Implicit Heat Conduction in M3D and Recent Scaling Results

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Background

The parallel heat transport model in M3D has historically been the "artificial sound wave": the MHD-like energy equation

$$\frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p + \gamma p \nabla \cdot \mathbf{v} = \tfrac{2}{3} \nabla_\perp \cdot \left[n \chi_\perp \nabla_\perp \left(\frac{p}{\rho} \right) \right] + \text{heating terms}$$

where

$$\nabla_\perp \equiv \hat{R} \frac{\partial}{\partial R} + \hat{z} \frac{\partial}{\partial z}$$

is supplemented by a pair of wave equations for temperature and an auxiliary variable u:

$$\frac{\partial T}{\partial t} = s \frac{\mathbf{B} \cdot \nabla u}{n}$$

$$\frac{\partial u}{\partial t} = s \mathbf{B} \cdot \nabla T + \nu \nabla_\perp^2 u$$

for sound speed s and artificial viscosity ν.

Drawbacks of the Artificial Sound Approach

- This model is not a part of standard MHD, and not directly comparable to results from codes that implement the standard model (unclear what the equivalent $\chi_{||}$ should be).

- Because the perpendicular operator is perpendicular to the ϕ direction rather than **B**, parallel and perpendicular transport are not cleanly separated.

- The implementation of the parallel operator is explicit in time, unlike the perpendicular one, and so can restrict the time step when *s* is large.

Parallel Heat Diffusion

The MHD energy equation with anisotropic heat conduction can be written

$$\frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p + \gamma p \nabla \cdot \mathbf{v} = -\tfrac{2}{3} \nabla \cdot \mathbf{q} + \text{heating terms}$$

where the heat flux $\mathbf{q}$ is given by

$$\mathbf{q} = -n\left[\left(\chi_{\|} - \chi_{\perp}\right)\hat{\mathbf{b}}\hat{\mathbf{b}} \cdot \nabla T + \chi_{\perp} \nabla T\right].$$

Straightforward solution of this equation using finite differences or low-order finite elements is susceptible to numerical pollution of perpendicular heat transport by parallel when $\chi_{\|} / \chi_{\perp} \gg 1$, as is typical.

Günter, *et al.*, have a 2nd-order scheme based on centered differences that largely avoids this problem[1].

[1]S. Günter, K. Lackner, and C. Tichmann, *J. Comp. Phys.* **226** (2007) 2306-2316.

Günter's Method for Finite Elements

The Galerkin integral of the heat conduction term against a test function is

$$-\int \lambda_i \nabla \cdot \mathbf{q} dV = \int \mathbf{q} \cdot \nabla \lambda_i dV + \text{surface term}$$

Substituting in the expression for **q**, we rewrite the integral on the RHS as

$$-\int n\left(\chi_{||} - \chi_{\perp}\right) \tilde{q}_{||} \hat{\mathbf{b}} \cdot \nabla \lambda_i dV - \int n \chi_{\perp} \nabla T \cdot \nabla \lambda_i dV$$

The key procedure is the replacement of the factor $\hat{b} \cdot \nabla T$ in the first integral with

$$\tilde{q}_{||m} \equiv \frac{\int_{\Delta_m} \hat{\mathbf{b}} \cdot \nabla T dV}{\int_{\Delta_m} dV},$$

reducing the order of the representation by one, in this case from a C^0 bilinear function to a C^{-1} piecewise constant function over element m.

M3D Implementation

New routine advances

$$\frac{\partial \tilde{T}}{\partial t} = \nabla \cdot \left\{ n \left[\left(\chi_{\|} - \chi_{\perp} \right) \hat{\mathbf{b}} \hat{\mathbf{b}} \cdot \nabla \tilde{T} + \chi_{\perp} \nabla \tilde{T} \right] \right\}$$

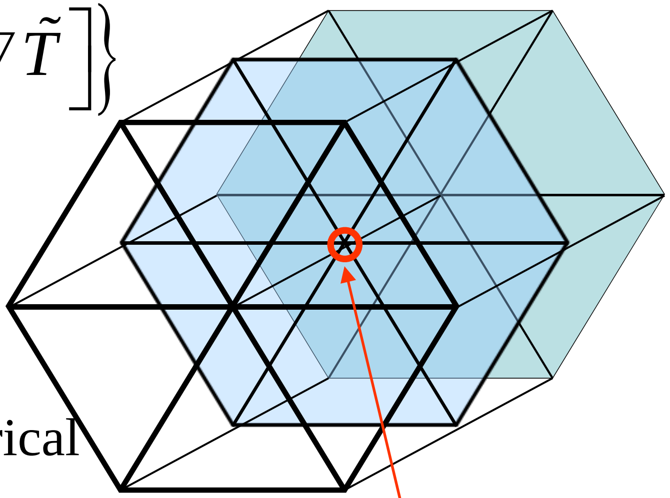
where

$$\tilde{T} = T - T_0$$

with arbitrary source term T_0; performs 3D numerical Galerkin integration (3×7-point quadrature) using trilinear test functions to construct global mass matrix **M** and heat conduction operator matrix **Q**; solves

$$\left(\bar{\mathbf{M}} - \theta \delta t \bar{\mathbf{Q}} \right) \cdot \tilde{\mathbf{T}}^{n+1} = \left[\bar{\mathbf{M}} + \left(1 - \theta \right) \delta t \bar{\mathbf{Q}} \right] \cdot \tilde{\mathbf{T}}^{n}$$

using GMRES, θ=1/2 for 2nd-order accurate implicit time advance.



Vertex values affect function over 12 adjoining triangular prisms

Qualitative Comparison with Artificial Sound Wave Method

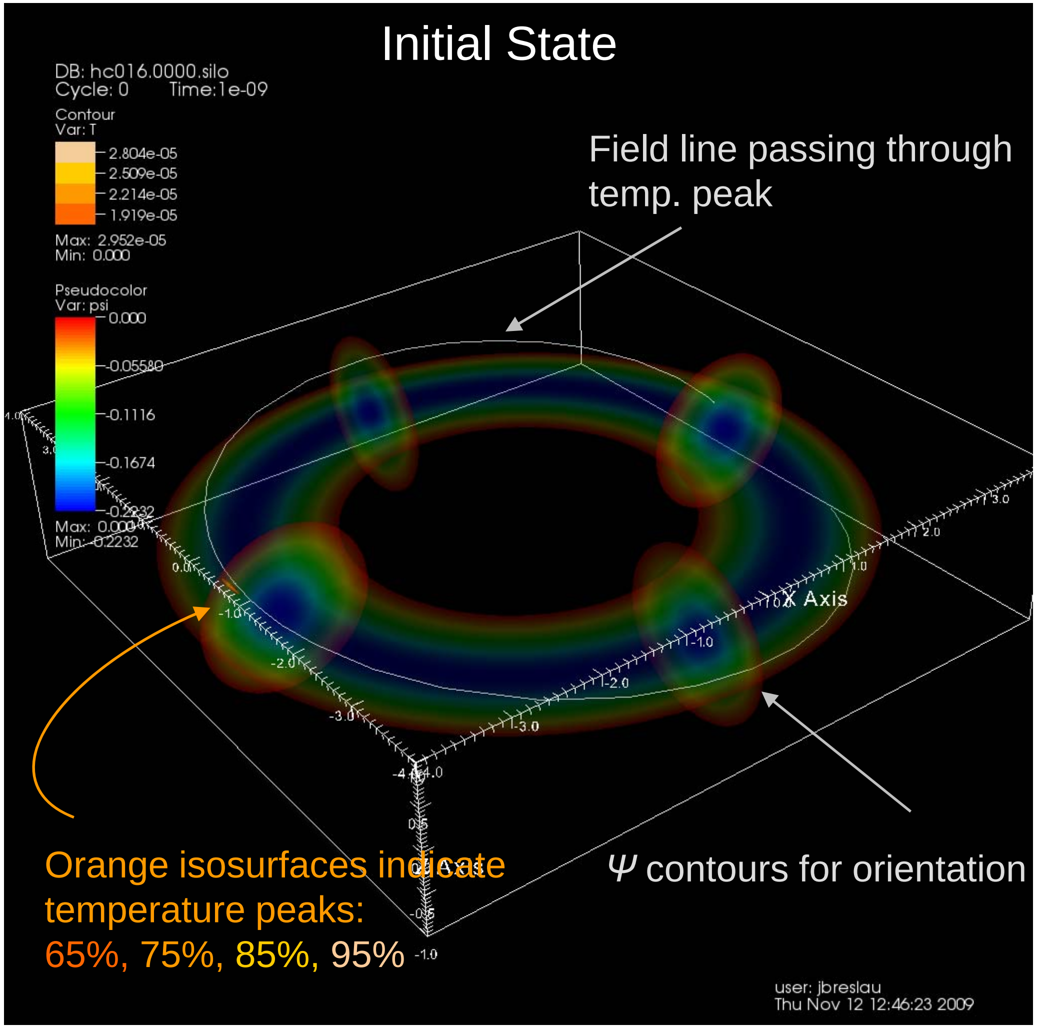
- Use circular cross-section equilibrium, aspect ratio 3; $1.33 < q < 4.79$.

- Peak $T = 3.1\times10^{-7}$ near axis.

- Add temperature perturbation

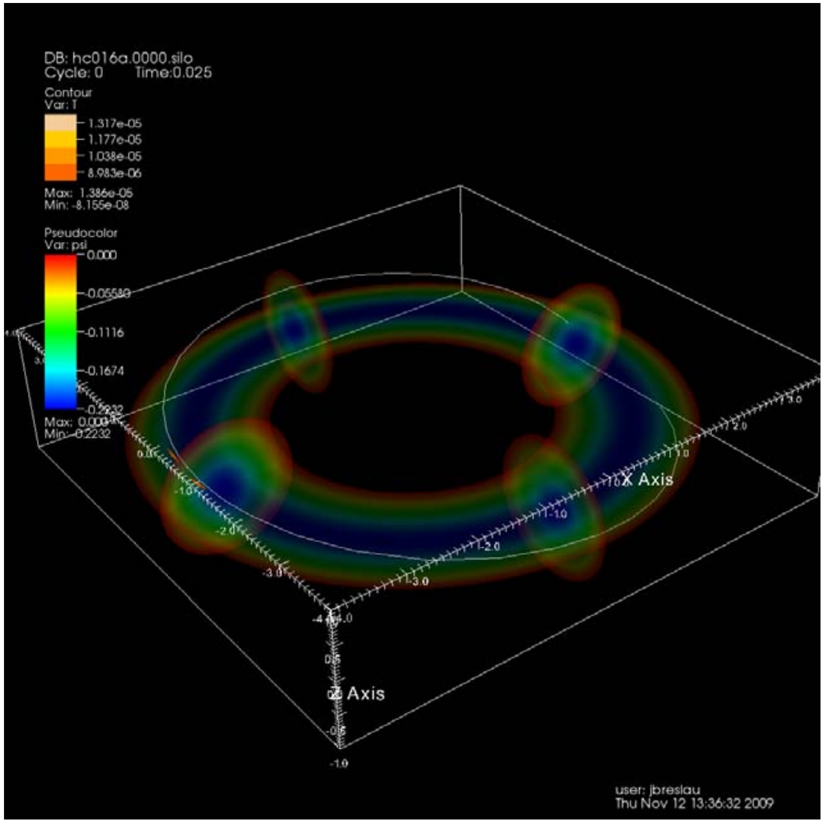
$$\delta T = 3\times10^{-5}\exp\left\{-\left(\frac{\varphi-\pi}{0.07709}\right)^2 - \left[\frac{(R-3.53)^2+(z-0.53)^2}{(0.04)^2}\right]\right\}$$

- Freeze density and **B** and **v** fields, evolve T only;
  $\chi_\perp = 10^{-50}$ and either
  $s=6$, $\nu=10^{-3}$
  or
  $\chi_\parallel = 60$

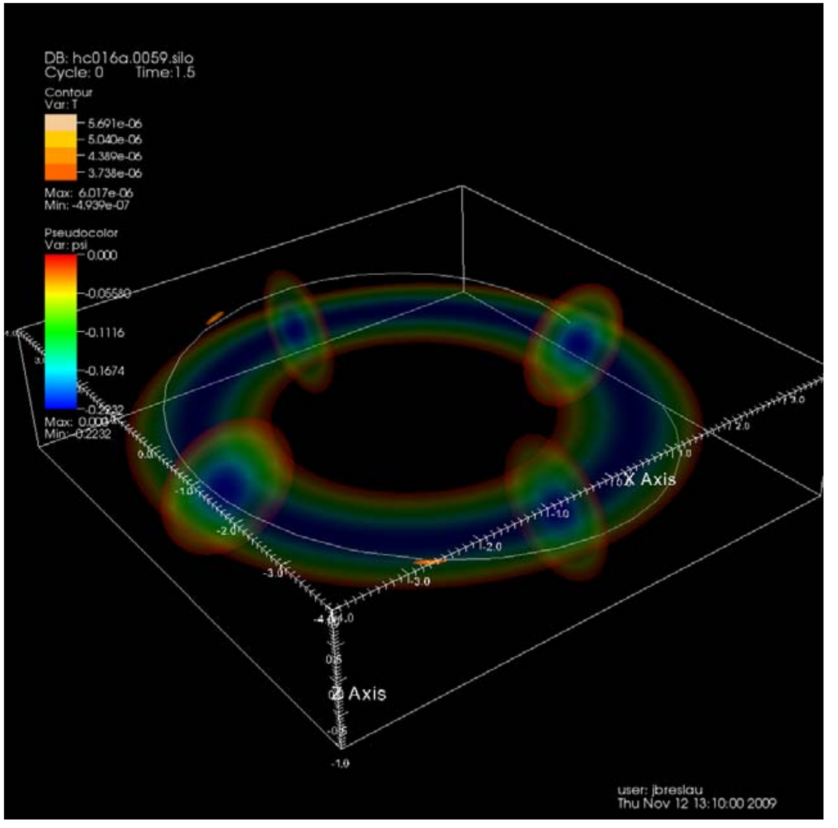


Artificial Sound Results

t = 0.025

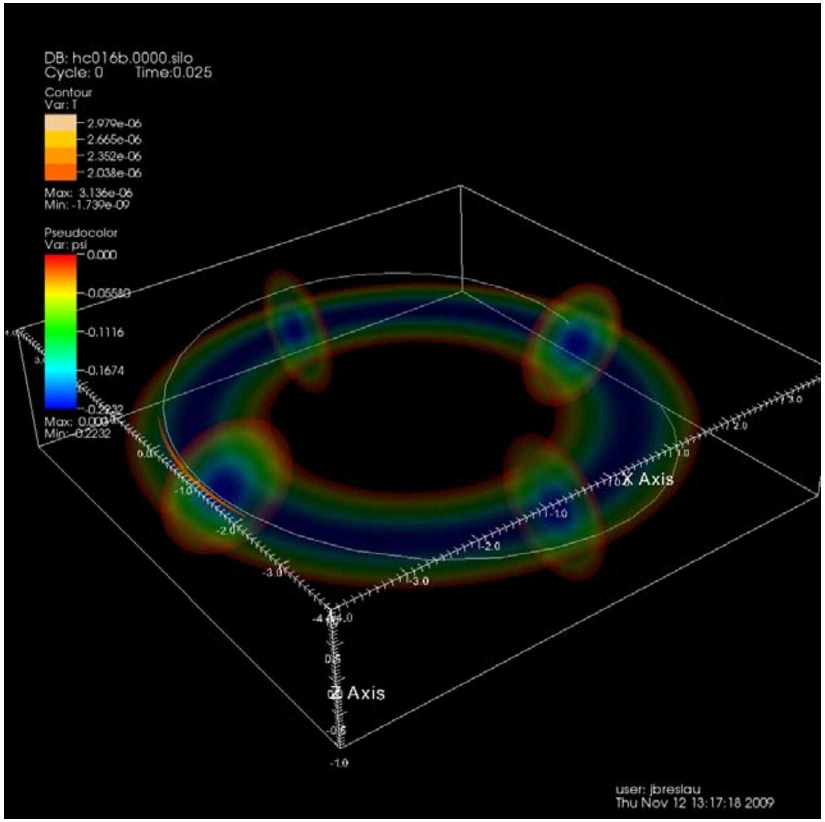


t = 1.5

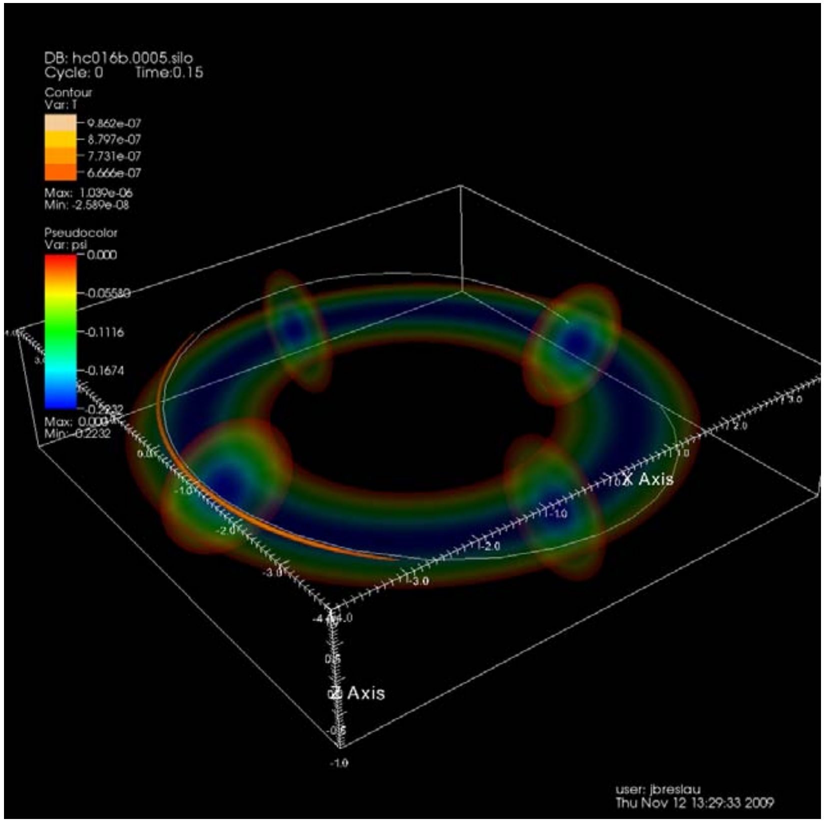


Implicit $\chi_{||}$ Results

t = 0.025

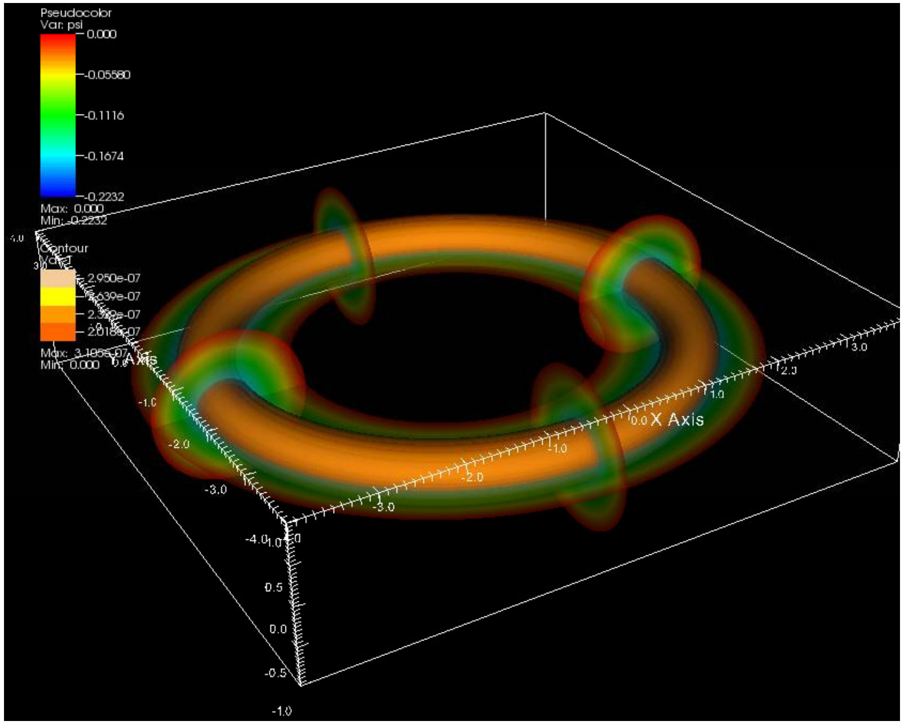


t = 0.15

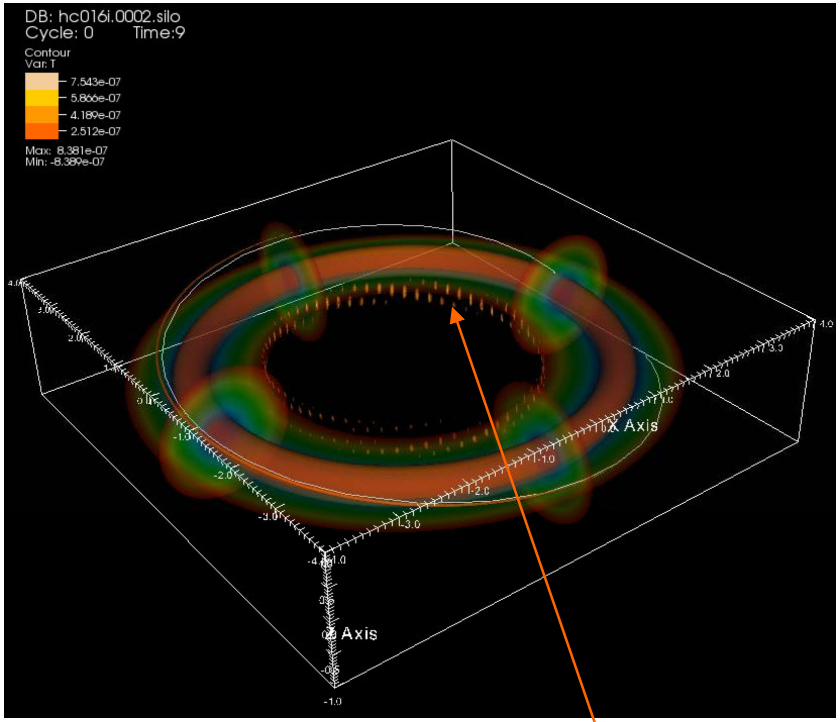


Late Time States

Implicit $\chi_{||}$, t = 15.0



Artificial sound, t = 9.0

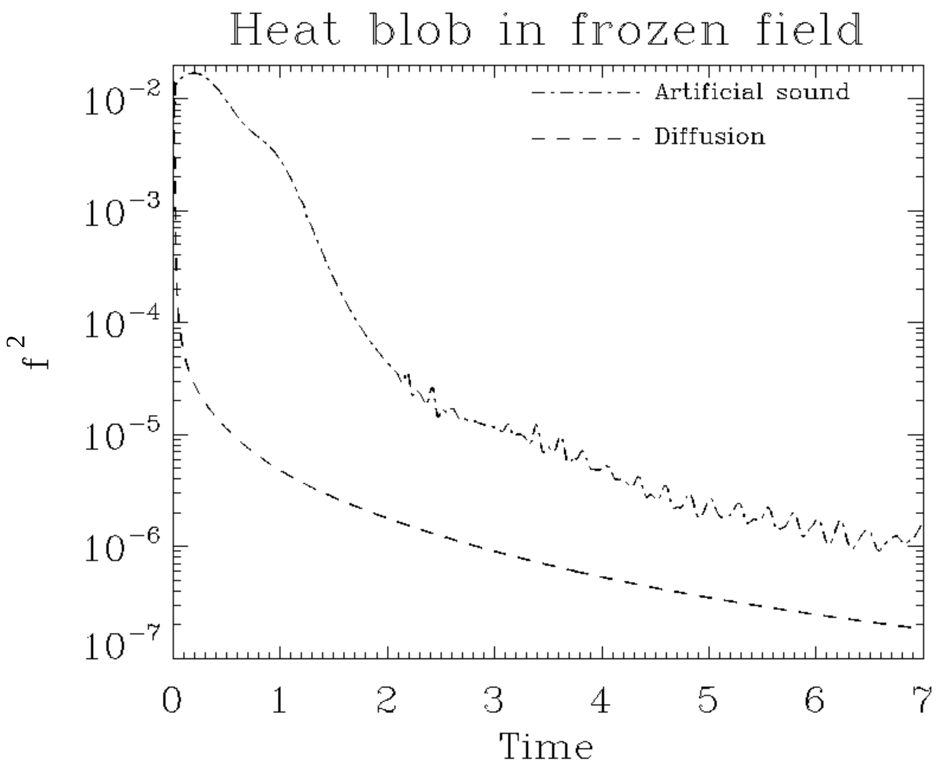


Numerical instability

Quantitative Test of Accuracy

The figure of merit is the normalized RMS parallel temperature gradient, defined as

$$f(t) \equiv \sqrt{\frac{\iiint \left|\mathbf{B}\cdot\nabla T\right|^2}{\iiint \left|\mathbf{B}\right|^2 \left|\nabla T\right|^2}}$$

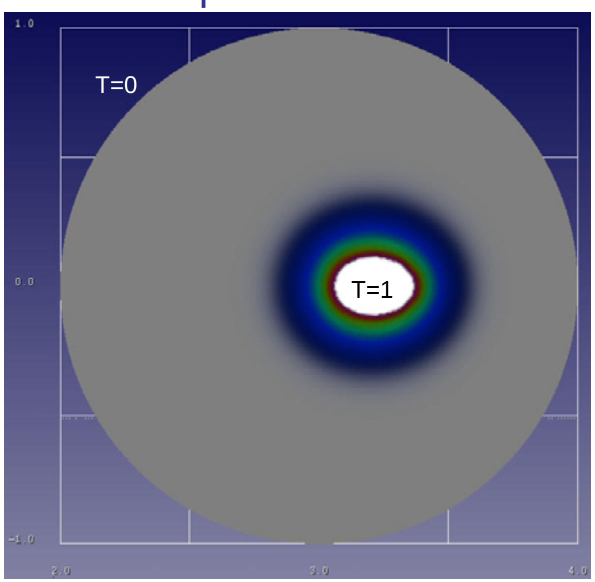


Artificial sound method goes unstable here

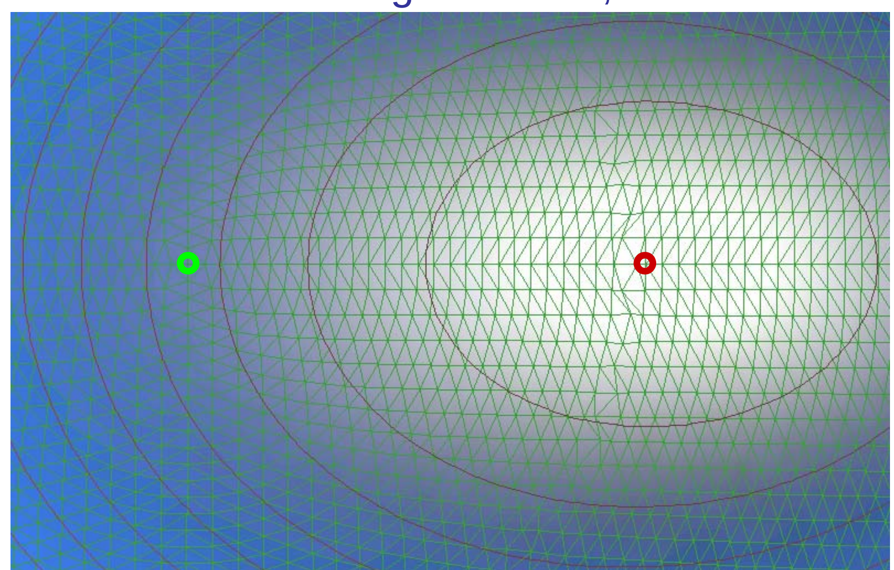
2^{nd} Test: Find steady state using misaligned grid with inhomogeneous bcs

- Start with circular cross-section equilibrium, aspect ratio three.
- Add 1,1 helical perturbation to poloidal flux to shift surfaces away from mesh.
- Use boundary condition T=0 on outer surface; T=1 on inner surface defined by ψ=-0.235.
- Run to steady state using 32 planes, 141 radial zones.

Initial temperature distribution

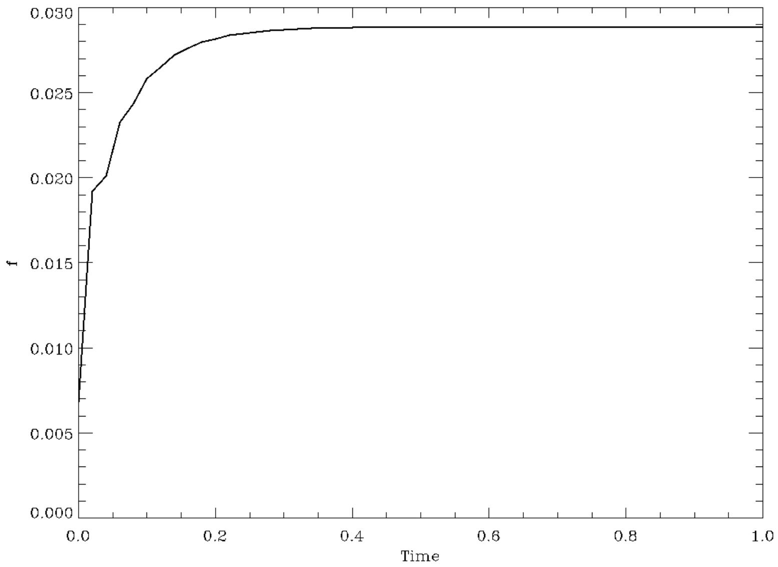


Detail of misaligned mesh, surfaces

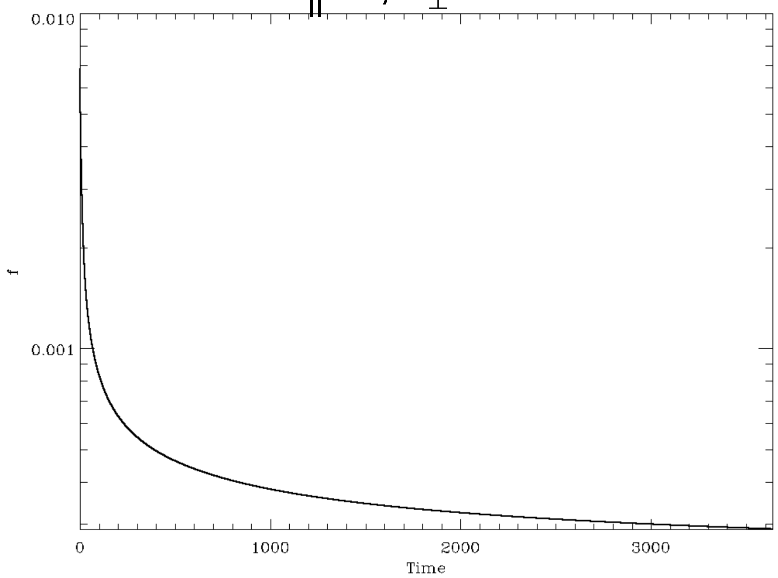


Extreme Cases

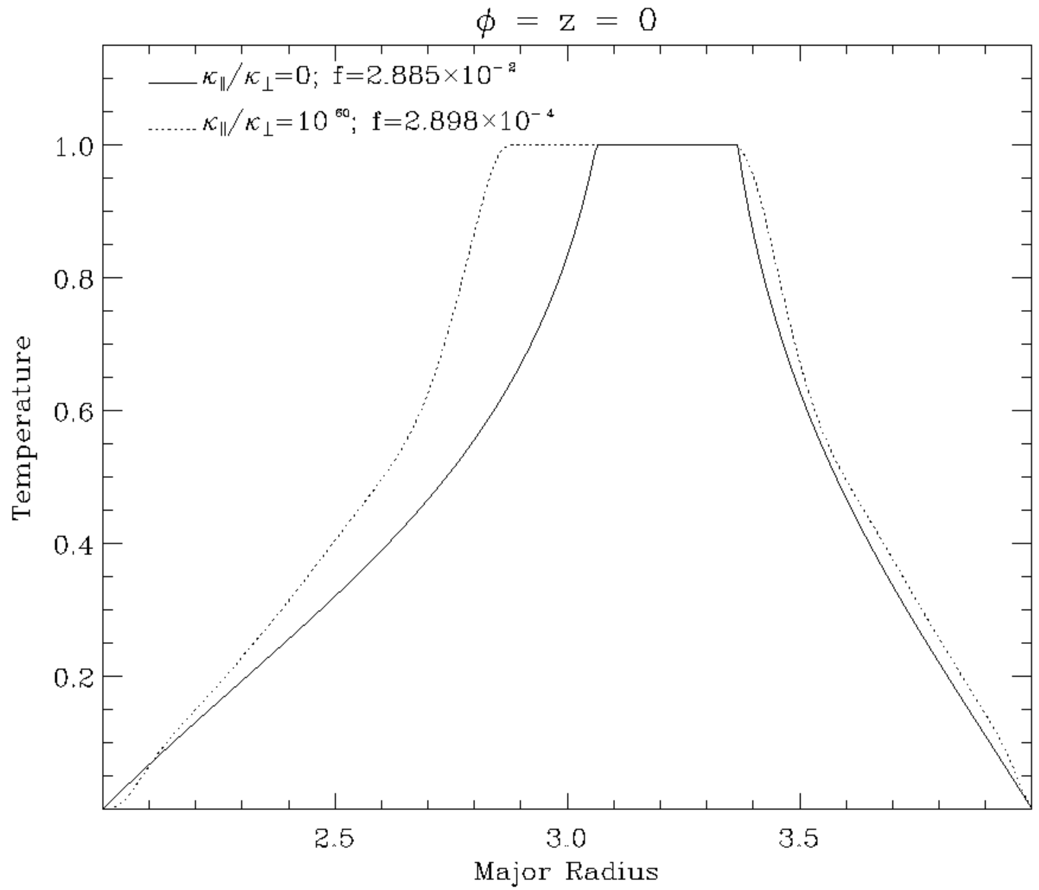
$\kappa_{||}$=0, $\kappa_{\perp}$=2



$\kappa_{||}$=1, $\kappa_{\perp}$=10^{-60}

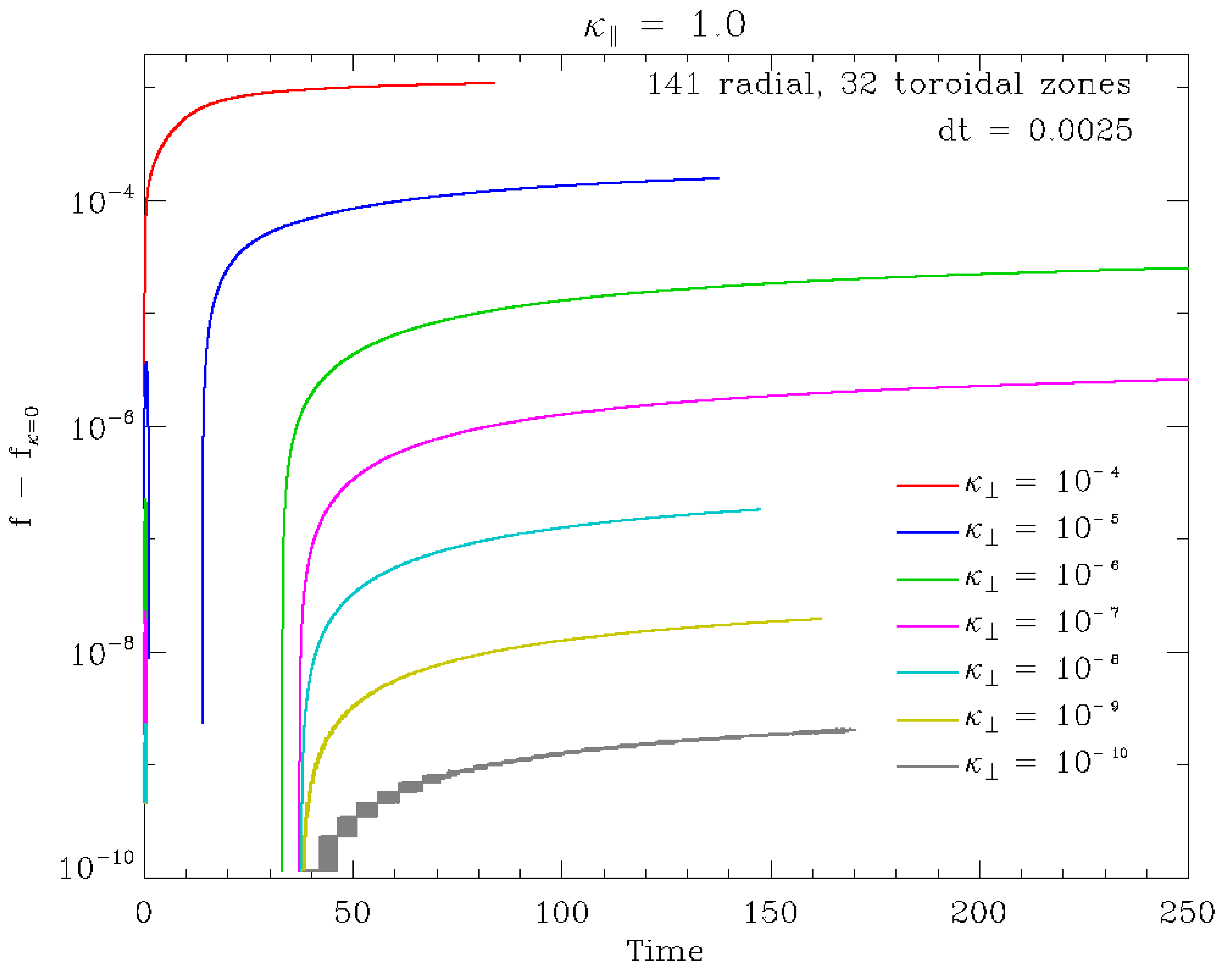


Final profile



Next: compare *f* history using other conductivity ratios to determine effective $\kappa_{\perp}$ due to pollution from parallel conduction.

Numerical $\kappa_\perp/\kappa_{||} < 10^{-10}$



Summary

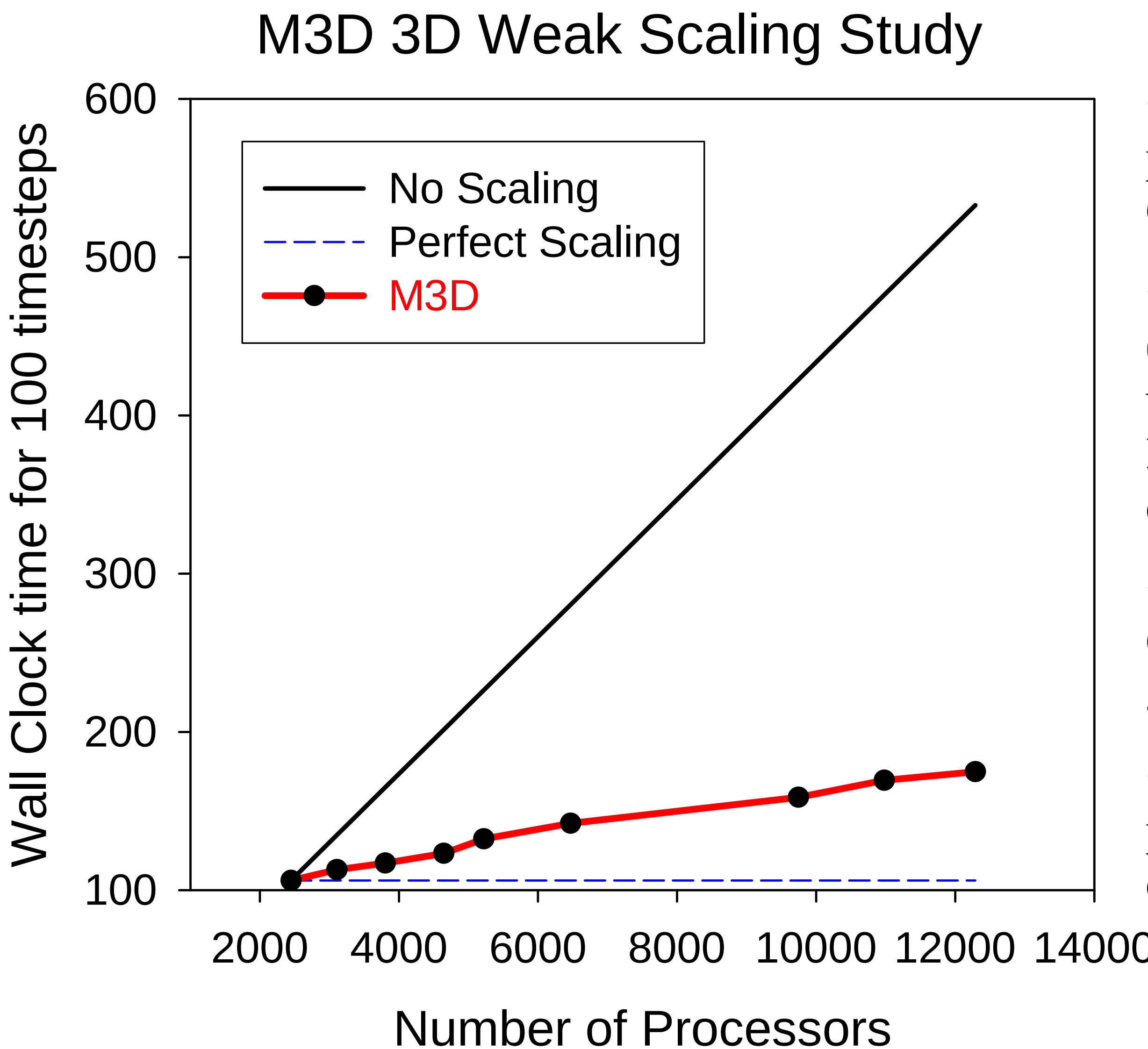
- True implicit parallel and perpendicular heat conduction have been implemented in M3D.

- Use of Günter’s method appears to allow high accuracy with linear finite elements even when tensor is highly anisotropic and mesh is misaligned.

- The new operator is an improvement on the old one in some respects.

- Further verification is needed. Because cases with analytic solutions are scarce, benchmarking with other codes would be useful.

M3D Scales to 12k+ Franklin Processors



- Algebraic multigrid preconditioner used for GMRES solves.
- Reverse Cuthill-McKee (RCM) matrix re-ordering used to reduce fill-in in ILU preconditioning for other linear solves.
- Base case is nonlinear C-Mod sawtooth with 24,000 vertices/CPU.
- ~200 toroidal CPUs, ~50 poloidal CPUS for largest cases.

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