Implementation of Implicit-Explicit Time Integration for the Kinetic Modeling of Tokamak Plasma Edge

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Background and Motivation

Inner edge: Adjacent to the core

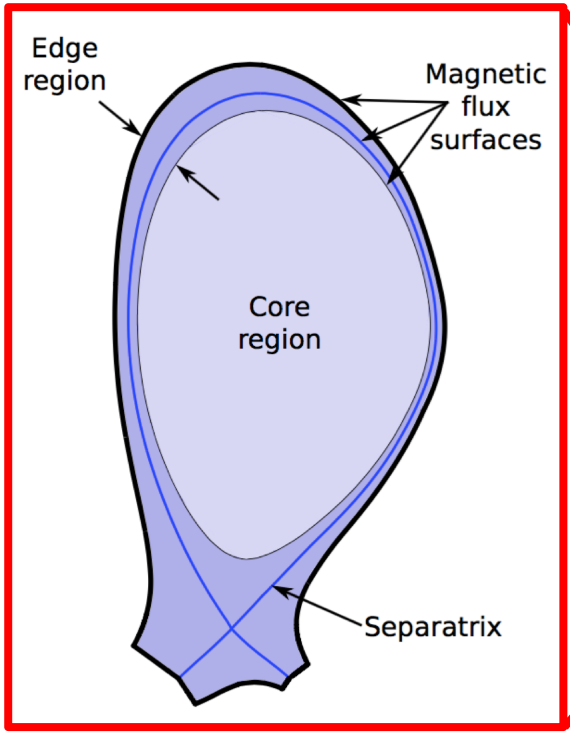
- High temperature and density
- Mean free paths comparable to density/temperature gradients
- Weakly collisional

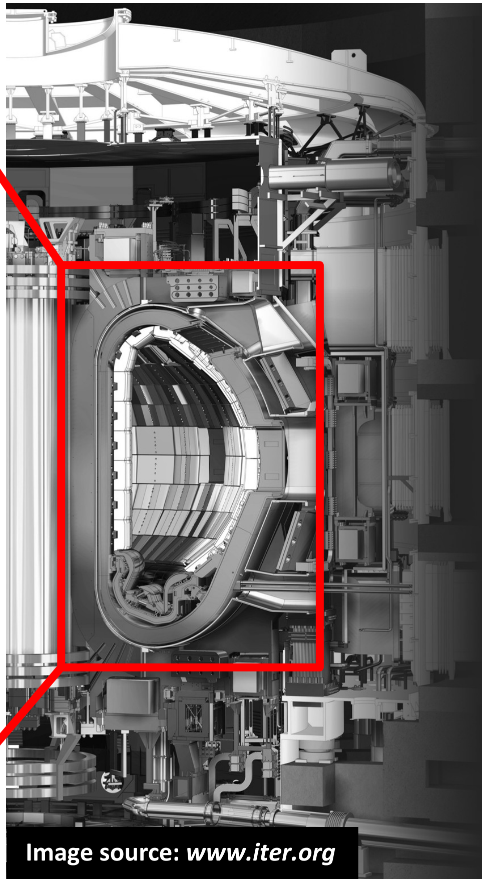
Requires kinetic simulation with collision model

Outer edge: Near tokamak wall

- Low temperature and density
- Short mean free paths compared to density/temperature gradients
- Strongly collisional

Introduces very small time scales





ITER tokamak

Plasma dynamics in the edge region is characterized by a large range of temporal scales

Governing Equations

Full-*f* gyrokinetic Vlasov equation for each ion species

$$\frac{\partial B^*_{\parallel,\alpha} f_\alpha}{\partial t} + \underbrace{\nabla_{\mathbf{R}} \cdot \left(\dot{\mathbf{R}}_\alpha B^*_{\parallel,\alpha} f_\alpha \right) + \frac{\partial}{\partial v_\parallel} \left(\dot{v}_{\parallel,\alpha} B^*_{\parallel,\alpha} f_\alpha \right)}_{\text{Vlasov}} = \underbrace{\sum_\beta c\left[f_\alpha, f_\beta \right]}_{\text{Collisions}}$$

where

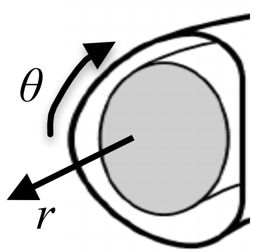
$$\dot{\mathbf{R}}_\alpha \equiv \dot{\mathbf{R}}_\alpha \left(\mathbf{R}, v_\parallel, \mu, t \right) = \frac{1}{B^*_{\parallel,\alpha}} \left[v_\parallel \mathbf{B}^*_\alpha + \frac{1}{Z_\alpha e} \hat{\mathbf{b}} \times \left(Z_\alpha e \mathbf{E} + \mu \nabla_{\mathbf{R}} B \right) \right] \quad \text{Velocity}$$

$$\dot{v}_{\parallel,\alpha} \equiv \dot{v}_{\parallel,\alpha} \left(\mathbf{R}, v_\parallel, \mu, t \right) = -\frac{1}{m_\alpha B^*_{\parallel,\alpha}} \mathbf{B}^*_\alpha \cdot \left(Z_\alpha e \mathbf{E} + \mu \nabla_{\mathbf{R}} B \right) \quad \text{Acceleration}$$

4D (2D-2V) phase space

$$\mathbf{R} \equiv \{ r, \theta \}$$

$$v_\parallel, \;\; \mu = \frac{1}{2} \frac{m_\alpha v_\perp^2}{B}$$



Electric field **E** can be specified or computed from f_α using the Poisson equation for electrostatic potential

We consider *single-species cases* in this study.

Fokker-Planck Collision Model

Fokker-Planck-Rosenbluth equation

$$c\left[f_\alpha, f_\beta\right] = \lambda_c \left(\frac{4\pi Z_\alpha Z_\beta e^2}{m_\alpha}\right)^2 \nabla_{(v_\parallel,\mu)} \cdot \left[\vec{\gamma}_\beta f_\alpha + \overleftrightarrow{\tau}_\beta \nabla_{(v_\parallel,\mu)} f_\alpha\right]$$

where the advective and diffusive coefficients are given by

$$\vec{\gamma}_\beta = \begin{bmatrix} \frac{\partial \varphi_\beta}{\partial v_\parallel} & 2\mu \frac{m_\beta}{B} \frac{\partial \varphi_\beta}{\partial \mu} \end{bmatrix}, \quad \overleftrightarrow{\tau}_\beta = \begin{bmatrix} -\frac{\partial^2 \varrho_\beta}{\partial v_\parallel^2} & -2\mu \frac{m_\beta}{B} \frac{\partial^2 \varrho_\beta}{\partial v_\parallel \mu} \\ -2\mu \frac{m_\beta}{B} \frac{\partial^2 \varrho_\beta}{\partial v_\parallel \mu} & -2\mu \left(\frac{m_\beta}{B}\right)^2 \left\{2\mu \frac{\partial^2 \varrho_\beta}{\partial \mu^2} + \frac{\partial \varrho_\beta}{\partial \mu}\right\} \end{bmatrix}$$

Rosenbluth potentials are related to f_β by the Poisson equations

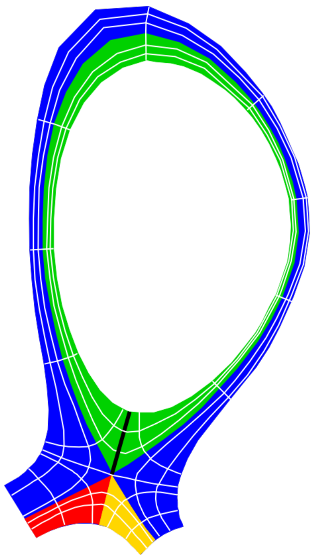
$$\frac{\partial^2 \varphi_\beta}{\partial v_\parallel^2} + \frac{m_\beta}{B} \frac{\partial}{\partial \mu} \left(2\mu \frac{\partial \varphi_\beta}{\partial \mu}\right) = f_\beta$$

$$\frac{\partial^2 \varrho_\beta}{\partial v_\parallel^2} + \frac{m_\beta}{B} \frac{\partial}{\partial \mu} \left(2\mu \frac{\partial \varrho_\beta}{\partial \mu}\right) = \varphi_\beta$$

Non-linear, integro-differential term

Each evaluation of the Fokker-Planck term requires Poisson solve in the velocity space

COGENT: Spatial Discretization



Vlasov term

- Mapped, multi-block grids for complex geometries
- 4^{th} order finite-volume discretization
- 5^{th} order WENO scheme for reconstruction at cell faces
- *Colella, et al., J. Comput. Phys., 2011; McCorquodale, et al., J. Comput. Phys., 2015*

Fokker-Planck collision term

- Conservative finite-difference discretization on Cartesian velocity grid
- 5^{th} order upwind discretization for the advective terms; 4^{th} order central discretization for the diffusive terms
- Poisson equations for Rosenbluth potentials discretized using 2^{nd} order central differences (*Dorf, et al., Contrib. Plasma Phys., 2014*)
- Energy-conserving modification implemented (*Taitano, et al., J. Comput. Phys., 2015*)

Time Integration

Spatial discretization yields **semi-discrete ODE in time**

$$\frac{d\tilde{f}}{dt} = \mathcal{R}\left(\tilde{f}\right) \equiv \underbrace{\mathcal{V}\left(\tilde{f}\right)} + \underbrace{\mathcal{C}\left(\tilde{f}\right)}$$

Spatially-discretized **Vlasov** and **collisions** terms

Explicit time integration:
Runge-Kutta methods

$$\Delta t \left(\lambda \left[\frac{d\mathcal{R}\left(\tilde{f}\right)}{d\tilde{f}} \right] \right) \in \{ z : |R(z)| \leq 1 \}$$

Time step constrained by eigenvalues (time scales) of *entire RHS*

Implicit-Explicit (IMEX) time integration:
Additive Runge-Kutta (ARK) methods

$$\mathcal{R}\left(\tilde{f}\right) = \underbrace{\mathcal{R}_{\text{stiff}}\left(\tilde{f}\right)}_{\text{Implicit}} + \underbrace{\mathcal{R}_{\text{nonstiff}}\left(\tilde{f}\right)}_{\text{Explicit}}$$

$$\Delta t \left(\lambda \left[\frac{d\mathcal{R}_{\text{stiff}}\left(\tilde{f}\right)}{d\tilde{f}} \right] \right) \in \{ z : |R(z)| \leq 1 \}$$

IMEX: time step constrained by eigenvalues (time scales) of *stiff component of RHS*

Temporal Scales at Tokamak Edge

Eigenvalues (time scales) of the entire RHS, and the Vlasov and collision terms separately

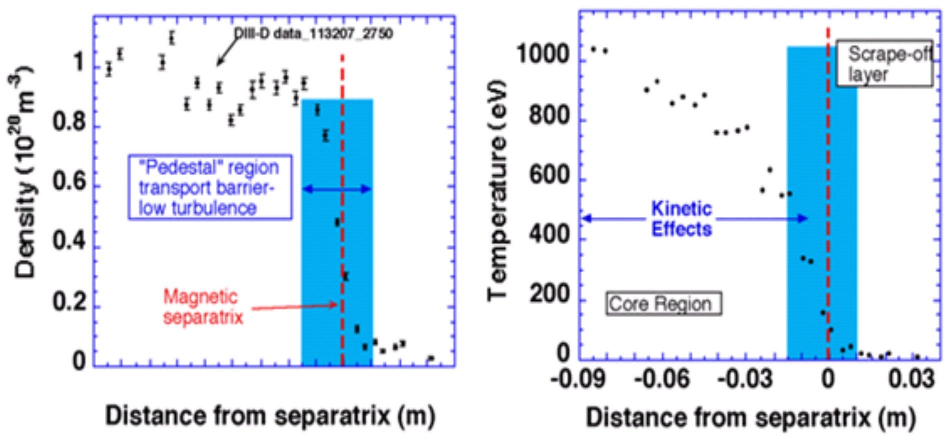
$$\lambda_R \equiv \lambda\left[\frac{d\mathcal{R}\left(\tilde{f}\right)}{d\tilde{f}}\right]$$

$$\lambda_V \equiv \lambda\left[\frac{d\mathcal{V}\left(\tilde{f}\right)}{d\tilde{f}}\right]$$

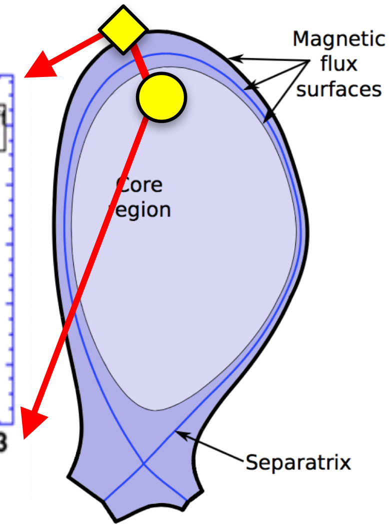
$$\lambda_C \equiv \lambda\left[\frac{d\mathcal{C}\left(\tilde{f}\right)}{d\tilde{f}}\right]$$

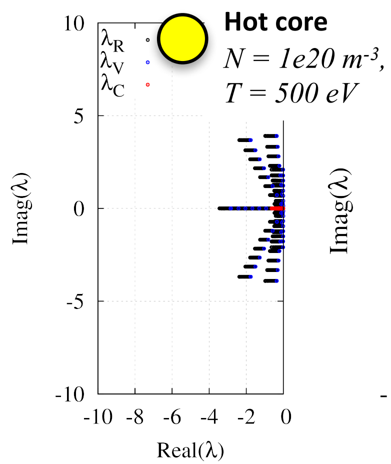
Jacobians computed using finite-differences on a very small grid

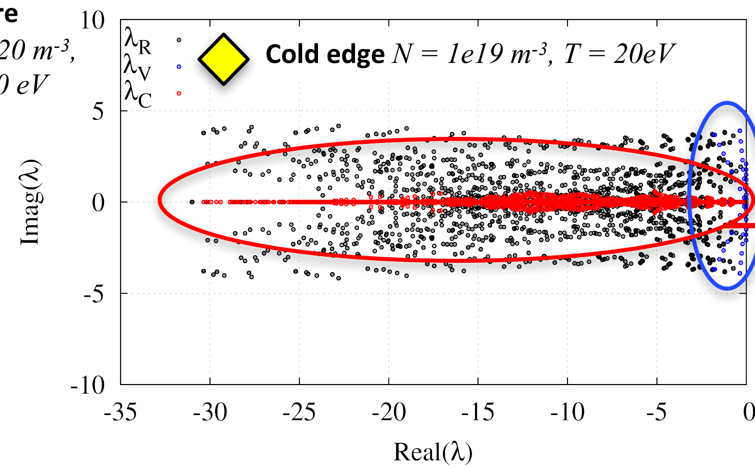
Tokamak edge density and temperature



Reference: *Porter, et al., Physics of Plasmas, 2000*







At the cold edge

$$|\lambda_V| \ll |\lambda_C|$$

$$\mathcal{R}_{\rm stiff} \equiv \mathcal{C}\left(\tilde{f}\right)$$
$$\mathcal{R}_{\rm nonstiff} \equiv \mathcal{V}\left(\tilde{f}\right)$$

Implicit-Explicit (IMEX) Time Integration

High-order, conservative multistage ***Additive Runge-Kutta (ARK)*** methods

Explicit method for non-stiff component (Explicit RK)

$$\begin{array}{c|ccccc} 0 & 0 & & & & \\ c_2 & a_{21} & 0 & & & \\ \vdots & \vdots & \ddots & 0 & & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & \cdots & \cdots & b_s \end{array}$$

+

Implicit method for stiff component (ESDIRK)

$$\begin{array}{c|ccccc} 0 & 0 & & & & \\ \tilde{c}_2 & \tilde{a}_{21} & \gamma & & & \\ \vdots & \vdots & \ddots & \gamma & & \\ \tilde{c}_s & \tilde{a}_{s1} & \cdots & \tilde{a}_{s,s-1} & \gamma \\ \hline & b_1 & \cdots & \cdots & b_s \end{array}$$

s → number of stages

Time step: $t_n \rightarrow t_{n+1} = t_n + \Delta t$

Stage solutions ⟶ $$\tilde{f}^{(i)} = \tilde{f}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} \mathcal{V}\left(\tilde{f}^{(j)}\right) + \Delta t \sum_{j=1}^{i} \tilde{a}_{ij} \mathcal{C}\left(\tilde{f}^{(j)}\right),\ i = 1, \cdots, s$$

Step completion ⟶ $$\tilde{f}_{n+1} = \tilde{f}_n + \Delta t \sum_{i=1}^{s} b_i \left\{ \mathcal{V}\left(\tilde{f}^{(i)}\right) + \mathcal{C}\left(\tilde{f}^{(i)}\right) \right\}$$

ARK2
- 2^{nd} order, 3 stage
- *Giraldo, et al., SIAM J. Sci. Comput., 2013*

ARK3
- 3^{rd} order, 4 stage
- *Kennedy & Carpenter, J. Comput. Phys., 2003*

ARK4
- 4^{th} order, 6 stage
- *Kennedy & Carpenter, J. Comput. Phys., 2003*

Implicit Stage Solution

Implicit stages require the solution to a ***nonlinear system of equations***

$$\underbrace{\frac{1}{\Delta t \tilde{a}_{ii}} \tilde{f}^{(i)} - \mathcal{C}\left(\tilde{f}^{(i)}\right) - \left[\tilde{f}_n + \Delta t \sum_{j=1}^{i-1} \left\{ a_{ij} \mathcal{V}\left(\tilde{f}^{(j)}\right) + \tilde{a}_{ij} \mathcal{C}\left(\tilde{f}^{(j)}\right) \right\} \right] = 0}$$

$$\mathcal{F}(y) = 0 \quad \text{where} \quad y \equiv \tilde{f}^{(i)}$$

Jacobian-free Newton-Krylov method (*Knoll & Keyes, J. Comput. Phys., 2004*):

Initial guess: $y_0 \equiv \tilde{f}_0^{(i)} = \tilde{f}^{(i-1)}$

Newton update: $y_{k+1} = y_k - \mathcal{J}(y_k)^{-1} \mathcal{F}(y_k)$

GMRES solver:
$\mathcal{J}(y_k)\,\Delta y = \mathcal{F}(y_k)$

Action of the Jacobian on a vector approximated by directional derivative

$$\mathcal{J}(y_k)\, x = \left. \frac{d\mathcal{F}(y)}{dy} \right|_{y_k} x \approx \frac{1}{\epsilon} \left[\mathcal{F}(y_k + \epsilon x) - \mathcal{F}(y_k) \right]$$

Preconditioning

Preconditioner *(sparse matrix)*		Exact Jacobian *(never assembled)*
$\left[\alpha\mathcal{I} - \frac{d\bar{\mathcal{C}}\left(\tilde{f}\right)}{d\tilde{f}}\right]$	$\approx$	$\left[\alpha\mathcal{I} - \frac{d\mathcal{C}\left(\tilde{f}\right)}{d\tilde{f}}\right]$

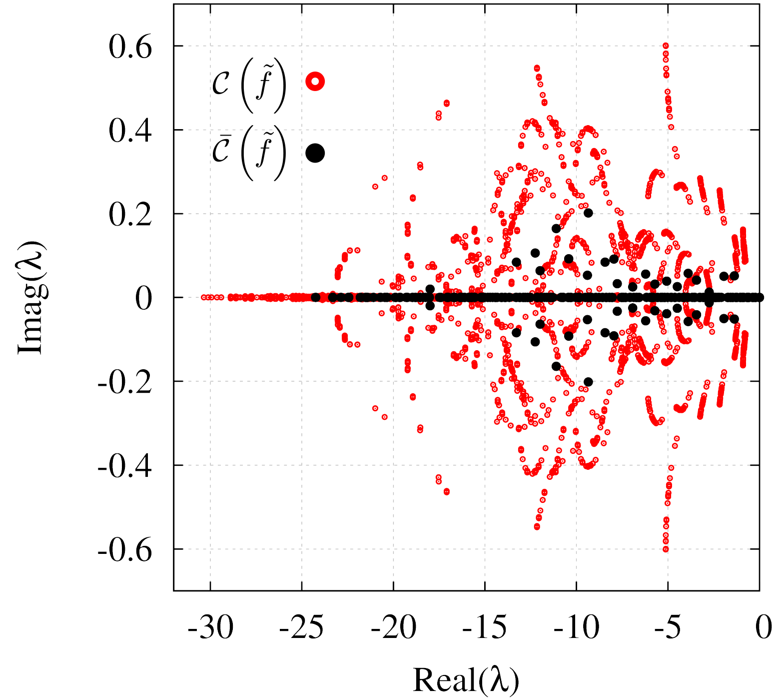
- Use lower order finite differences to construct the preconditioning matrix
- More sparse than the actual Jacobian
- Assembled and stored as a sparse matrix

$\mathcal{C}\left(\tilde{f}\right)$
- 5^{th} order upwind for advective terms
- 4^{th} order central for diffusion terms

$\bar{\mathcal{C}}\left(\tilde{f}\right)$
- 1^{st} order upwind for advective terms
- 2^{nd} order central for diffusion terms

Results in a 9-banded matrix

Eigenvalues of the Jacobian of the actual collisions term and the approximation for preconditioning



The preconditioner is inverted using the *Gauss-Seidel method* (computationally inexpensive)

Test Problem: Ion Parallel Heat Transport

A 2D slab (in configuration space), ***representative of cold edge***

$$\left.\begin{array}{l} n = 10^{20}\ m^{-3} \\ T = 20\ eV \end{array}\right\} \quad k_{\parallel}\lambda = 0.065$$

Highly collisional

Periodic

1 unit

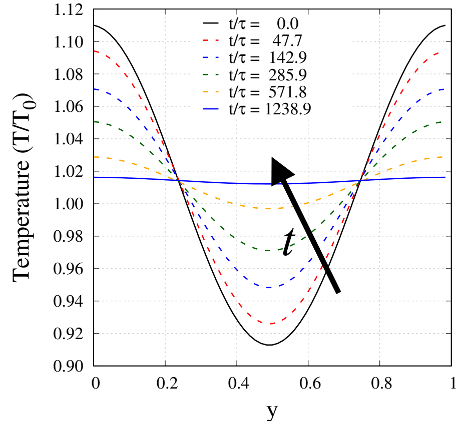
1 unit

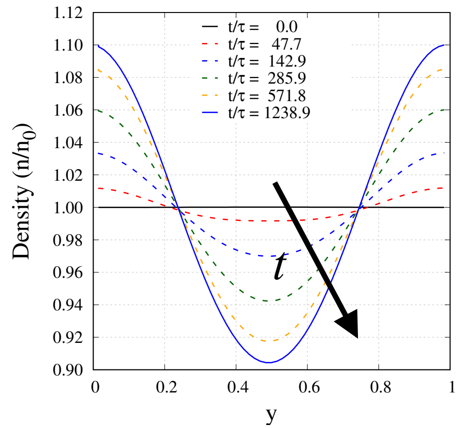
$$\frac{\partial\,(\cdot)}{\partial x} = 0$$

$$T(x, y, 0) = T_0\,(1 + 0.1\cos 2\pi y)$$
$$n(x, y, 0) = n_0$$
$$\phi(x, y, t) = -0.1\frac{T_0}{Ze}\cos 2\pi y$$

$$\mathbf{B} = B_y\hat{\mathbf{y}} + B_z\hat{\mathbf{z}} = \text{constant}$$

Periodic



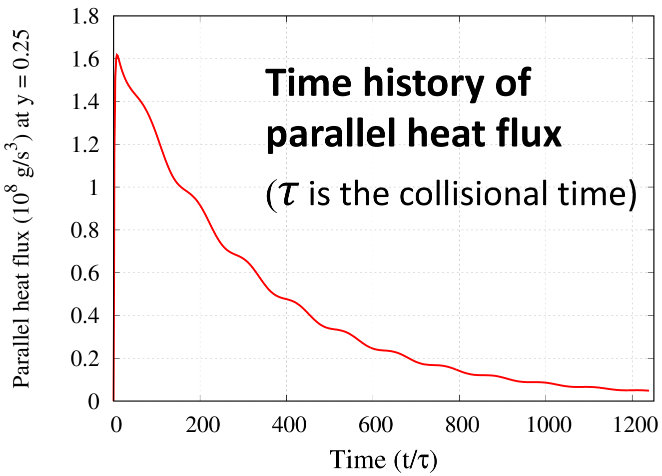


Transport time scale

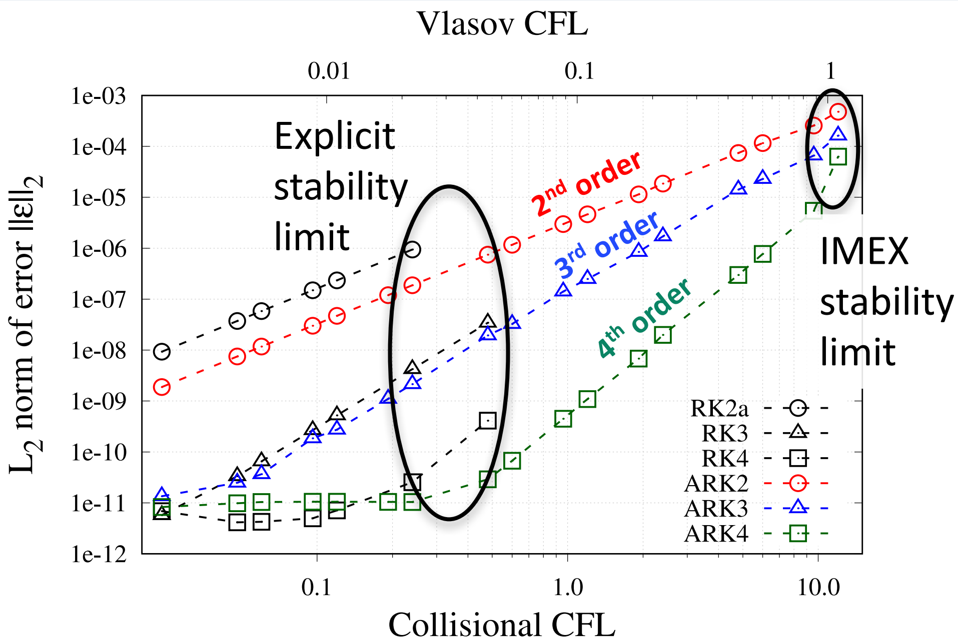
- Temperature equilibrates to constant value
- Density assumes cosine shape to balance electrostatic potential

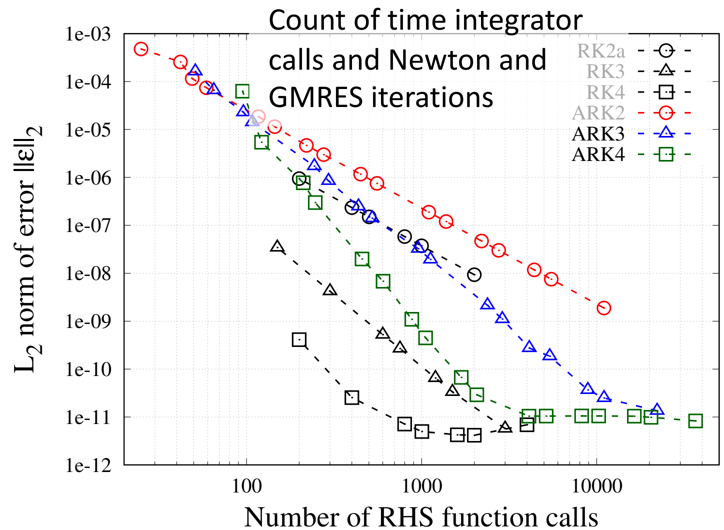
Collisional time scale

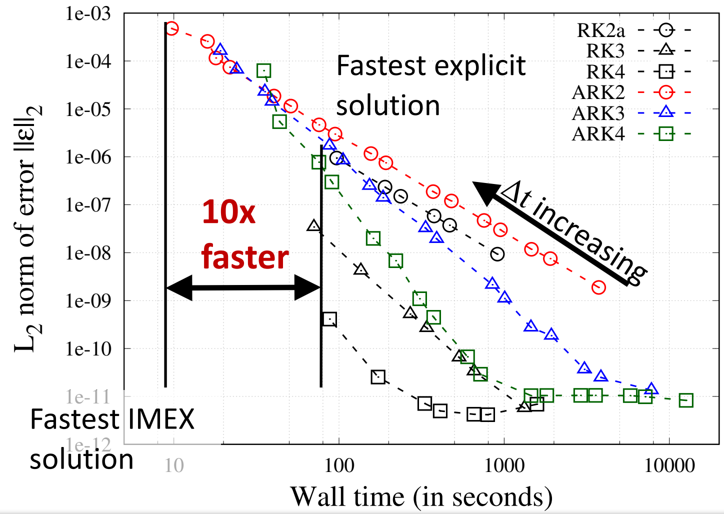
- Heat flux attains values consistent with temperature gradient



Performance of IMEX Time Integrators







- Problem setup:
  - Grid size: $6\ (x) \times 64\ (y) \times 36\ (v_{||}) \times 24\ (\mu)$
  - Reference solution computed with RK4 using very low Δt
- IMEX methods achieve theoretical orders of convergence
- ***Fastest stable solution***: IMEX schemes are 4x (ARK4) to 10x (ARK2) faster with 25x larger time steps.

Effect of Preconditioner

Computational cost of ARK4 with and without preconditioner

Gauss-Seidel solver with 80 iterations

Vlasov CFL	Collision CFL	Number of Function Calls *			Wall time (seconds)		
		No PC	With PC	Ratio	No PC	With PC	Ratio
0.04	**0.5**	*2164*	*2067*	***0.96***	711.33	719.1	**1.01**
0.11	**1.2**	*991*	*879*	***0.89***	321.5	307.9	**0.96**
0.22	**2.4**	*586*	*457*	***0.78***	190.5	161.2	**0.85**
0.55	**6.0**	*355*	*211*	***0.59***	123.1	75.5	**0.61**
1.10	**12.0**	*190*	*95*	***0.50***	63.3	35.1	**0.55**

* Number of function calls = Calls from time integrator (time steps × stages) + number of Newton iterations + number of GMRES iterations

- Preconditioner results in significant speed-up
- Overhead of assembling and inverting the preconditioning matrix is relatively small

Conclusions and Future Work

- IMEX approach for highly-collisional tokamak edge plasma
  - ✓ Collisions integrated in time implicitly while Vlasov term integrated in time explicitly
  - ✓ Wall time for fastest stable solution significantly reduced
  - ✓ Low order preconditioning results in lower computational cost at high collision CFL numbers

- Future work
  - More efficient solver for inverting the preconditioning matrix (Gauss-Seidel needs 80 iterations!)
  - Implement IMEX for other fast scales (*electrostatic Alfven waves, parallel electron transport, ion acoustic modes, parallel ion transport*)

Thank you.
Questions?

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