Particle-based neoclassical closure relations for NTM simulations

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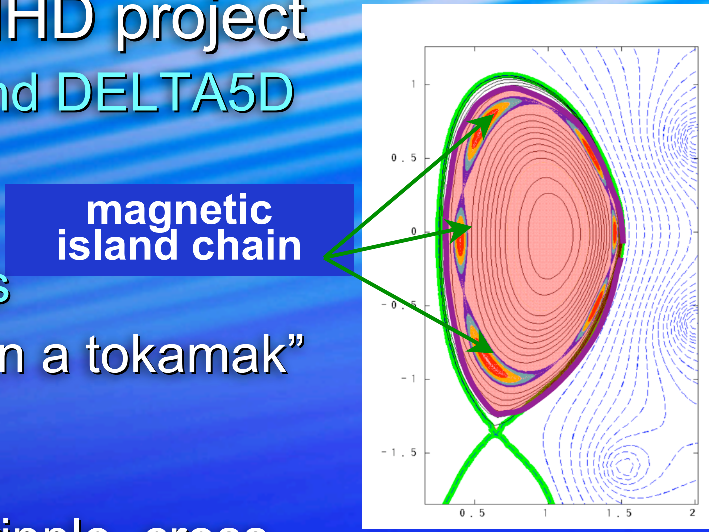
NTM simulation requires MHD closure relations with long-mean free path effects in localized 3–dimensional regions (magnetic islands)

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
- 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



Neoclassical transport particle 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

Our computational method for NTM closures includes three components:

- M3D to DELTA5D coupling
  - data compression (3D SVD method)
  - noise reduction, smoothing
  - particles assigned to processors
- Particle closure relation
  - new δf method
  - preserves fluid flow velocities from M3D
  - calculates viscosities
- DELTA5D to M3D coupling
  - data compression
  - noise reduction, smoothing (3D SVD method)

MHD to particle coupling

- Need for following particles multiple steps between MHD steps
  - Physics reason: collisional evolution
  - Computational reason: noise reduction, filtering
- Data compression
  - Improved scatter operations
  - Assign particles to processors or regions
- Discretization error smoothing in MHD code data
- Performance issues
  - Cache paging

SVD data compression method

- SVD (Singular Value Decomposition)
- POD (Principal Orthogonal Decomposition)
  - Extracts “dominant features” and coherent structures
  - Compresses information into a few low order weights and orthonormal eigenfunctions
  - 2D data - standard method

$$A_{ij} = \sum_{k=1}^{N_J} w_k u_k(x_i) v_k(y_j) \qquad \text{data compression ratio} = R_c = \frac{N_I N_J}{r(N_I + N_J + 1)}$$

$$r = \text{ \# of terms in k summation}$$

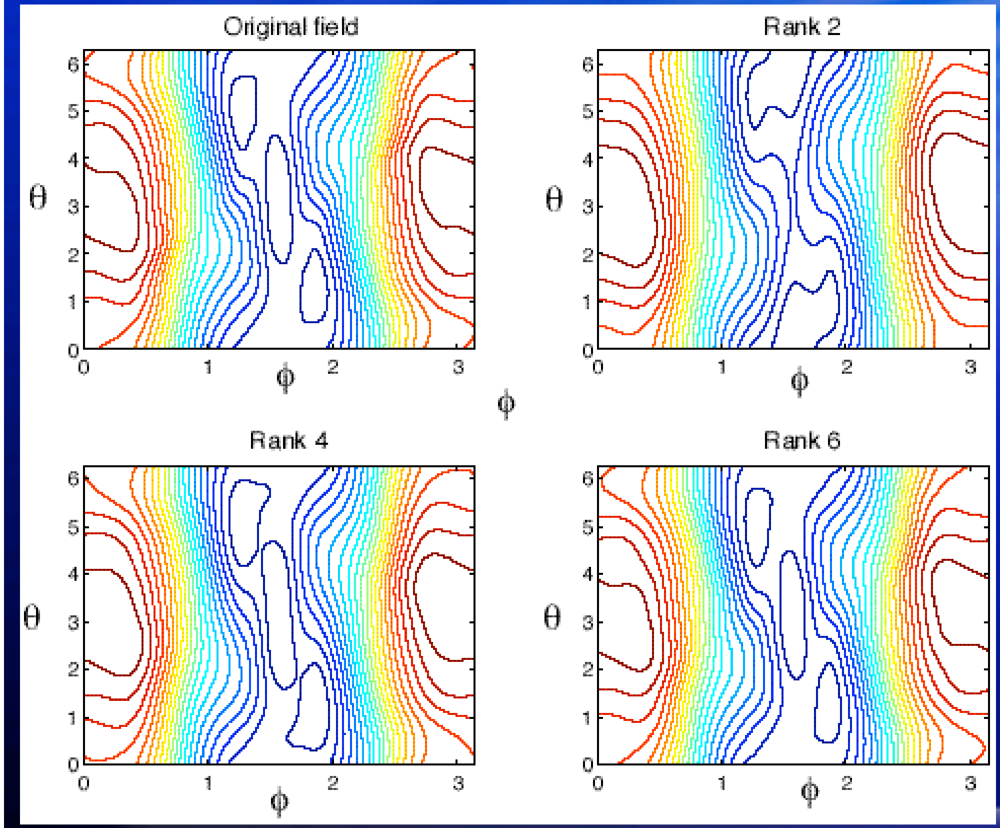
  - 3D data
    - Generalized low rank approximation (GLRA)
    - Stacking (folding) methods
    - 2D SVD + Fourier decomposition in toroidal angle

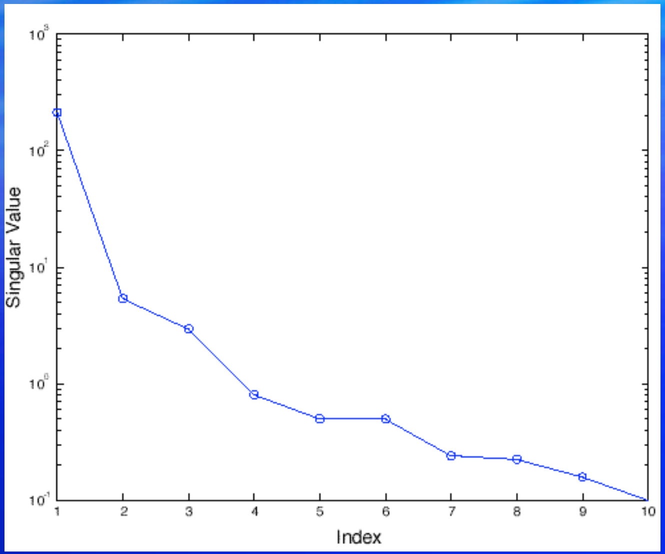
High performance + small memory footprint SVD* fits of magnetic/electric field data have been developed

$$B_{ij} = B\left(\theta_i, \phi_j\right)$$ N x N matrix

$$B_{ij}^{\lambda} = \sum_{k=1}^{\lambda} w_k \, g_k\left(\theta_i\right) f_k\left(\phi_j\right)$$ 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

SVD data compression method for three-dimensional data

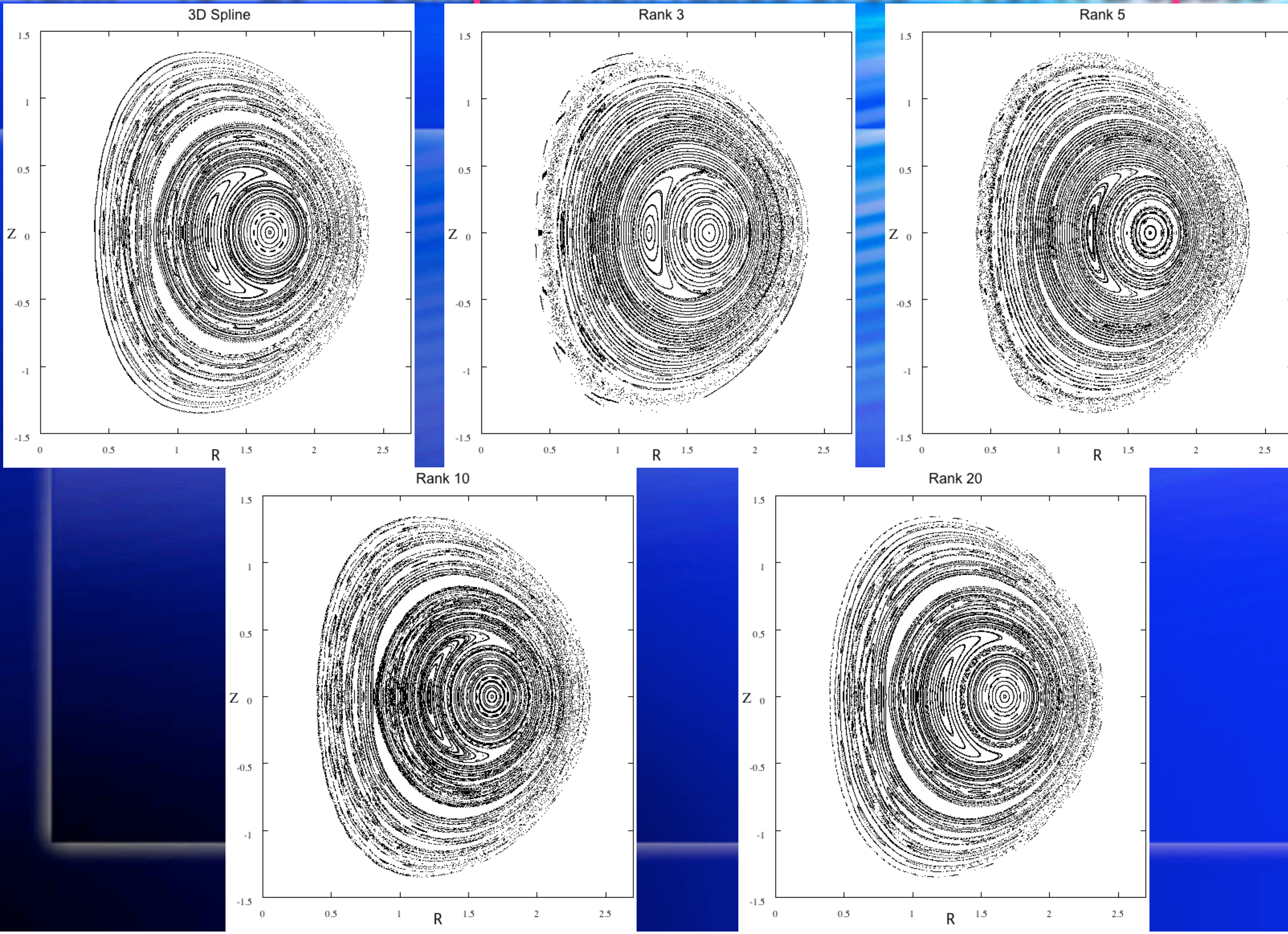
- GLRA (Generalized Low Rank Approximation) method recently developed
  - J. Ye in *21st International Conference on Machine Learning (2004)*
  - *D. del-Castillo Negrete, D. Spong, E. D'Azevedo, S. Hirshman, "Compression of MHD Simulation Data Using SVD," in preparation*
- Iterative algorithm for minimizing Frobenius norm between 3D data and GLRA matrix form:

$$\sum_{k=1}^{N_K} \left\| a_k - L D_k R^T \right\|^2 \qquad (a_k)_{ij} \equiv A_{ijk}$$

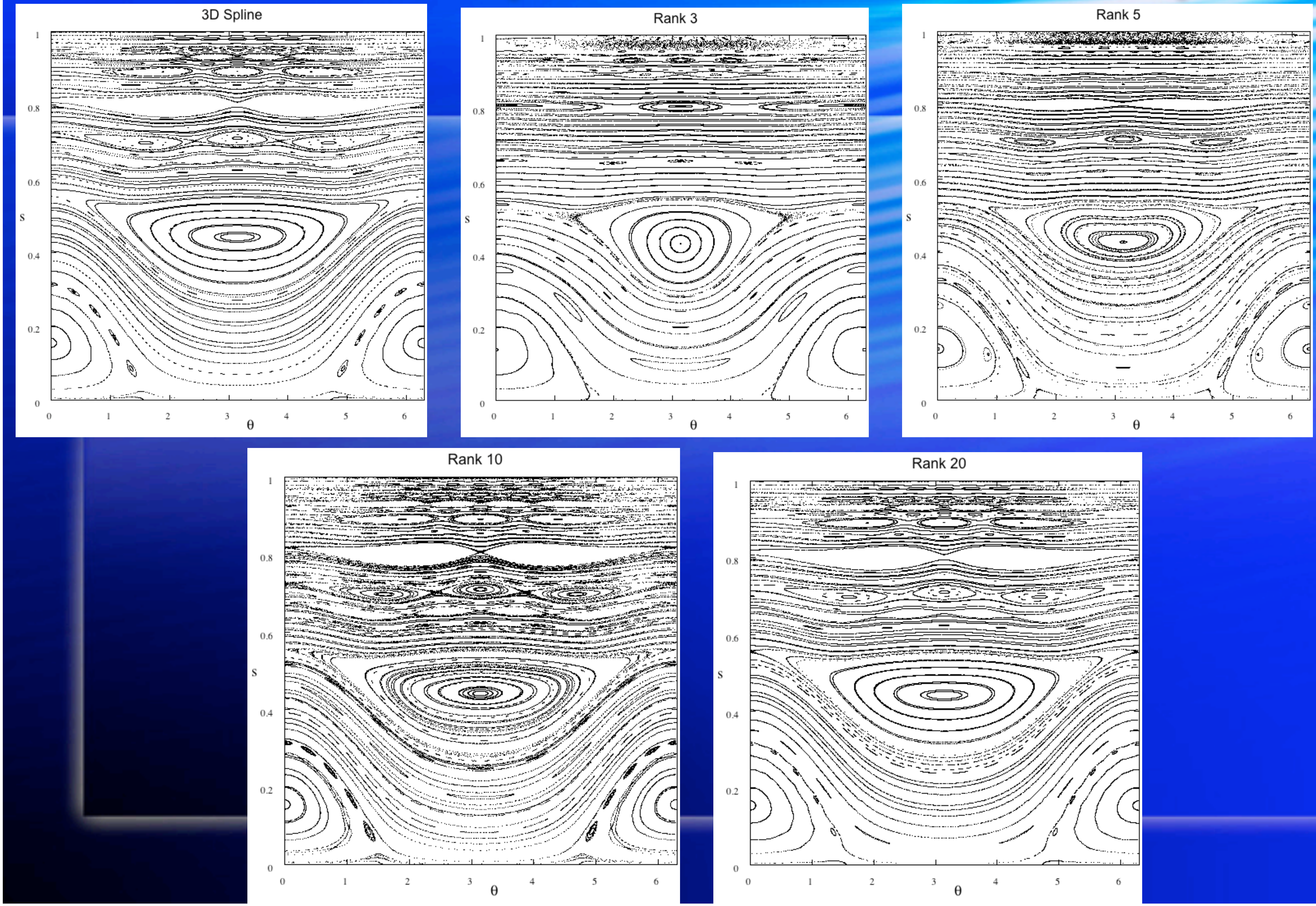
$$L \in R^{I \times r_1} \quad and \quad L \in R^{J \times r_2} \text{ are 2D matrices independent of k}$$

  - Analogous to 2D SVD (N_k = 1 limit), but iteration required and D_k matrices are not diagonal

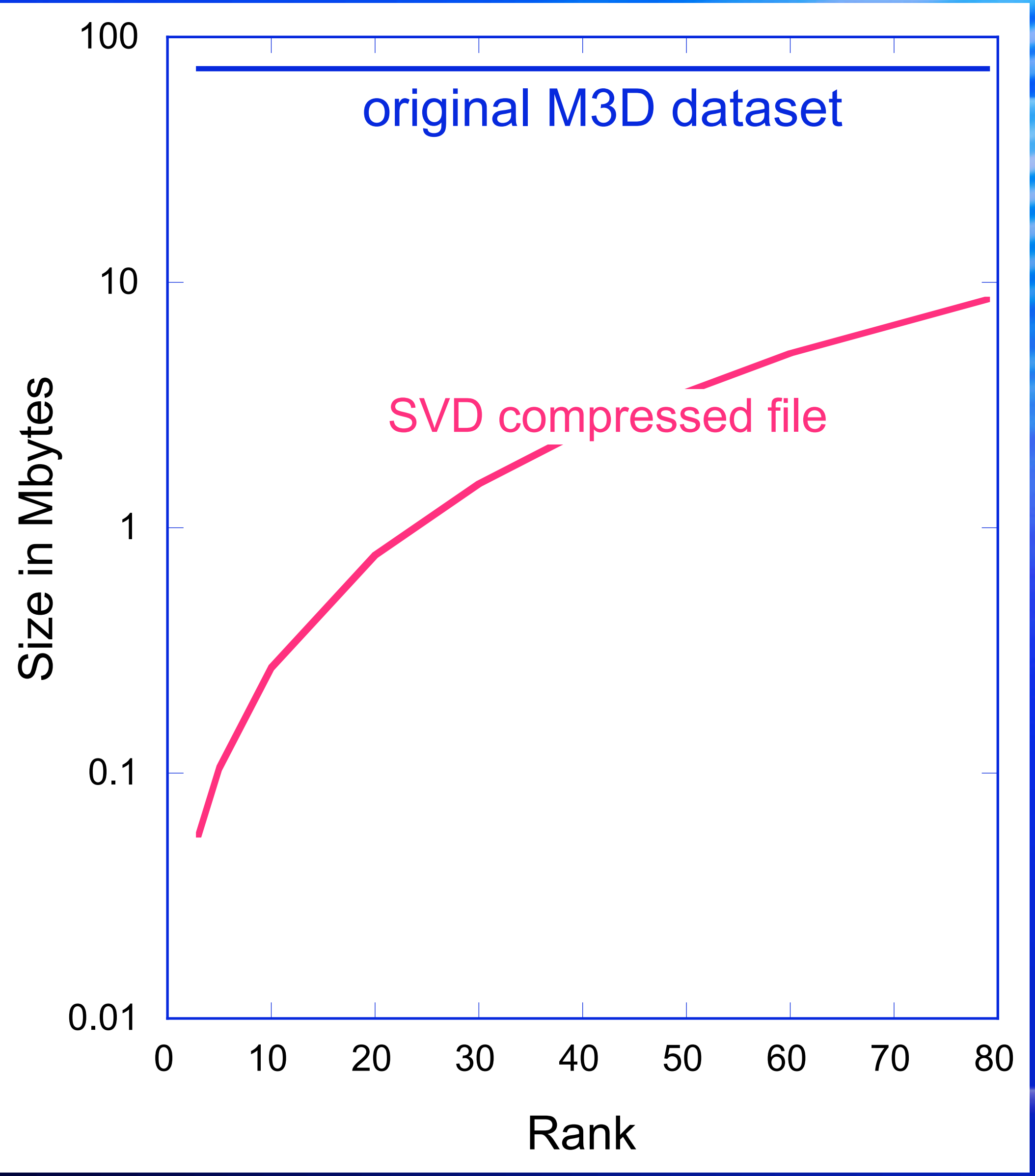
SVD fits of M3D dataset reproduce more exact fits for rank = 10 - 20 -> compression ratios of 35 - 100: R-Z space



SVD fits of M3D dataset reproduce more exact fits for rank = 10 - 20 -> compression ratios of 35 - 100: s-θ space



Significant compressions can be achieved while retaining all significant data features



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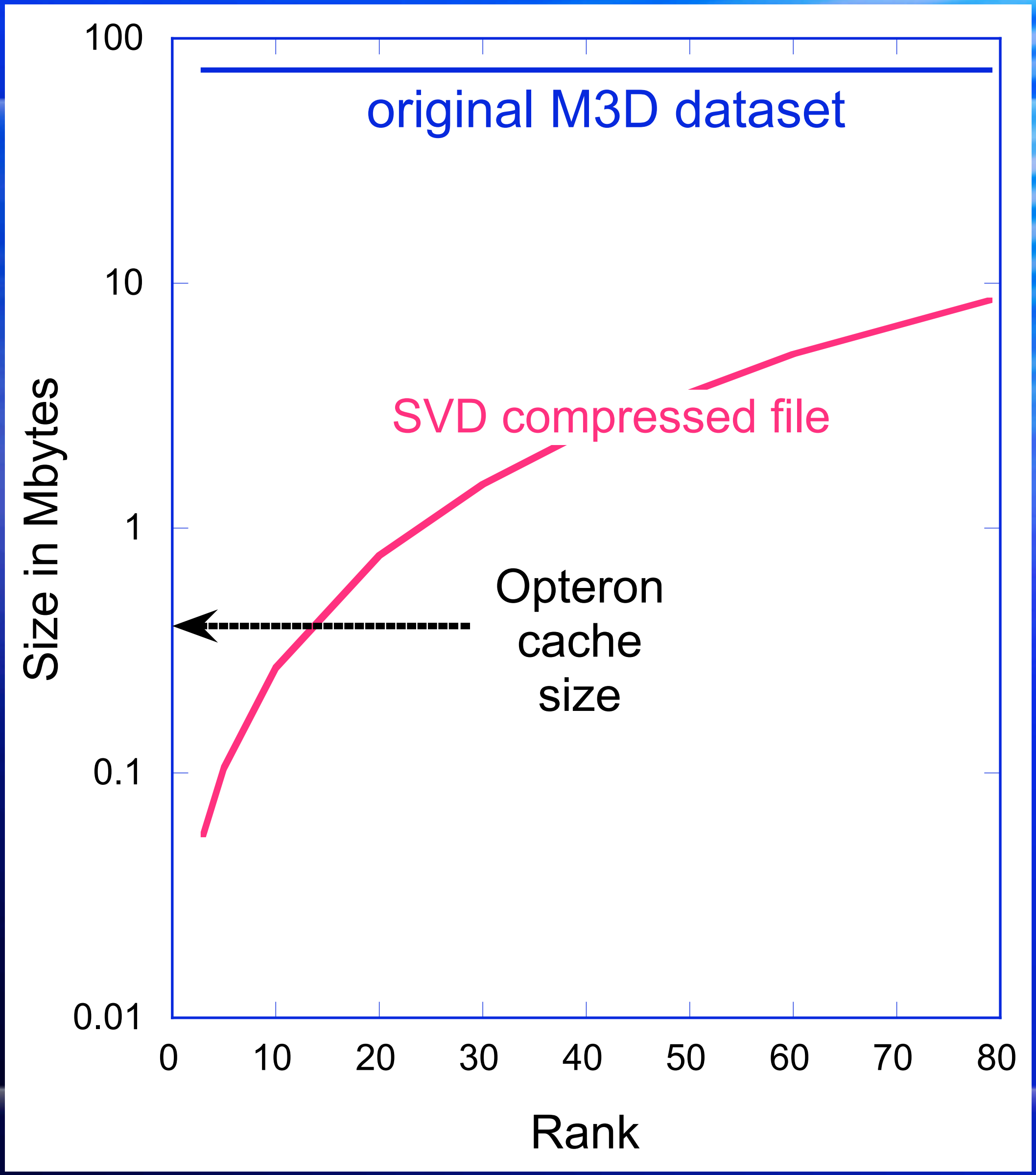


Neoclassical Closure Relations

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**

DELTA5D equations were converted from magnetic to cylindrical coordinates
Uses 3D cubic B-spline fit to data from VMEC

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

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

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

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

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

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

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

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

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

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)

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

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

$$\sigma^{EE} = 2\,m^{2} v_{\perp}^{2} \Delta v_{0} \qquad \sigma^{\lambda\lambda} = 2\left(\frac{k_{\parallel}}{\omega} - \frac{v_{\parallel}}{v^{2}}\right)^{2} \frac{v_{\perp}^{3}\Delta v_{0}}{v^{2}}$$

$$\mu^{E} = 2\left(1 - \frac{k_{\parallel} v_{\parallel}}{\omega}\right) m v_{\perp} \Delta v_{0} \qquad \mu^{\lambda} = \left\{2\left[\left(1 - \frac{k_{\parallel} v_{\parallel}}{\omega}\right) - \frac{v_{\perp}^{2}}{v^{2}}\right]\left(\frac{k_{\parallel}}{\omega} - \frac{v_{\parallel}}{v^{2}}\right) + \frac{v_{\parallel}}{v^{2}}\frac{v_{\perp}^{2}}{v^{2}}\right\}\frac{v_{\perp}\Delta v_{0}}{v}$$

where

$$\Delta v_{0} = \frac{1}{v_{\perp}}\left(\frac{eZ}{2m}\left|E_{+} J_{n-1}(k_{\perp}\rho) + E_{-} J_{n+1}(k_{\perp}\rho)\right|\right)^{2} \frac{2\pi}{n\left|\dot{\Omega}\right|}$$

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

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

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

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

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

$$(V - C)\delta f_U = \sigma_U = -mv^2 P_2(v_{\parallel}/v)\vec{B}\bullet\vec{\nabla}\ln B$$

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

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

From these δf components, either the Sugama/Nishimura M*, N*, L* or DKES D11, D13, D33 coeffiecients can be obtained

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

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

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

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

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

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

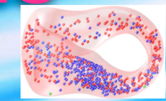
D_{11}, D_{13}, D_{33} from M*, N*, L*:

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

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

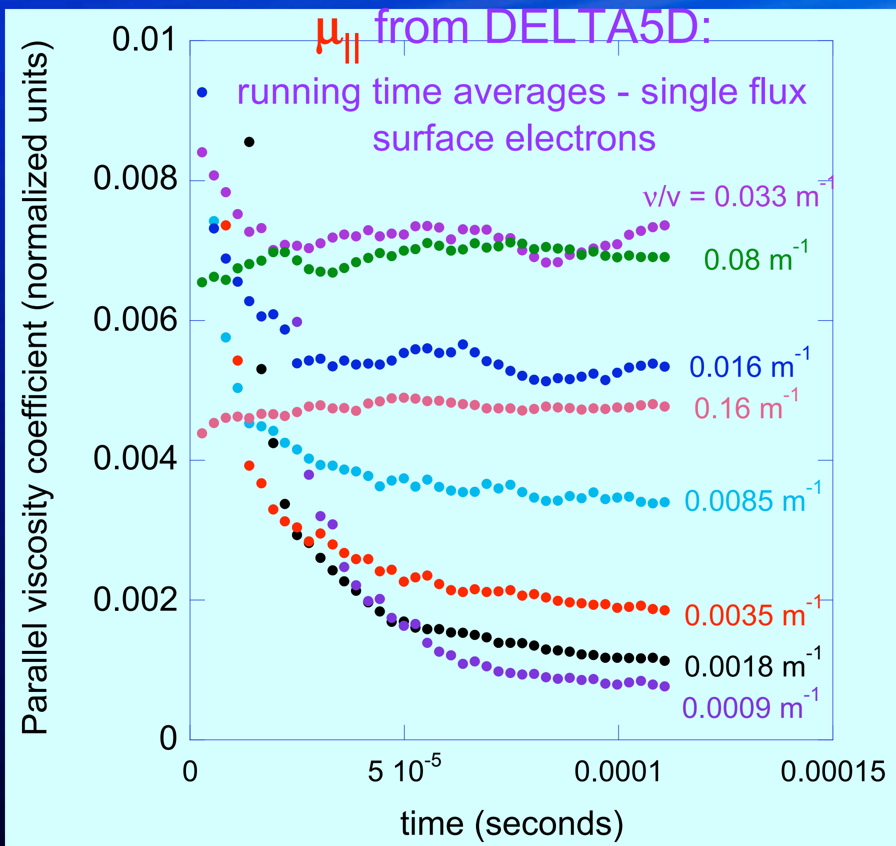
$$D_{11} = L^* + \frac{2}{3}\frac{v}{\mathrm{v}}\tilde{U}^2 - \frac{3}{2}\left(\frac{v}{\mathrm{v}}\right)^3 D\frac{(N^*)^2}{\langle B^2\rangle}$$

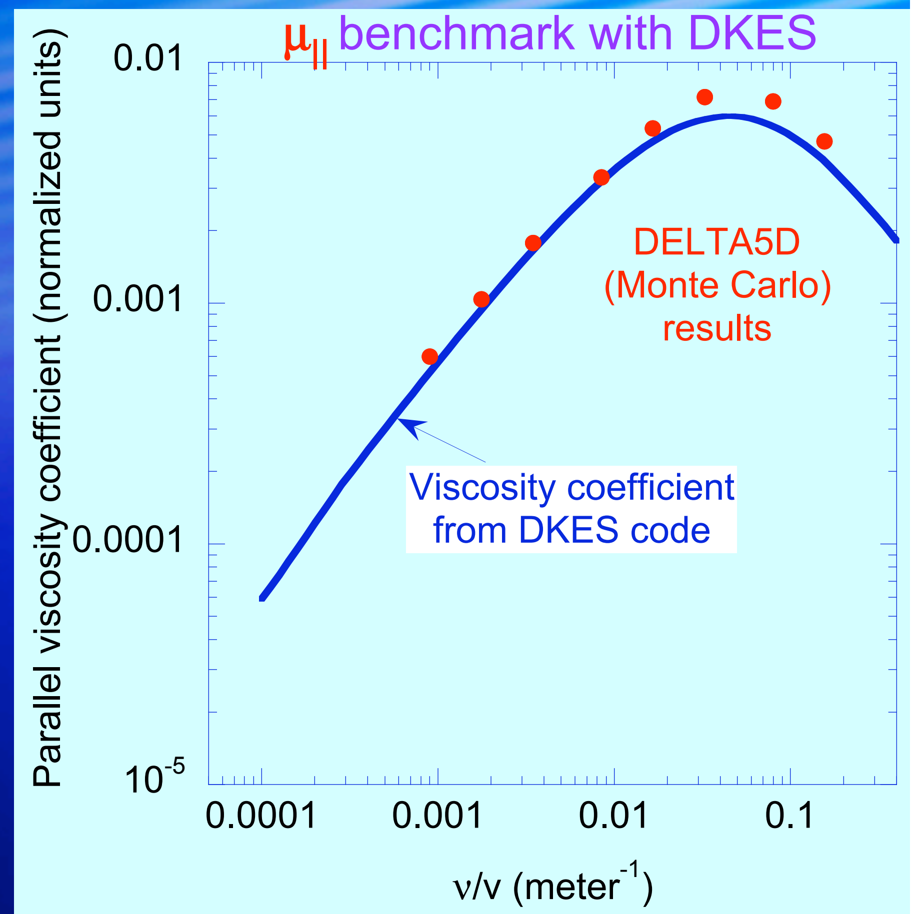
New MHD viscosity-based closure relations are more consistent with the MHD model



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

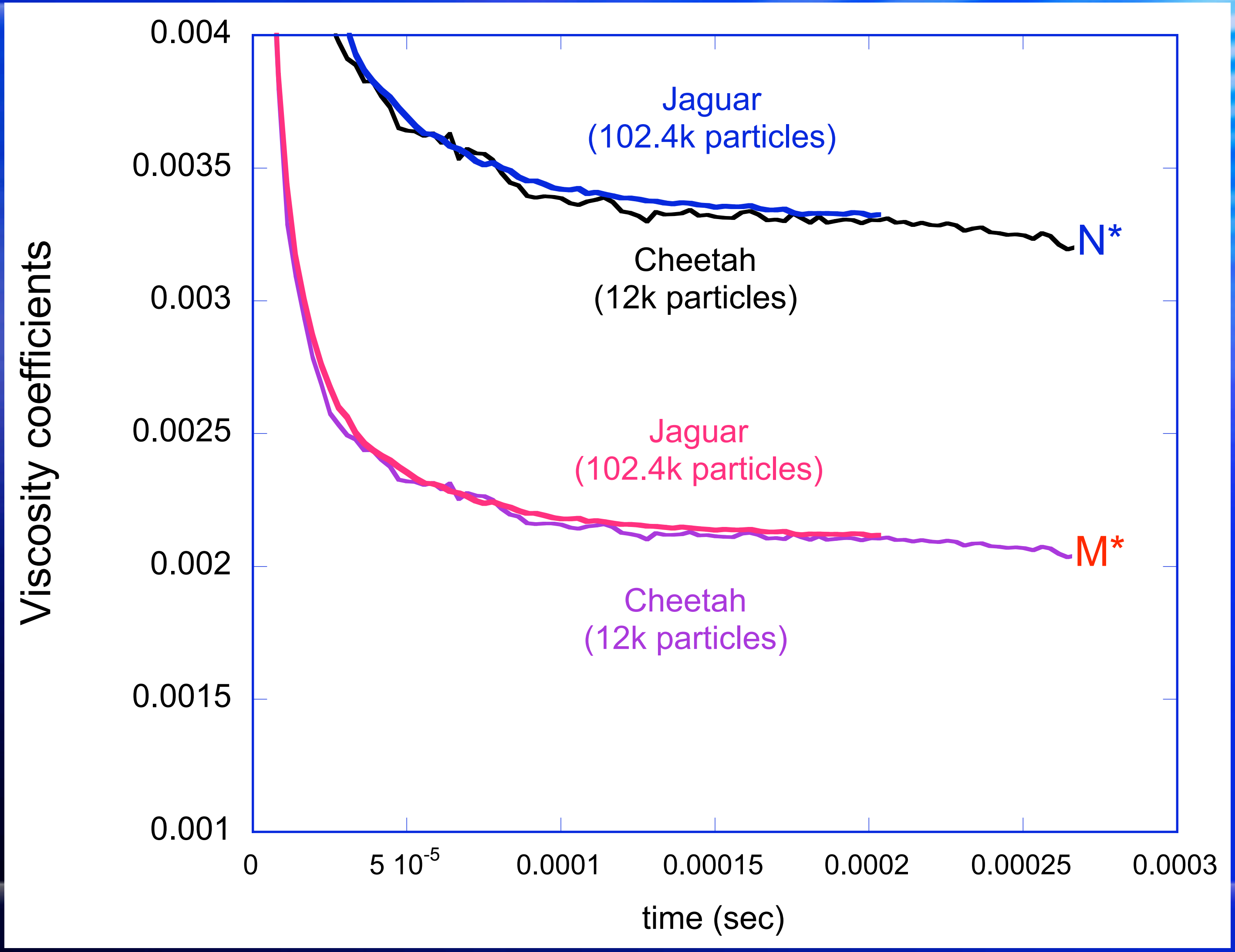
where $M_j, N_j \propto \int_0^\infty dE\, e^{-E/kT}\sqrt{E}\left(E-\frac{5}{2}kT\right)^{j-1}$ $\mu_\parallel, N(E)$



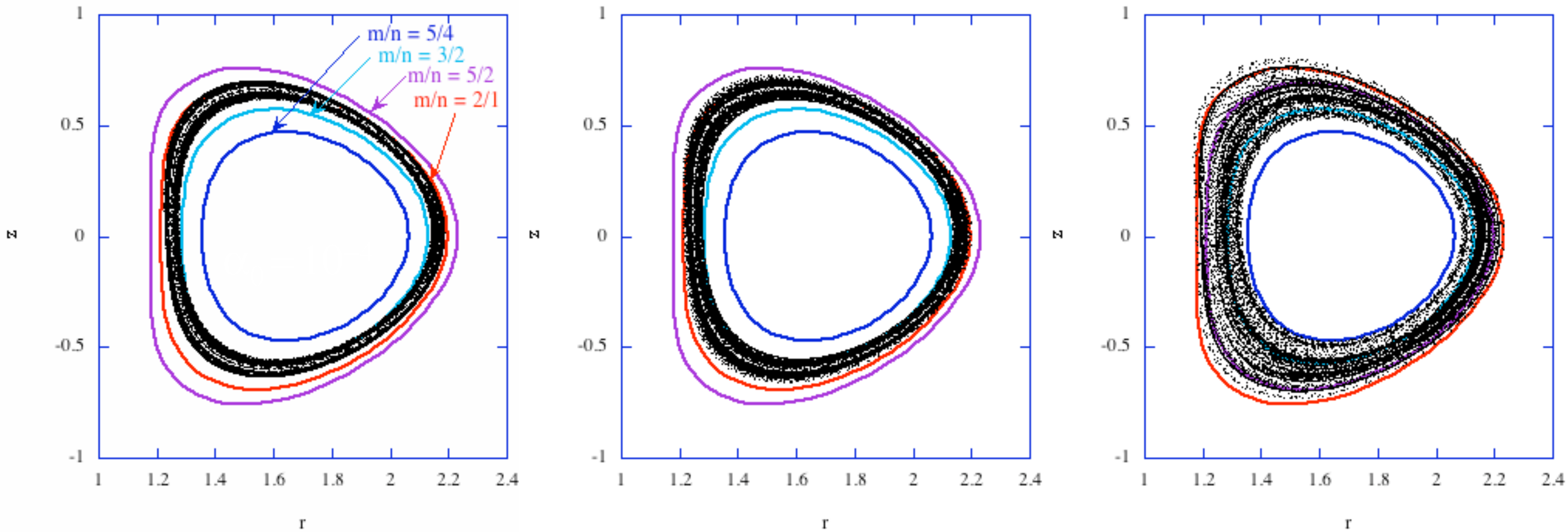


* DKES: Drift Kinetic Equation Solver

Viscosities show convergence with increasing number of particles
(single flux surface)

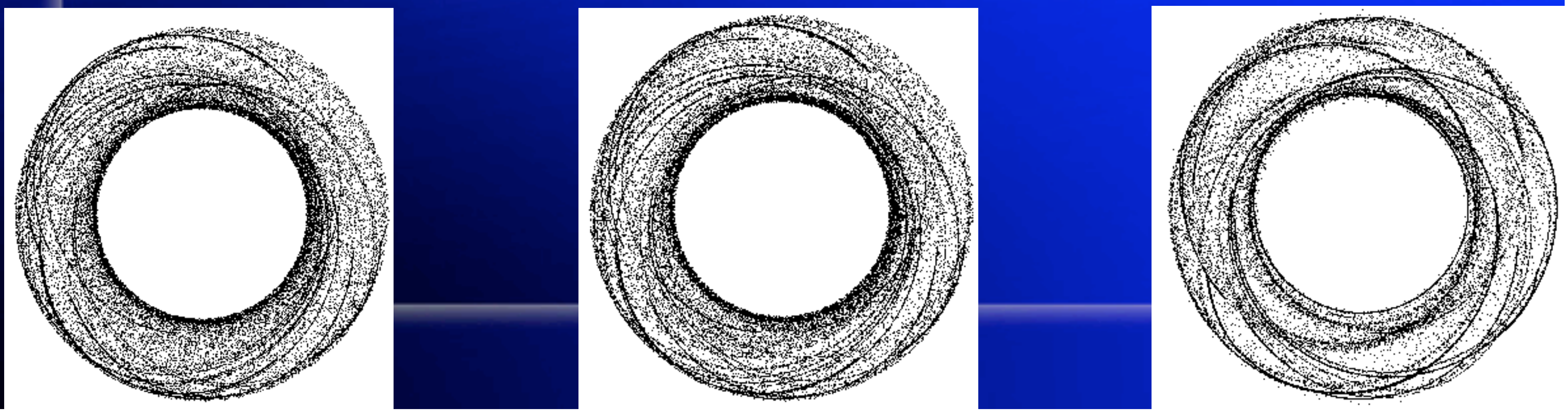


A model perturbed field has been added to mock up tearing modes: $\mathbf{B} = \mathbf{B}_{VMEC} + \nabla\times(\alpha\mathbf{B}_{VMEC})$:



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

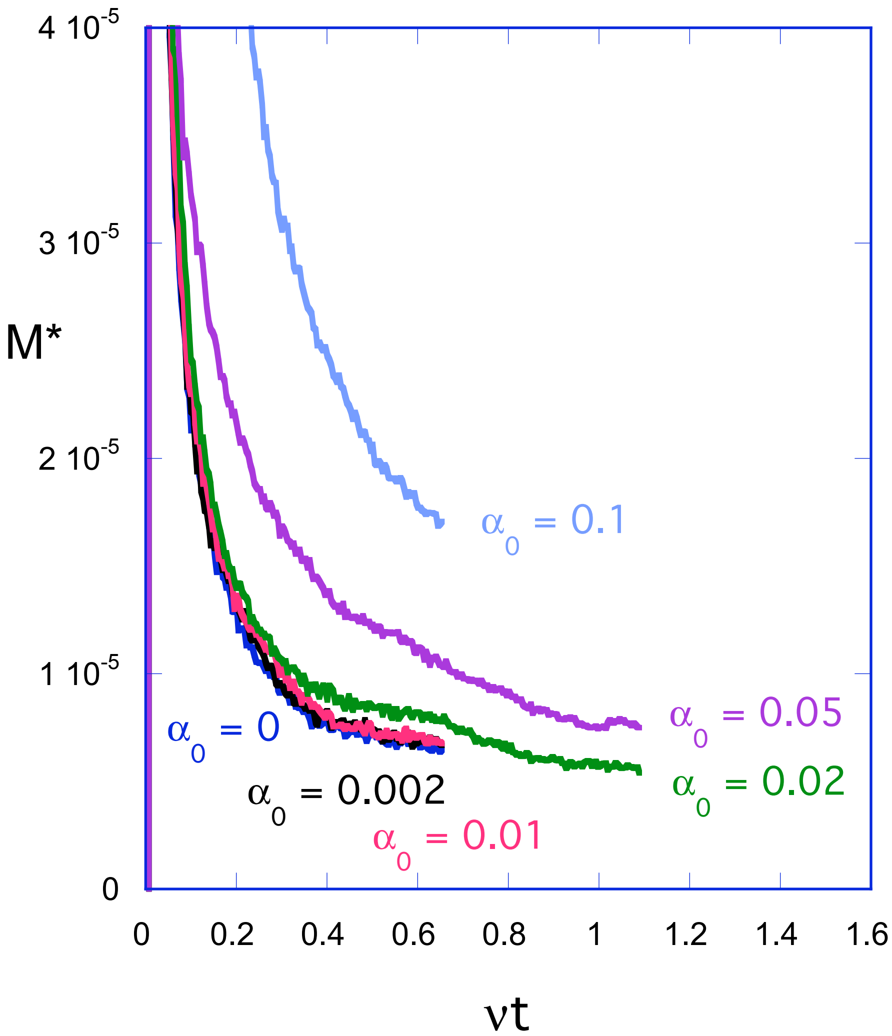
$$\alpha_{mnc,s}(\psi) = \alpha_0 e^{-(\psi-\psi_0)^2/\Delta^2}$$



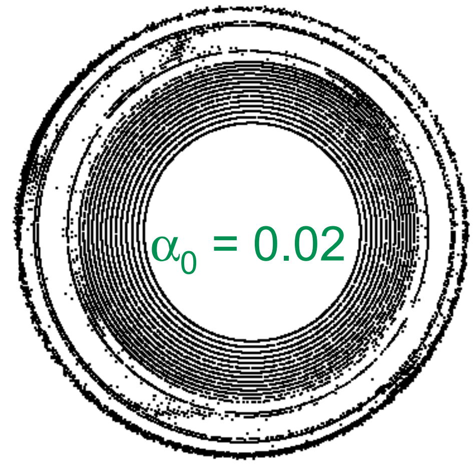
Magnetic perturbations increase viscosity

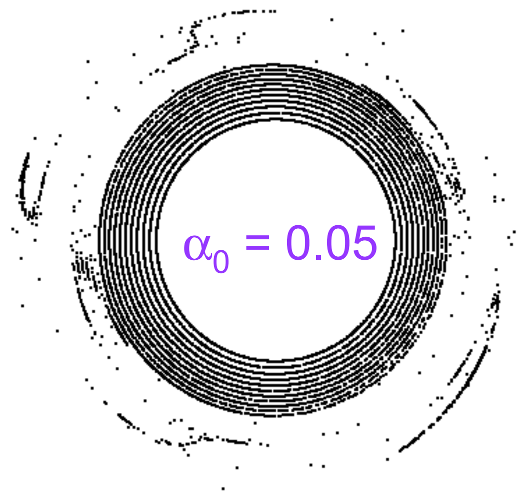
$$\alpha = \sum_{m,n}\left[\alpha_{mnc}(\psi)\cos(m\theta - n\phi) + \alpha_{mns}(\psi)\sin(m\theta - n\phi)\right]$$

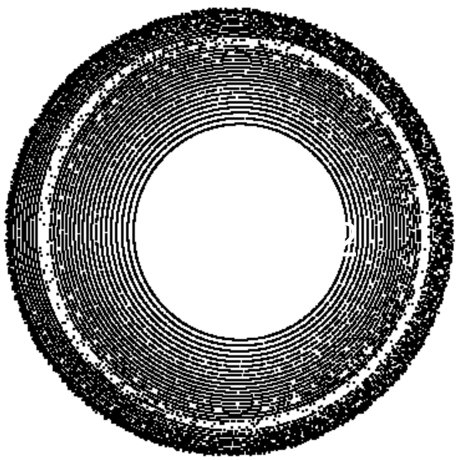
$$\alpha_{mnc,s}(\psi) = \alpha_0 e^{-(\psi-\psi_0)^2/\Delta^2}$$



field line puncture plots:





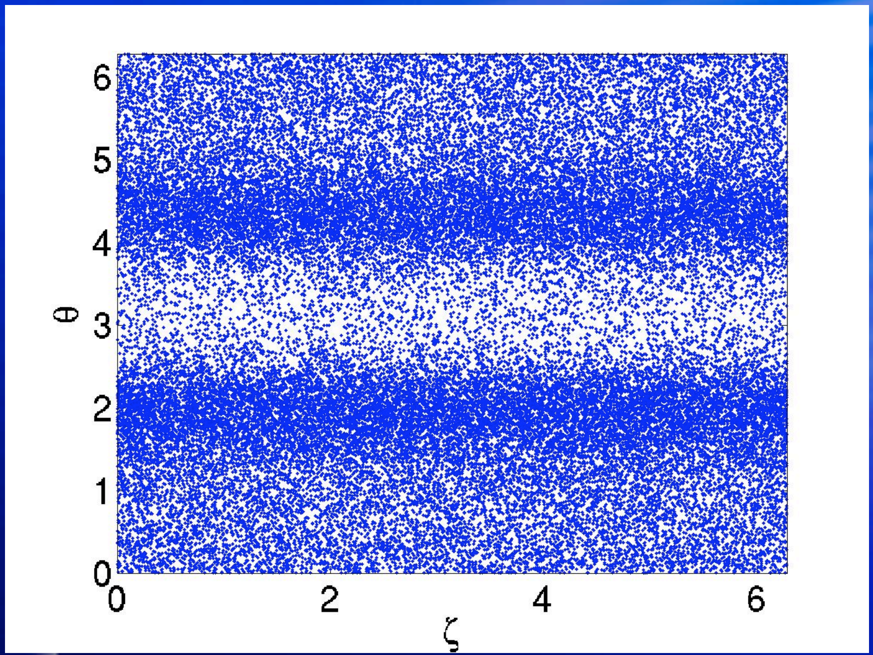


Particle to MHD coupling

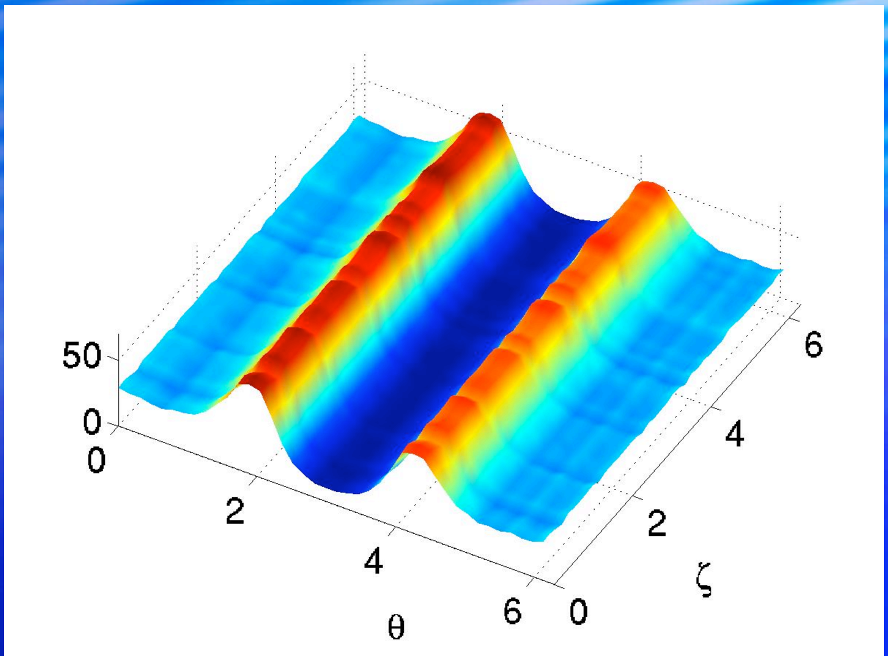
- Data compression
  - Improved gather operations
- Particles discreteness smoothing
  - Systematic method for removing high frequency noise

SVD data smoothing and compression

Raw particle
Monte Carlo data



Rank-1 SVD
40x40 coarse grained
Distribution function



Data representation

Individual particle coordinates

$$\left(\zeta_i, \vartheta_i\right)$$

Size $2 \times 51{,}200 \sim 10^5$

Tensor product of 1-D SVD eigenfunctions

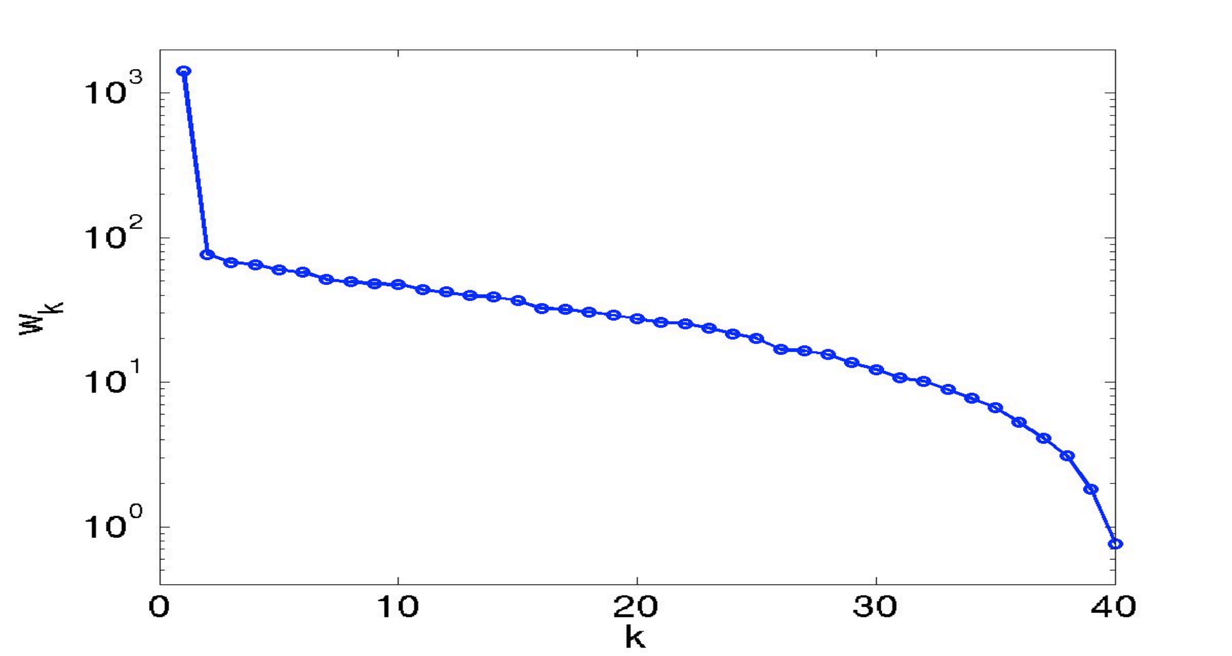
$$f = w^1\, u_1(\zeta) \otimes v_1(\vartheta)$$

Size $1 + 2 * 40 \sim 10^2$

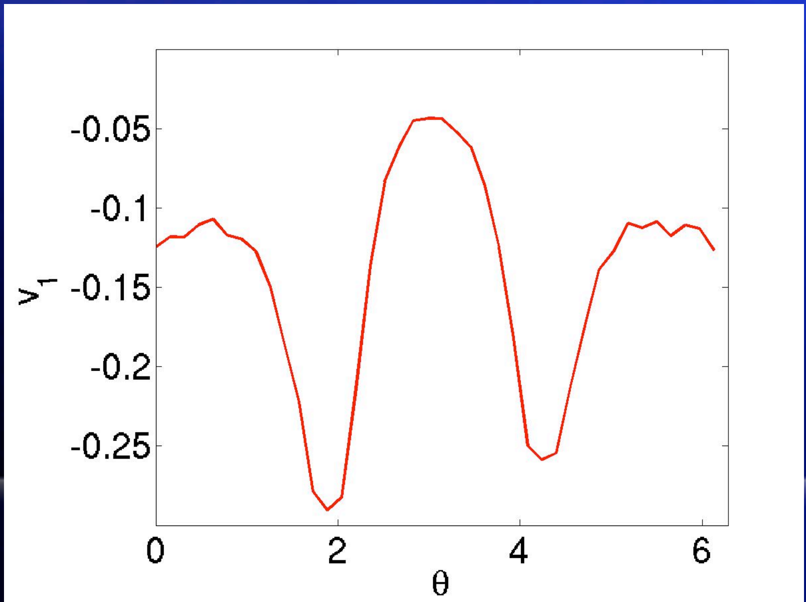
SVD data smoothing and compression

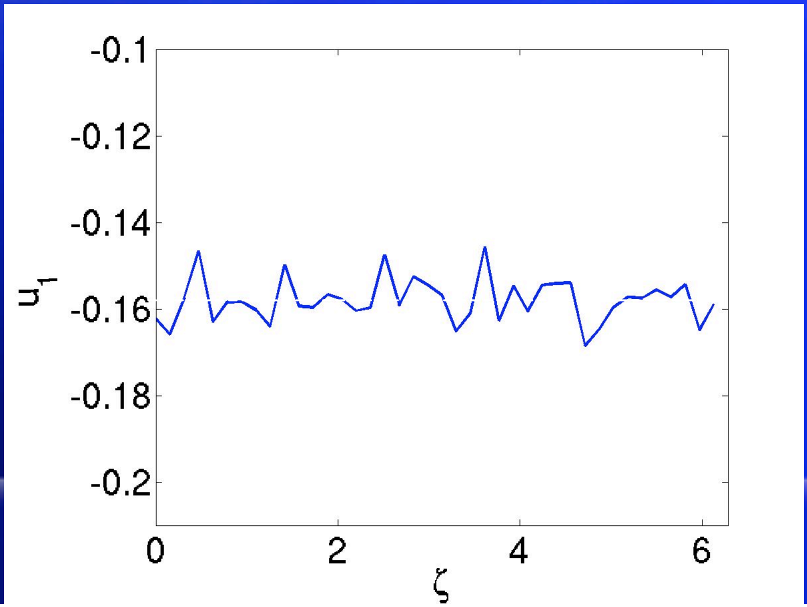
SVD spectrum

$$f = w^1\, u_1(\zeta) \otimes v_1(\vartheta)$$



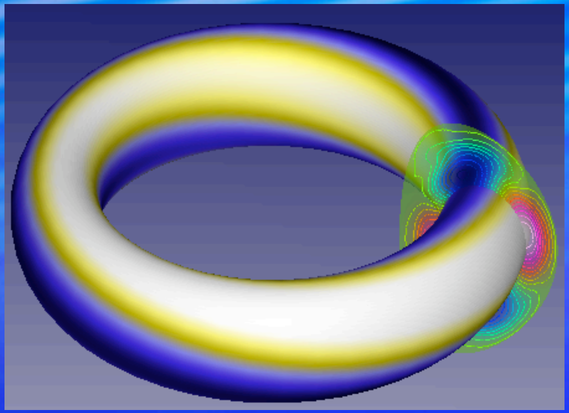
SVD rank-one eigenfunctions





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

Summary

- SVD data compression methods developed for 3D data
  - Typical M3D single timestep dataset compressed by factor of 35-100 while preserving main island features
  - Systematic, controllable noise reduction/smoothing
  - Attractive for particle gather/scatter operations
  - Should minimize cache paging
- Particle-based closure methods developed for neoclassical viscosities
  - Extension of stellarator methods - applicable to 3D fields
  - Benchmarked for axisymmetric tokamaks and tokamak + islands
  - Delta-f method fixes plasma flows and calculates viscosities
  - Avoids redundant incorporation of MHD flows into particle population