electrons viscous stress tensors, Π, and the conductive heat flows, $\vec{q}$ are required to close the system.

- **For nearly collisionless, magnetized plasmas, form of needed closures are [2]:**

$$\Pi_{\|} \equiv m \int d^3v \left(v_{\|}^2 - \frac{v_{\perp}^2}{2}\right) f,$$

$$q_{\|} \equiv T \int d^3v \left(\frac{v^2}{v_{th}^2} - \frac{5}{2}\right) v_{\|} f,$$

where $v_{\perp}$ and $v_{\|}$ are perpendicular and parallel particle speeds.

[2] Z. Chang and J. D. Callen, Phys Fluids B **4 , 1167 (1992).**

Previous expressions for parallel heat flux valid in collisional and collisionless limits.

- **Collisional flux,** [3]

$$q_{\|} = -3.16\left(\frac{n_e T_e \tau_e}{m_e}\right)\vec{\nabla}_{\|} T_e.$$

- **Collisionless heat flux,** [4,5]

$$q_{\|}(L') = \frac{n_e v_{th}}{\pi^{3/2}} \int_0^\infty dL \frac{T(L'-L) - T(L'+L)}{L/2}.$$

- **Solve electron drift kinetic equation allowing for $\frac{\partial}{\partial t} \sim \nu \sim k_{\|} v_{th}$.**

  1. **mode frequency, $\omega \sim \tau_r^{-1} \sim 10^{-3} - 10^{1}$,**
  2. **collision frequency, $\nu_e \sim 10^{-5}$,**
  3. **transit frequency, $k_{\|} v_{the} \sim 10^{-5}$ in island, for example, and $k_{\|} v_{the} \sim 0$ at X-point**

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[3] S.I. Braginskii, *"Transport processes in a plasma,"* **1**, edited by M.A. Leontovich, Consultants Bureau, New York, 1965

[4] B.W. Hammett and F.W. Perkins, Phys. Rev. Lett. **64**, 3019 (1990).

[5] R.D. Hazeltine, Phys. Plasmas **5**, 3282 (1998).

Collisional or collisionless parallel transport?

- **Nature of parallel transport in vicinity of magnetic island varies.**

  Collisional near X-points: $k_{\parallel} v_{th}/\nu \to 0$.

  Moderately collisional inside island: $k_{\parallel} v_{th}/\nu \geq 1$

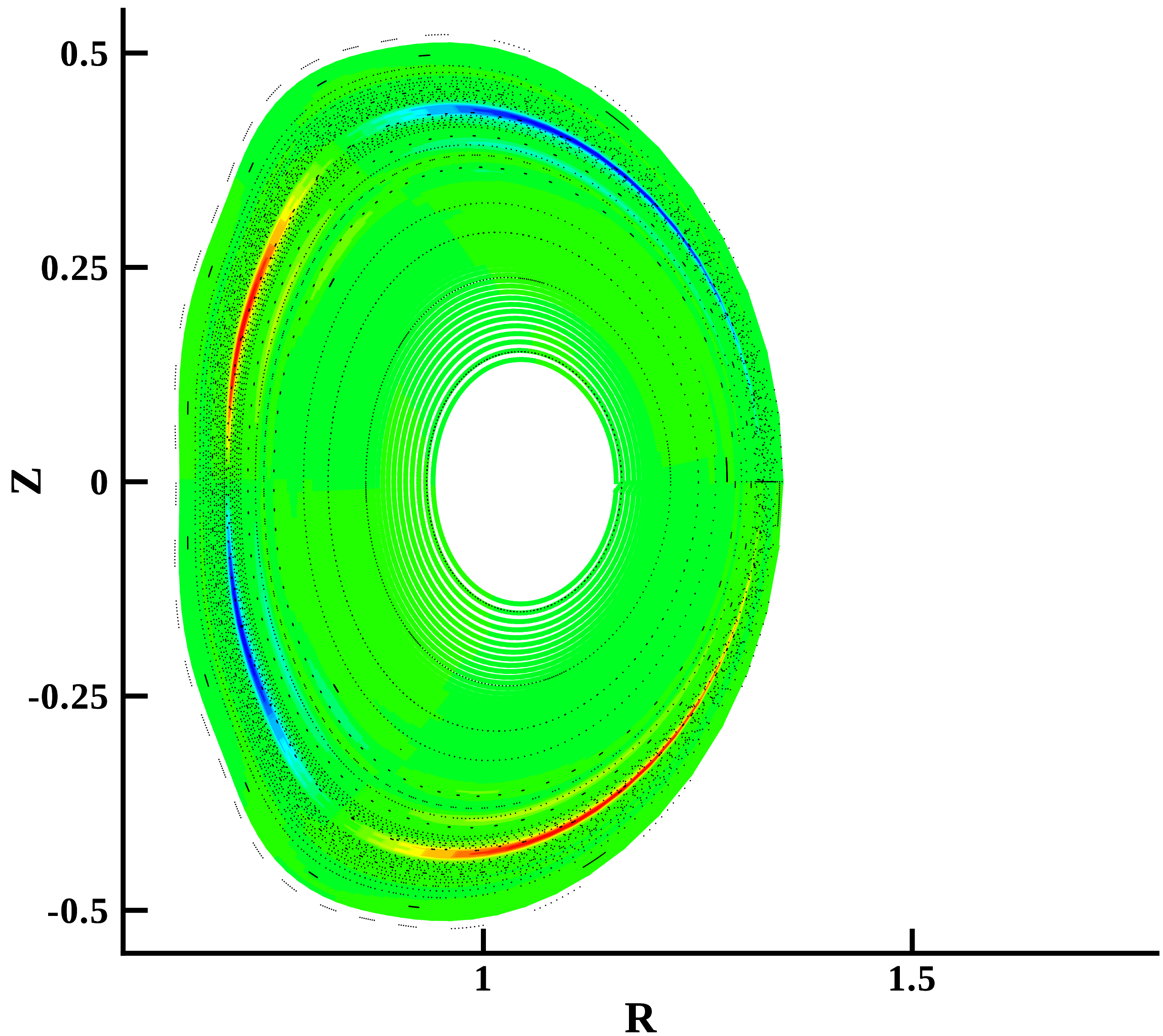


Figure 1: Perturbed heat flow contours due to a **2/1** magnetic island.

- **Closures should allow for arbitrary collisionality.**

General $\Rightarrow$ Intractable?

- **Model requirements for closures.**
  1. **Relevant electron and ion kinetic equations**

     Drift kinetic equations (DKE)
  2. **Good collision operator**

     Lorentz pitch-angle scattering operator
  3. **Free-streaming and time-dependent physics**

     Integration involving characteristics.
  4. **General geometry**

     Arbitrary, axisymmetric toroidal geometry

- **Closures must also be numerically tractable.**
  1. **Time spent calculating closures $\sim$ time for nonlinear step.**
  2. **Closures must be robust, i.e., numerically stable.**

Take Chapman-Enskog-like (CEL) approach.

- **Write f as the sum of Maxwellian, f_M, and kinetic distortion, F:**

$$f = f_M + F = n(\vec{x},t)\left[\frac{m}{2\pi T(\vec{x},t)}\right]^{\frac{3}{2}} exp\left[-\frac{m(\vec{v}-\vec{V})^2}{2T(\vec{x},t)}\right] + F,$$

and insert in

$$\frac{df}{dt} = C(f).$$

- **Use 3 lowest moment equations to write full CEL kinetic equation:**

$$\frac{\partial F}{\partial t} + \vec{v}\cdot\vec{\nabla}F + \frac{e}{m}\left(\vec{E}+\vec{v}\times\vec{B}\right)\cdot\vec{\nabla}_{\vec{v}'}F - C(f) =$$

$$m\left(\vec{v}'\vec{v}' - \frac{v'^2}{3}\mathrm{I}\right) : \vec{\nabla}\vec{V}\frac{f_M}{T} + \vec{v}'\cdot\left(\vec{\nabla}\cdot\Pi - \vec{R}\right)\frac{f_M}{p} -$$

$$\frac{2}{3}L_1^{(\frac{1}{2})}\left(\Pi : \vec{\nabla}\vec{V} + \vec{\nabla}\cdot\vec{q} - Q\right)\frac{f_M}{p} + L_1^{(\frac{3}{2})}\vec{v}'\cdot\vec{\nabla}T\frac{f_M}{T}.$$

- **Why 5-moment CEL approach?**

  1. **Keeps fluid and kinetic physics separate.**
  2. **$\vec{V}$ and T (or p) readily available in most plasma fluid codes.**
  3. **Density does not appear directly as drive.**
  4. **Fewer fluid equations.**

WARNING: 5-moment approach is less messy but requires better solution of kinetic equation.

Gyroaverage full CEL kinetic equation, ignore drifting and solve for parallel dynamics.

- Gyroaveraging and projecting out dominant parallel part yields

$$\left(\frac{\partial}{\partial t} + \vec{v}_{\parallel} \cdot \vec{\nabla}\right) \bar{F} - \left\langle C(\bar{F} + f_M)\right\rangle =$$

$$-mv^2 P_2(v_{\parallel}/v) \left(\hat{b}\hat{b} - \frac{\mathrm{I}}{3}\right) : \vec{\nabla}_{\parallel} \vec{V}_1 \frac{f_M}{T} + \vec{v}_{\parallel} \cdot \left(\vec{\nabla} \cdot \Pi_{\parallel 1} - \vec{R}\right) \frac{f_M}{p} -$$

$$\frac{2}{3} L_1^{(\frac{1}{2})} \left(\nabla_{\parallel} q_{\parallel} - Q\right) \frac{f_M}{p} + L_1^{(\frac{3}{2})} \vec{v}_{\parallel} \cdot \vec{\nabla} T \frac{f_M}{T}.$$

  where $\vec{v}_{\parallel} \cdot \vec{\nabla}$ will be written $\hat{\mathrm{b}} v_{\parallel} \partial / \partial L$.

- Employ Lorentz scattering operator

$$\left\langle C(\bar{F} + f_M)\right\rangle = L(F) = \frac{\nu_L}{2} \frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial F}{\partial \xi}$$

  where $\xi = v_{\parallel}/v$, and expand in Legendre polynomials

$$\bar{F}_L = \sum_{n=0}^{N} F_n(v, L, t) P_n(\xi) f_{M0}.$$

- Integrate along characteristics, $\tau = L \pm vt$, to invert the advective operator.

Heat flow calculation involves integration along field lines.

- Parallel heat flow definition was

  $$q_\parallel \equiv T \int d^3v \left(\frac{v^2}{v_{th}^2} - \frac{5}{2}\right) v_\parallel F.$$

$$\begin{pmatrix} dt & v\epsilon_{0,1}dL & 0 & 0 & \dots & & & \\ v\epsilon_{1,0}dL & dt+\lambda_1\nu & v\epsilon_{1,2}dL & 0 & & & & \\ 0 & v\epsilon_{2,1}dL & dt+\lambda_2\nu & v\epsilon_{2,3}dL & 0 & \dots & & \\ \vdots & & \vdots & & & & & \\ \dots & & & & 0 & v\epsilon_{N,N-1}dL & dt+\lambda_N\nu \end{pmatrix} \begin{pmatrix} F_0 \\ F_1 \\ F_2 \\ \vdots \\ F_N \end{pmatrix} =$$

$$\begin{pmatrix} g_0 dL(q_\parallel) \\ g_1 dL(T) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- Ignoring $\partial q_\parallel/\partial L$ in inhomogeneous term and taking time-asymptotic limit yields

  $$q_\parallel(L') = \int_0^\infty dL\,[T(L'-L) - T(L'+L)]\,\frac{\partial K}{\partial(\ln L)}$$

  $$K(s) = \frac{4n_0 v_{th}}{3\sqrt{\pi}} s^3 \left(s^2 - \frac{5}{2}\right)^2 \sum_{i=0}^{N} a_i \exp\left(-s^2 - \bar{k}_i L\right).$$

- Recall that collisionless and collisional forms were

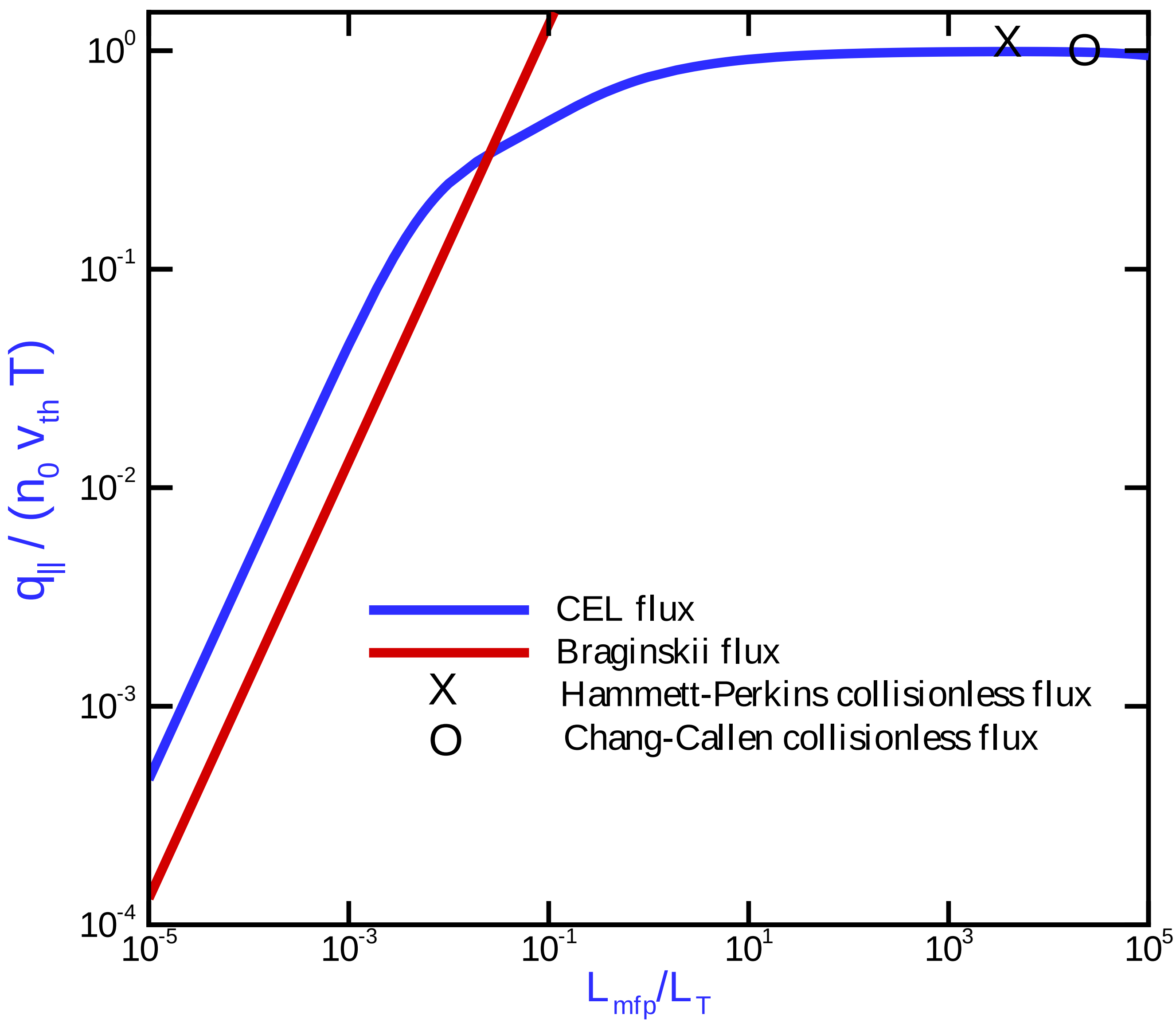
  $$q_\parallel(L') = \frac{n_e v_{th}}{\pi^{3/2}} \int_0^\infty dL'(T(L'-L) - T(L'+L))K$$

  where $K(s) = 2/L$, and

  $$q_\parallel = -3.16\left(\frac{n_e T_e \tau_e}{m_e}\right)\vec{\nabla}_\parallel T_e.$$

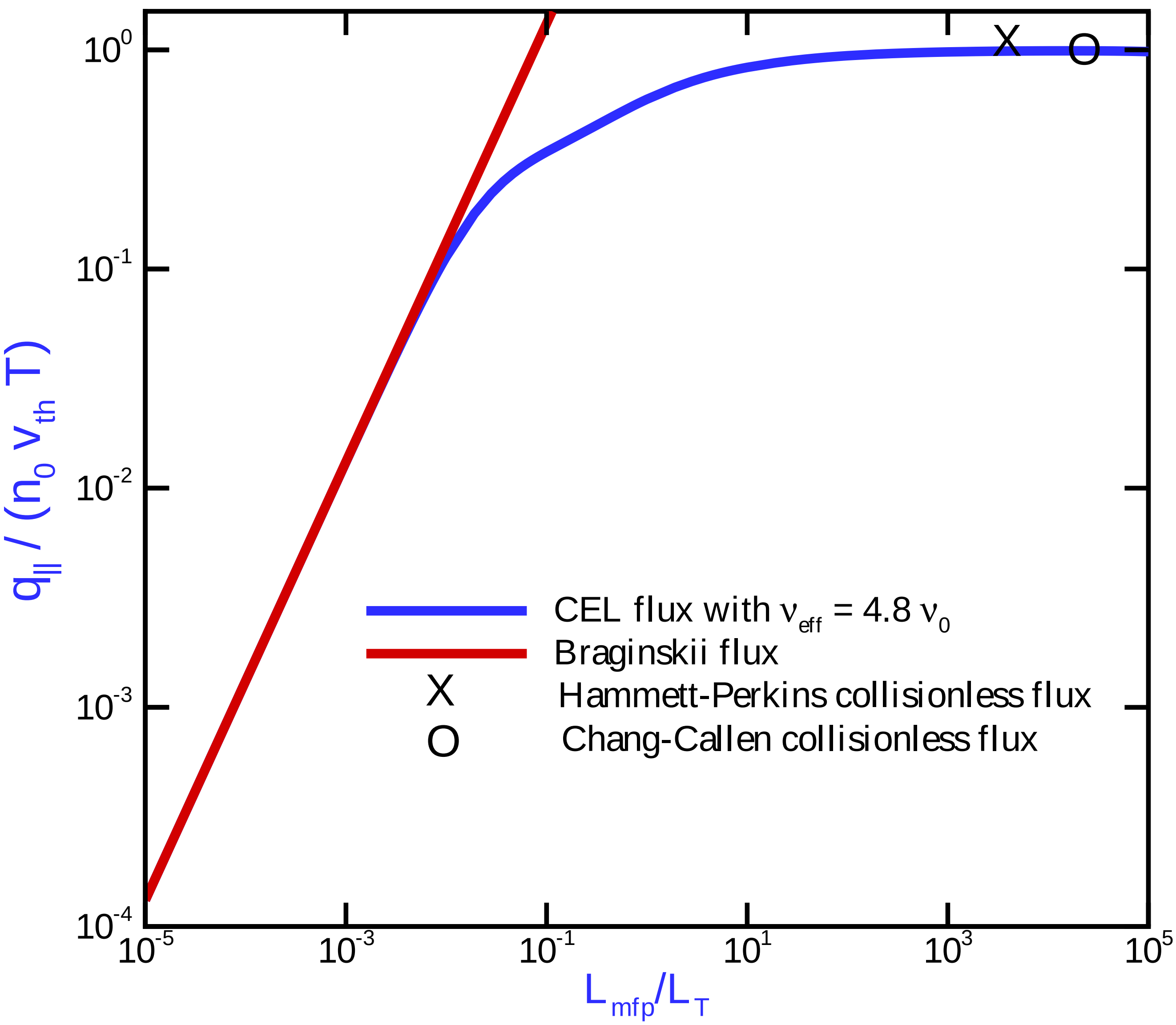
Heat flux closure is approximate for arbitrary collisionality.

- **Heat flux for homogeneous magnetic field and sinusoidal temperature perturbations.**



Modified heat flux closure is "exact" for arbitrary collisionality.

- **Ad hoc effective collision frequency, $\nu_{eff} = 4.8\nu_0$, brings heat flux into agreement with collisional version.**

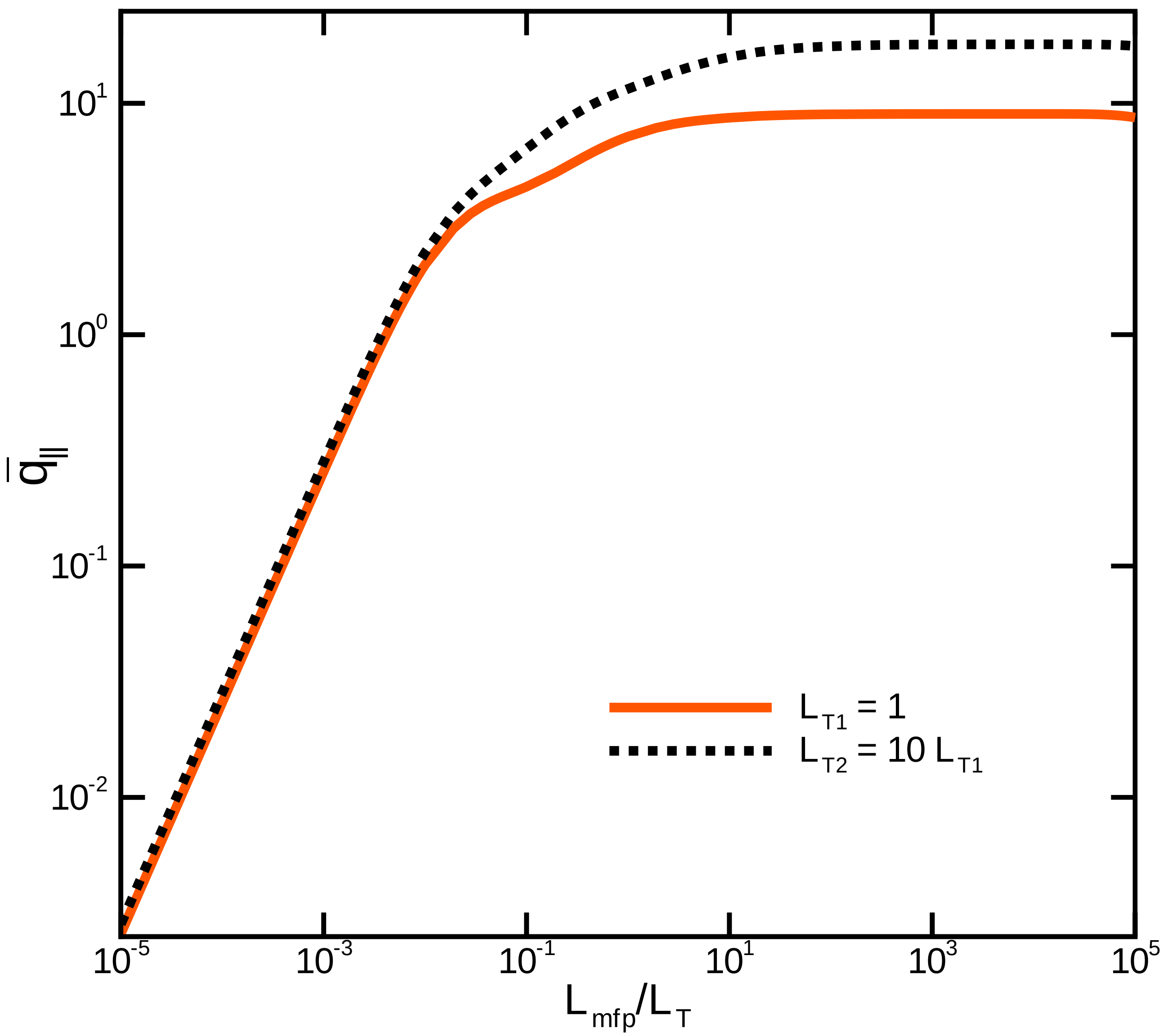


Multiple scalelengths add in nearly collisionless regime.

- **Doubling of heat flux in nearly collisionless regime due to additional sinusoidal perturbation**

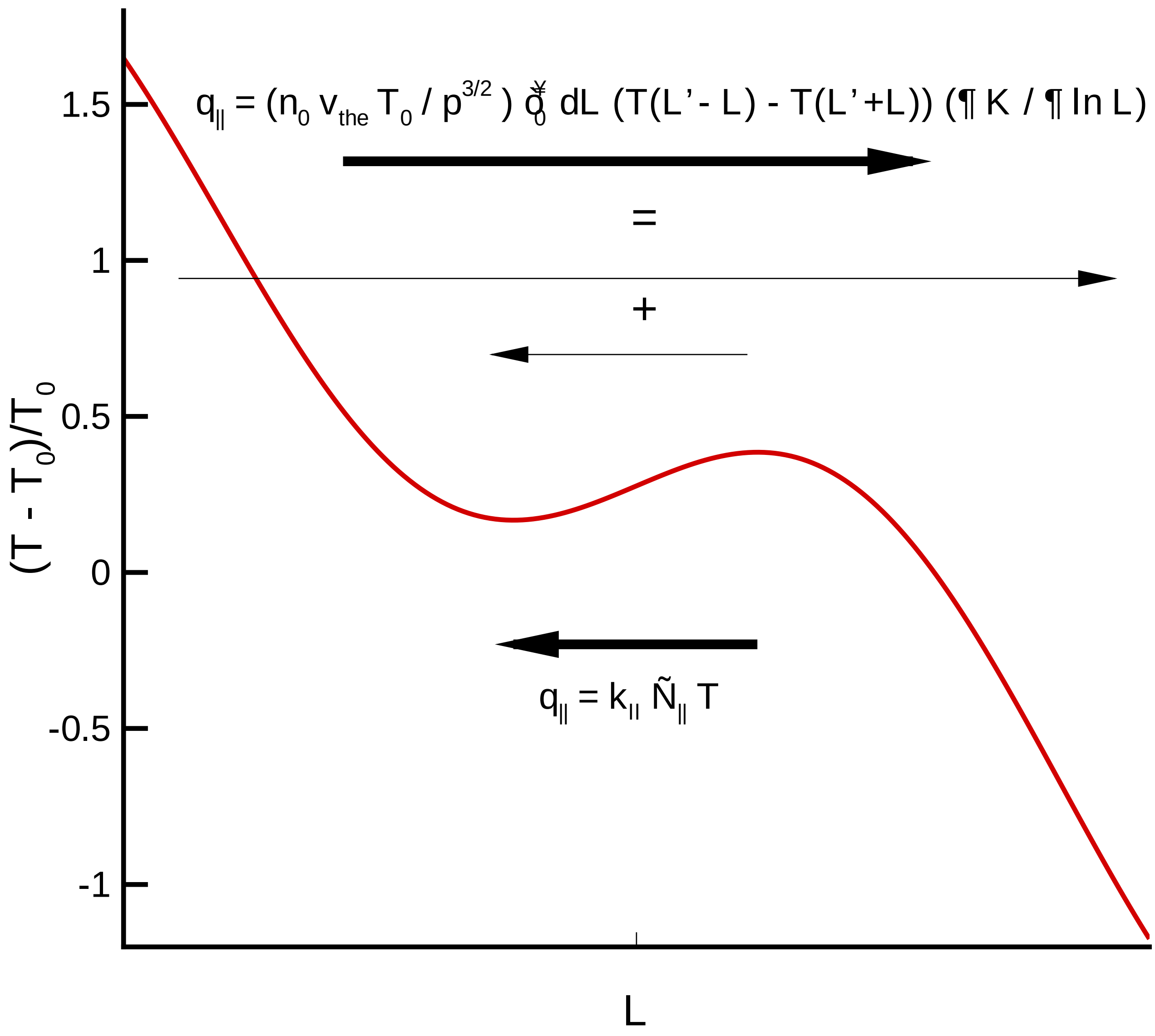
  $\tilde{T} = \sin(2\pi L/L_{T1} + \pi) + \underline{\sin(2\pi L/L_{T2} + \pi)}$,

  where $L_{T2} = 10 L_{T1}$.



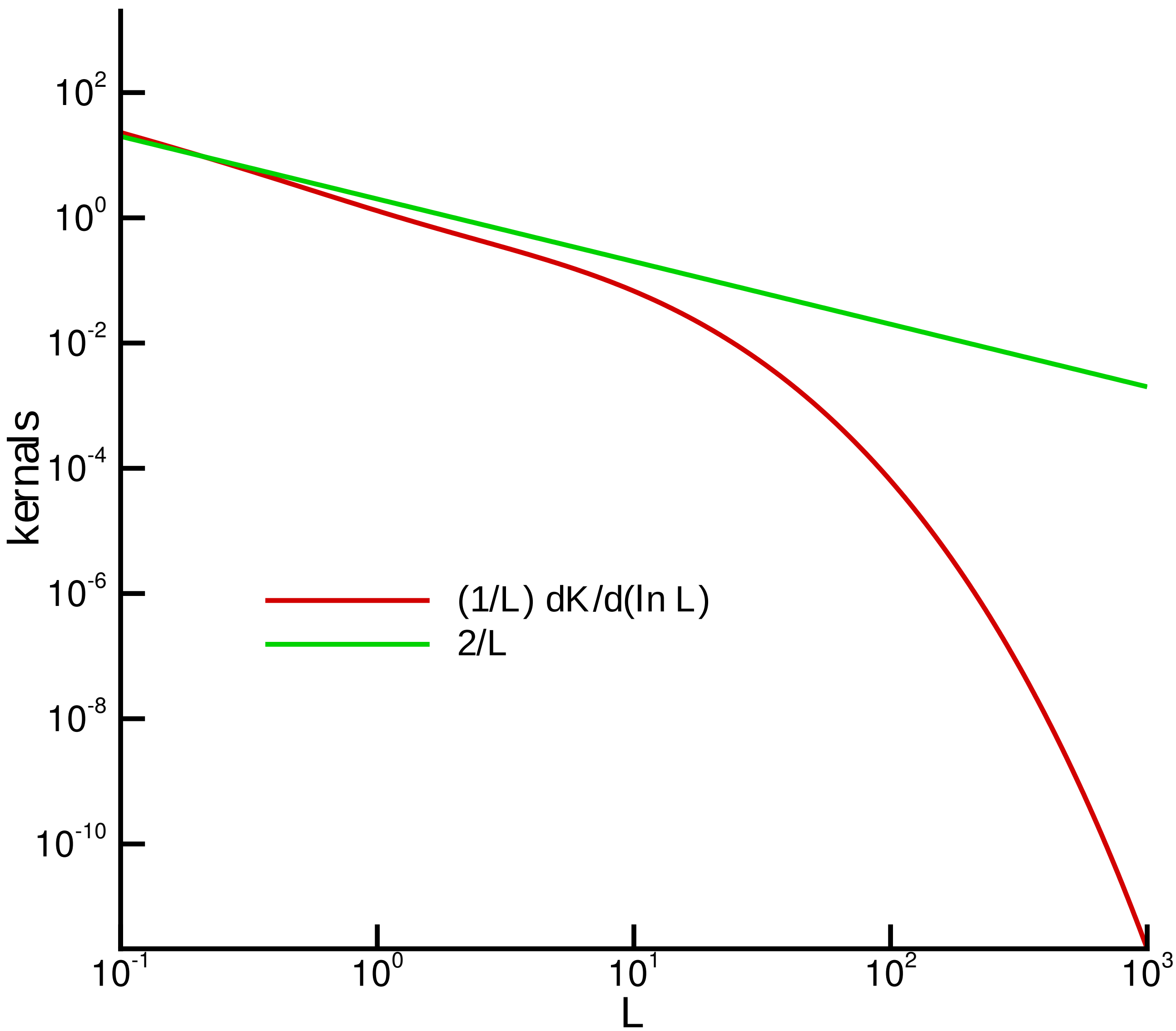
Important to account for long wavelength features of temperature along field lines.

- **General heat flux closure predicts heat can flow up local gradients by accounting for perturbations over longer scale lengths.**



Nearly collisionless closure truncates more rapidly than collisionless closure.

- **Kernal of nearly collisionless closure falls off more rapidly than kernal of colliisonless closure. Here it was assumed that $L_{mfp} = 1$.**

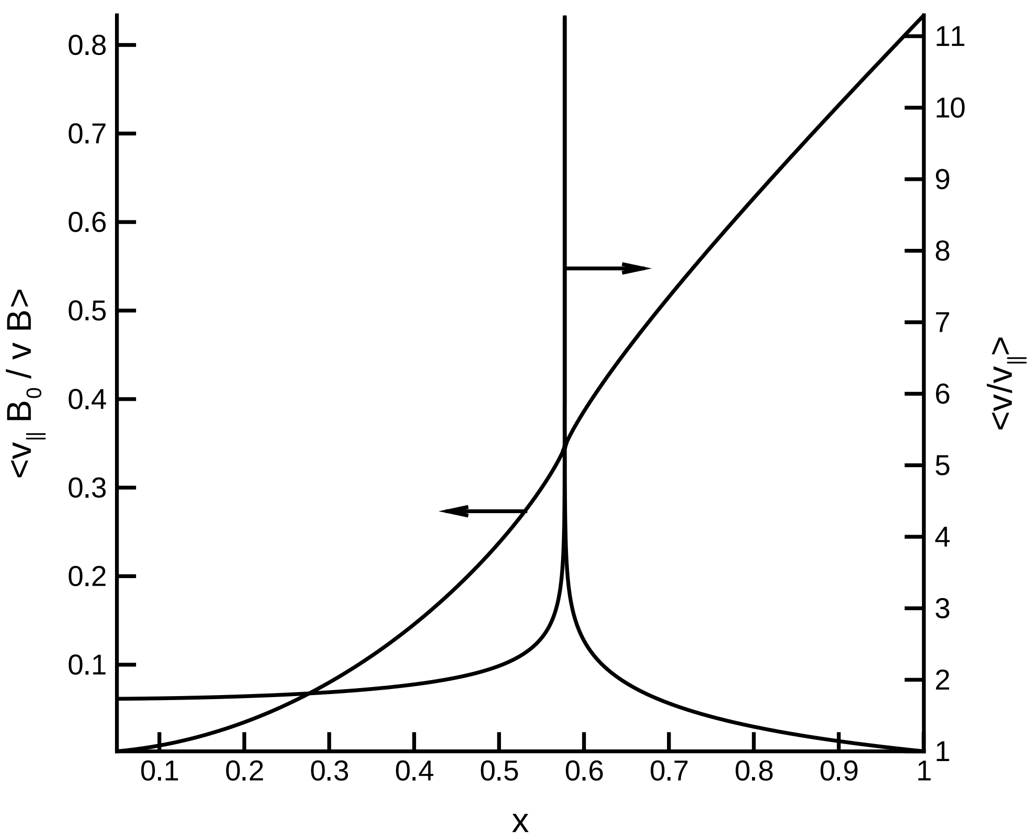


Bounce-averaged Lorentz collision operator treated with expansion in pitch-angle eigenfunctions.

- **Introduce pitch-angle variable, $\xi = \pm\sqrt{1-\lambda B_0}$, and solve following eigenvalue equation:** [6]

$$\frac{1}{\xi}\langle\frac{v}{v_\parallel}\rangle^{-1}\frac{\partial}{\partial\xi}\frac{1-\xi^2}{\xi}\langle\frac{v_\parallel B_0}{vB}\rangle\frac{\partial C_n}{\partial\xi} + \gamma_n C_n = 0,$$

Here the C_n replace the Legendre polynomials, P_n, in expansion in pitch-angle basis functions.



[6] J. G. Cordey, Nuclear Fusion **16**, 499 (1976).

Parallel closures for finite $|\vec{B}|$ have same form as $|\vec{B}| = 0$ case.

- **Define bounce-averaged parallel heat flux as**

$$\left\langle q_{\|} \right\rangle \equiv -T^{eq} \left\langle \int d^3v L_1^{(\frac{3}{2})} v_{\|} F \right\rangle$$

- **Summing over odd pitch-angle basis functions again yields**

$$q_{\|}(L') = \int_0^{\infty} dL \left[T(L' - L) - T(L' + L) \right] \frac{\partial K}{\partial(\ln L)}$$

$$K(s) = \frac{4 n_0 v_{th}}{3\sqrt{\pi}} s^3 \left(s^2 - \frac{5}{2} \right)^2 \sum_{i=0}^{N} a_i \exp\left(-s^2 - \bar{k}_i L \right),$$

Here a_i's and k_i's contain collisional and passing particle information.

- **Could multiply collisionless and collisional forms by passing particle fraction, f_p.**

$$q_{\|}(L') = f_p \frac{n_e v_{th}}{\pi^{3/2}} \int_0^{\infty} \frac{dL' (T(L' - L) - T(L' + L))}{L/2}$$

$$q_{\|} = -3.16 f_p \left(\frac{n_e T_e \tau_e}{m_e} \right) \vec{\nabla}_{\|} T_e.$$

Incorporate $|\vec{B}|$ variations into closures for trapped particle effects

- **Only passing electrons carry heat over longer temperature gradient scale lengths. In addition, trapped electrons act viscously to slow down passing electrons.**

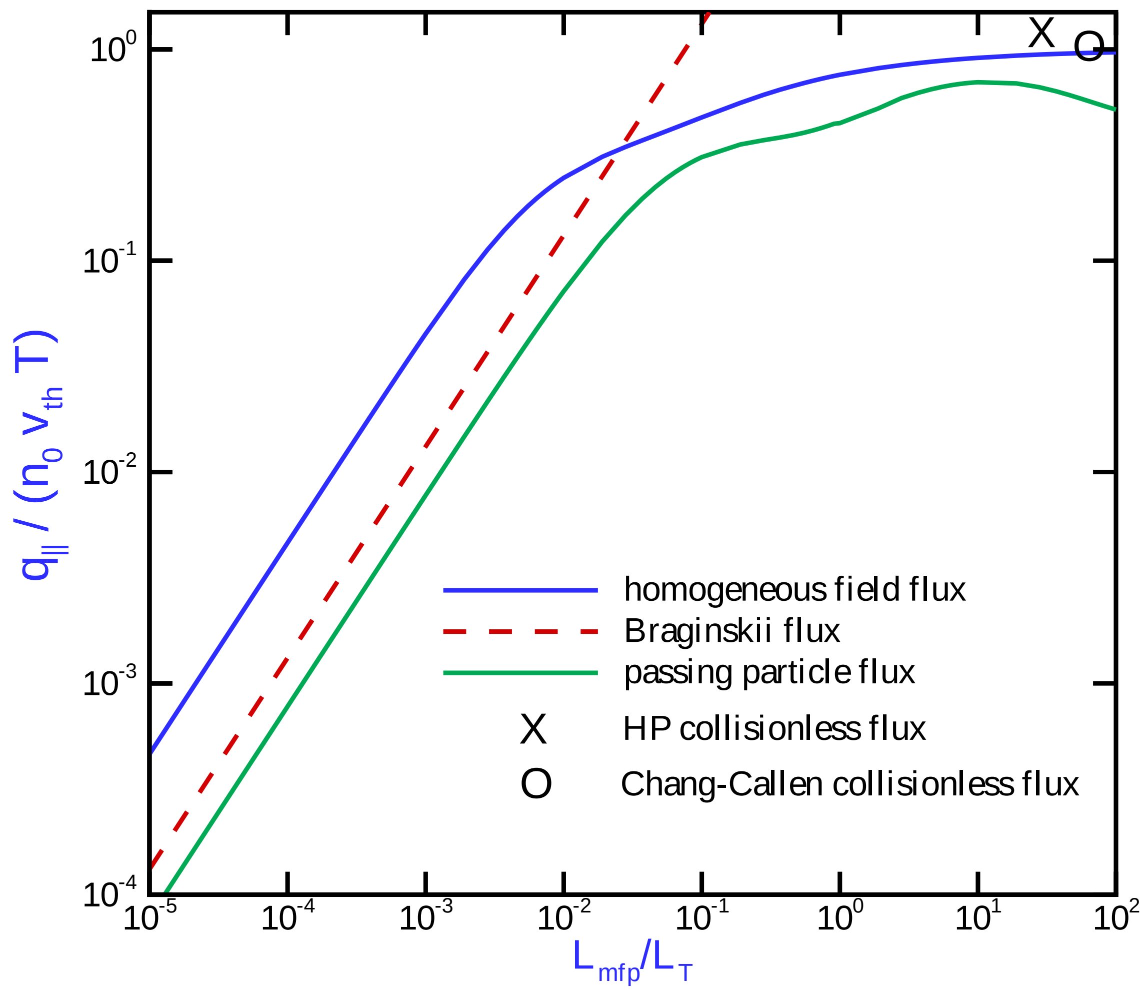
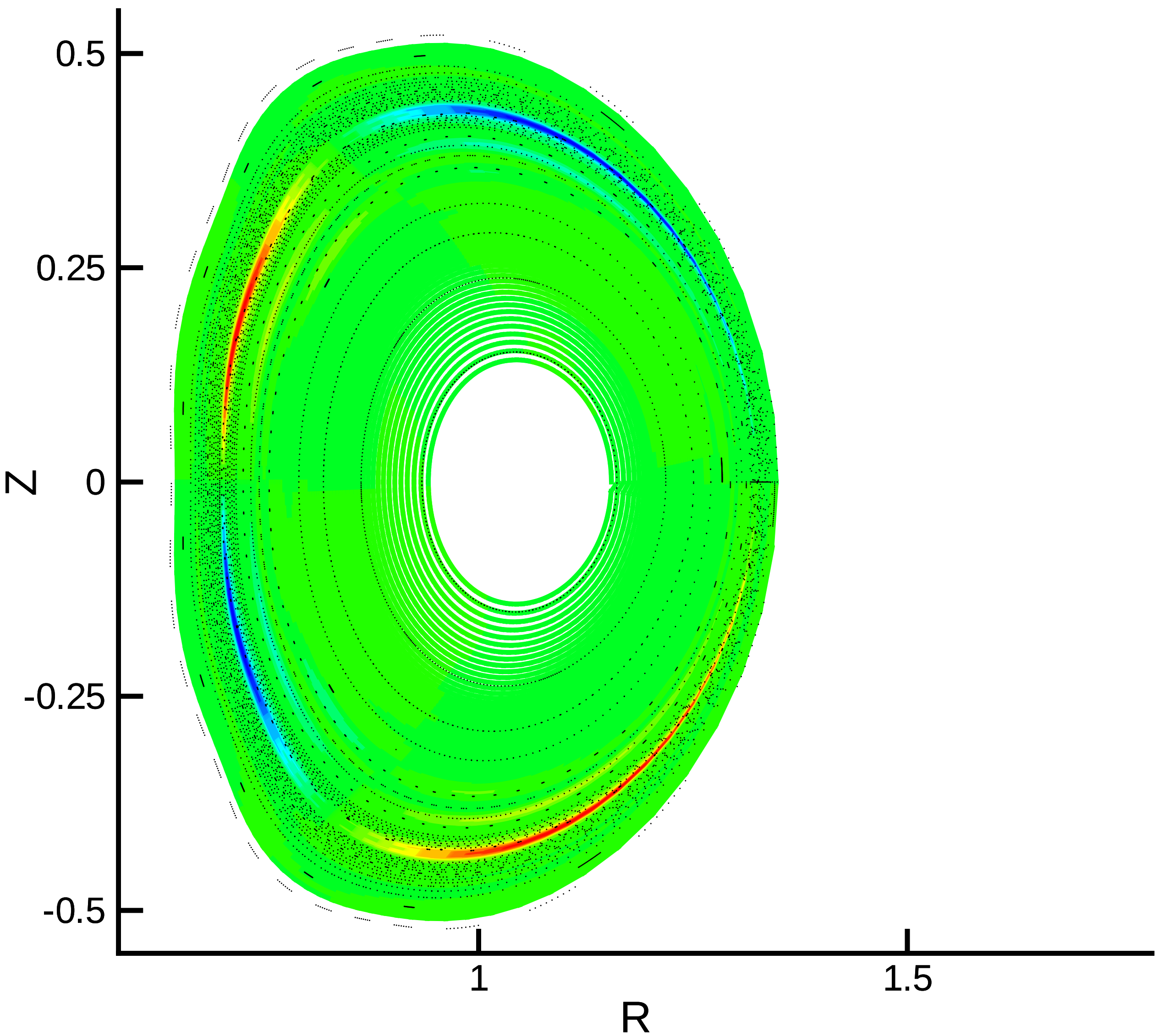


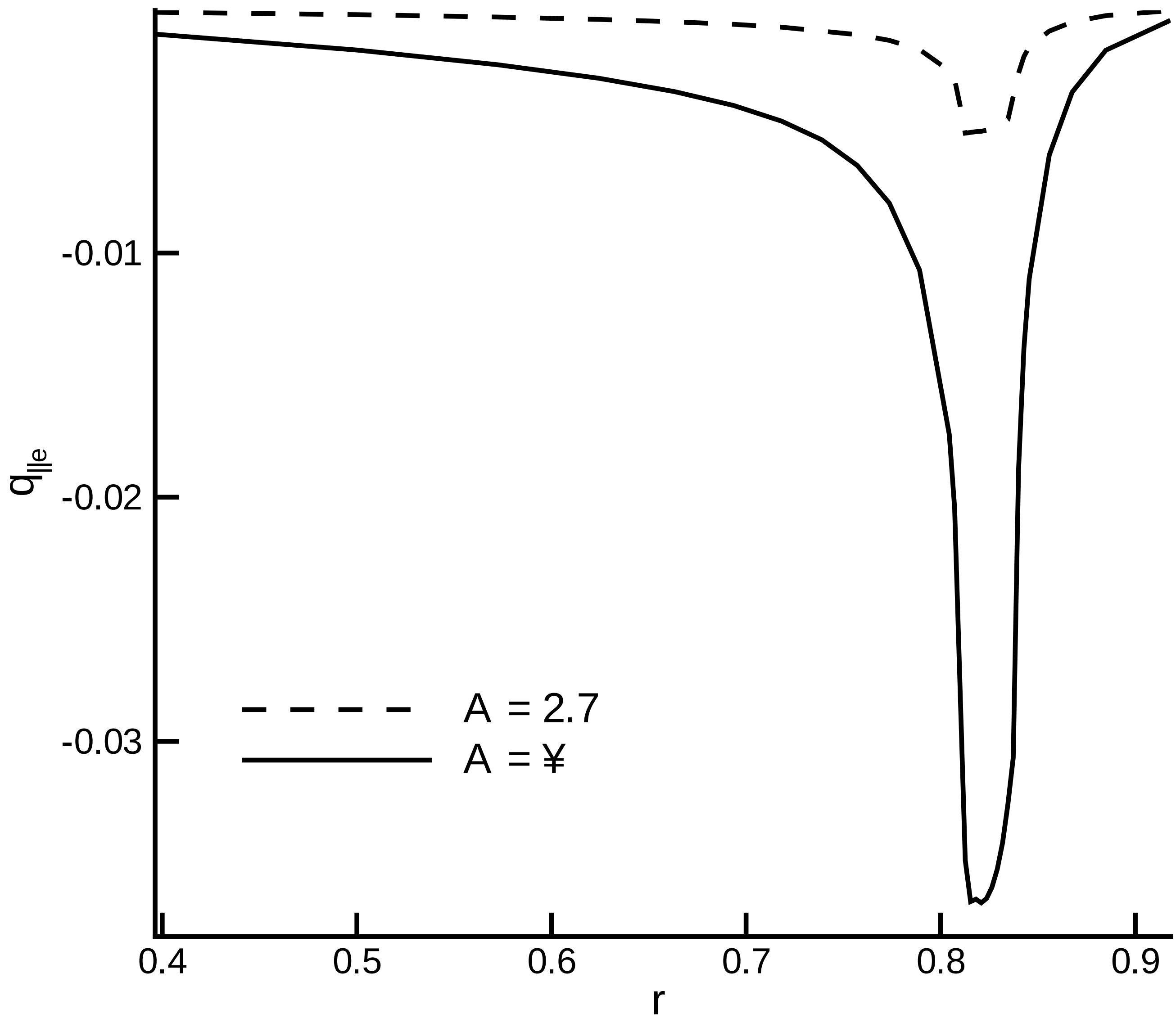
Figure 2: Heat flux for inhomogeneous magnetic field and sinusoidal temperature perturbation.

Perturbed parallel heat flow contours due to a 2/1 magnetic island.



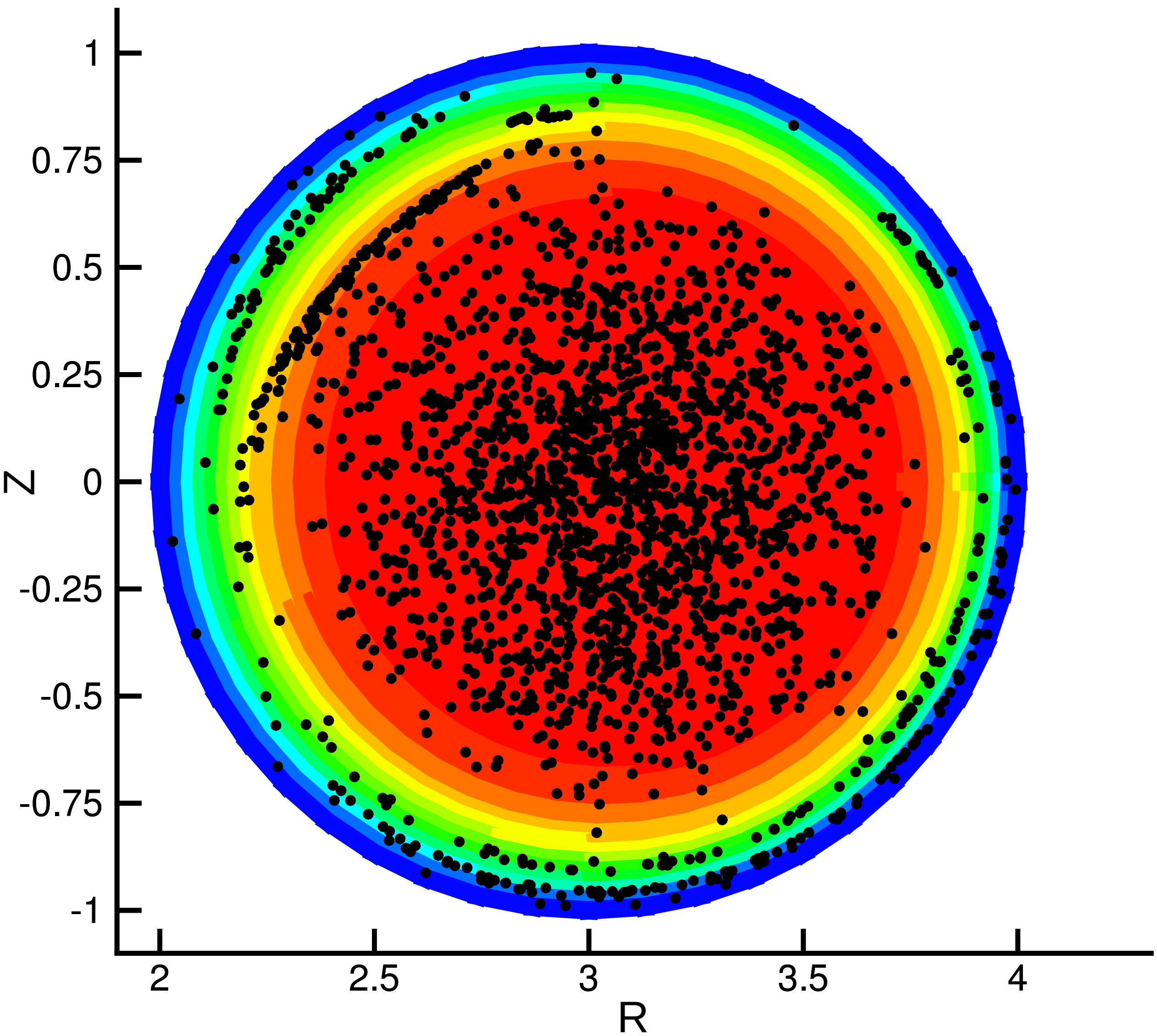
Particle trapping significantly reduces parallel heat transport inside islands in finite-aspect-ratio tori.

- **Heat flux due to helical magnetic island shows order-of-magnitude reduction in heat flux between $A = \infty$ and $A = 2.7$.**

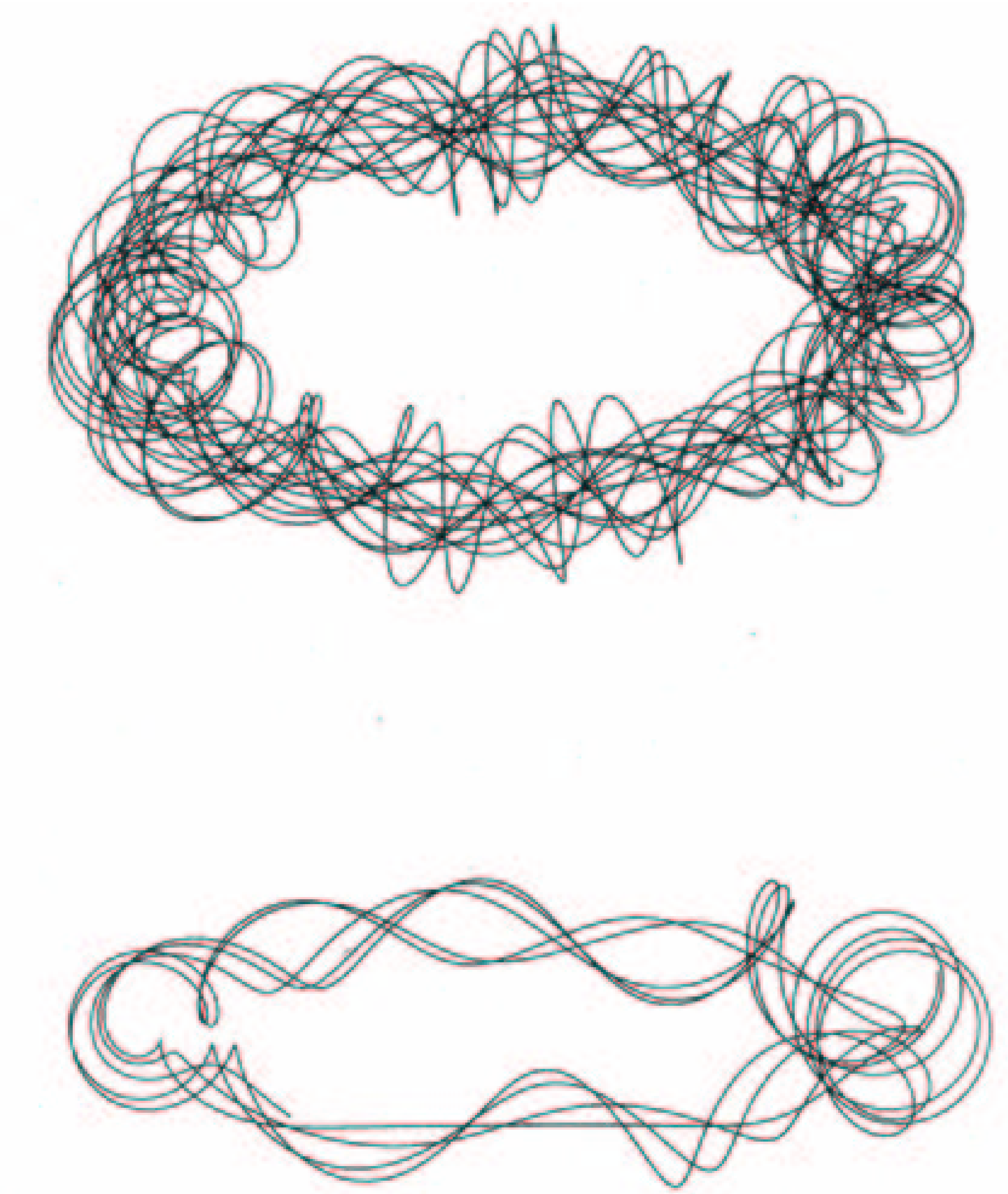


Previously poor electron heat confinement in RFP's interpreted as enhanced effective radial thermal diffusivity, χ_ψ.

- **Magnetic field line chaos responsible for electron temperature flattening inside reversal surface.**

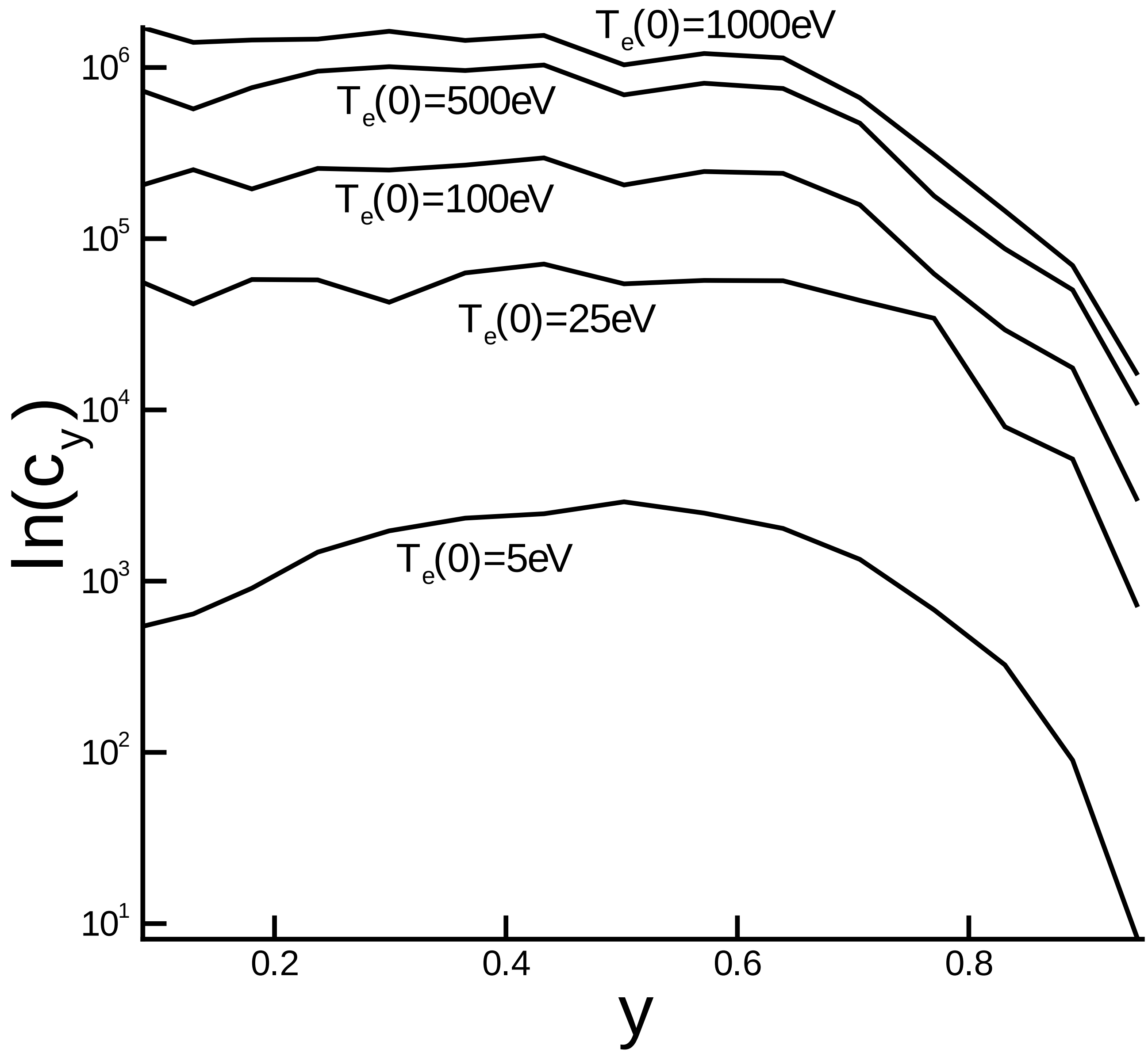


Single magnetic field line ergodically fills volume inside reversal surface.



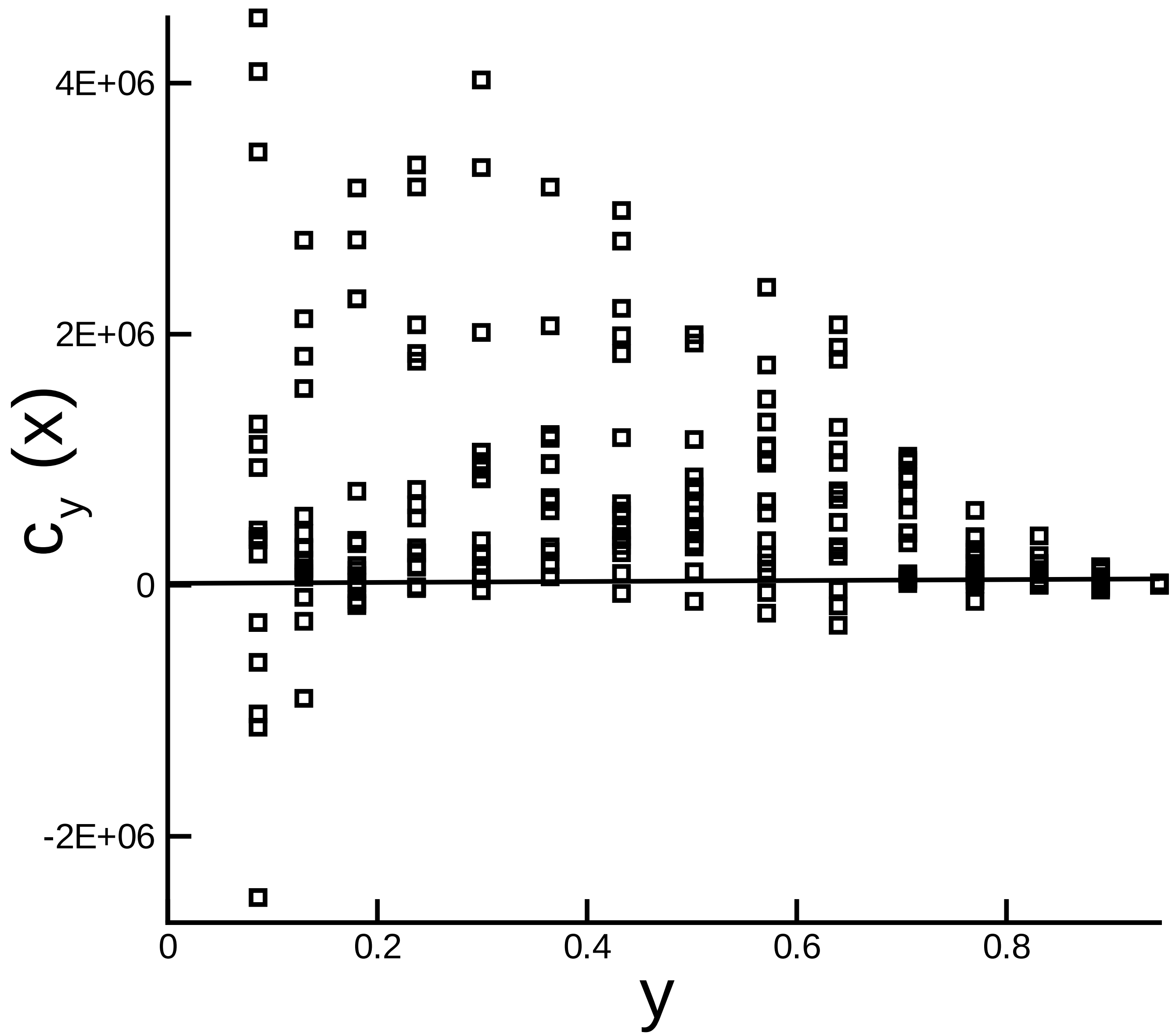
In static calculation with $|\vec{B}| = 0$, collisionality controls χ_ψ.

- **χ_ψ increases with decreasing collisionality as more mobile electrons become more efficient carriers of heat.**



General heat flux closure predicts heat flow against local gradients.

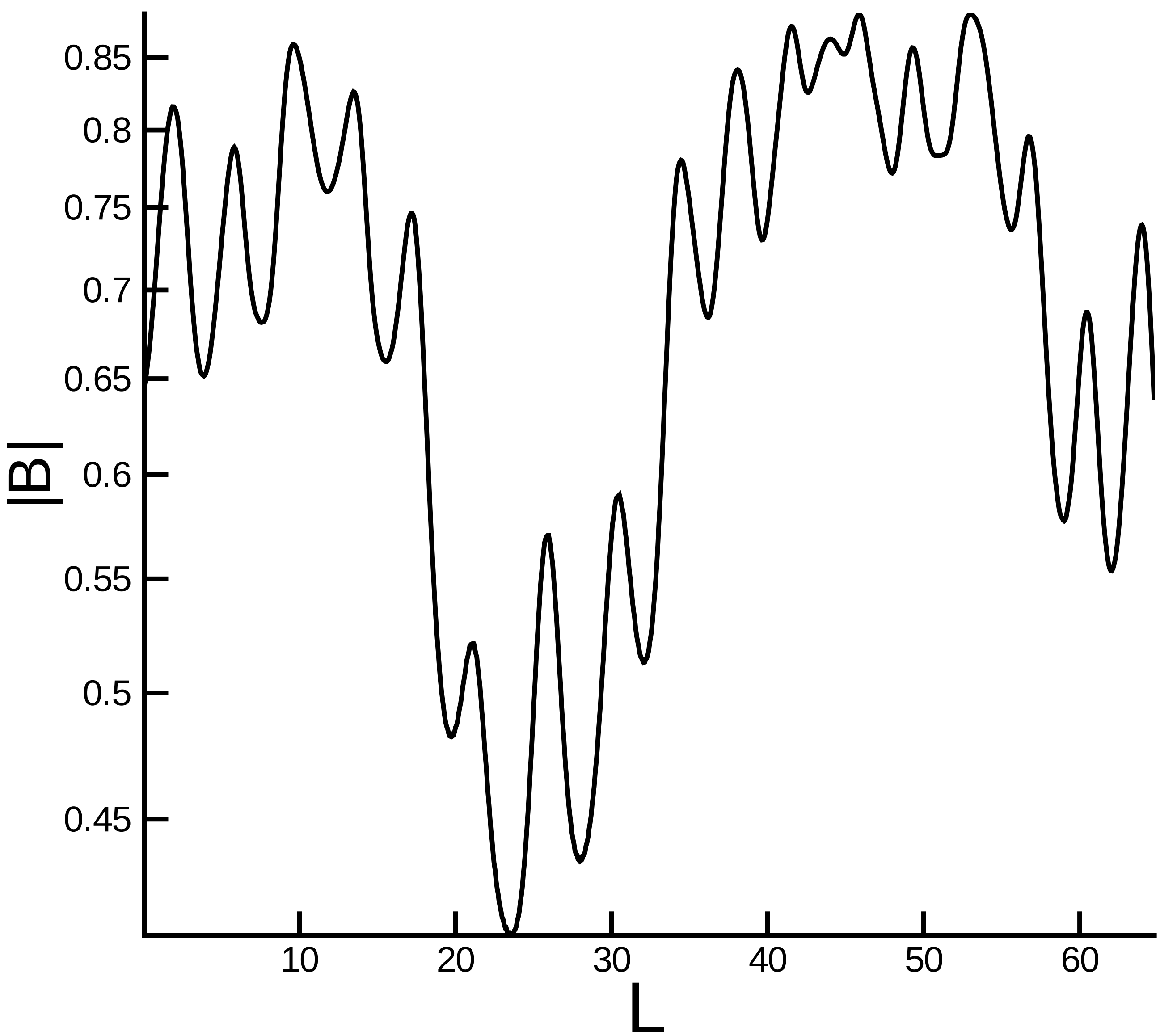
- **In small subset of cases heat flows against local gradients for superimposed axisymmetric temperature profile.** [7]



[7] E. D. Held, J. D. Callen, C. C. Hegna and C. R. Sovinec, Phys. Plasmas **8**, 1171 (2001)

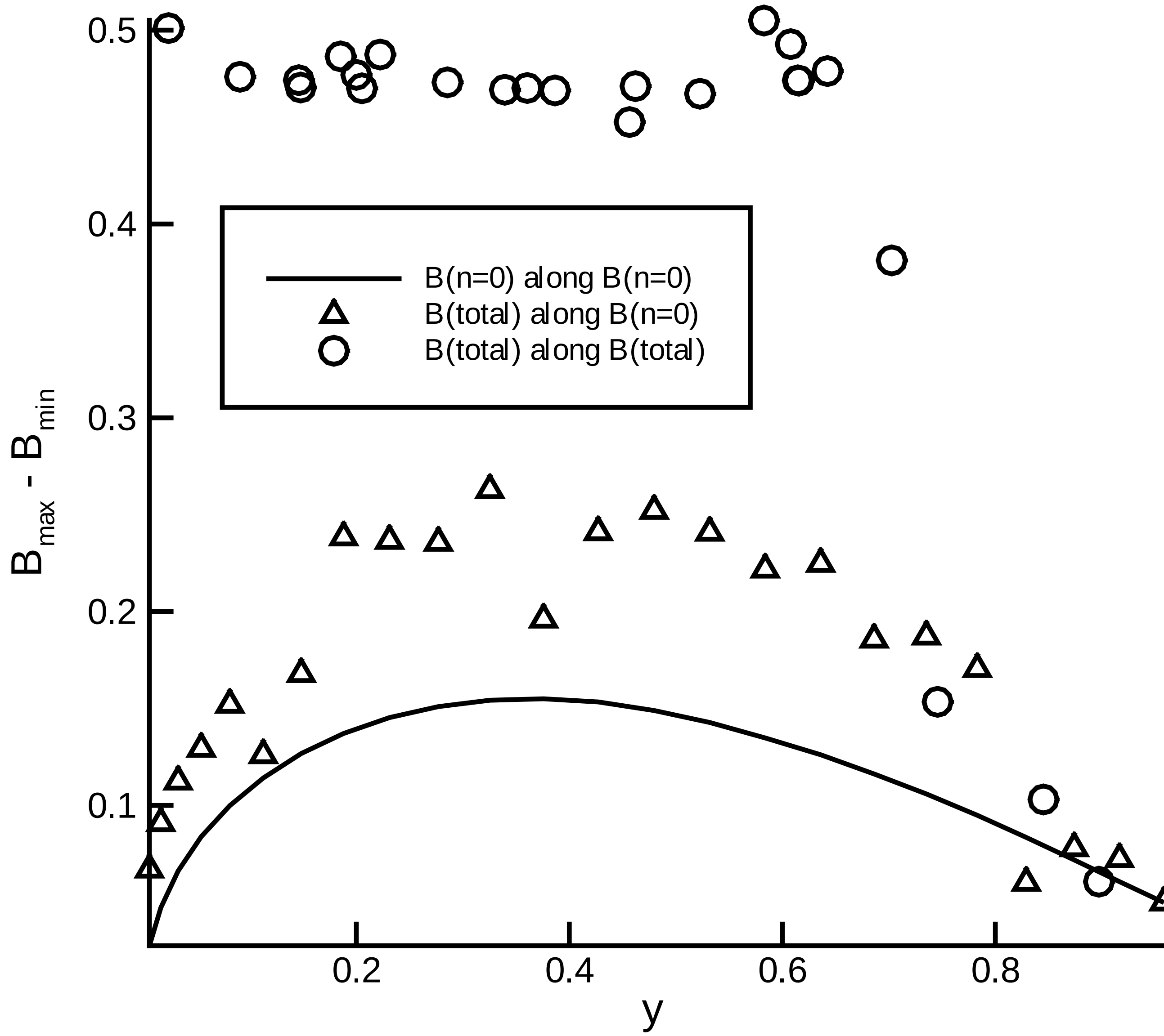
Along single field line electrons see chaotic distribution of short and long magnetic mirrors.

- **Short scale wiggles of axisymmetric field superimposed upon longer wells delineated by the reversal surface.**



Perturbed magnetic field contributes significantly to structure of trapped/passing space.

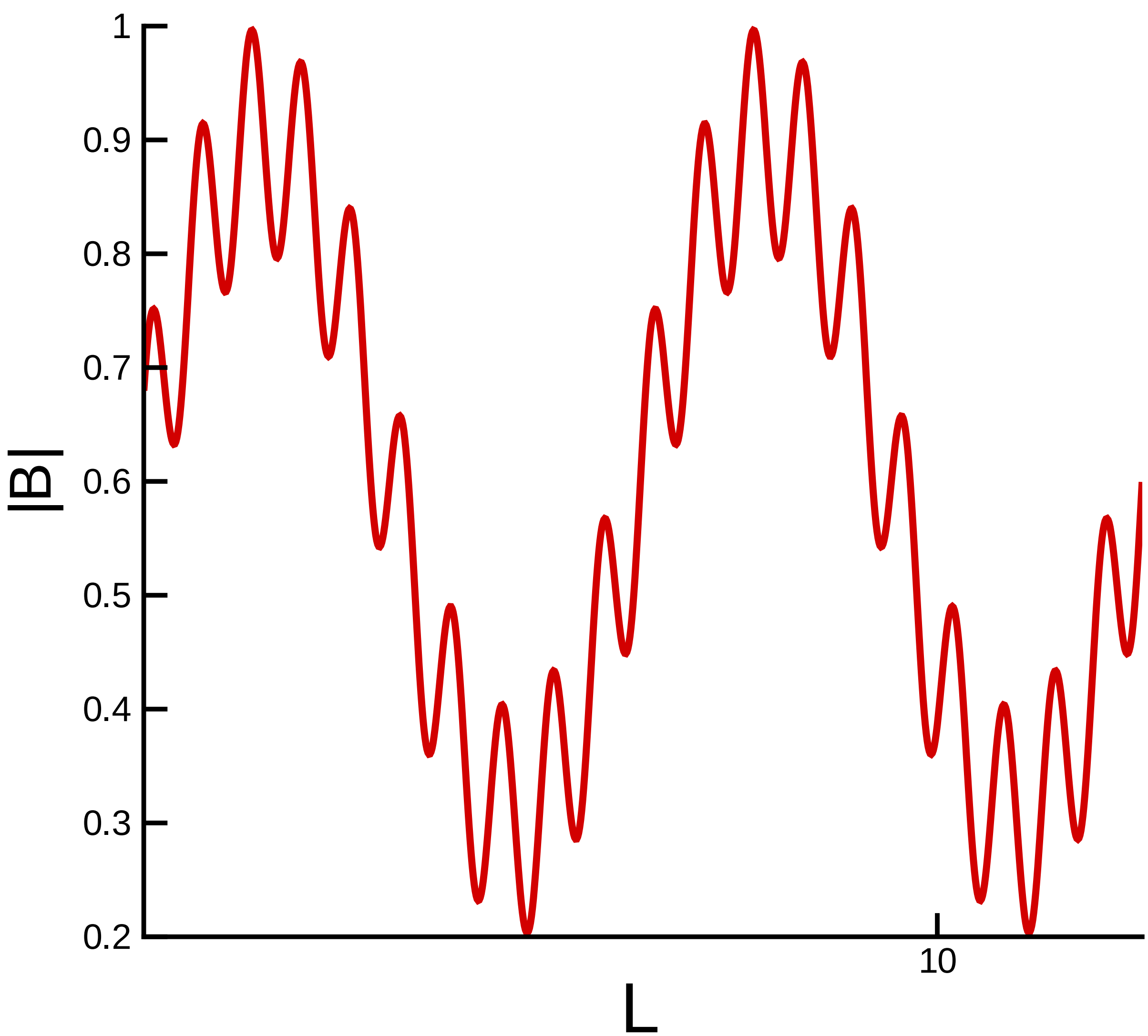
- **Variations in $|\vec{B}|$ along single field line depend upon field line trajectories.**



Model short and long magnetic mirrors as ideal sinusoidal perturbations in $|\vec{B}|$.

- **Model pitch-angle space by separating into two trapped distributions and one set of passing electrons to handle following idealization:**

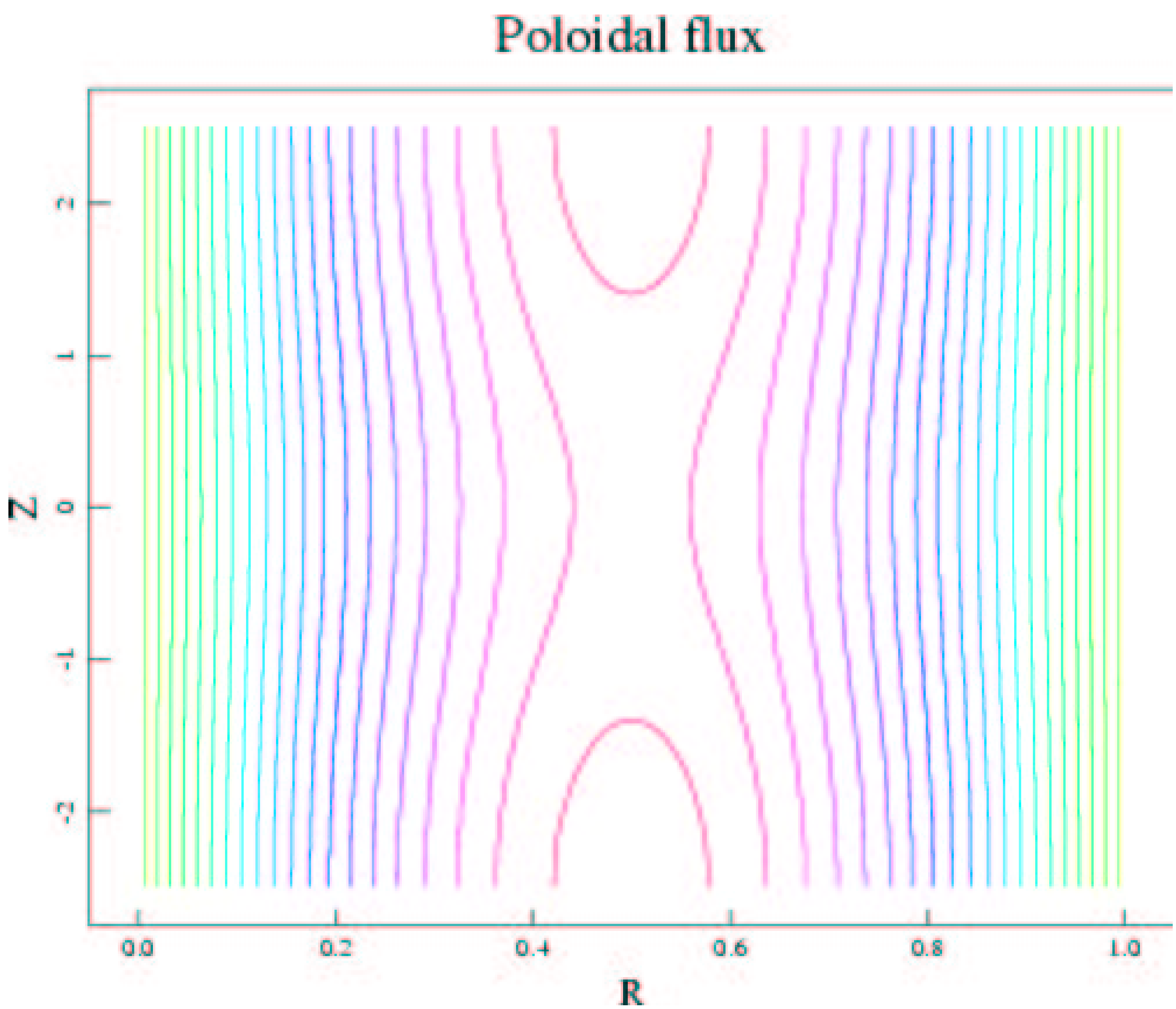
  $|\vec{B}| = B_1 \cos 2\pi L + B_2 \cos 20\pi L.$



Islands in slab geometry good testbed for heat flux closure.

- **Single-helicity island in slab geometry, periodic in Z and into plane.**

- **Heat flux boundary condition imposed at $R = 0$.**



Diffusive and CEL closures take different forms.

- Want to solve

$$\frac{3}{2}n\frac{\partial T}{\partial t} = -\vec{\nabla}\cdot\vec{q}.$$

- Diffusive heat flow uses

$$\vec{\nabla}\cdot\vec{q} = \vec{\nabla}\cdot\kappa\vec{\nabla}T = \kappa_\perp\nabla^2 T + \vec{\nabla}\cdot(\kappa_\parallel - \kappa_\perp)\hat{\mathrm{b}}\hat{\mathrm{b}}\cdot\vec{\nabla}T,$$

where $\kappa_\parallel$ and $\kappa_\perp$ are the parallel and perpendicular scalar conductivities.

- CEL closure expressible as

$$\vec{\nabla}\cdot\vec{q} = \kappa_\perp\nabla^2 T - \vec{\nabla}\cdot\kappa_\perp\hat{\mathrm{b}}\hat{\mathrm{b}}\cdot\vec{\nabla}T + \vec{\nabla}\cdot\vec{q}_\parallel,$$

where $\vec{q}_\parallel = q_\parallel\hat{\mathrm{b}}$.

- Temperature equation stabilized numerically with self-adjoint, semi-implicit operator, G, on left side.

$$(1 + \Delta t f \mathrm{G})\frac{\partial T}{\partial t} = \mathrm{K}(T).$$

- Time-discretized equation written as

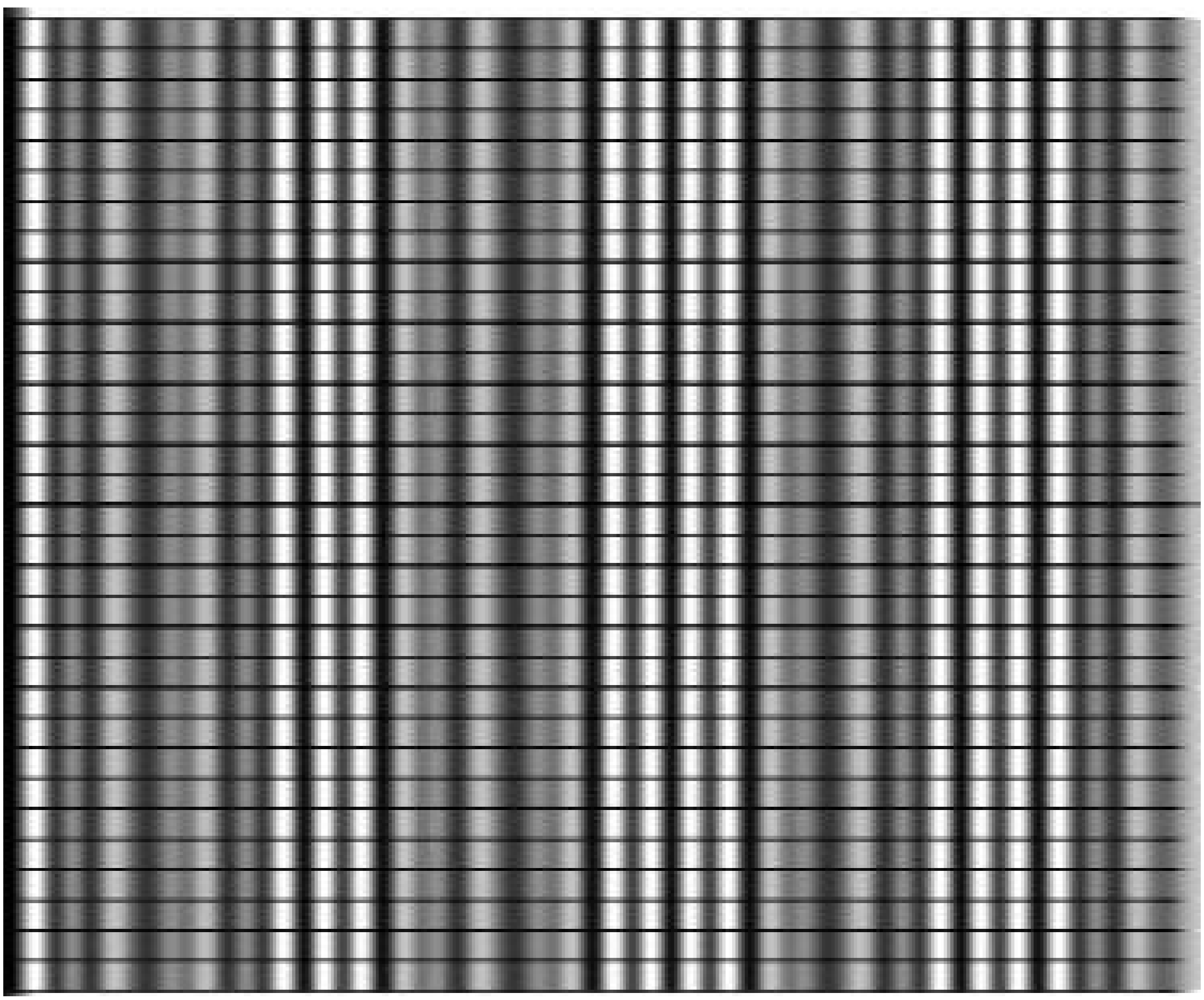
$$\left[\mathrm{I} - \Delta t f\left(\kappa_\perp\nabla^2 + \vec{\nabla}\cdot(\kappa_\parallel - \kappa_\perp)\hat{\mathrm{b}}\hat{\mathrm{b}}\cdot\vec{\nabla}\right)\right]\Delta T = \Delta t\left[\kappa_\perp\nabla^2 T - \vec{\nabla}\cdot\kappa_\perp\hat{\mathrm{b}}\hat{\mathrm{b}}\cdot\vec{\nabla}T + \vec{\nabla}\cdot\vec{q}_\parallel\right]$$

Closure calculations require significant computational effort.

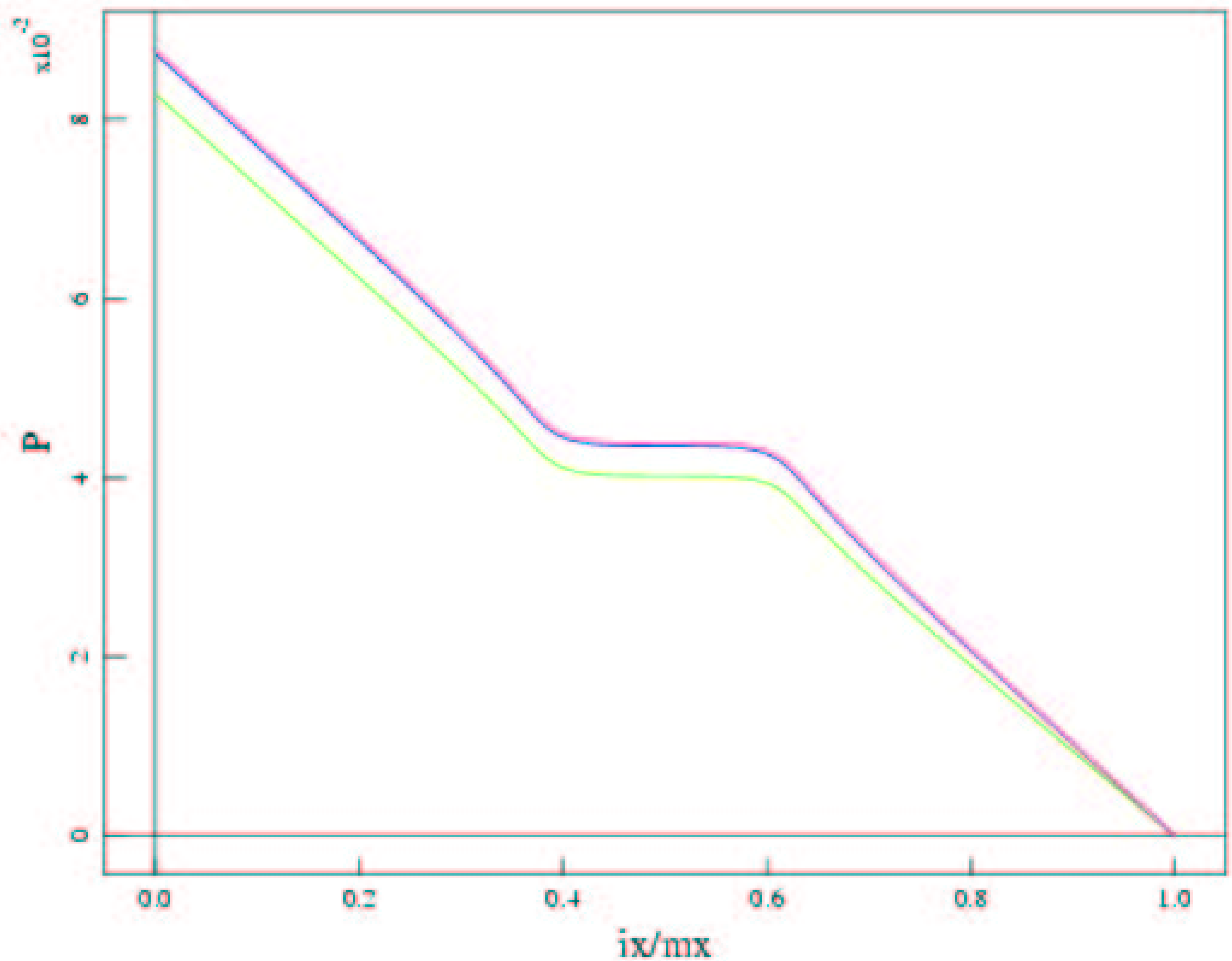
- **Processors integrate $\sim 10^3$ m for single heat flux calculation to converge with $T_e \sim 1000$eV, $v_{the} \sim 2 \times 10^7$ and $L_{mfp} \sim 100$m.**

- **Require 10^4 $q_{\|}$ calculations per toroidal harmonic performed at 10^3 timesteps involves integrating**

  $10^{10}m$ per simulation.



Evolution of temperature profile across O-point shows significant flattening with $T_{0e} = 1000eV$, $n_{0e} = 5 \times 10^{13}$ *and* $dt = .1ms$.



Semi-implicit operator slows down temperature evolution with $dt = 1ms$.

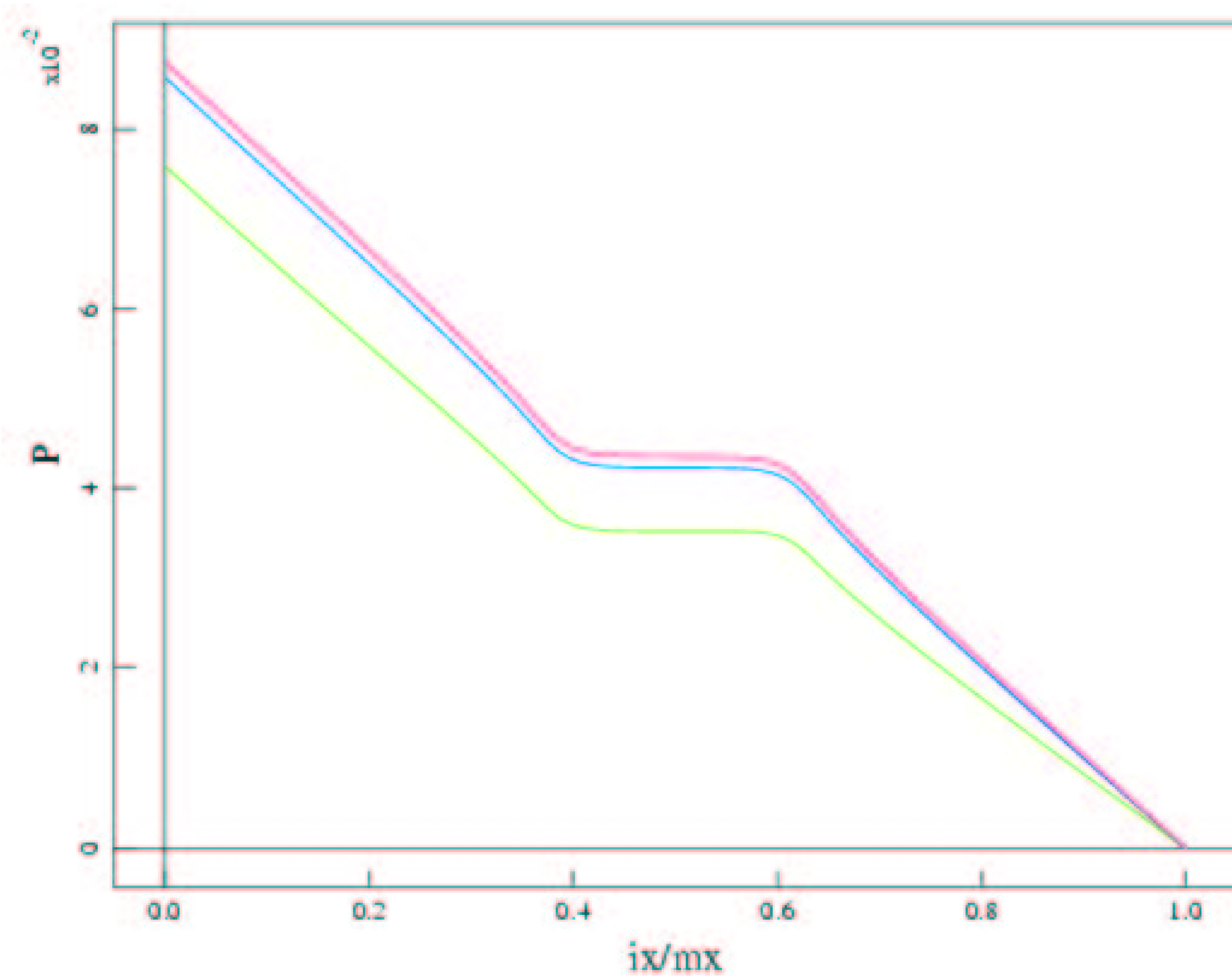


Figure 3: Temperature profile evolution with $dt = 1.0ms$, $T_{0e} = 1000eV$ and $n_{0e} = 10^{13}$.

At large time steps ($dt = 10ms$) semi-implicit operator introduces errors into evolution but generates correct equilibrium solution.

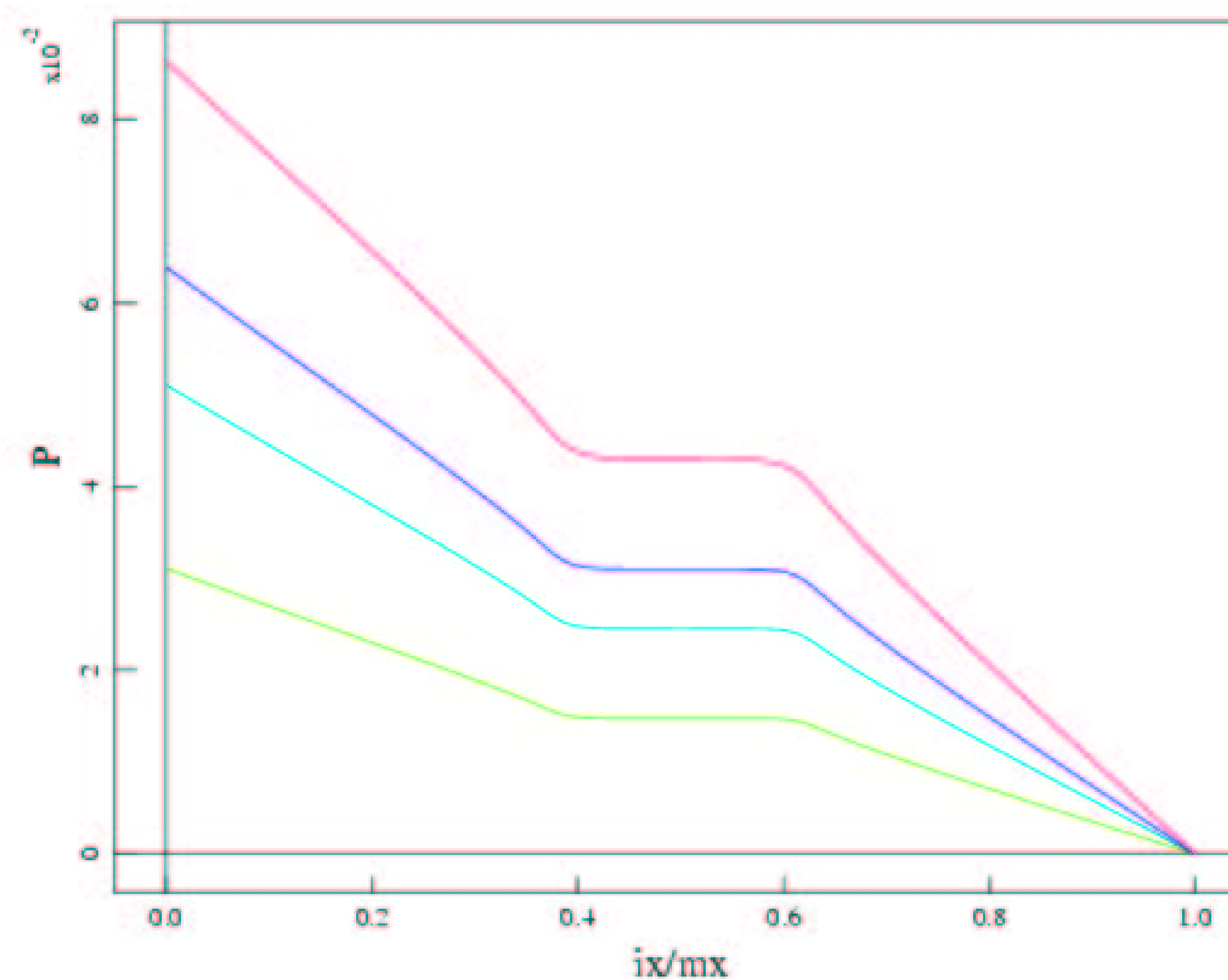


Figure 4: Temperature profile evolution with $dt = 10.0ms$, $T_{0e} = 1000eV$ and $n_{0e} = 10^{13}$.

Errors introduced by semi-implicit operator scale linearly with timestep.

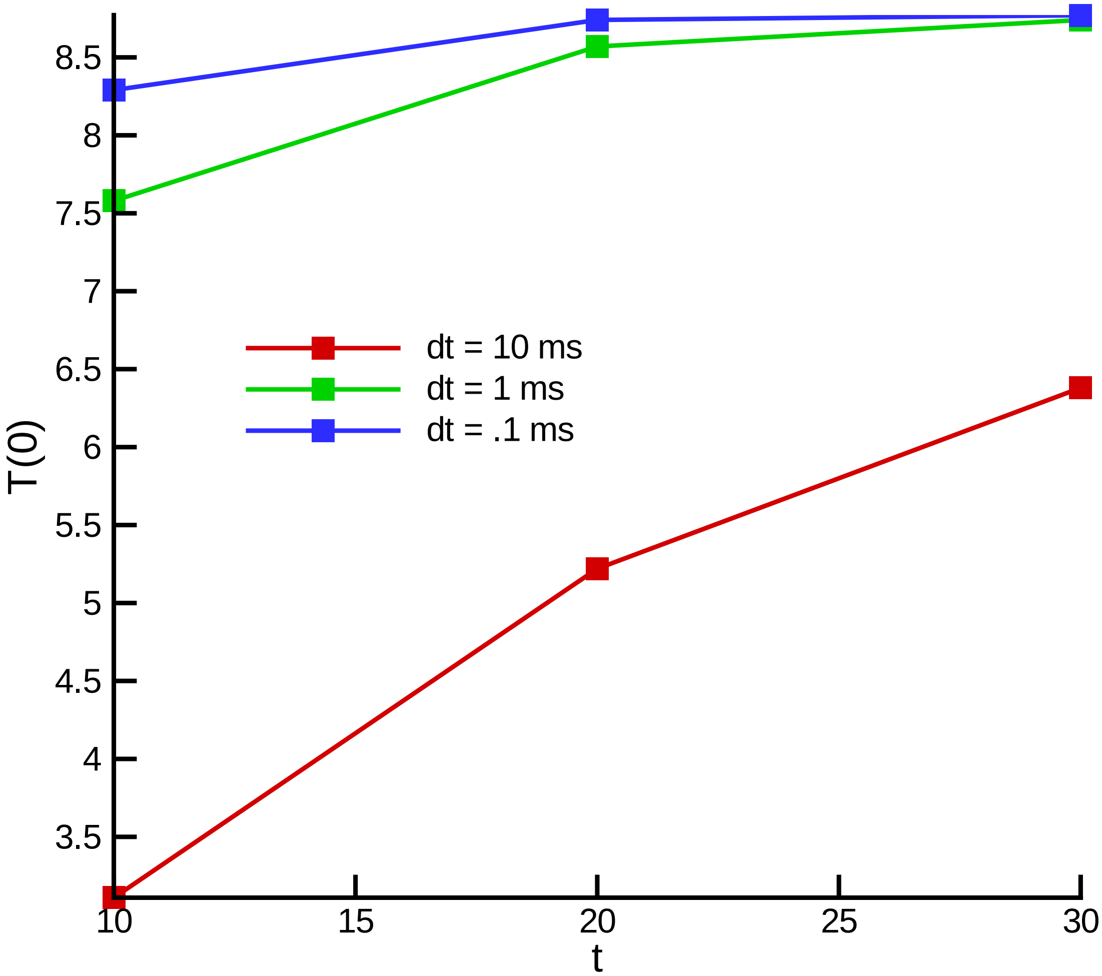


Figure 5: On axis temperature versus time for $dt = .1, 1$, and $10ms$.

Conclusions

- General parallel closure scheme devised to allow for arbitrary collisionality and trapped particle effects.

- Preliminary calculations of parallel heat flow along chaotic magnetic field and in vicinity of helical island show importance of proper treatment of collisionality and $|\vec{B}|$ variations.

- Robust temperature flattening inside islands predictied by parallel heat flow closure.

- CEL heat flow time $\sim$ temperature equation solve time

- Full implementation of complete closure model promises novel results from NIMROD simulations of plasmas confined by resistively evolving magnetic fields.