Particle-based neoclassical closure relations for NTM simulations

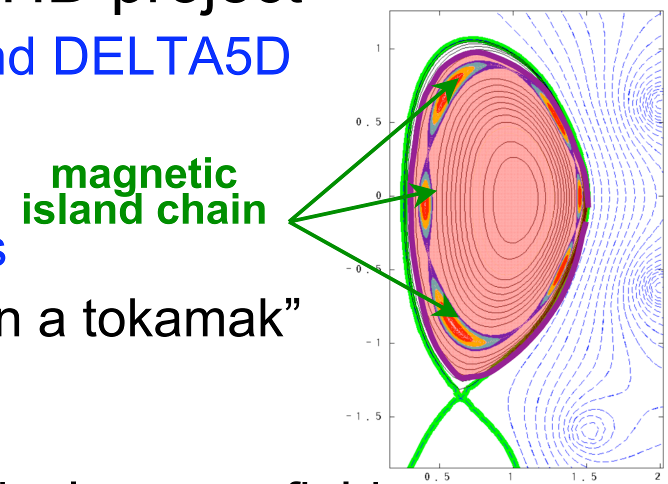
D. A. Spong[*], E. F. D'Azevedo[†], D. B. Batchelor[*],
D. del-Castillo-Negrete[*], M. Fahey[‡], S. P. Hirshman[*], R. T. Mills[‡]
[*]Fusion Energy Division, [†]Computer Science and Mathematics Division,
[‡]National Center for Computational Sciences
Oak Ridge National Laboratory

S. Jardin, W. Park, G.Y.Fu, J. Breslau, J. Chen,
S. Ethier, S. Klasky
Princeton University Plasma Physics Laboratory

NTM simulation requires MHD closure relations with long-mean free path effects in localized 3–dimensional regions (magnetic islands)

ORNL/PPPL LDRD terascale/multiscale MHD project

– Improved efficiency of M3D (extended MHD) and DELTA5D (neoclassical transport in 3D systems)
  - Cray X1E, Cray XT3 NLCF systems

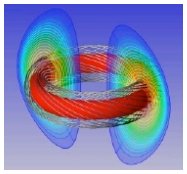


– Development of particle-based closure relations
  - Island regions analogous to “stellarator within a tokamak”
    – K. C. Shaing, Phys. Plasmas **11**, 625 (2004); **10**, 4728 (2003), **9**; 3470 (2002)
  - 3D variation of |B| significantly modify local ripple, cross-field transport, local bootstrap current, flow damping
  - New δf model avoids redundant calculation of flows, pressure variations, etc. provided by the MHD model

– Merging of extended MHD with neoclassical particle closure
  - New data compression, noise reduction techniques developed based on principal orthogonal decomposition/SVD methods
  - Applicable both to data from MHD -> particles and particles-> MHD

Optimization of DELTA5D and M3D for vector architectures

New sparse matrix-vector multiply routine (vectorized) developed: 10 times faster



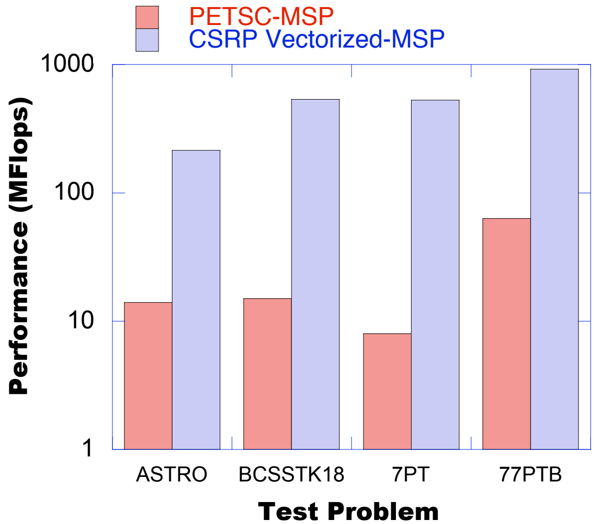
M3D

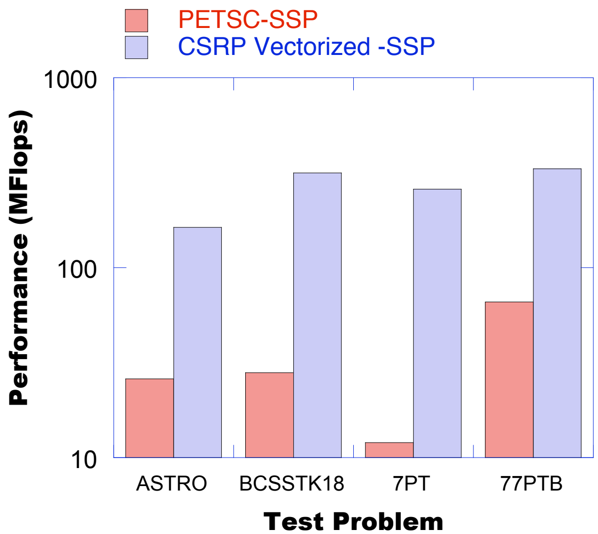
- M3D spends much time in:

  Sparse elliptic equation solvers

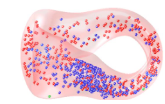
  Matrix-vector multiplies | **ILU preconditioner (forward/backward solves)**

- PETSC matrix storage
  - **CSR (Compressed Sparse Row)**
  - **Unit stride good for scalar/poor for vector processors**
- CSRP (CSR with permutation)
  - **Reorders/groups rows to match vector register size**
  - **“strip-mining” breaks up longer loops**
- CSRP algorithm encapsulated into a new PETSC matrix object

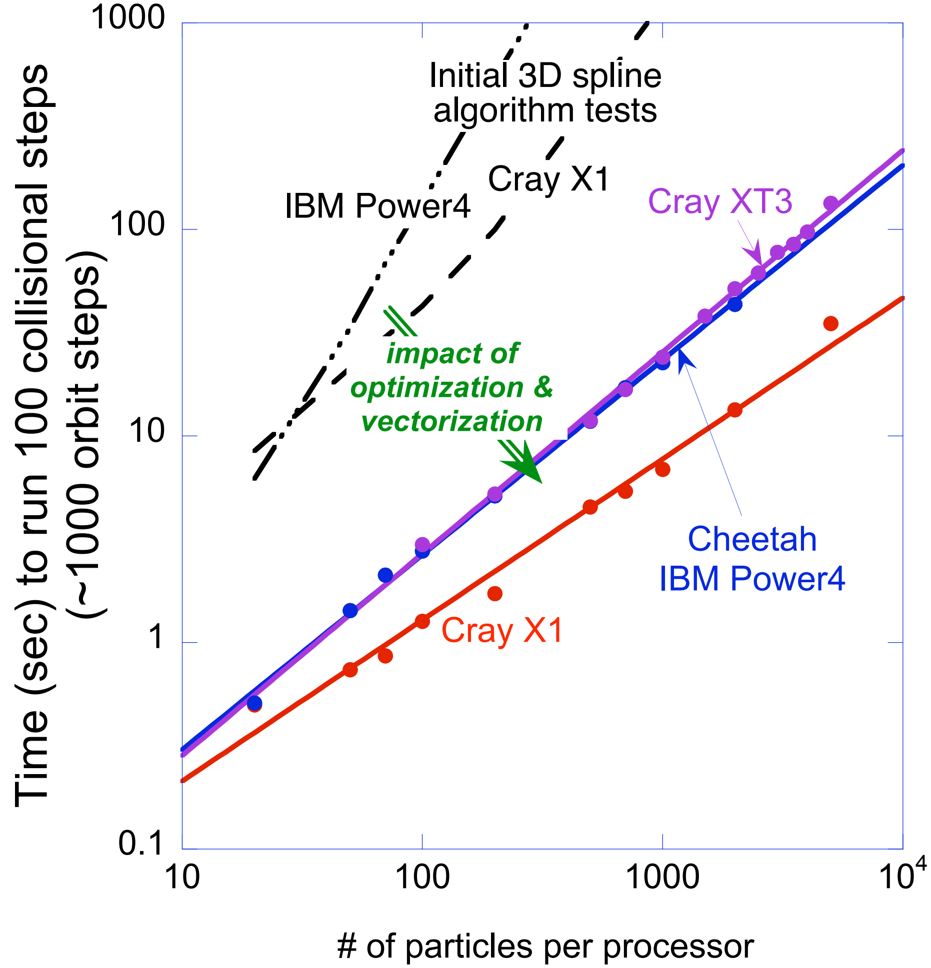




Particle simulation performance has been significantly improved by optimizing the magnetic field evaluation routines:


DELTA5D

- DELTA5D converted to cylindrical geometry for compatibility with M3D
- 3D B-spline routine optimized by vectorization
- For larger problems, spline memory requirements will limit number of particles per processor
- New data compression techniques developed



Neoclassical Closure Relations

Our goal is to couple kinetic transport effects with an MHD model - important for long collisional path length plasmas such as ITER

- **Closure relations: enter through the momentum balance equation and Ohm's law:**

$$nm\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla\right)\mathbf{V}=-\nabla p-\nabla\cdot\Pi+\mathbf{J}\times\mathbf{B}$$

$$\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla\right)p=-\gamma p\nabla\cdot\mathbf{V}+(\gamma-1)(Q-\nabla\cdot\mathbf{q})$$

$$\mathbf{E}=-\mathbf{V}\times\mathbf{B}+\eta\mathbf{J}+\frac{1}{ne}\left(\mathbf{J}\times\mathbf{B}-\nabla p_e-\nabla\cdot\Pi_{\parallel e}\right)$$

$$\frac{\partial\mathbf{B}}{\partial t}=-\nabla\times\mathbf{E},\qquad \nabla\cdot\mathbf{B}=0,\qquad \mu_0\mathbf{J}=\nabla\times\mathbf{B}$$

- **Moments hierarchy closed by Π = function of** *n, T,* V**,** B**,** E
- **Requires solution of Boltzmann equation: f = f(**x,v**,t)**
- **High dimensionality: 3 coordinate + 2 velocity + time**

Neoclassical transport closures introduce new challenges:

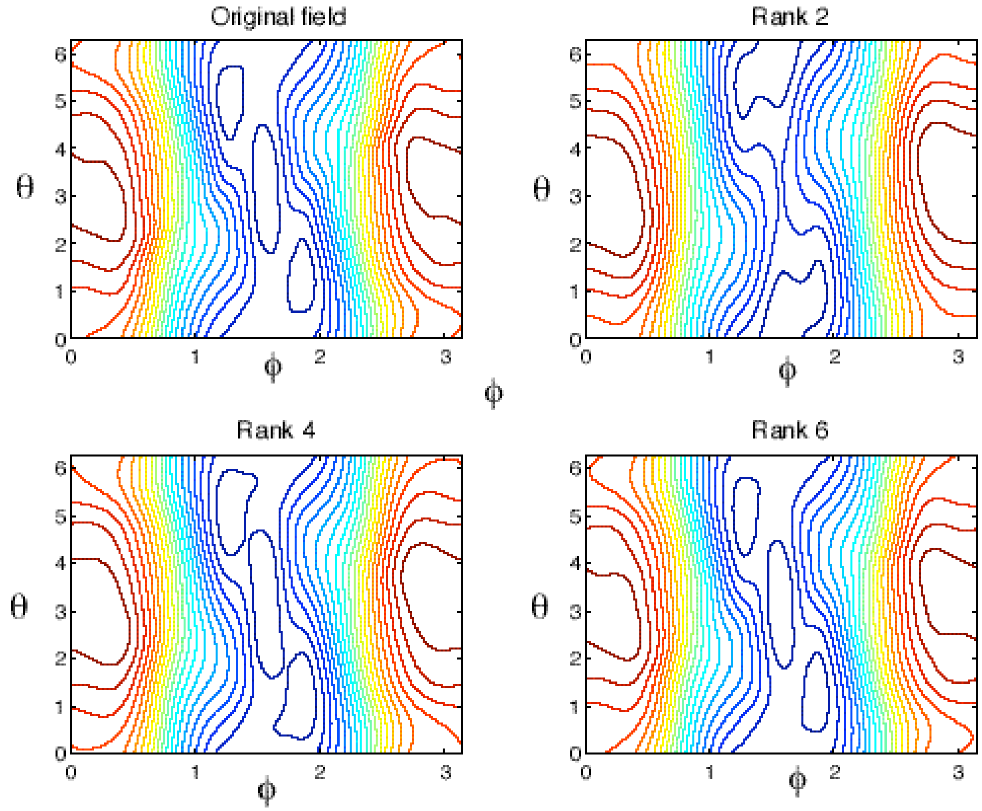
- Collisions introduce new timescales
  - lengthy evolution to steady state, especially at low collisionalities
  - Time-averaging needed to remove noise introduced by Langevin collision operator
- New δf partitioning
  - Want to avoid calculating quantities (flows, macroscopic gradients) that are already evolved by the MHD model
- New data compression/smoothing methods
  - Interpolated M3D data noisy, not local to each processor
  - Particle data noisy, scattered over many processors
  - Need to package data for heterogeneous systems

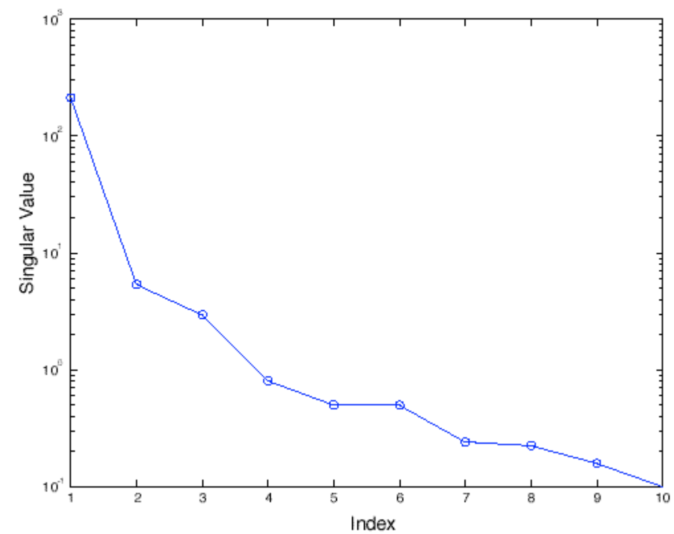
High performance + small memory footprint SVD* fits of magnetic/electric field data have been developed

$$B_{ij} = B\left(\theta_i, \phi_j\right) \quad N \text{ x } N \text{ matrix} \qquad B_{ij}^{\lambda} = \sum_{k=1}^{\lambda} w_k \, g_k\left(\theta_i\right) f_k\left(\phi_j\right)$$

λ-rank approximation

$2\lambda N$ *terms* $\quad \lambda << N$

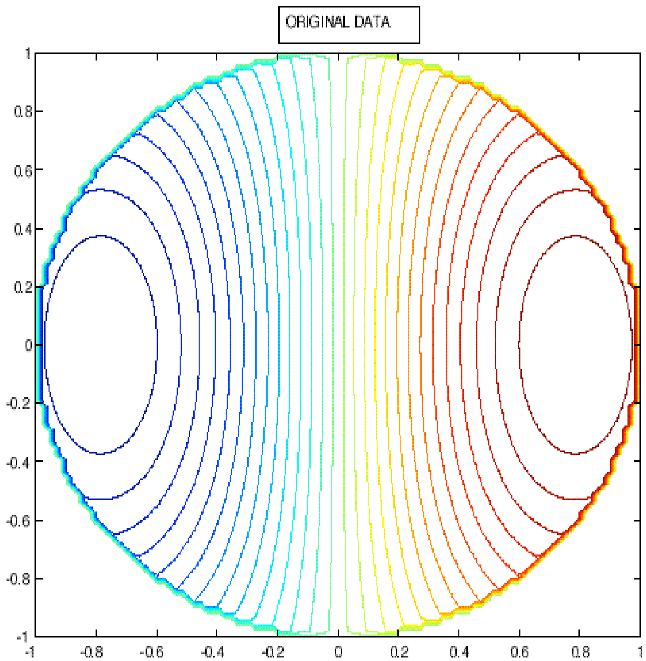


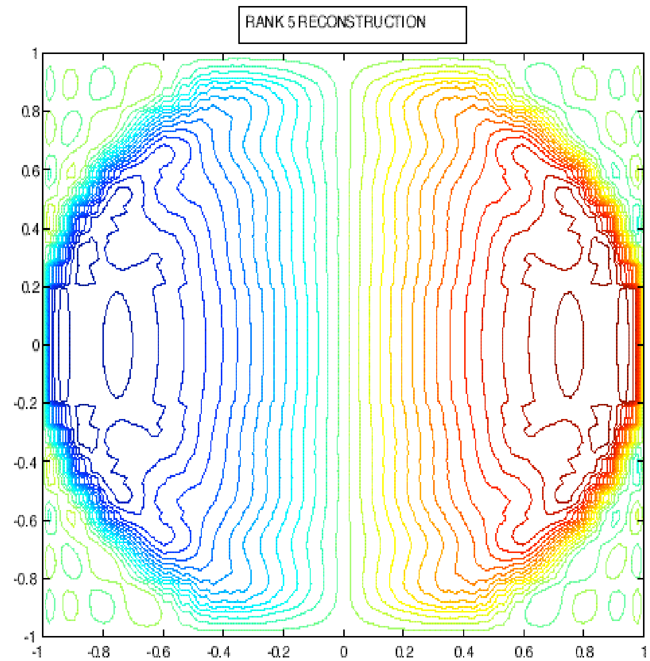


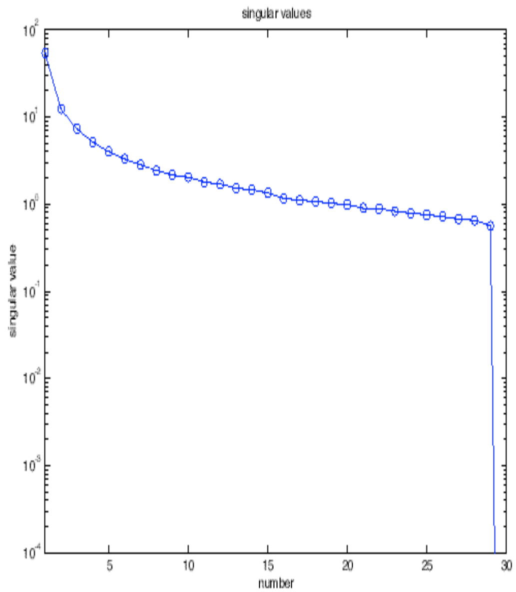
Strategy: combine 2-D SVD* fit (R,Z) with 1-D Fourier series (ϕ)

*SVD: Singular value decomposition

However, SVD method has problems with non-Cartesian boundaries



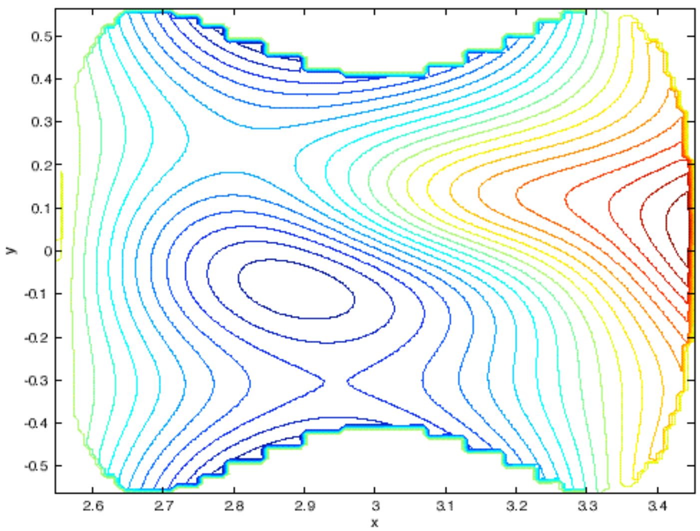




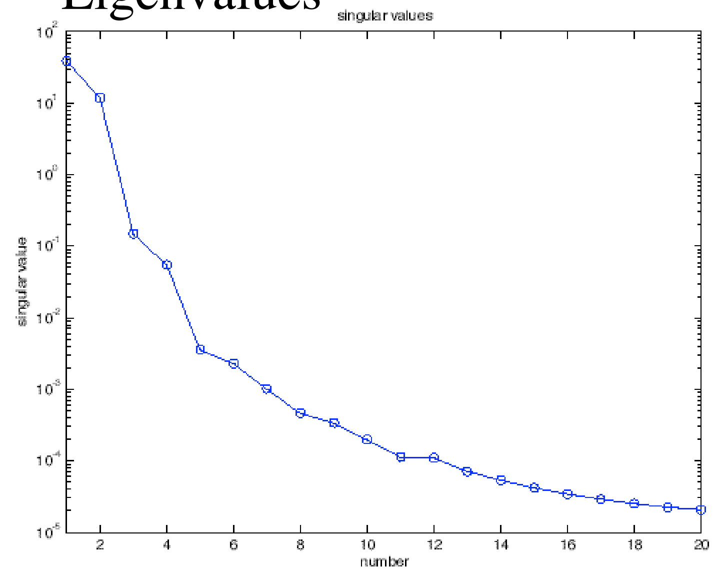
Proposed alternative: Create an extension of the field in the vacuum and apply SDV compression to the total resulting field.

Test of crystal growth algorithm

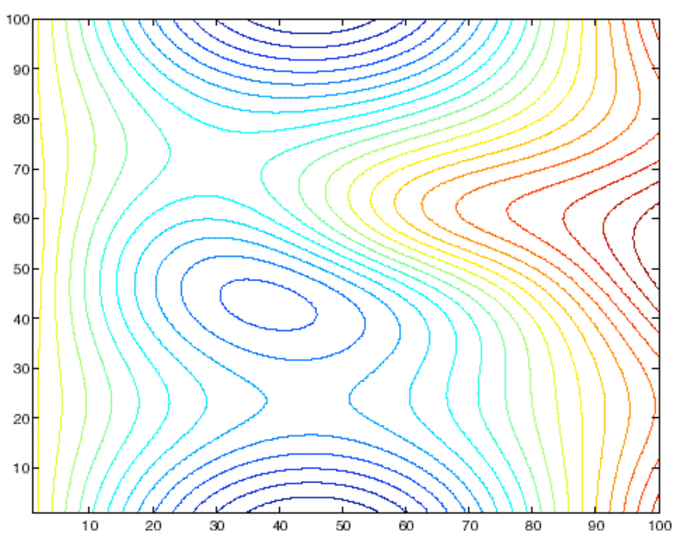
Original data



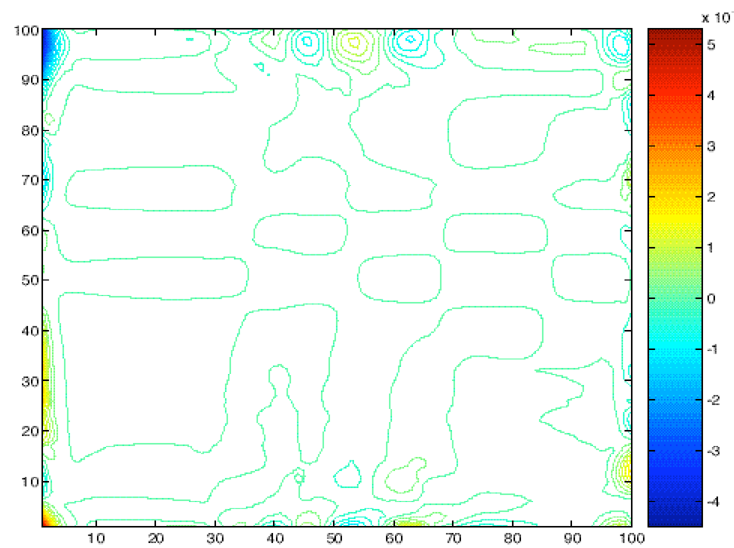
Eigenvalues



Extended data

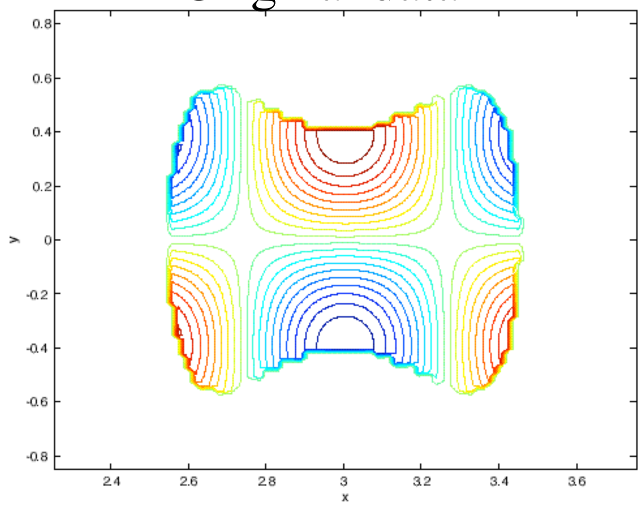


Rank 5 approximation error

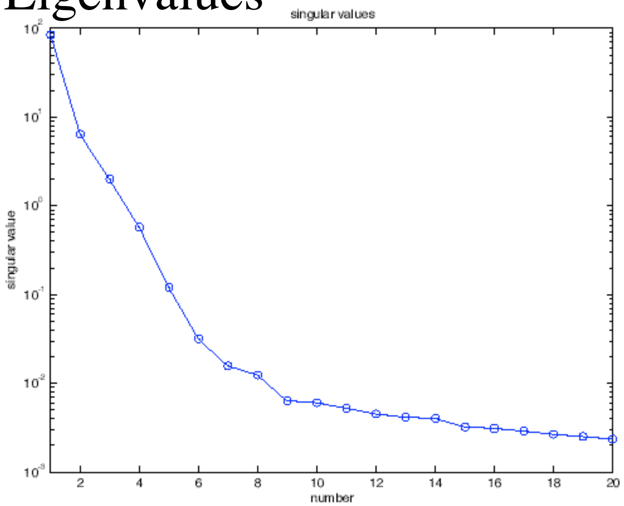


Test of grid extension algorithm

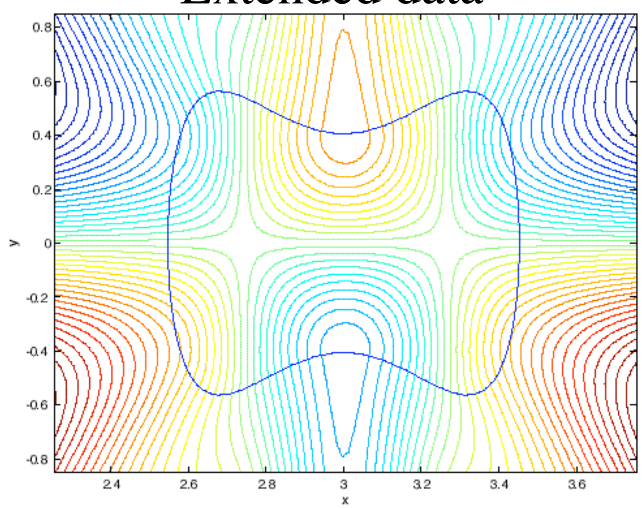
Original data



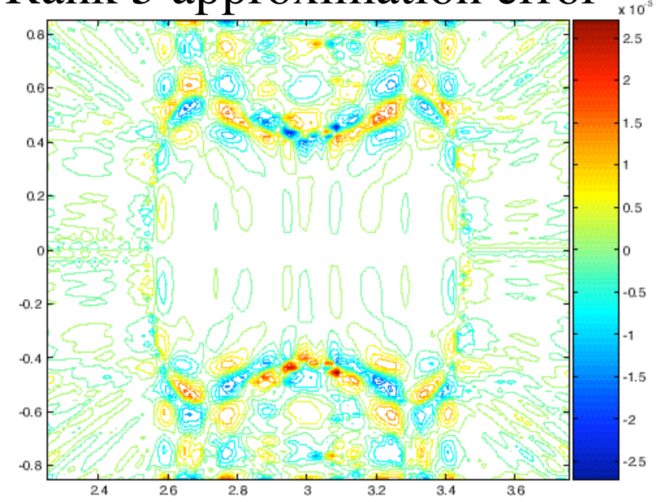
Eigenvalues



Extended data



Rank 5 approximation error



DELTA5D equations were converted from magnetic to cylindrical coordinates

Uses bspllib 3D cubic B-spline fit to data from VMEC

$$\frac{d\vec{R}}{dt} = \frac{1}{B_{\parallel}^{*}}\left[v_{\parallel}\vec{B}^{*} - \hat{b}\times\left(\vec{E}^{*} - \frac{1}{Ze}\mu\vec{\nabla}\left|\vec{B}\right| \right)\right]$$

$$m\frac{dv_{\parallel}}{dt} = \frac{\vec{B}^{*}}{B_{\parallel}^{*}}\bullet\left(Ze\vec{E}^{*} - \mu\vec{\nabla}\left|\vec{B}\right| \right)$$

$$where \quad B_{\parallel}^{*} = \hat{b}\bullet\vec{B}^{*} \qquad \hat{b} = \vec{B}/\left|\vec{B}\right| \qquad \mu = \frac{mv_{\perp}^{2}}{2\left|\vec{B}\right|}$$

$$\vec{B}^{*} = \vec{B} + \frac{mv_{\parallel}}{Ze}\vec{\nabla}\times\hat{b} = \vec{B} - \frac{mv_{\parallel}}{Ze}\hat{b}\times\left(\hat{b}\bullet\vec{\nabla}\hat{b}\right)$$

$$\vec{E}^{*} = \vec{E} - \frac{mv_{\parallel}}{Ze}\frac{\partial\hat{b}}{\partial t} \approx \vec{E} \quad (if\ \partial B/\partial t \ll \Omega_{c})$$

In M3D variables, $\vec{B} = \vec{\nabla}\psi\times\vec{\nabla}\phi + \frac{1}{F}\nabla_{\perp}F + \left(R_{0} + \tilde{I}\right)\vec{\nabla}\phi$

Coulomb collision operator for collisions of test particles (species a) with a background plasma (species b):

$$C_{ab}f_a = \frac{\nu_D^{ab}}{2}\frac{\partial}{\partial\lambda}(1-\lambda^2)\frac{\partial f_a}{\partial\lambda} + \frac{1}{v^2}\frac{\partial}{\partial v}\left\{v^2\left[2\nu_\varepsilon\alpha_{ab}f_a + \frac{\nu_\varepsilon}{v}\alpha_{ab}^3\frac{\partial f_a}{\partial v}\right]\right\}$$

where

$$\nu_D^{ab} = \frac{\nu_0^{ab}}{(v/\alpha_{ab})^3}\left[\phi\left(\frac{v}{\alpha_b}\right) - G\left(\frac{v}{\alpha_b}\right)\right] \qquad \nu_\varepsilon = \nu_0^{ab}G\left(\frac{v}{\alpha_b}\right)$$

$$\phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x dt\; t^{1/2}\; e^{-t} \qquad G(x) = \frac{1}{2x^2}[\phi(x) - x\phi'(x)]$$

$$\alpha_{ab} = \sqrt{\frac{2T_{b0}}{m_a}} \qquad \alpha_b = \sqrt{\frac{2T_{b0}}{m_b}} \qquad \nu_0^{ab} = \frac{4\pi n_b \ln\Lambda_{ab}(e_a e_b)^2}{(2T_b)^{3/2}m_a^{1/2}}$$

Monte Carlo (Langevin) Equivalent of the Fokker-Planck Operator

[A. Boozer, G. Kuo-Petravic, Phys. Fl. **24** (1981)]

$$\lambda_n = \lambda_{n-1}(1 - \nu_d \Delta t) \pm \left[\left(1 - \lambda_{n-1}^2\right)\nu_d \Delta t\right]^{1/2}$$

$$E_n = E_{n-1} - (2\nu_\varepsilon \Delta t)\left[E_{n-1} - \left(\frac{3}{2} + \frac{E_{n-1}}{\nu_\varepsilon}\frac{d\nu_\varepsilon}{dE}\right)T_b\right] \pm 2\left[T_b E_{n-1} \nu_\varepsilon \Delta t\right]^{1/2}$$

Local Monte-Carlo equivalent quasilinear ICRF operator (developed by J. Carlsson)

$$E^{+} = E^{-} + \mu^{E} + \zeta\sqrt{\sigma^{EE}} \qquad \lambda^{+} = \lambda^{-} + \mu^{\lambda} + \zeta\sqrt{\sigma^{\lambda\lambda}}$$

$\zeta = $ a zero-mean, unit-variance random number (i.e., $\mu^{\zeta} = 0$ and $\sigma^{\zeta} = 1$)

$$\sigma^{EE} = 2\,m^2 v_\perp^2 \Delta v_0 \qquad \sigma^{\lambda\lambda} = 2\left(\frac{k_{||}}{\omega} - \frac{v_{||}}{v^2}\right)^2 \frac{v_\perp^3 \Delta v_0}{v^2}$$

$$\mu^{E} = 2\left(1 - \frac{k_{||} v_{||}}{\omega}\right) m v_\perp \Delta v_0 \qquad \mu^{\lambda} = \left\{2\left[\left(1 - \frac{k_{||} v_{||}}{\omega}\right) - \frac{v_\perp^2}{v^2}\right]\left(\frac{k_{||}}{\omega} - \frac{v_{||}}{v^2}\right) + \frac{v_{||}}{v^2}\frac{v_\perp^2}{v^2}\right\}\frac{v_\perp \Delta v_0}{v}$$

where

$$\Delta v_0 = \frac{1}{v_\perp}\left(\frac{eZ}{2m}\left|E_+ J_{n-1}(k_\perp \rho) + E_- J_{n+1}(k_\perp \rho)\right|\right)^2 \frac{2\pi}{n|\dot{\Omega}|}$$

as $\dot{\Omega} \to 0$

$$\frac{2\pi}{n|\dot{\Omega}|} \to 2\pi^2 \left|\frac{2}{n\ddot{\Omega}}\right|^{2/3} \times \mathrm{Ai}^2\left(-\frac{n^2\dot{\Omega}^2}{4}\left|\frac{2}{n\ddot{\Omega}}\right|^{4/3}\right)$$

A new δf partitioning method is used that separates not only the Maxwellian, but also $E_{||}$, $u_{||}$, $q_{||}$, and diamagnetic flow distortions of f_M:

$$f = f_M \left[1 + \frac{e}{T} \int \frac{dl}{B} \left(BE_{\parallel} - \frac{B^2}{\langle B^2 \rangle} \langle BE_{\parallel} \rangle \right) \right]$$

Extension of H. Sugama, S. Nishimura, Phys. Plasmas 9, 4637 (2002) to δf particle method

$$+ \frac{2}{v_{th}} \frac{v_{\parallel}}{v} x \; f_M \left[u_{\parallel} + \left(x^2 - \frac{5}{2} \right) \frac{2q_{\parallel}}{p} \right]$$

$$+ \frac{f_M}{T} \left[\delta f_U \left\{ \frac{\langle u_{\parallel} B \rangle}{\langle B^2 \rangle} + \left(x^2 - \frac{5}{2} \right) \frac{2 \langle q_{\parallel} B \rangle}{p \langle B^2 \rangle} \right\} + \delta f_X \left\{ X_1 + X_2 \left(x^2 - \frac{5}{2} \right) \right\} + \alpha \left(\delta f_U + m v_{\parallel} B \right) \right]$$

$$(V - C) \delta f_U = \sigma_U = -m v^2 P_2(v_{\parallel} / v) \vec{B} \bullet \vec{\nabla} \ln B \qquad (V - C) \delta f_X = \sigma_X = -\frac{v^2}{2\Omega} P_2(v_{\parallel} / v) \vec{B} \bullet \vec{\nabla} \left(B \tilde{U} \right)$$

$$where \quad x = v / v_{th}, \;\; \tilde{U} = Pfirsch - Schlüter \;\; flow = \frac{B_{\zeta}}{B} \left[1 - \frac{B^2}{\langle B^2 \rangle} \right] \;\; for \;\; tokamak, \;\; P_2(y) = \frac{3}{2} y^2 - \frac{1}{2}$$

From these δf components, either the Sugama/Nishimura M*, N*, L* or DKES D_{11}, D_{13}, D_{33} coeffiecients can be directly obtained

$$\text{M*, N*, L* viscosity coefficients = functions of : } (\delta f_U, \sigma_U);\ (\delta f_X, \sigma_X);\ (\delta f_U, \sigma_X)$$

$$with\ \ (\cdots,\cdots) = \frac{1}{2}\int_{-1}^{1} d(v_\parallel / v) \oiint_{\theta,\zeta} (\cdots,\cdots)\sqrt{g}\, / V'$$

M*, N*, L* from D_{11}, D_{13}, D_{33}:

$$M^* = \left(\frac{\nu}{\mathrm{v}}\right)^2 \frac{D_{33}}{D} \qquad where \quad D = 1 - \frac{3}{2}\frac{\nu}{\mathrm{v}}\frac{D_{33}}{\langle B^2 \rangle}$$

$$N^* = \left(\frac{\nu}{\mathrm{v}}\right)\frac{D_{13}}{D}$$

$$L^* = D_{11} - \frac{2}{3}\frac{\nu}{\mathrm{v}}\tilde{U}^2 + \frac{3}{2}\frac{\nu}{\mathrm{v}}\frac{D_{13}^2}{D\langle B^2 \rangle}$$

D_{11}, D_{13}, D_{33} from M*, N*, L*:

$$D_{33} = \frac{M^*}{\left(\frac{\nu}{\mathrm{v}}\right)^2 + \frac{3}{2}\frac{\nu}{\mathrm{v}}\frac{M^*}{\langle B^2 \rangle}} \qquad D = 1 - \frac{3}{2}\frac{\nu}{\mathrm{v}}\frac{D_{33}}{\langle B^2 \rangle}$$

$$D_{13} = \left(\frac{\nu}{\mathrm{v}}\right)^{-1} D N^*$$

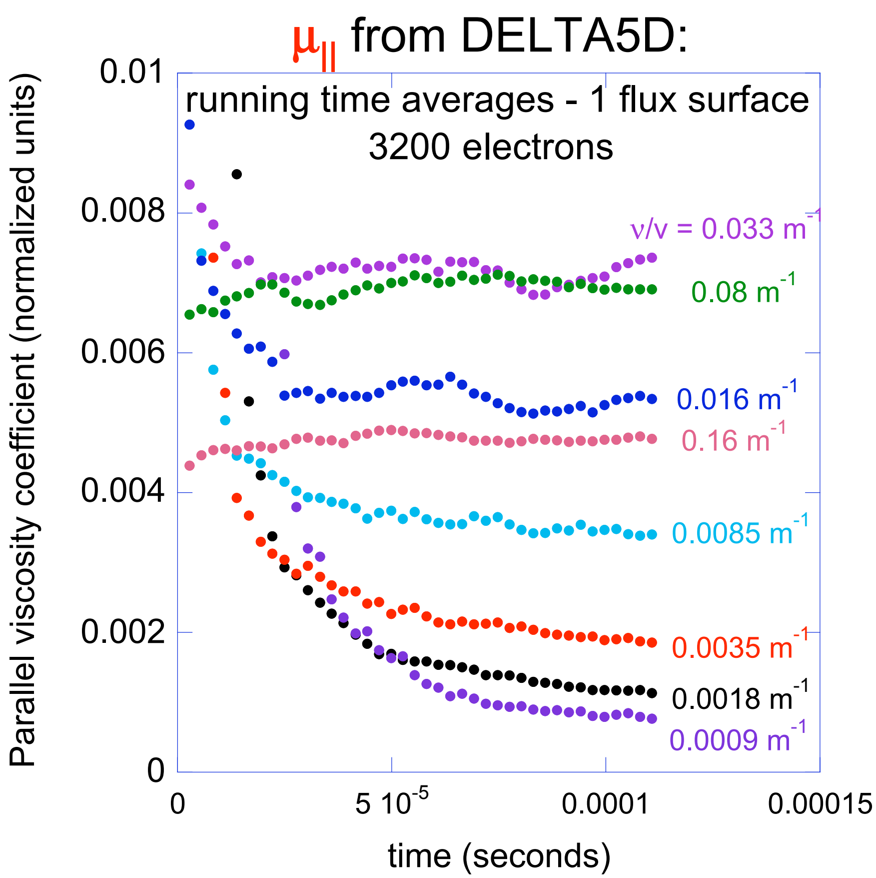
$$D_{11} = L^* + \frac{2}{3}\frac{\nu}{\mathrm{v}}\tilde{U}^2 - \frac{3}{2}\left(\frac{\nu}{\mathrm{v}}\right)^3 D \frac{(N^*)^2}{\langle B^2 \rangle}$$

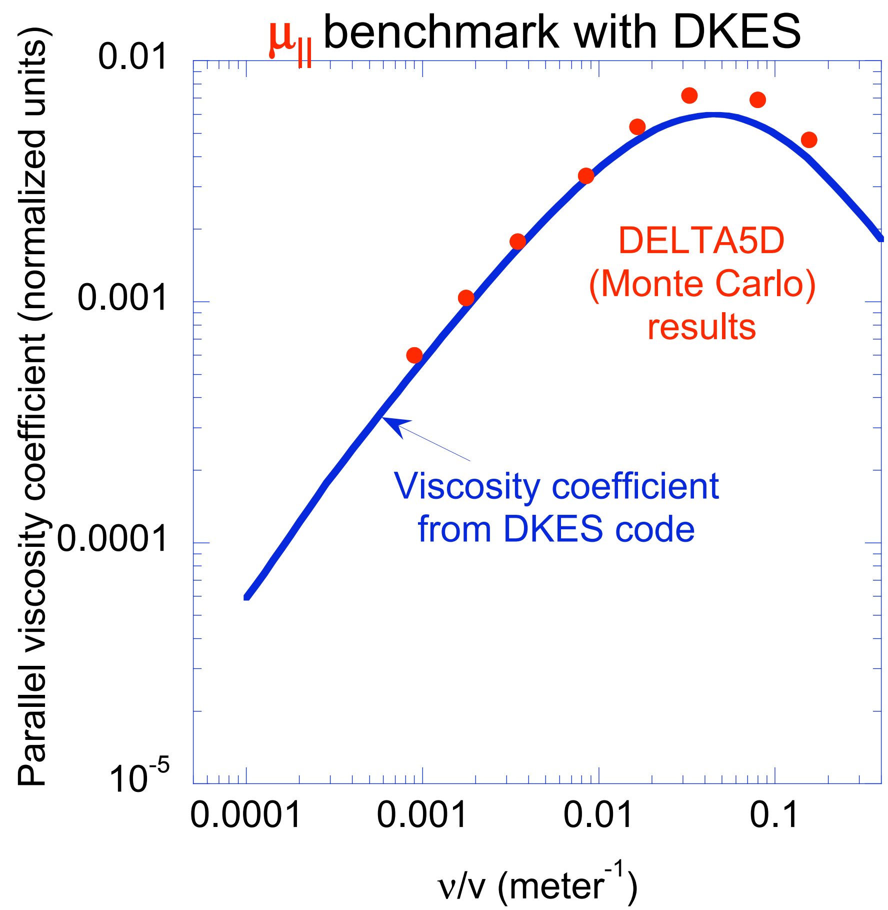
New MHD viscosity-based closure relations are more consistent with the MHD model

DELTA5D

$$\begin{bmatrix} \mathbf{B}\cdot(\nabla\cdot\Pi) \\ \mathbf{B}\cdot(\nabla\cdot\Theta) \end{bmatrix} = \begin{bmatrix} M_1 & M_2 \\ M_2 & M_3 \end{bmatrix} \begin{bmatrix} V_{\|} \\ Q_{\|} \end{bmatrix} + \begin{bmatrix} N_1 & N_2 \\ N_2 & N_3 \end{bmatrix} \begin{bmatrix} \frac{1}{n}\frac{\partial p}{\partial s} - e\frac{\partial \phi}{\partial s} \\ -\frac{\partial T}{\partial s} \end{bmatrix}$$

$$\text{where } M_j, N_j \propto \int_0^\infty dE\, e^{-E/kT}\sqrt{E}\left(E - \frac{5}{2}kT\right)^{j-1} \mu_{\|}, N(E)$$



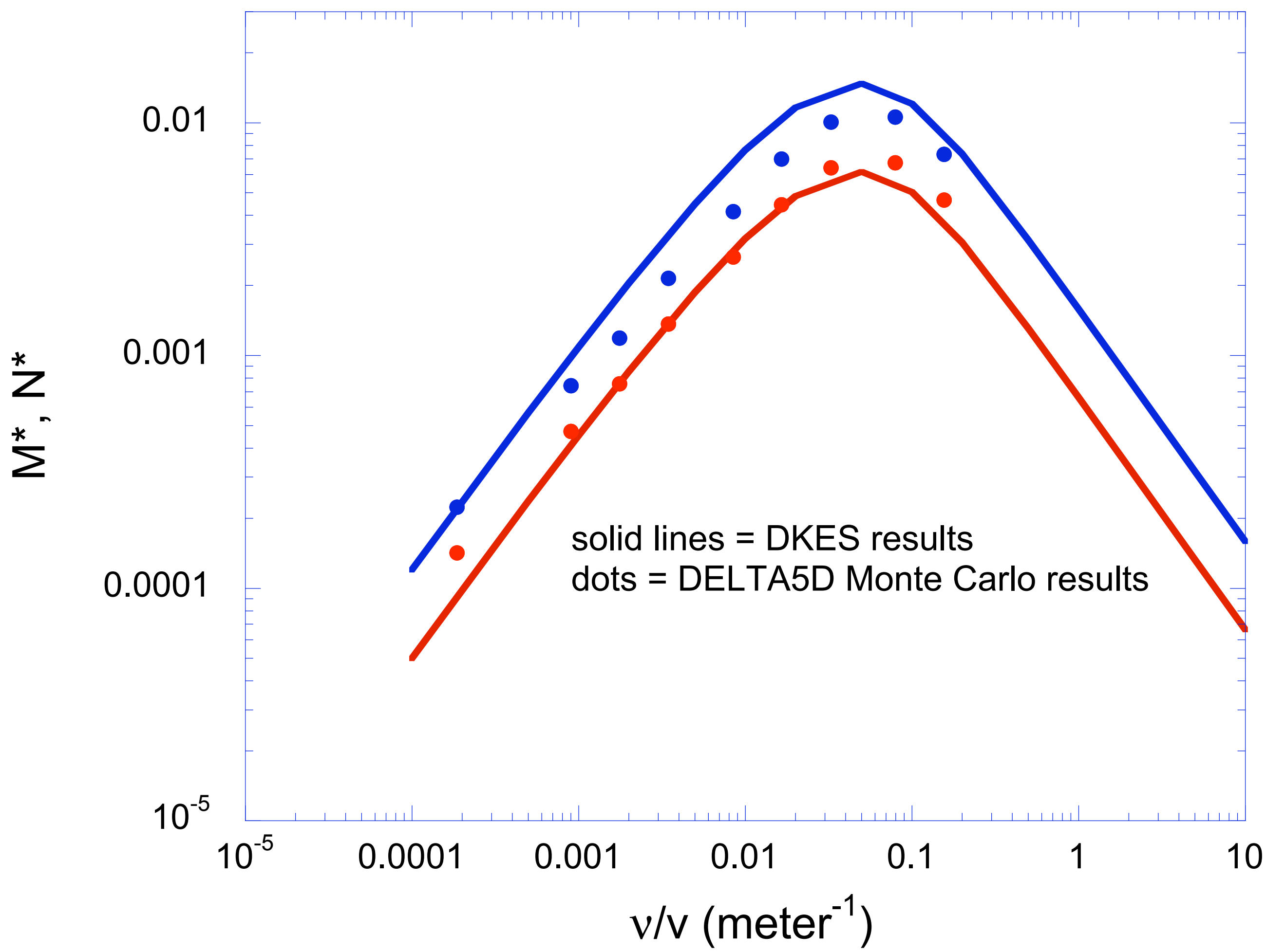


* DKES: Drift Kinetic Equation Solver

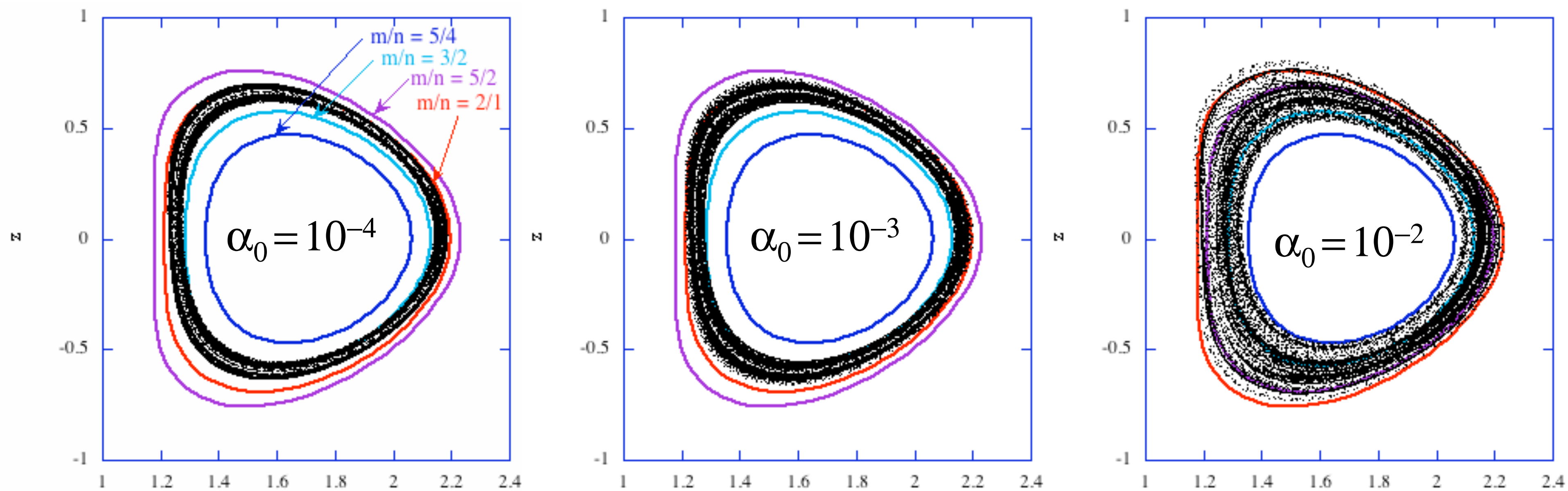
This comparison has recently been extended to the N* coefficient and extended to lower collisionality

$$\begin{bmatrix} \mathbf{B}\cdot\left(\nabla\cdot\Pi\right) \\ \mathbf{B}\cdot\left(\nabla\cdot\Theta\right) \end{bmatrix} = \begin{bmatrix} M_1 & M_2 \\ M_2 & M_3 \end{bmatrix} \begin{bmatrix} V_{\parallel} \\ Q_{\parallel} \end{bmatrix} + \begin{bmatrix} N_1 & N_2 \\ N_2 & N_3 \end{bmatrix} \begin{bmatrix} \frac{1}{n}\frac{\partial p}{\partial s} - e\frac{\partial \phi}{\partial s} \\ -\frac{\partial T}{\partial s} \end{bmatrix}$$

$$\text{where } M_j, N_j \propto \int_0^\infty dE\, e^{-E/kT}\sqrt{E}\left(E - \frac{5}{2}kT\right)^{j-1} \quad M^*, N^*(E)$$

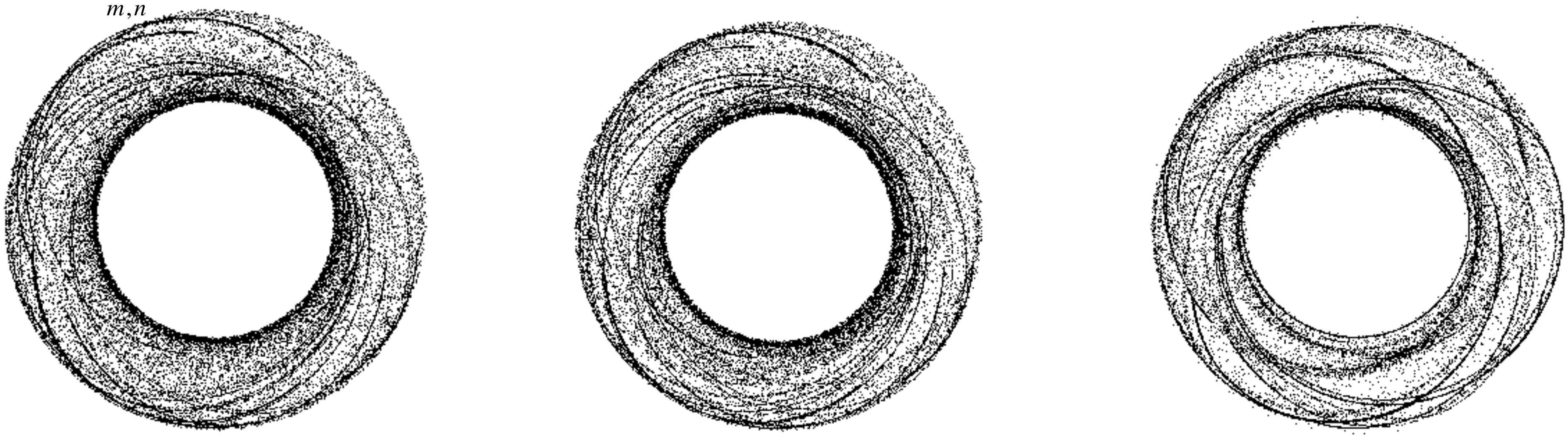


A model perturbed field has been added to mock up tearing modes: $\mathbf{B} = \mathbf{B}_{VMEC} + \nabla\times(\alpha\mathbf{B}_{VMEC})$:



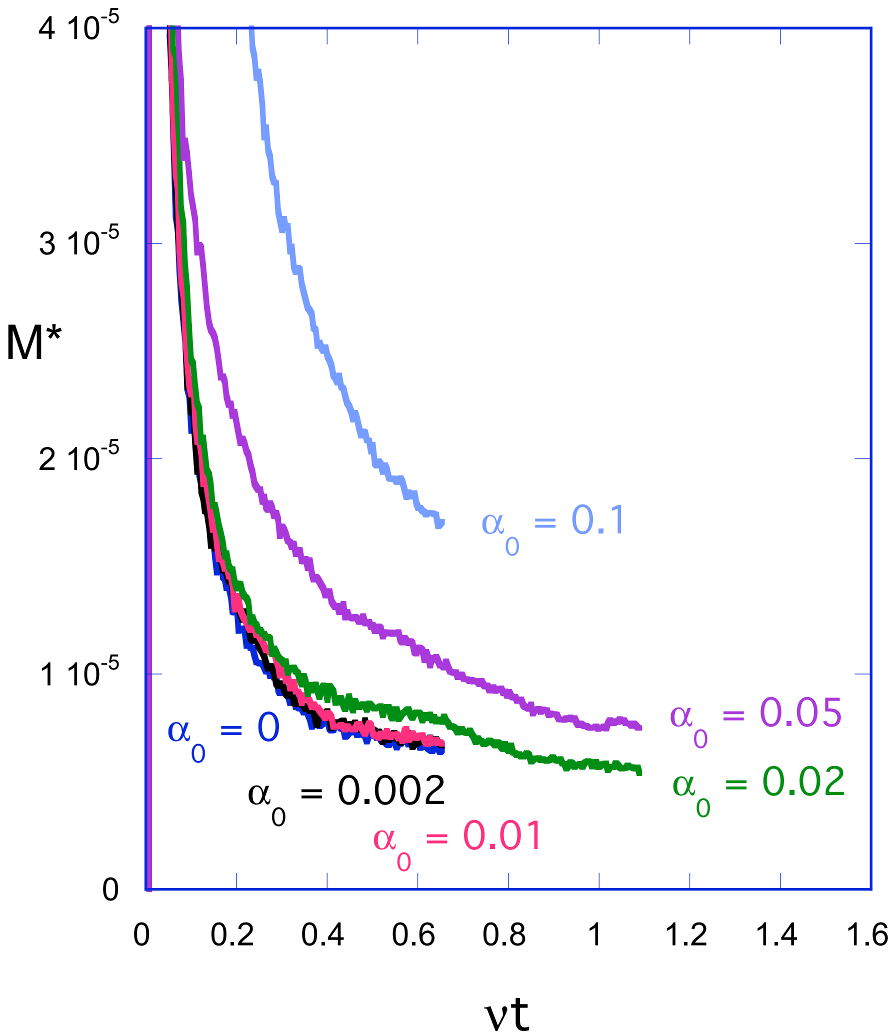
$$\alpha = \sum_{m,n}\left[\alpha_{mnc}(\psi)\cos(m\theta - n\phi) + \alpha_{mns}(\psi)\sin(m\theta - n\phi)\right]$$

$$\alpha_{mnc,s}(\psi) = \alpha_0 e^{-(\psi-\psi_0)^2/\Delta^2}$$

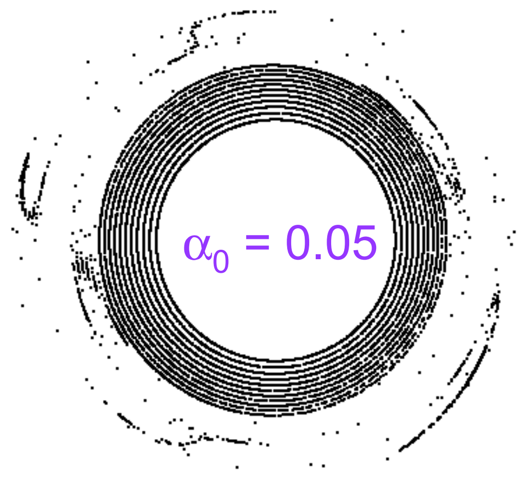


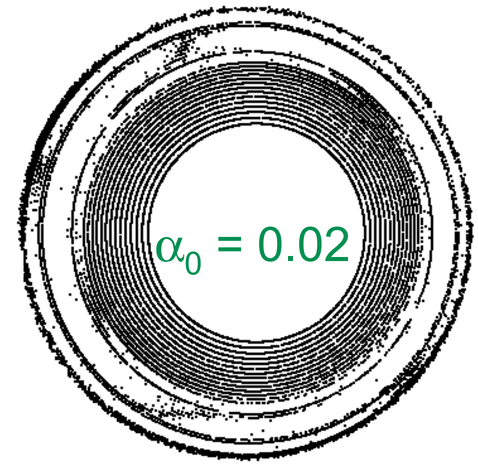
Magnetic perturbations increase viscosity

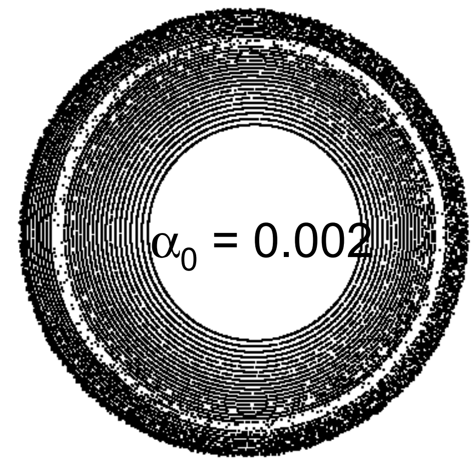
$$\alpha = \sum_{m,n} \left[\alpha_{mnc}(\psi)\cos(m\theta - n\phi) + \alpha_{mns}(\psi)\sin(m\theta - n\phi) \right] \qquad \alpha_{mnc,s}(\psi) = \alpha_0 e^{-(\psi-\psi_0)^2/\Delta^2}$$



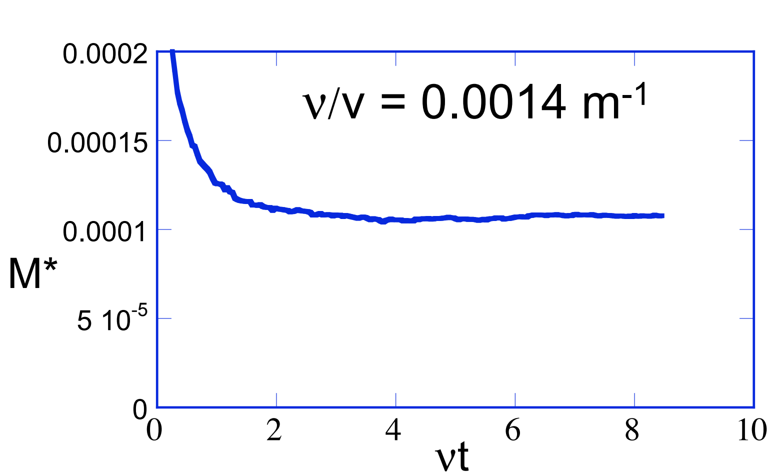
field line puncture plots:

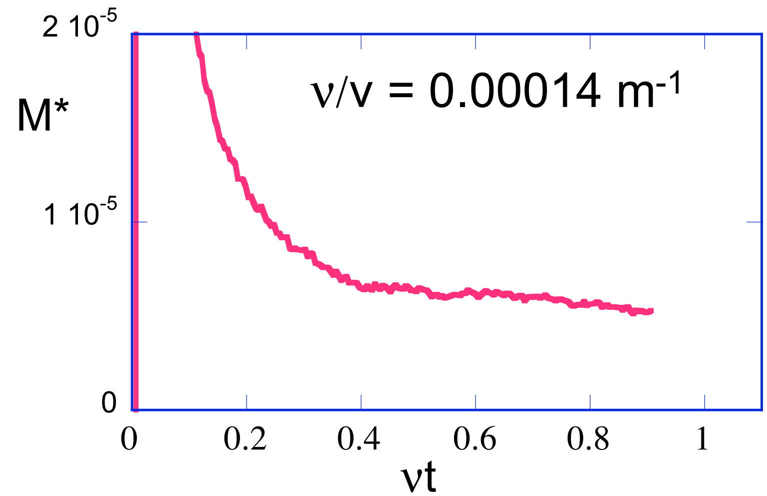




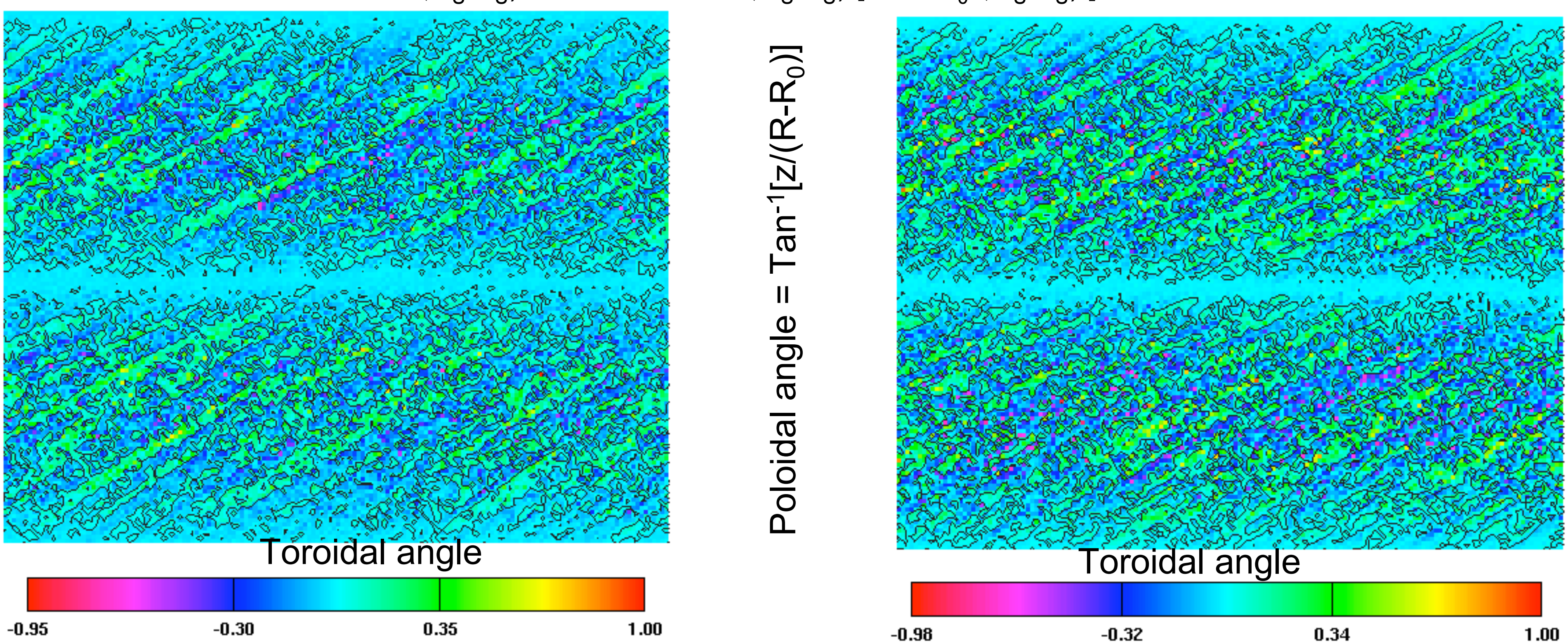


Local viscosity variation within a flux surface



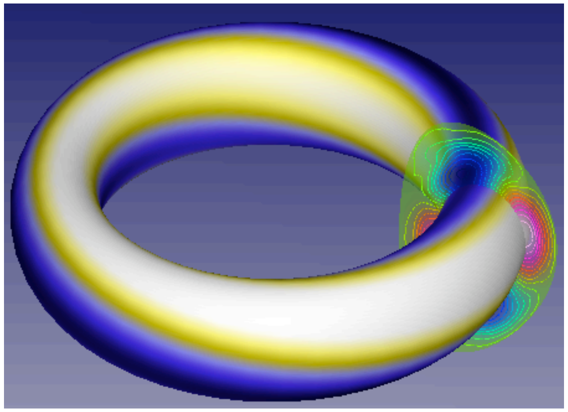


($\delta f_U,\sigma_U$) contours, $M^* \sim (\delta f_U,\sigma_U)/[1\text{-}1.5C_0\ (\delta f_U,\sigma_U)\ ]$



In the next phase, kinetic closure relations will be further developed and coupled with the MHD model:

Nonlinear M3D 2/1 tearing mode



- **Closure relations**
  - Calculate using fields from M3D tearing mode
    - Recent data from W. Park, G-Y. Fu
  - Study 2D/3D variation of stress tensor
  - Time-varying stress tensor - rotating island
  - Accelerate slow collisional time evolution of viscosity coefficients
    - Test pre-converged restarts
    - Equation-free projective integration extrapolation methods
  - Green-Kubo molecular dynamics methods - direct viscosity calculation
- **DELTA5D/M3D coupling**
  - Interface, numerical stability, data compression, gather/scatter

Open Closure Issues:

Increasing
Island
size

- Your suggestions are welcome
- Do we forge ahead with existing moments method for general toroidal systems (small island limit)?
- Identify island regions and define local coordinate sytems within them (“stellarator within a tokamak” model)?
  - Maintenance of ambipolarity and charge neutrality within islands
- Can these particle closure methods be extended to more general magnetic field models:

$$\vec{B} = \psi' \ \vec{\nabla}\rho \times \vec{\nabla}\theta + \chi' \ \vec{\nabla}\zeta \times \vec{\nabla}\rho \qquad \Rightarrow \qquad \vec{B} = \vec{\nabla}\alpha \times \vec{\nabla}\beta$$