# 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

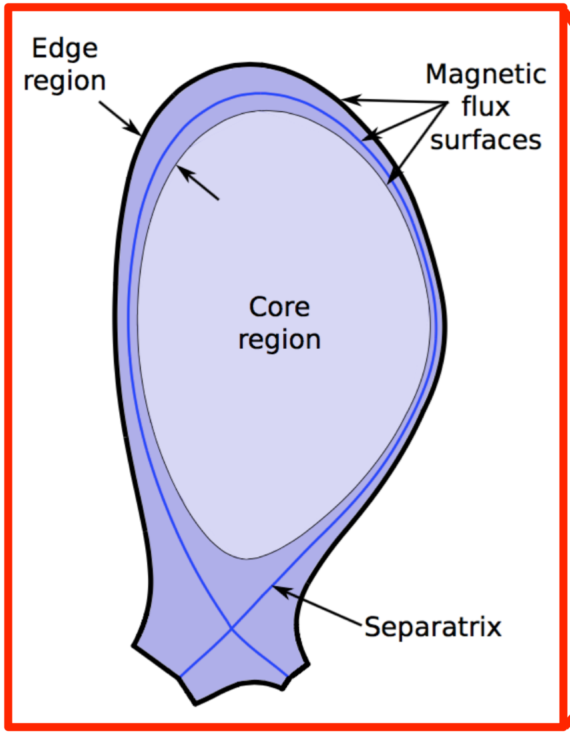
- High temperature and density
- Mean free paths comparable to density/temperature gradients
- Weakly collisional

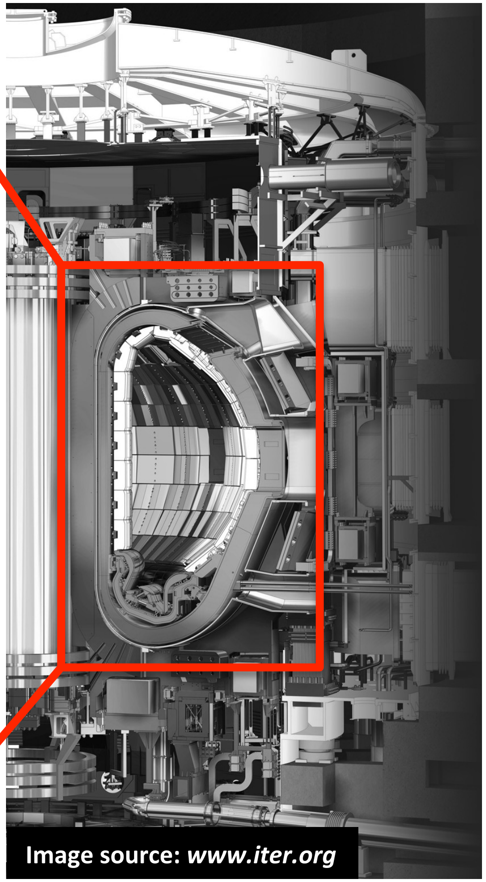
*Requires kinetic simulation with collision model*

***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

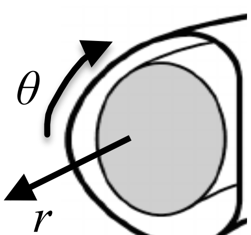
$$\dot{\mathbf{R}}_\alpha \equiv \dot{\mathbf{R}}_\alpha\left(\mathbf{R}, v_\parallel, \mu, t\right) = \frac{1}{B^*_{\parallel,\alpha}}\left[v_\parallel \mathbf{B}^*_\alpha + \frac{1}{Z_\alpha e}\hat{\mathbf{b}} \times \left(Z_\alpha e \mathbf{E} + \mu \nabla_{\mathbf{R}} B\right)\right] \quad \text{Velocity}$$

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

## 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 $f_\alpha$ 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

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

**Rosenbluth potentials** are related to $f_\beta$ by the Poisson equations

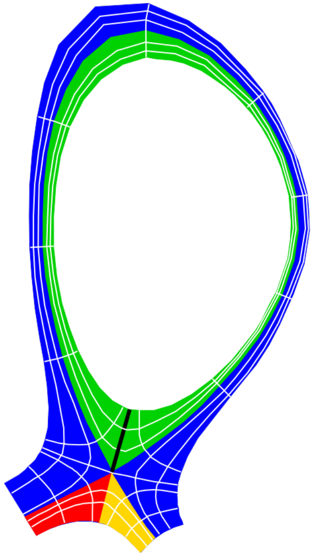
$$\frac{\partial^2 \varphi_\beta}{\partial v_\parallel^2} + \frac{m_\beta}{B}\frac{\partial}{\partial \mu}\left(2\mu \frac{\partial \varphi_\beta}{\partial \mu}\right) = f_\beta$$

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

**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

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

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

**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

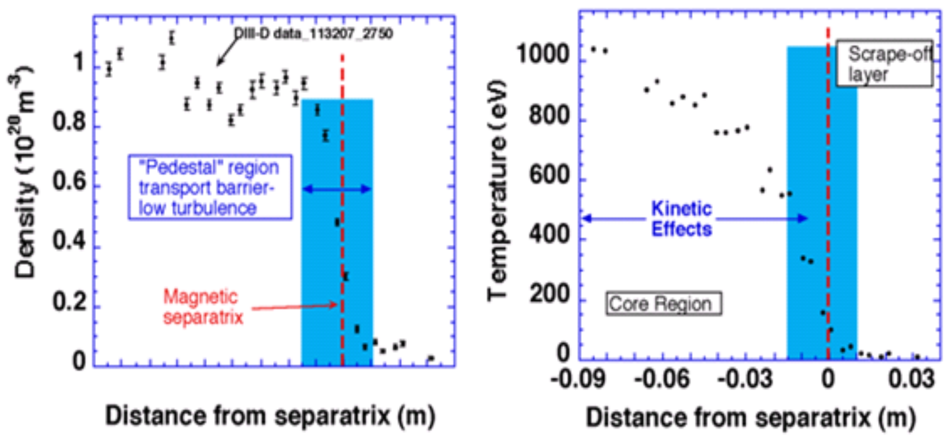
$$\lambda_R \equiv \lambda \left[ \frac{d\mathcal{R}\left(\tilde{f}\right)}{d\tilde{f}} \right]$$

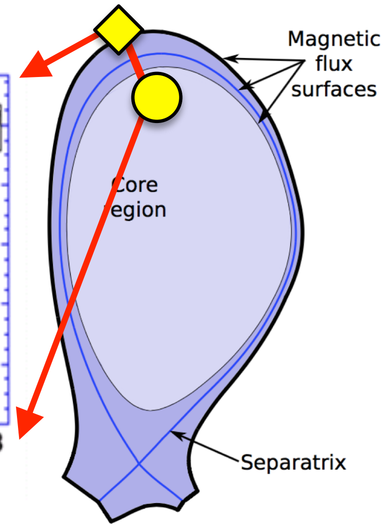
$$\lambda_V \equiv \lambda \left[ \frac{d\mathcal{V}\left(\tilde{f}\right)}{d\tilde{f}} \right]$$

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

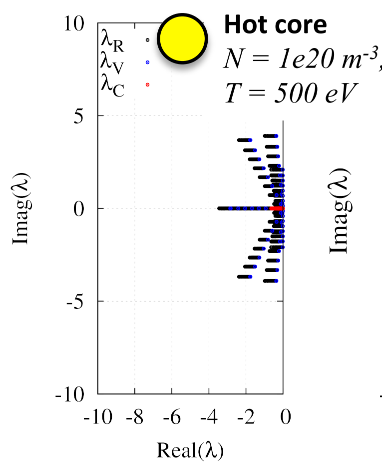
Jacobians computed using finite-differences on a very small grid

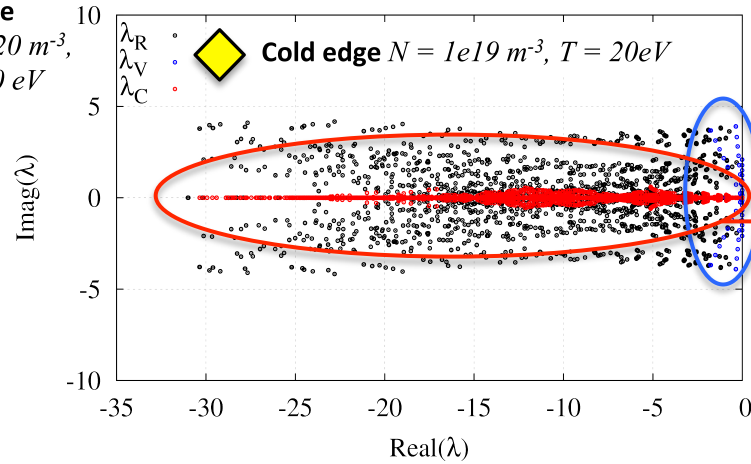
## Tokamak edge density and temperature




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




**At the cold edge**

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

$$\boxed{\begin{aligned} \mathcal{R}_{\text{stiff}} &\equiv \mathcal{C}\left(\tilde{f}\right) \\ \mathcal{R}_{\text{nonstiff}} &\equiv \mathcal{V}\left(\tilde{f}\right) \end{aligned}}$$

# Temporal Scales at Tokamak Edge

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

$\lambda$

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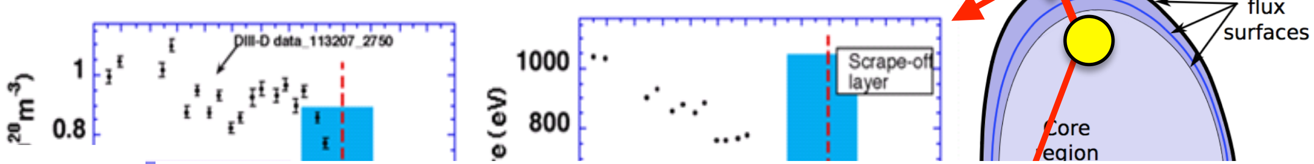
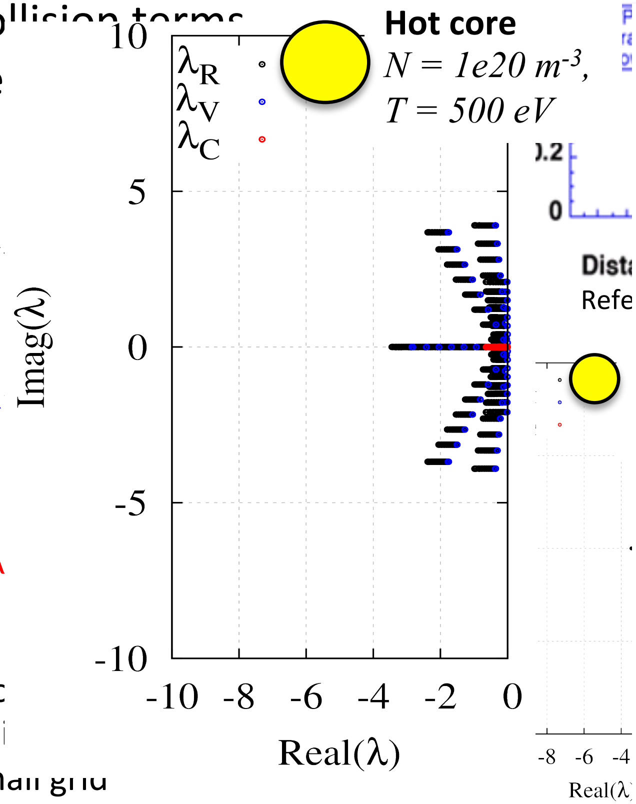
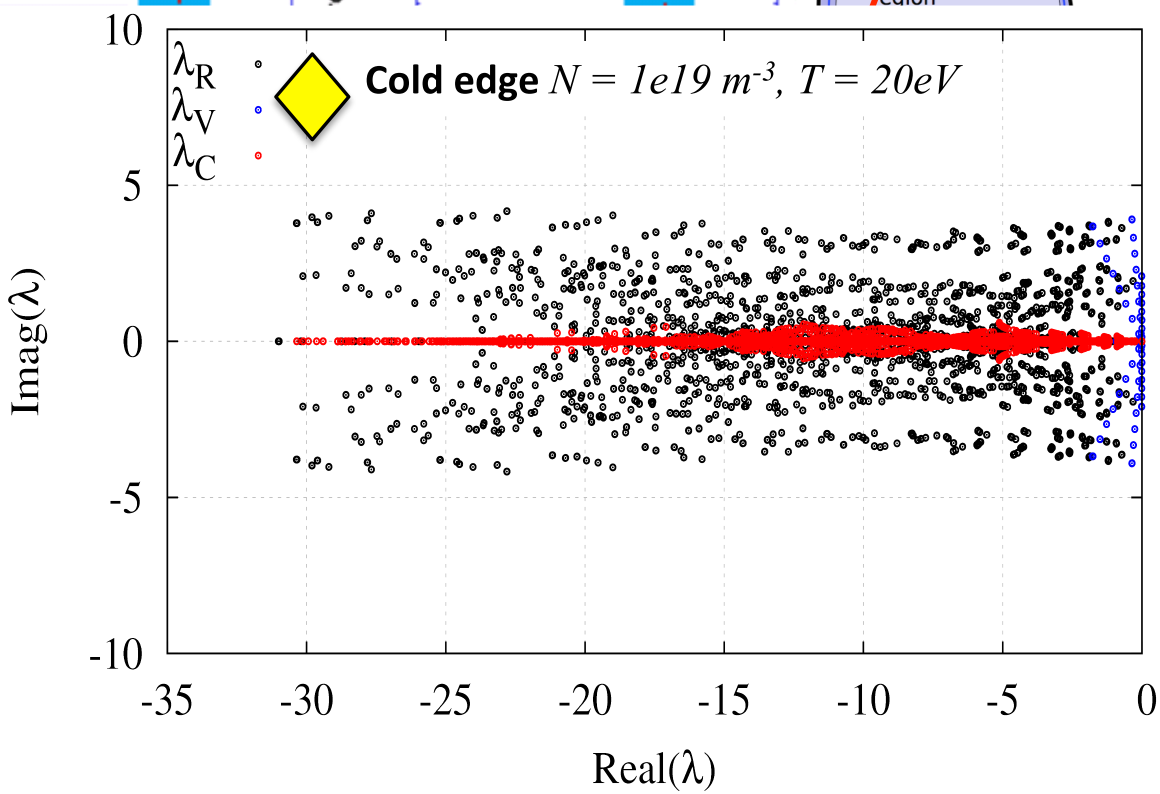
Jac
fini
small grid

**Tokamak edge density and temperature**



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

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

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

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

# Implicit Stage Solution

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

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

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

*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: $y_{k+1} = y_k - \mathcal{J}\left(y_k\right)^{-1} \mathcal{F}\left(y_k\right)$

GMRES solver:

$\mathcal{J}\left(y_k\right) \Delta y = \mathcal{F}\left(y_k\right)$

Action of the Jacobian on a vector approximated by directional derivative

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

# Preconditioning

**Preconditioner** *(sparse matrix)* $\approx$ **Exact Jacobian** *(never assembled)*

$$\left[\alpha\mathcal{I} - \frac{d\bar{\mathcal{C}}\left(\tilde{f}\right)}{d\tilde{f}}\right] \approx \left[\alpha\mathcal{I} - \frac{d\mathcal{C}\left(\tilde{f}\right)}{d\tilde{f}}\right]$$

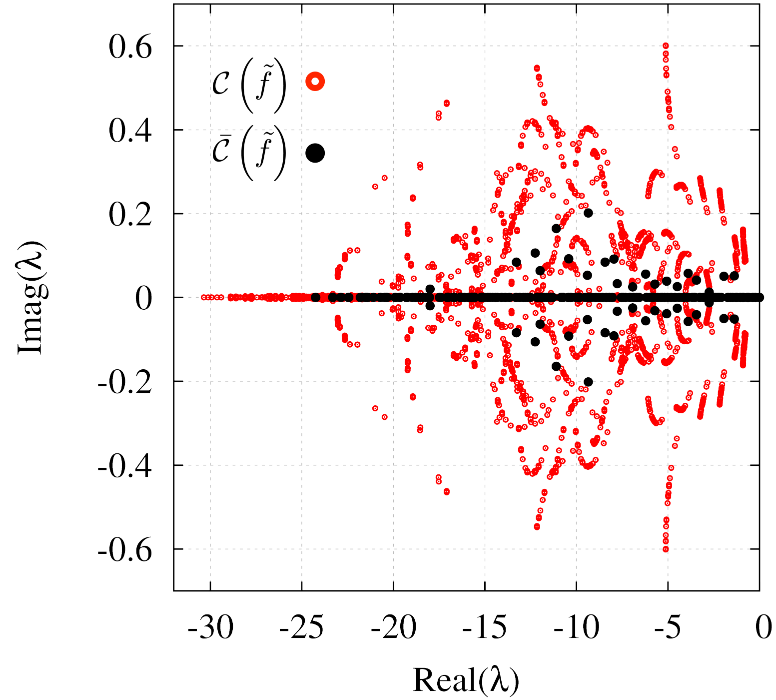
- Use lower order finite differences to construct the preconditioning matrix
- More sparse than the actual Jacobian
- Assembled and stored as a sparse matrix

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

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



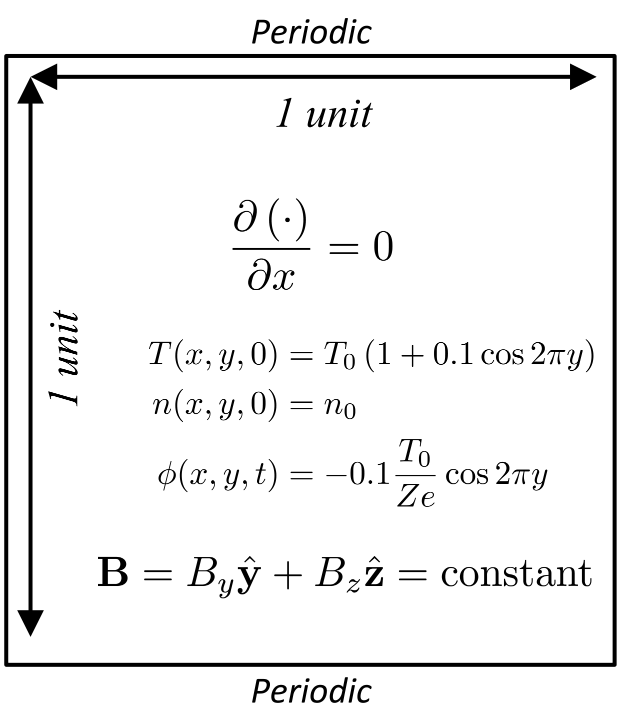

The preconditioner is inverted using the *Gauss-Seidel method* (computationally inexpensive)

# Test Problem: Ion Parallel Heat Transport

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

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

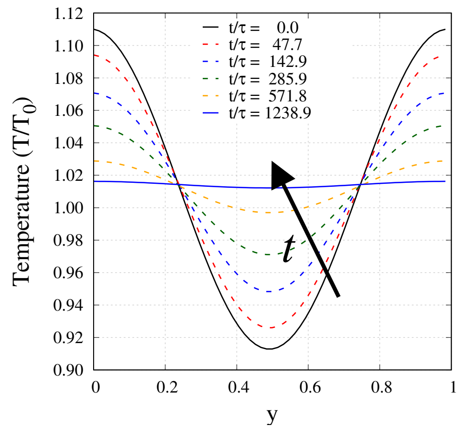
**Highly collisional**

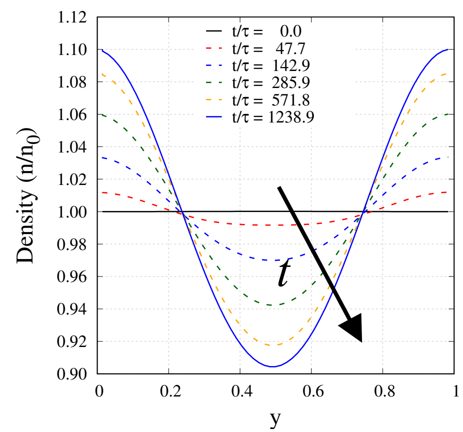



$$\frac{\partial\left(\cdot\right)}{\partial x} = 0$$

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

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



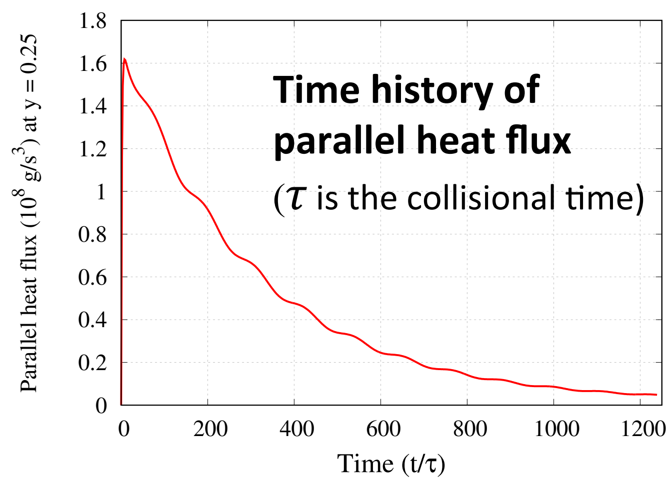




**Transport time scale**

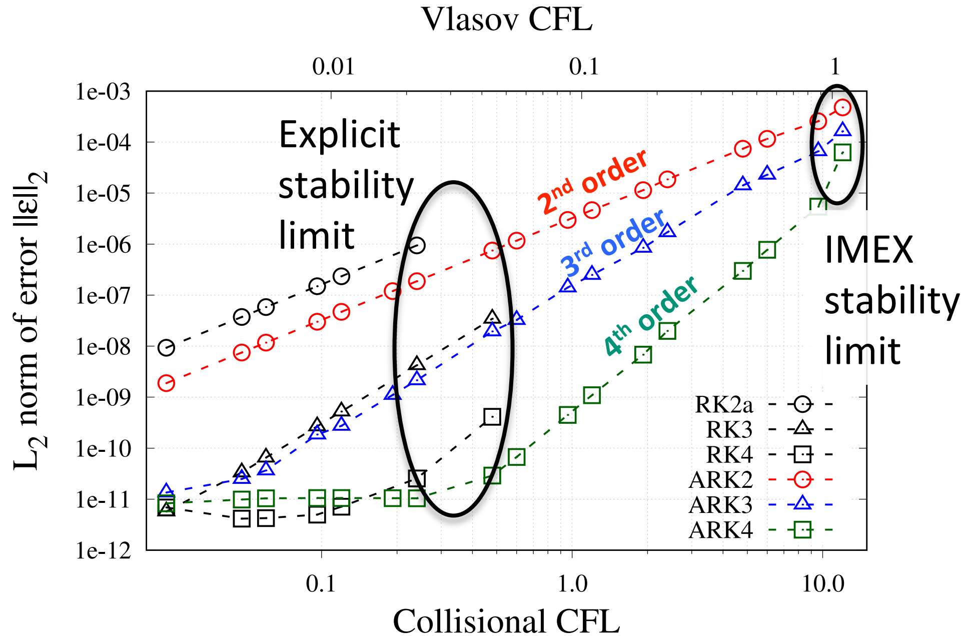
- Temperature equilibrates to constant value
- Density assumes cosine shape to balance electrostatic potential

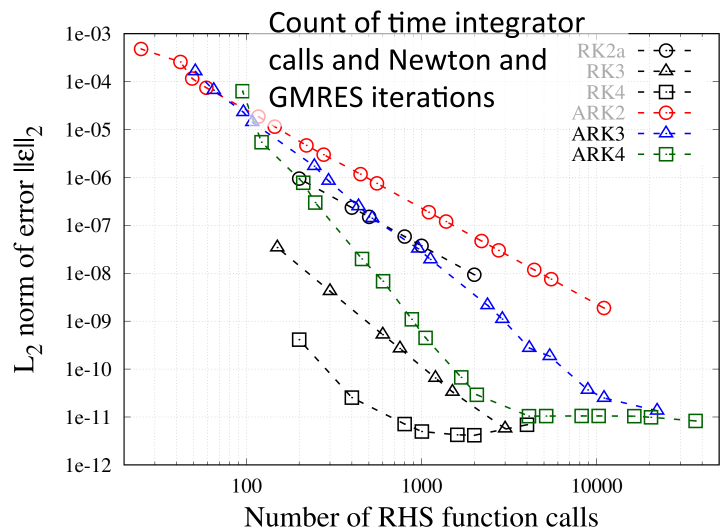
**Collisional time scale**

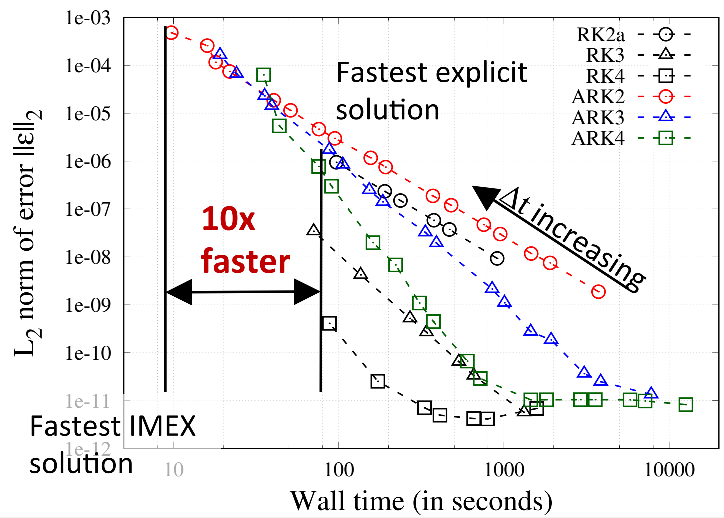
- Heat flux attains values consistent with temperature gradient



# Performance of IMEX Time Integrators




- Problem setup:
  - Grid size: 6 $(x)$ × 64 $(y)$ × 36 $(v_{||})$ × 24 $(\mu)$
  - Reference solution computed with RK4 using very low $\Delta t$
- 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?