Continuum drift kinetics applied to parallel heat transport*

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Abstract

The Chapman-Enskog like electron drift kinetic equation* provides kinetic closure of fluid equations and extends to the long mean free path regime of magnetized plasmas. In this work we discuss the application of a continuum numerical solution to this equation to provide closure for parallel heat flux in NIMROD. Accuracy is improved by expressing the equation in velocity coordinates using pitch-angle and speed normalized by the thermal speed. This leads to a tight coupling of temperature, T, to kinetic distortion, F, and demands a careful semi-implicit time advance for large time steps. Results are obtained from two integration schemes applied to a simultaneous advance of T and F: 1) Picard iteration, and 2) Newton's method. We compare the computational efficiency of both approaches. Additional parallelism was recently developed parallelizing the preconditioning step in the linear solver over speed collocation points in the velocity domain. We present the parallel scaling performance of this development. Using NIMROD we explore the effects of particle trapping on thermal transport in toroidal geometry in the presence of magnetic islands.

*J. J. Ramos, Phys Plasmas **17**, 082502 (2010).

Objective: Include kinetics in NTM simulations

Continuum kinetic tools in NIMROD:

- The Chapman-Enskog-like (CEL) drift-kinetic equation can be solved simultaneously with fluid equations to provide closures such as parallel heat-flux.
- The CEL method partitions the velocity distribution function into a Maxwellian and kinetic distortion in a self-consistent way that is preserved over time. Taking fluid moments of the kinetic distortion checks this partitioning.

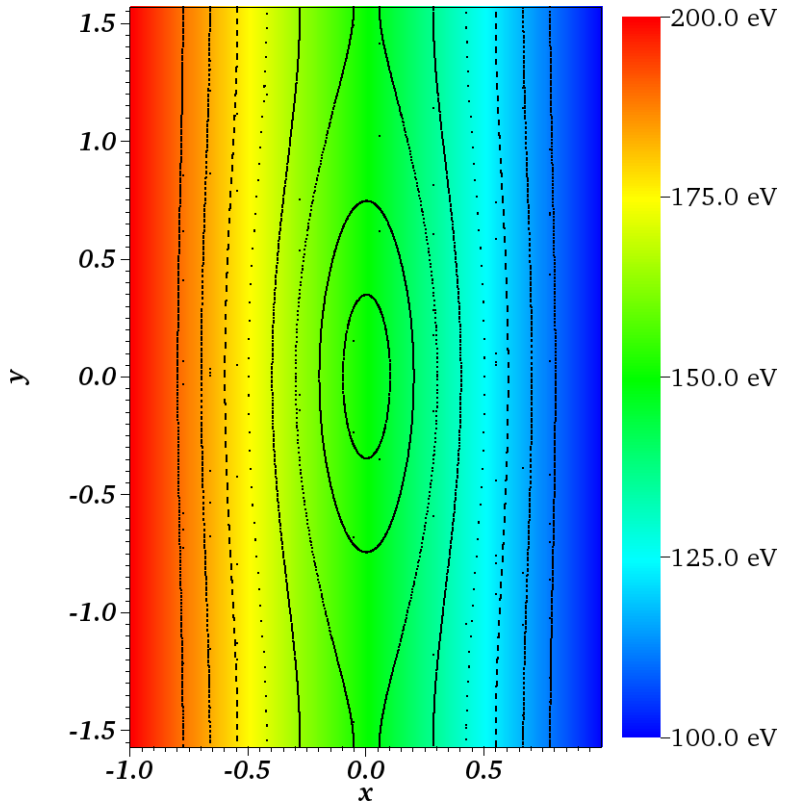
Research Objective: Understand challenges of solving the fluid + CEL kinetic system

- Strong nonlinear coupling between fluid quantities and kinetic distortion
- Scaling velocity by thermal speed
- Implicit advance for large time steps

Start with a simplified coupling: thermal transport with kinetic parallel closure:

$$\frac{3}{2}n\frac{\partial T}{\partial t} = \kappa_\perp \nabla \cdot [(\mathbf{I} - \mathbf{bb}) \cdot \nabla T] - \nabla \cdot \mathbf{q}_\parallel + Q$$

A simple model of a magnetic island



Initial linear T profile flattens across island

Kinetic electron parallel thermal transport in slab island geometry

- $\nu_e / (v_{T_e}/L) \sim 1/5$
- Boundary condition: periodic in Z direction
- Use fluid closure for ions
- Use steady state solution with fluid parallel heat flux as initial condition
- Take large implicit time steps to rapidly find new steady state with kinetic parallel heat flux

Continuum kinetics in NIMROD used to study thermal transport

- Temperature equation $\frac{3}{2}n\frac{\partial T}{\partial t} = \kappa_\perp \nabla\cdot[(\mathbf{I}-\mathbf{bb})\cdot\nabla T] - \nabla\cdot\mathbf{q}_\parallel$

- Two options for closures (fluid or kinetic):
  1) Fourier conduction $\mathbf{q}_\parallel = -\kappa_\parallel (\mathbf{b}\cdot\nabla T)\,\mathbf{b}$ (using mixed finite element formulation)
  2) Kinetic heat flux $\mathbf{q}_\parallel = \frac{m}{2}\int d\mathbf{v} v^2 v_\parallel F$

     Chapman-Enskog-Like (CEL) DKE for kinetic distortion, F

$$\frac{\partial F}{\partial t} + \mathbf{v}_\parallel\cdot\nabla F - \frac{1-\xi^2}{2\xi}\mathbf{v}_\parallel\cdot\nabla \ln B\frac{\partial F}{\partial \xi} - \frac{s}{2}\left(\mathbf{v}_\parallel\cdot\nabla + \frac{\partial}{\partial t}\right)\ln T\frac{\partial F}{\partial s}$$
$$= C + \left(\frac{3}{2}-s^2\right)\mathbf{v}_\parallel\cdot\nabla \ln T f^{\mathrm{M}} + \frac{2}{3nT}\left(s^2-\frac{3}{2}\right)(\nabla\cdot\mathbf{q}_\parallel) f^{\mathrm{M}}$$

(red terms have T dependence) where $(s,\xi) \equiv \left(|\mathbf{v}|/v_T, \mathbf{v}_\parallel/|\mathbf{v}|\right)$

Recent developments in NIMROD's contiuum kinetics

- Newton's method for fully nonlinear, implicit F/T solves
- Full preconditioner
- New block preconditioner
- Parallelism over speed collocation points
- Reusing preconditioner when appropriate

Discretization uses NIMROD's FEM and novel velocity representation*

NIMROD's **spatial** discretization is FE (poloidally) + Fourier (toroidally):

$$T\left(R,Z,\phi,t\right)=\sum_{i}\left\{T_{i,n=0}\left(t\right)+2\Re e\left[\sum_{n>0}T_{i,n}\left(t\right)\mathrm{e}^{in\phi}\right]\right\}\alpha_{i}\left(R,Z\right)$$

$$F\left(R,Z,\phi,s,\xi,t\right)=\sum_{i}\left\{F_{i,n=0}\left(s,\xi,t\right)+2\Re e\left[\sum_{n>0}F_{i,n}\left(s,\xi,t\right)\mathrm{e}^{in\phi}\right]\right\}\alpha_{i}\left(R,Z\right)$$

Lagrange or GLL polynomials

Pitch-angle discretization is FE:

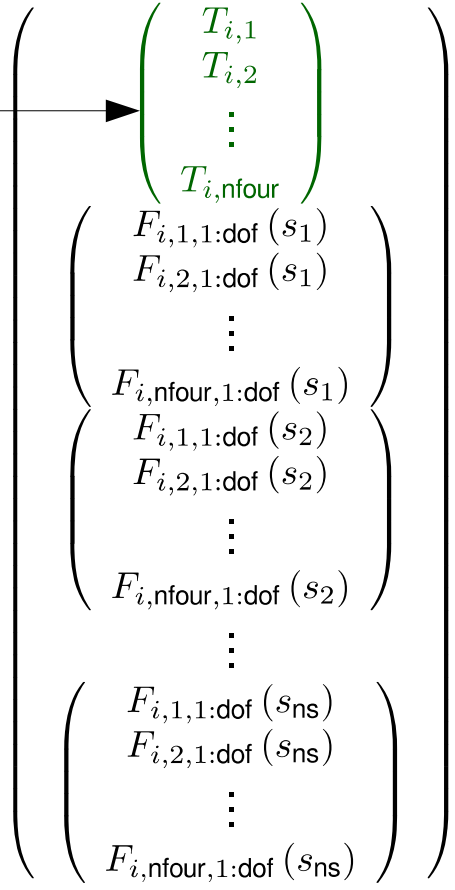
$$F_{i,n}\left(s,\xi,t\right)\equiv\sum_{\xi_{j}}F_{i,n,\xi_{j}}\left(s,t\right)P_{\xi_{j}}\left(\xi\right)$$

where $F_{i,n,\xi_{j}}\left(s\right)$ are solved at a set of collocation points in **Speed**

*E. D. Held, *et al*, Phys Plasmas **22**, 032511 (2015).

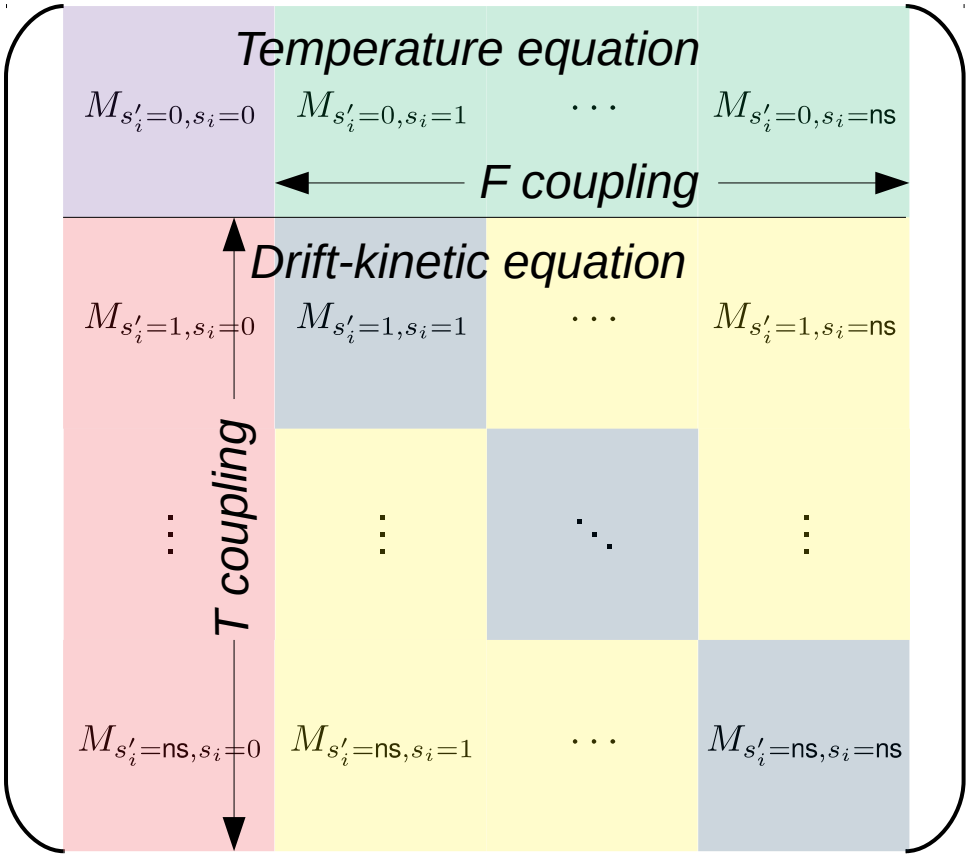
T & F are coupled for semi-implicit advance with both centered at the same time

Fluid quantities prepend to distribution function solution vector



- Electron collision operator mostly couples pitch-angle nodes gives natural speed-block structure
- If constructing full preconditioner, speed index combines with pitch-angle index as a ”vector component”
- Can be extended to other fluid variables

The linear operator's toroidal-blocks can be written in the following matrix form



A few preconditioning strategies implemented:

1) Full preconditioner includes all terms
2) Block Jacobi inverts ▢ & ▢ s-blocks excluding:
   - ✗ off-diagonal collision operator terms
   - ✗ thermodynamic drives
   - ✗ s-derivative
   - ✗ heat-flux in temperature equation
3) New block preconditioner uses ▢, ▢ & ▢ s-blocks is similar, but includes:
   - ✔ heat-flux in temperature equation

s-blocks are tailored to pitch-angle scattering operator and low-collisionality

Newton's method is working well

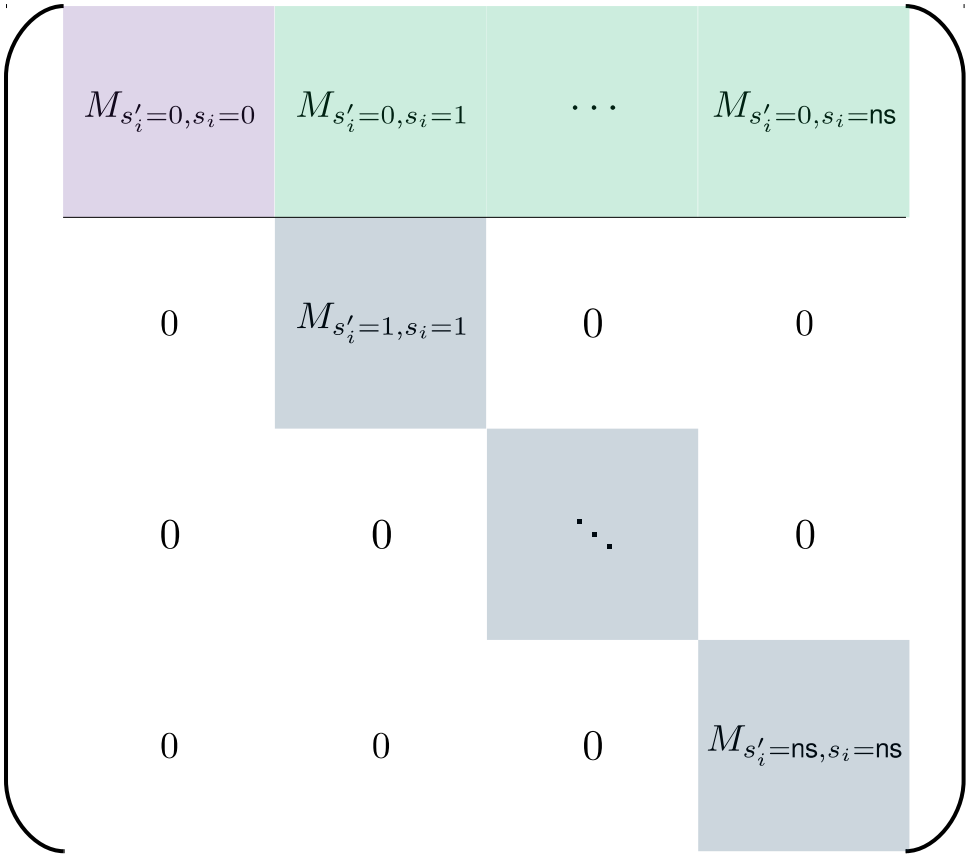
- Pseudo code:

```
Evaluate RHS, b (initially x_0 = A(x_0) = 0)
Construct preconditioner for linearized operator
Start
    Call GMRES iterative solver to solve J(x_i) · (x_{i+1} − x_i) = b − A(x_i)
    If linear system takes only 1 GMRES iteration
        Exit loop
    Else
        Evaluate nonlinear operator, A(x_{i+1})
        Update right hand side
```

$$\mathbf{A}\left(\mathbf{x}^{k+1}\right) = \mathbf{x}^{k+1} - \mathbf{x}^{k} - \theta\Delta t\left[\mathbf{b}\left(\mathbf{x}^{k+1}\right) - \mathbf{b}\left(\mathbf{x}^{k}\right)\right]$$

- Only adds substantial computational time when nonlinear residual is large
- For slab island problem with 32x32 spatial grid, polynomial degree 4, ns=4, 3 ξ cells, ξ polynomial degree 3, dt=10μs, run for 1ms, most time steps take **3 iterations**, and reaches a peak of **11 iterations**.
- Run time with Newton iterations is roughly half for same problem, running with only 1 Newton iteration (linear operator) each time step.

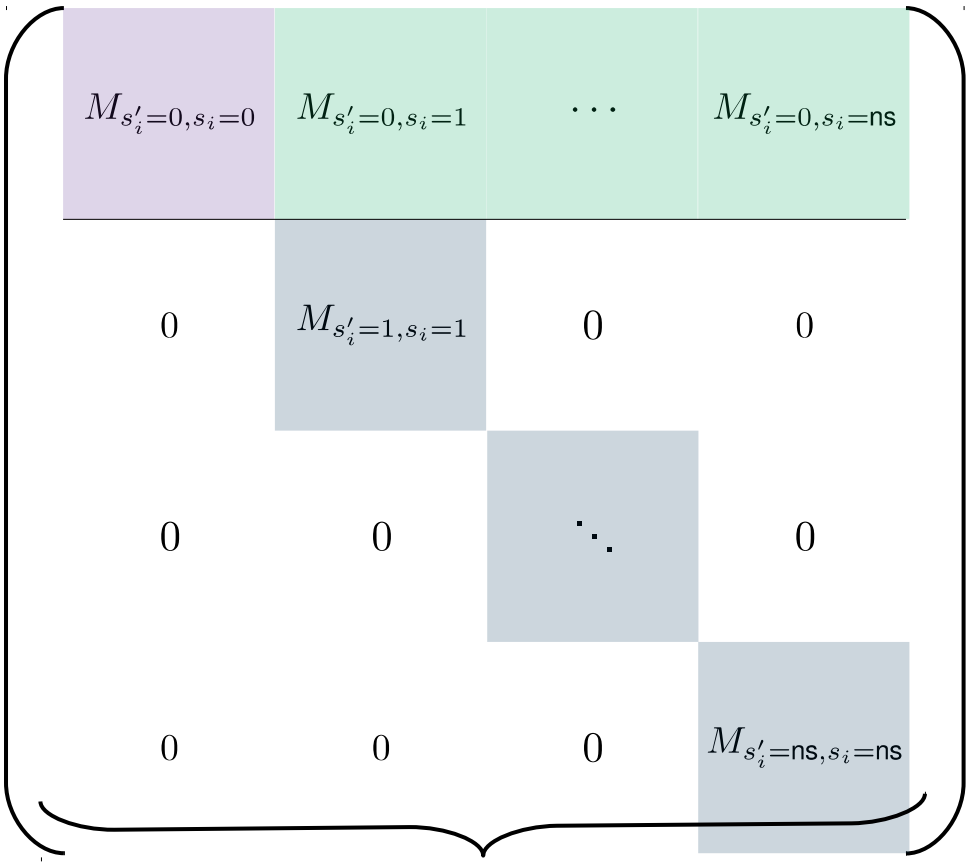
New block preconditioner has some advantages



Computational advantages:

- Inverse easily written by hand (back substitution)
- Like successive over relaxation (used for toroidal preconditioning), only diagonal blocks need be factored
- Easy modification to existing preconditioning subroutine
- Factoring diagonal blocks can be skipped over multiple time steps, while off-diagonal blocks are inexpensive to update every Newton iteration

Block decomposition of matrix facilitates parallelism



- ns+1 groups of processors used (each group having as many as running serial-in-s)
- Each group of processors is assigned a speed index, $0 \leq s_i \leq \text{ns}$
- Group $s_i = 0$ computes first block and factors
- Each group $s_i \geq 1$ computes a single off-diagonal block and a single diagonal block and factors
- Each group owns a piece of the vector being preconditioned and the result
- Data gets passed from the $s_i \geq 1$ groups to the $s_i = 0$ group (back substitution).
- Communication is similar to successive over relaxation

New block preconditioner has pros and cons

Example 1ms run

- 32x32 poloidal grid
- 4^{th} order polynomial FE basis
- 3 ξ cells, 3^{rd} order polynomials
- ns=4 speed collocation points
- starting from fluid steady state
- taking 100x10μs time steps

	Block Jacobi	New Approach
Total GMRES its on 1^{st} Newton it	2328	590
Total GMRES its	3415	2840
Total Newton its	300	436

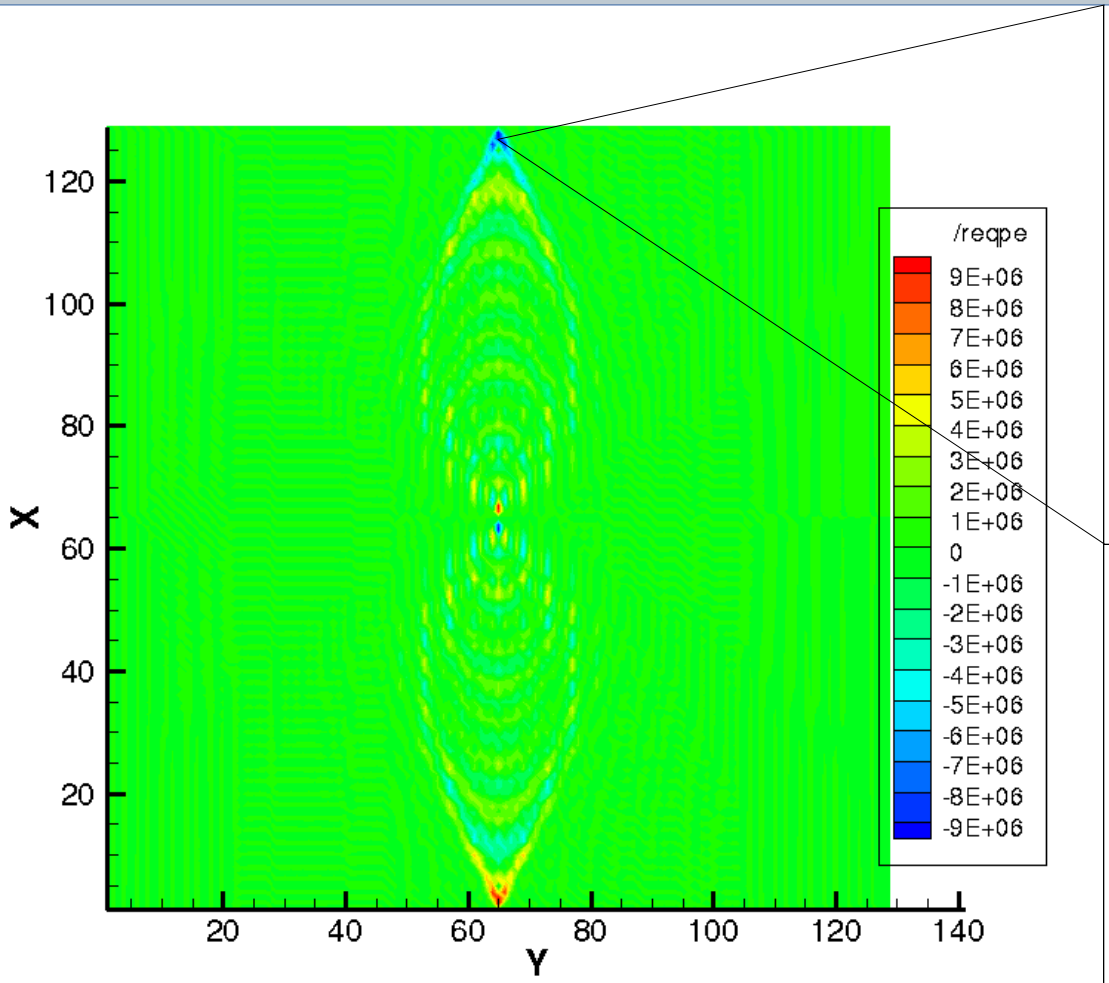
Large implicit time steps are possible

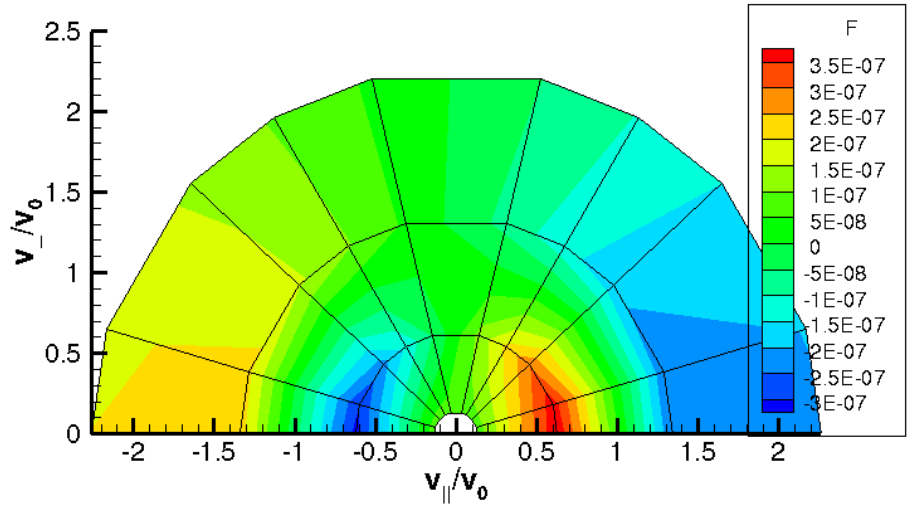
Some relevant time scales	
transit time	~1μs
collision time	~10μs
NTM in quasi-stationary state	~200ms*
locking dynamics	~15ms*
time locked before disruption	~300ms*

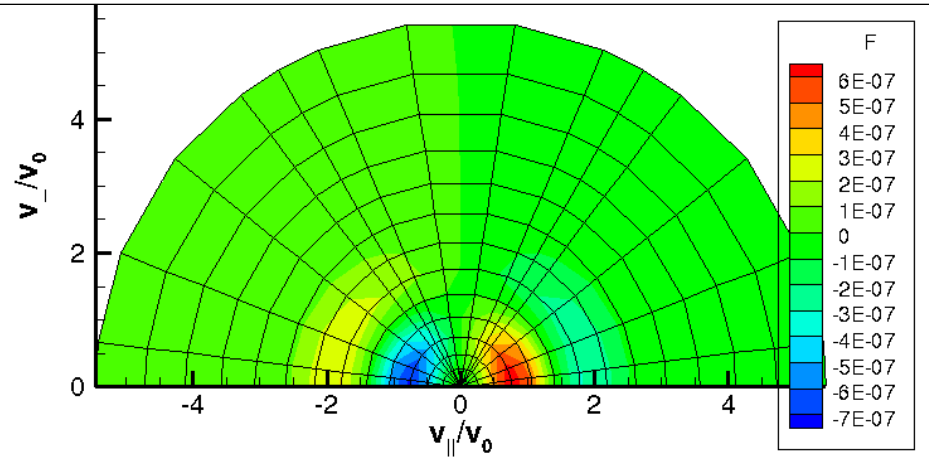
ns/ξ poly degree	4/3	7/4	15/5
time step	10μs	10μs	5μs
simulation time	1ms	1ms	40μs
MPI Tasks	64	512	1024
s-parallelism	No	Yes	Yes
wall clock time	1.9hrs	2.8hrs	2.3hrs

*R. Sweeney, W. Choi, R. LaHaye, *et al*, Nucl. Fusion **57**, 016019 (2017).

Convergence in velocity space to be investigated







Upcoming work

- Cleanup s-parallelization for smaller memory footprint
- Implement additional parallelization in pitch-angle
  - Domain decomposition (can collision operator be done implicitly?)
  - Static condensation
- Add artificial anisotropic diffusion
- Adaptive time step
- Examine needed velocity grid for electron-ion collisions
- Use developed code in a tearing mode simulation with evolving $\mathbf{B}$, n, $\mathbf{V}$