Semi-Implicit Time Integration for Multiscale Tokamak-Edge Plasma Dynamics

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CASC
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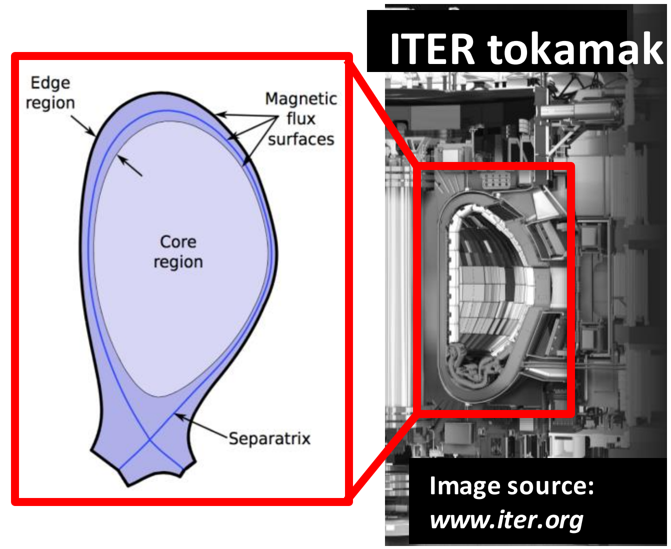
Challenges in Simulating Tokamak-Edge Plasma Dynamics

Kinetic effects are essential

- Strong deviations from the Maxwellian distribution
- Large poloidal variation in the electrostatic potential

High-dimensionality of governing equations

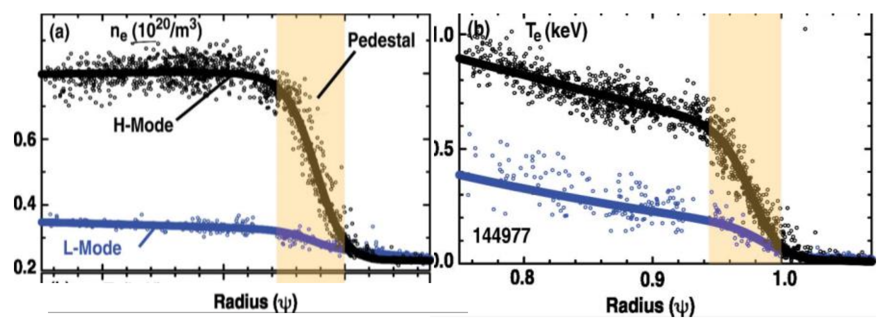


Complicated geometry and anisotropy

- Magnetic separatrix and X-point
- Physical boundaries
- **Strong magnetic field** implies parallel advection much larger than perpendicular drifts

Collision regimes vary rapidly

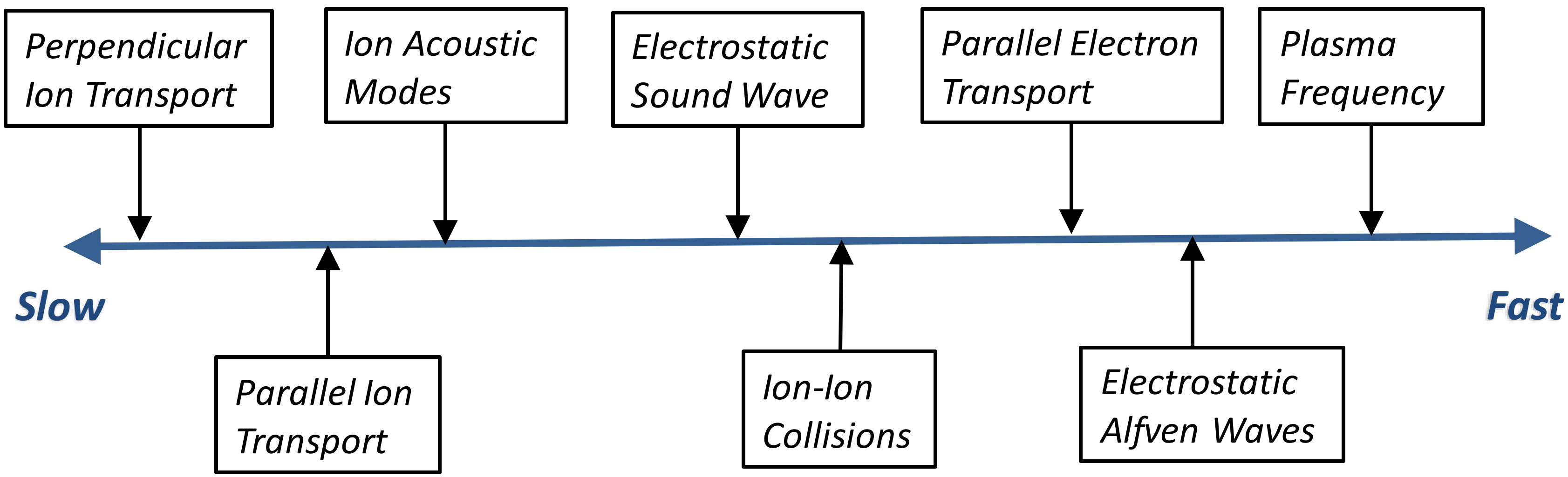
- Weakly-collisional in the hot core
- Strongly-collisional in the cold edge



A. W. Leonard, Phys. Plasmas 21, 090501 (2014)

Time Scales and Time Integration

Tokamak edge plasma dynamics is characterized by a **large range of time scales**



Explicit time-integration constrained by *fastest time scale in the model*

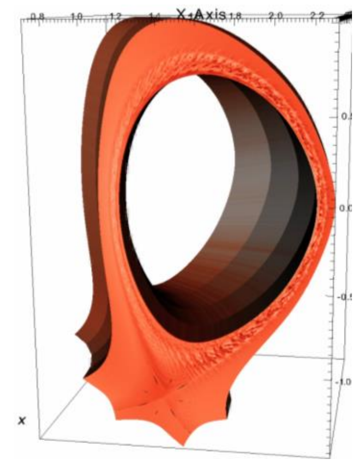
- *Inefficient when resolving slow dynamics*

Implicit time-integration requires solution to *nonlinear system of equations*

- *Unconditional stability*
- *Pay for inverting terms we want to resolve?*

Which time scales do we want to resolve? *(Usually, some of them)*

COGENT: *High-Order Finite-Volume Gyrokinetic Code for Magnetized Plasma Dynamics*



Physics/Mathematical characteristics	**Algorithm choice**
High dimensionality (kinetic modelling)	High-order spatial discretization
Numerical Conservation	Finite volume discretization; Conservative semi-implicit time integration
Complex geometry and anisotropy (tokamak edge, Z-pinch)	Mapped, multiblock, field-aligned grids
Multiple time scales	**Implicit-explicit (IMEX) time integration** (high-order additive Runge-Kutta methods)

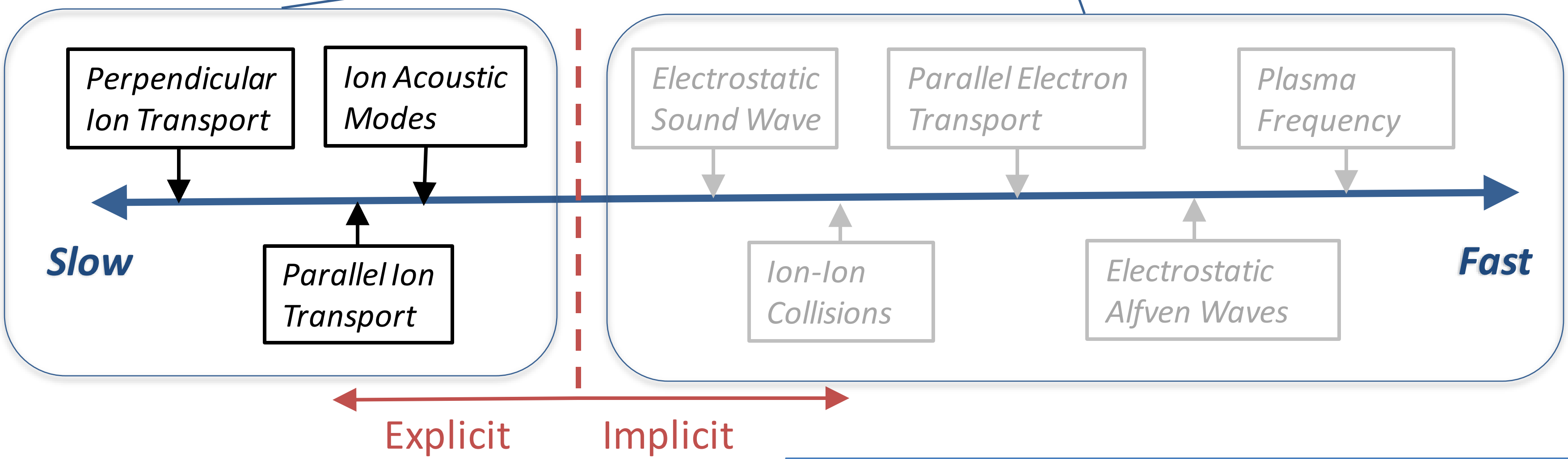
Implicit-Explicit (IMEX) Time Integration

Resolve scales of interest; Treat implicitly faster scales

ODE in time Resulting from spatial discretization of PDE $$\frac{d\mathbf{y}}{dt} = \mathcal{R}(\mathbf{y})$$

IMEX time integration:
partition RHS

$$\mathcal{R}(\mathbf{y}) = \mathcal{R}_{\text{nonstiff}}(\mathbf{y}) + \mathcal{R}_{\text{stiff}}(\mathbf{y})$$

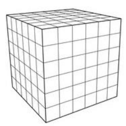


Time step constrained by *fastest explicit time scale*

Flexible, user-specified partitioning of various physics terms depending on the time scale of interest

Governing Equations: *Cross-Separatrix Transport Model with Self-Consistent Electric Fields*

Phase-space collisional drift-kinetic model (4D/5D) – *ion species*



$$\frac{\partial\left(B^*_{\parallel\alpha} f_\alpha\right)}{\partial t} + \nabla_{\mathbf{X}} \cdot \left(\dot{\mathbf{X}}_\alpha B^*_{\parallel\alpha} f_\alpha\right) + \frac{\partial}{\partial v_\parallel}\left(\dot{v}_{\parallel\alpha} B^*_{\parallel\alpha} f_\alpha\right) = \mathcal{C}\left[B^*_{\parallel\alpha} f_\alpha\right]$$

Fokker-Planck collision model

where

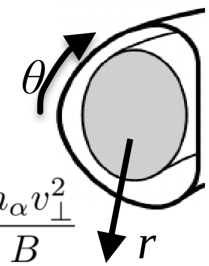
$$\dot{\mathbf{X}}_\alpha = \frac{1}{B^*_{\parallel\alpha}}\left[v_\parallel \mathbf{B}^*_\alpha + \frac{1}{Z_\alpha e}\mathbf{b} \times \left(Z_\alpha e \nabla\phi + \mu\nabla B\right)\right],$$

$$\dot{v}_{\parallel\alpha} = -\frac{1}{m_\alpha B^*_{\parallel\alpha}}\mathbf{B}^*_\alpha \cdot \left(Z_\alpha e \nabla\phi + \mu\nabla B\right)$$

Physical and velocity coordinates

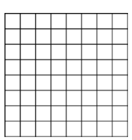
$$\mathbf{X} \equiv \{r, \theta\}$$

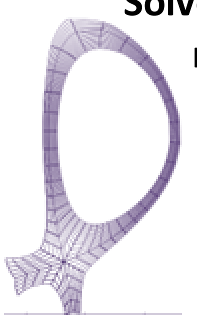
$$v_\parallel, \ \mu = \frac{1}{2}\frac{m_\alpha v_\perp^2}{B}$$



Configuration-space self-consistent, quasineutral model (2D/3D) – *electrostatic potential*

$$\frac{\partial}{\partial t}\left[\nabla_\perp \cdot \left(\frac{e^2 n_i}{m_i \Omega_i^2}\nabla_\perp\phi\right)\right] = \nabla_\perp \cdot \mathbf{j}_{i,\perp} + \nabla_\parallel\left[\sigma_\parallel\left(\frac{1}{e n_i}\nabla_\parallel P_e - \nabla_\parallel\phi + \frac{0.71}{e}\nabla_\parallel T_e\right)\right]$$
$$- \nabla_\perp \cdot \left(\frac{c^2 m_i n_i \nu_{ex}}{B^2}\nabla_\perp\phi\right)$$



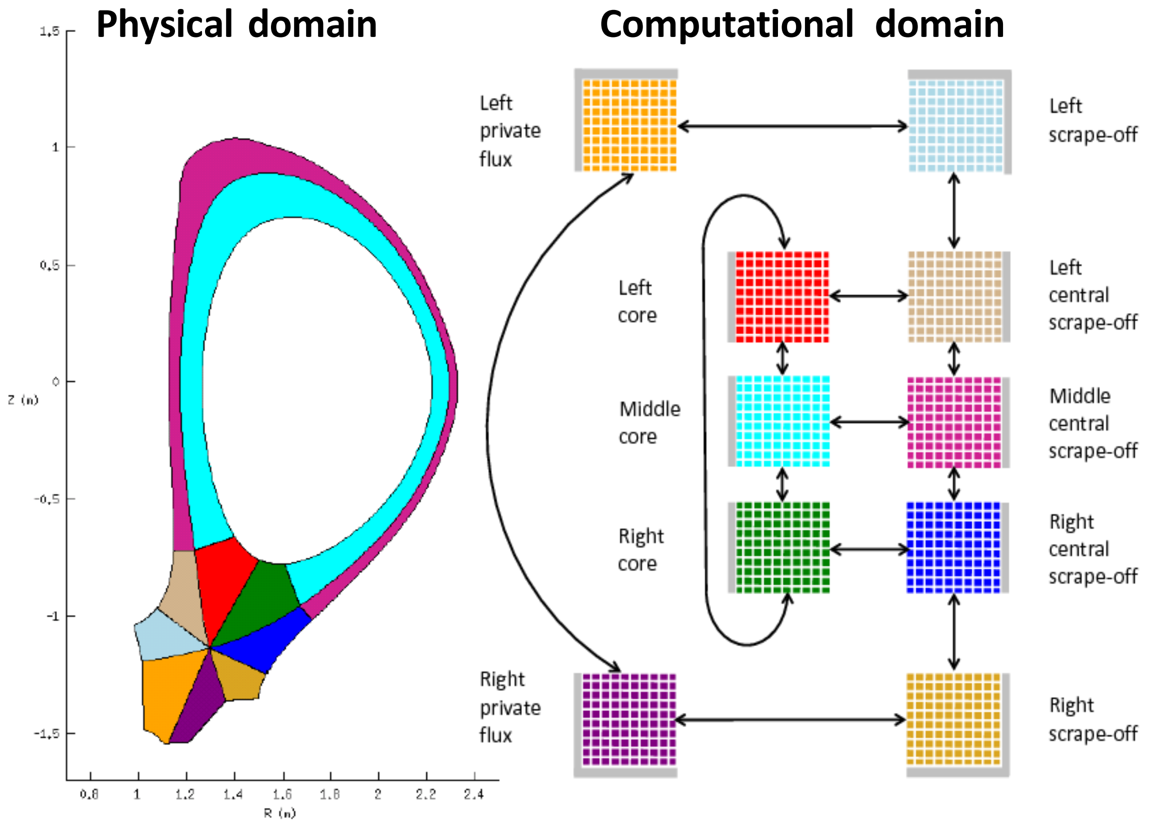


Solved on a mapped, multi-block mesh representing the tokamak edge

Reference: Dorf & Dorr, 2018, Contrib. Plasma Phys.

Spatial Discretization: Mapped Multiblock Grids

- Spatial discretization uses **Chombo**
- Domain decomposed into **multiple blocks**
- Each block mapped to a **Cartesian hypercube** with uniform grid
- High-order finite volume discretization requires extended **smooth block mappings**
- One of the coordinates is **aligned along the magnetic flux** lines (2D) or surfaces (3D)



Example: Ten-block grid for the DIII-D geometry

Reference: Dorr Et Al., 2018, J. Comput. Phys.

Semi-Discretized ODE and Stiff Terms

Semi-discrete ODE for the kinetic ions

$$\frac{d\mathbf{f}}{dt} = \mathcal{V}(\mathbf{f}, \mathbf{\Phi}) + \mathcal{C}(\mathbf{f})$$

Semi-discrete ODE for the electrostatic potential

$$\frac{d}{dt}\left[\mathcal{M}(\mathbf{f})\,\mathbf{\Phi}\right] = \mathcal{R}_{\perp}(\mathbf{f}, \mathbf{\Phi}) + \mathcal{R}_{\|}(\mathbf{f}, \mathbf{\Phi})$$

$$\nabla_{\perp} \cdot \left(\frac{e^2 n_i}{m_i \Omega_i^2} \nabla_{\perp} \phi\right) \rightarrow \mathcal{M}(\mathbf{f})\,\mathbf{\Phi}$$

ODE with nonlinear LHS operator

$$\mathbf{f} = \begin{bmatrix} \vdots \\ B^*_{\|\alpha} f_\alpha \\ \vdots \end{bmatrix}$$

$$\mathbf{\Phi} = \begin{bmatrix} \vdots \\ \phi \\ \vdots \end{bmatrix}$$

(vectors of solution at grid points)

Partitioned system of ODEs for IMEX time integration

$$\frac{d}{dt}\left[\mathbb{M}(\mathbf{U})\right] = \mathcal{R}_{\mathrm{nonstiff}}(\mathbf{U}) + \mathcal{R}_{\mathrm{stiff}}(\mathbf{U})$$

where $\mathbf{U} \equiv \begin{bmatrix} \mathbf{f} \\ \mathbf{\Phi} \end{bmatrix}$, $\mathbb{M} \equiv \begin{bmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{M} \end{bmatrix}$, $\mathcal{R}_{\mathrm{nonstiff}} \equiv \begin{bmatrix} \mathcal{V}(\mathbf{f}, \mathbf{\Phi}) \\ \mathcal{R}_{\perp}(\mathbf{f}, \mathbf{\Phi}) \end{bmatrix}$,

$$\mathcal{R}_{\mathrm{stiff}} \equiv \begin{bmatrix} \mathcal{C}(\mathbf{f}) \\ \mathcal{R}_{\|}(\mathbf{f}, \mathbf{\Phi}) \end{bmatrix}$$

***Fast timescales:* kinetic collisions and parallel current divergence**

Additive Runge-Kutta (ARK) Time Integration

Modified for nonlinear LHS term

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

Stage solutions

$$\mathbb{M}\left(\mathbf{U}^{(i)}\right) = \mathbb{M}\left(\mathbf{U}^{n}\right) + \Delta t \left[\sum_{j=1}^{i-1} a_{ij} \mathcal{R}_{\text{nonstiff}}\left(\mathbf{U}^{(j)}\right) + \sum_{j=1}^{i} \tilde{a}_{ij} \mathcal{R}_{\text{stiff}}\left(\mathbf{U}^{(j)}\right)\right], \quad i = 1, \ldots, s$$

Step Completion

$$\mathbb{M}\left(\mathbf{U}^{n+1}\right) = \mathbb{M}\left(\mathbf{U}^{n}\right) + \Delta t \sum_{i=1}^{s} b_i \left[\mathcal{R}_{\text{nonstiff}}\left(\mathbf{U}^{(i)}\right) + \mathcal{R}_{\text{stiff}}\left(\mathbf{U}^{(i)}\right)\right]$$

Standard ARK methods if $\mathbb{M}\left(\mathbf{U}\right) = \mathbf{U}$

Note: *"Explicit" stages and step completion* ***also require solution to nonlinear system of equations***

Butcher tableaux representation of time integrator

Explicit RK

$$\begin{array}{c|ccccc} 0 & 0 & & & \\ c_2 & a_{21} & 0 & & \\ \vdots & \vdots & \ddots & 0 & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & \cdots & \cdots & b_s \end{array} \quad + \quad \begin{array}{c|ccccc} 0 & 0 & & & \\ \tilde{c}_2 & \tilde{a}_{21} & \gamma & & \\ \vdots & \vdots & \ddots & \gamma & \\ \tilde{c}_s & \tilde{a}_{s1} & \cdots & \tilde{a}_{s,s-1} & \gamma \\ \hline & b_1 & \cdots & \cdots & b_s \end{array}$$

First-stage-explicit DIRK

ARK2c: 2nd order, 3-stage
(Giraldo, et al, 2013, SISC)

ARK3: 3rd order, 4-stage
(Kennedy & Carpenter, 2003, JCP)

ARK4: 4th order, 6-stage
(Kennedy & Carpenter, 2003, JCP)

Reference: Kennedy & Carpenter, 2003, J. Comput. Phys.

JFNK Solver for Nonlinear System

We need to solve a *nonlinear system of equations* at each time integration stage and at step completion

"Explicit" stages and step completion

$$\mathbb{M}\left(\mathbf{U}\right) = \mathbf{rhs}$$

Implicit stages

$$\alpha\mathbb{M}\left(\mathbf{U}\right) - \mathcal{R}_{\text{stiff}}\left(\mathbf{U}\right) = \mathbf{rhs}$$

where $\alpha = 1/\left(\tilde{a}_{ii}\Delta t\right)$

Jacobian-free Newton-Krylov (JFNK) method :

(Initial guess is *previous stage solution)*

Newton update:

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

Preconditioned GMRES

$$\mathcal{J}\mathcal{P}^{-1}\mathcal{P}\Delta y = \mathcal{F}\left(y_k\right)$$

Action of the Jacobian on a vector approximated by *directional derivative*

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

Reference: Knoll & Keyes, 2004, J. Comput. Phys.

Operator-Split Multiphysics Preconditioner (1)

The **implicit RHS** comprises an **arbitrary number of terms**

$$\mathcal{R}_{\text{stiff}}(\mathbf{U}) = \sum_k \mathcal{F}_k(\mathbf{U})$$

Jacobian

$$\left[\alpha\mathbb{M}'(\mathbf{U}) - \sum_k \mathcal{F}_k'(\mathbf{U})\right]$$

Approximation for Preconditioner

$$\left[\alpha\tilde{\mathbb{M}}'(\mathbf{U}) - \sum_k \tilde{\mathcal{F}}_k'(\mathbf{U})\right]$$

$$\tilde{\mathbb{M}}' \approx \mathbb{M}', \tilde{\mathcal{F}}_k' \approx \mathcal{F}_k'$$

Operator-split wrapper over preconditioners for each individual physics term(s)

$$\left[\alpha\tilde{\mathbb{M}}'(\mathbf{U}) - \sum_k \tilde{\mathcal{F}}_k'(\mathbf{U})\right]\mathbf{x} = \mathbf{b}$$

$$\Rightarrow \mathbf{x} = \prod_{k=N}^{2}\left(\left[\alpha\mathbb{M}' - \mathcal{F}_k'\right]^{-1}\left[\alpha\mathbb{M}'\right]\right)\left[\alpha\mathbb{M}' - \mathcal{F}_1'\right]^{-1}\mathbf{b}$$

- Operator-split approach **wraps multiple independent preconditioners for each term(s)** with fast time scales to precondition the complete implicit solve, *instead of a monolithic preconditioner*
- An **efficient preconditioning strategy** (matrix construction and solver) can be chosen specifically **for each implicit physics** *independent of other implicit terms*
- Applying (inverting) the preconditioner requires the **successive application of these individual preconditioners** on the solution vector

Operator-Split Multiphysics Preconditioner (2)

Implicit kinetic term: *Fokker-Planck-Rosenbluth collision term*

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

where the advective and diffusive coefficients are given by

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

$\mathcal{C}\left(\tilde{f}\right)$ 5th order upwind (advection)
4th order central (diffusion)

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

Results in a **9-banded matrix**; inverted with **Gauss-Seidel**

Implicit fluid terms: *Elliptic LHS Op and parallel current divergence*

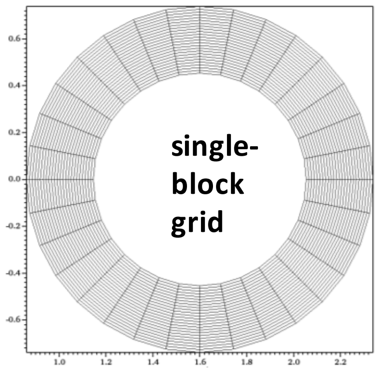
$$\nabla_\perp \cdot \left(\frac{e^2 n_i}{m_i \Omega_i^2} \nabla_\perp \phi\right) \qquad \nabla_\parallel \left[\sigma_\parallel \left(\frac{1}{e n_i} T_e \nabla_\parallel n_i - \nabla_\parallel \phi\right)\right]$$

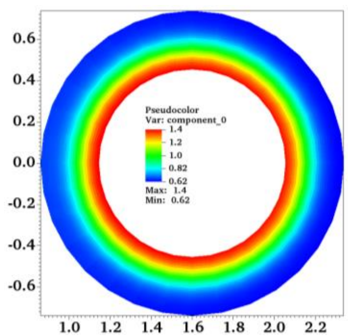
Discretized with 4th order mapped finite volume method
Jacobian approximation constructed with 2nd order mapped finite-difference discretization

Solved with the **Algebraic Multigrid (AMG) method** implemented in the *hypre* library

Test Cases: *Tokamak Edge Simulations*

Kinetic Ion Species with Fokker-Plank Collisions and Fluid Potential Model

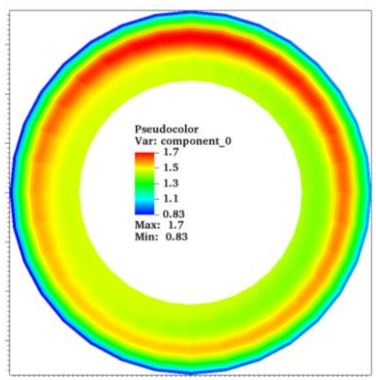




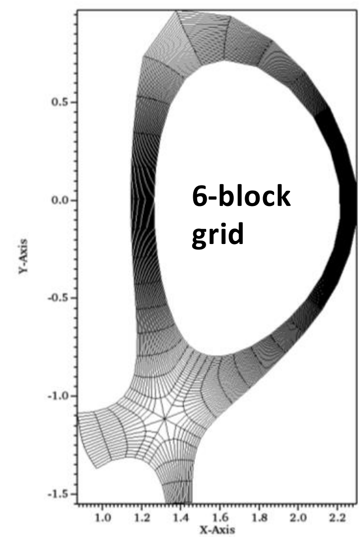
Initial Ion Temperature

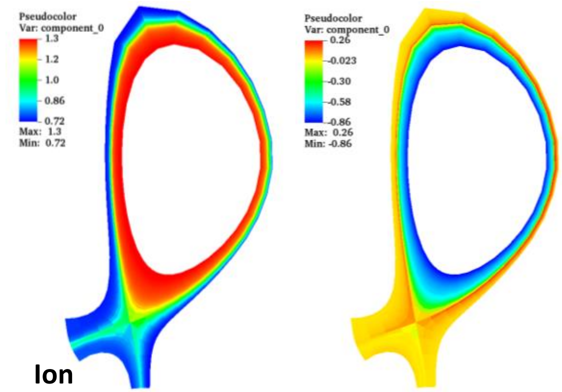
Neoclassical thermal relaxation in annular geometry

Ion Temperature @ 4ms



Plasma equilibration under H-mode parameters in DIII-D tokamak





Ion Temperature

Potential

Solution at $t = 2.8ms$

Reference: Dorf & Dorr, 2018, Contrib. Plasma Phys.

Weakly collisional simulations

Kinetic equation: *completely explicit*

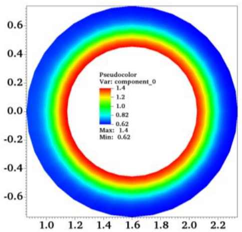
Fluid potential equation: ***parallel current divergence implicit***; perpendicular terms explicit

Strongly collisional simulations

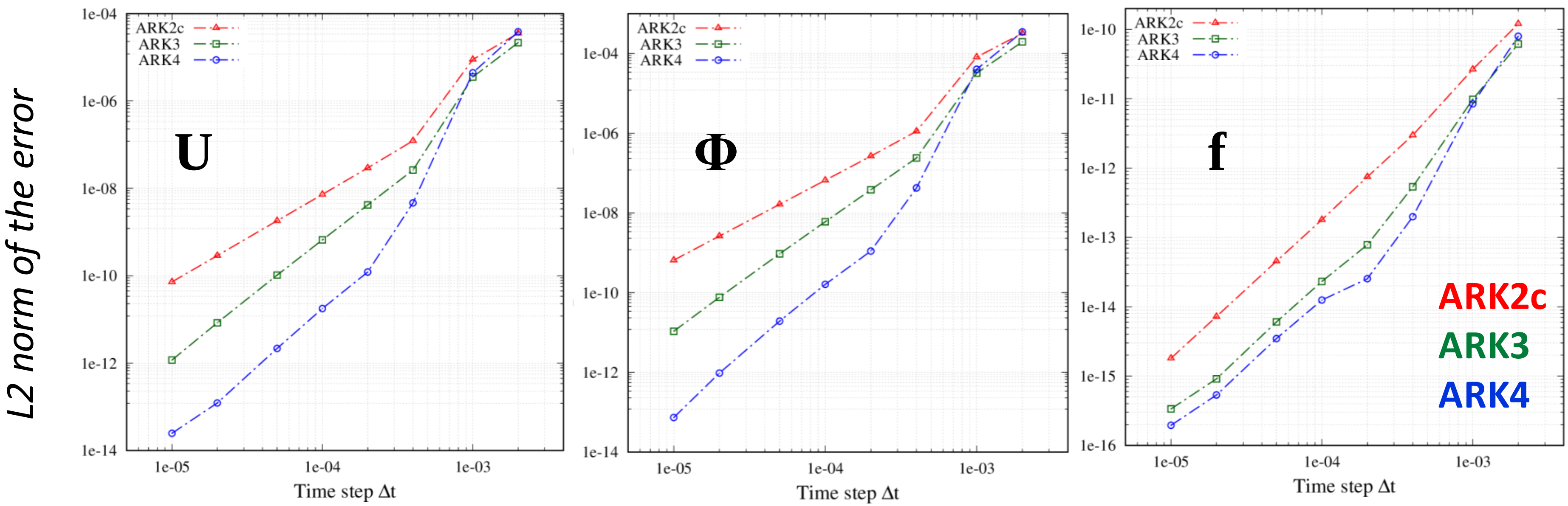
Kinetic equation: ***Collisions implicit***; Vlasov explicit

Fluid potential equation: ***parallel current divergence implicit***; perpendicular terms explicit

Test Case: Neoclassical Thermal Relaxation
Weakly-collisional

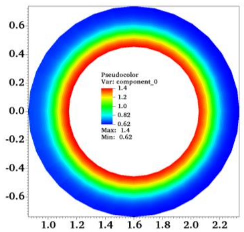


- **Electrostatic potential** (Φ) converges at the theoretical orders (*semi-implicit in time*, with ***nonlinear LHS operator***)
- **Distribution function** ($\mathbf{f}$) converges at ~***2nd order (?)*** (*completely explicit* in time)

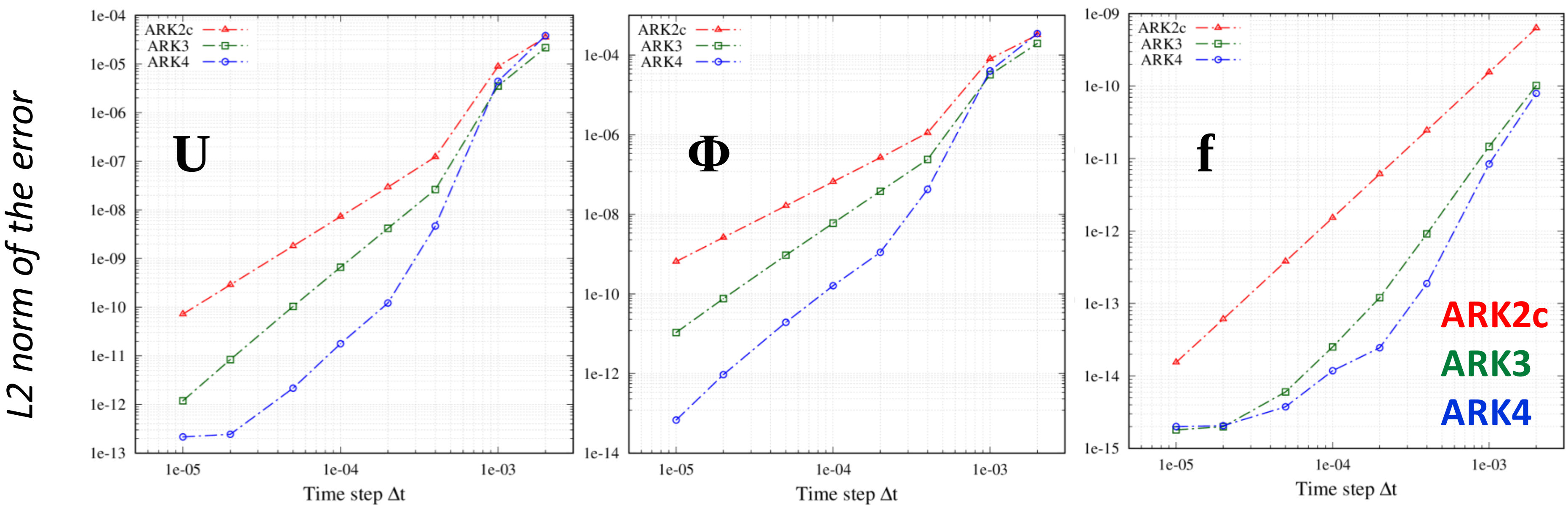


Final time $t_f = 0.002$ (normalized units); ***Timescales:*** ~ 0.1 (Vlasov), ~ 5 (Collisions)
Reference solution generated with ARK4 at $\Delta t_{ref} = 0.05 \Delta t_{min}$ in convergence study

Test Case: Neoclassical Thermal Relaxation
Strongly-collisional



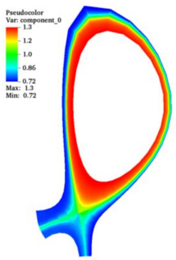
- **Electrostatic potential** (Φ) converges at the theoretical orders (*semi-implicit in time*, with ***nonlinear LHS operator***)
- **Distribution function** ($\mathbf{f}$) converges ***at theoretical order*** for ARK2c and ARK3 (*implicit collisions, explicit Vlasov* in time)



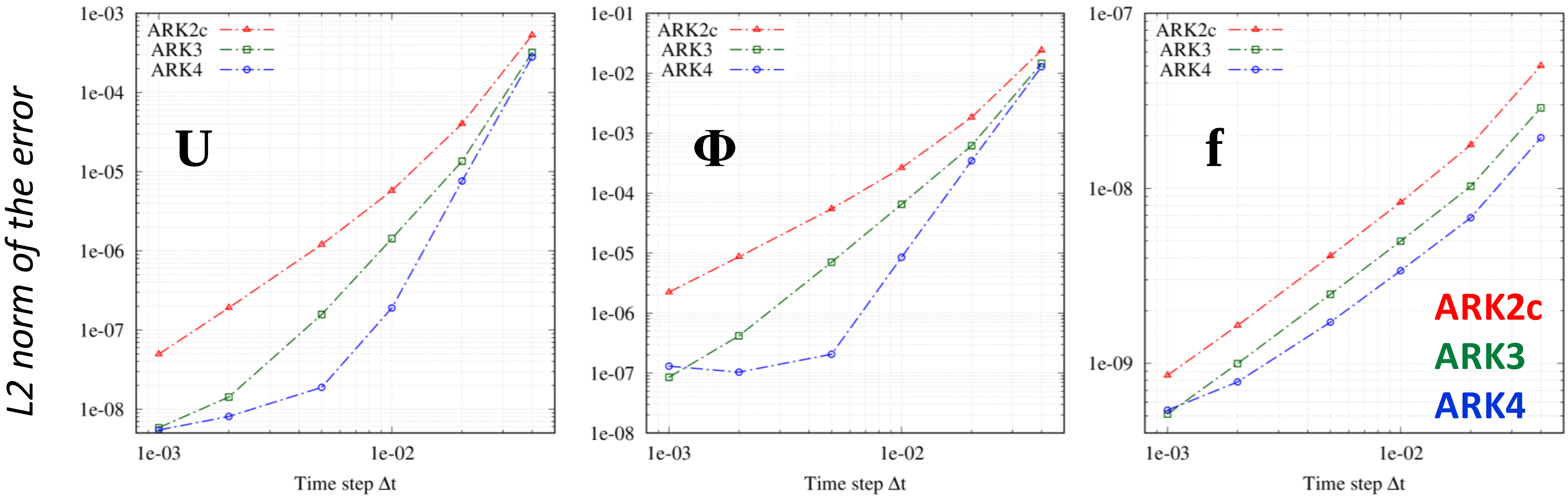
Final time $t_f = 0.002$ (normalized units); ***Timescales:*** ~0.1 (Vlasov), ~5e-3 (Collisions)

Reference solution generated with ARK4 at $\Delta t_{ref} = 0.05 \Delta t_{min}$ in convergence study

Test Case: DIII-D Tokamak H-Mode Simulation
Weakly-collisional



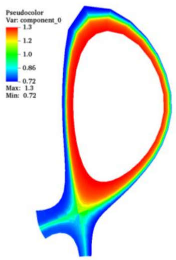
- **Electrostatic potential** (Φ) converges at the theoretical orders (*semi-implicit in time*, with ***nonlinear LHS operator***)
- **Distribution function** ($\mathbf{f}$) converges at ~***1st order*** (*completely explicit* in time)



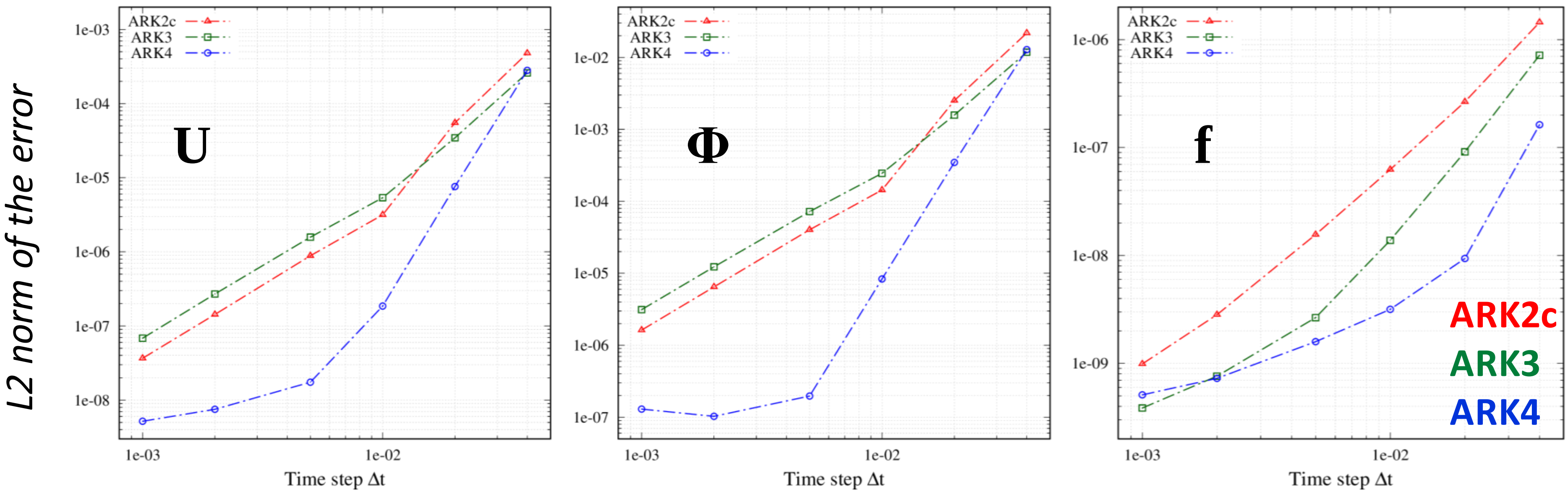
Final time $t_f = 0.040$ (normalized units); ***Timescales:*** ~7e-2 (Vlasov), ~0.7 (Collisions)

Reference solution generated with ARK4 at $\Delta t_{ref} = 0.05\Delta t_{min}$ in convergence study

Test Case: DIII-D Tokamak H-Mode Simulation
Strongly-collisional



- **Electrostatic potential** (**Φ**): ARK2c and ARK4 converge as expected; ARK3 converges at ***2nd order*** (*semi-implicit in time*, with ***nonlinear LHS operator***)
- **Distribution function** (**f**): ARK2c and ARK3 converge as expected; ARK4 converges at ***4th order*** initially, then ~***1st order*** (*completely explicit* in time)



Final time $t_f = 0.040$ (normalized units); ***Timescales:*** ~7e-2 (Vlasov), ~8e-3 (Collisions)
Reference solution generated with ARK4 at $\Delta t_{ref} = 0.05 \Delta t_{min}$ in convergence study

Summary

- **COGENT** is a high-order mapped multiblock code for tokamak-edge plasma dynamics
  - **Open source:** https://github.com/LLNL/COGENT
- We have implemented a **flexible implicit-explicit (IMEX) time integration framework** that allows user-specified partitioning of the various terms into the implicit and explicit sides.
  - Modified the standard Additive Runge-Kutta methods to allow for a ***nonlinear left-hand-side operator***
- **Operator-split preconditioning** acts as a wrapper for tailored preconditioners for each implicit term to precondition the complete implicit solve
- We are testing **time convergence** for simulations on **mapped multiblock grids**
  - Obtained **theoretical convergence** in some cases; currently investigating cause of sub-optimal convergence.

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Thank you.
Questions?

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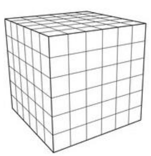
“Multiple-Dimensioned” Governing Equations

COGENT can evolve an arbitrary combination of PDEs of *varying dimensionality* (kinetic and fluid) with a high-order, consistent discretization

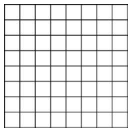
Phase-space kinetic equations (4D/5D) – *ions, electron*

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot \left(\dot{\mathbf{x}} \left[f, \phi \right] f \right) + \frac{\partial}{\partial v_{\parallel}} \left(\dot{v}_{\parallel} \left[f, \phi \right] f \right) = C \left[f \right]$$

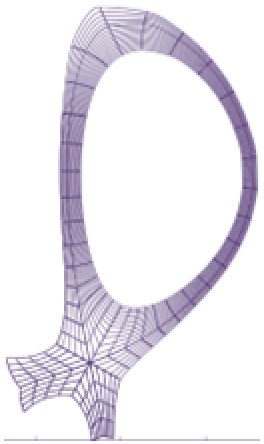


Configuration space fluid/field equations (2D/3D)
– *ions, electron, vorticity, neutrals*

$$\frac{\partial \phi}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{F} \left(f, \phi \right) = \nabla_{\mathbf{x}} \left(\nabla_{\mathbf{x}} \cdot \mathbf{G} \left(f, \phi \right) \right)$$



Solved on a mapped, multi-block mesh representing the tokamak edge



+ any closure equations (e.g., gyro-Poisson equation for electrostatic potential or any other equation to complete the system)

Number of kinetic and fluid equations is flexible and user-specified, including capability for kinetic-only or fluid-only simulations

COGENT is part of the Edge Simulation Laboratory collaboration between US DOE ASCR and FES

edge
simulation
laboratory

Math (ASCR)

CASC
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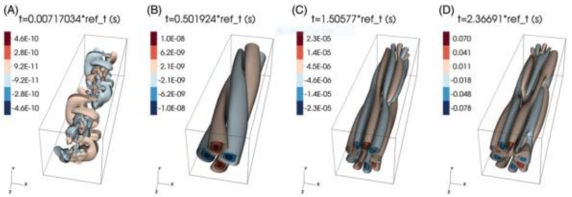
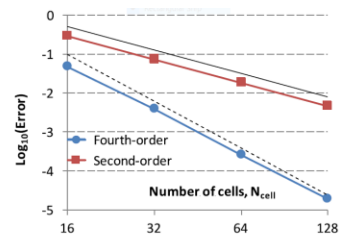
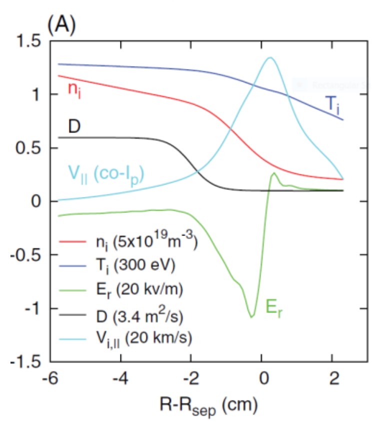
Kinetic drift-wave instability (Lee et al., Contrib. Plasma Phys., 58, 445-450, 2018)



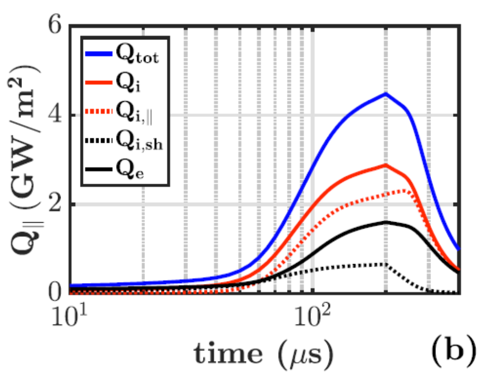
High-order drift wave modeling (Dorf et al., J. Comput. Phys., 373, 446-545, 2018)



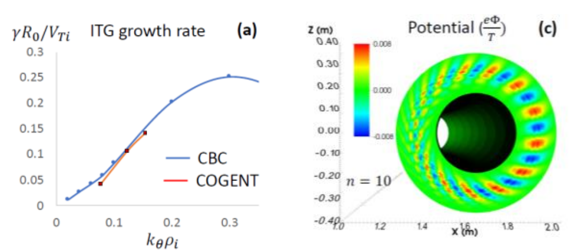
Cross separatrix transport (Dorf et al., Contrib. Plasma Phys.,58, 434-444, 2018)



ELM heat pulse (Joseph et al., Nucl. Mater. Energy, 19, 330-334, 2019)



5-D full-f gyrokinetic code COGENT (Dorf et al., Contrib. Plasma Phys.,2020)

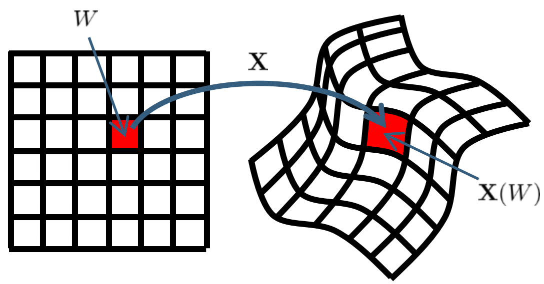


4^{th} Order Mapped Finite-Volume Discretization

Computational coordinates:

Spatial domain discretized by rectangular control volumes

$$V_{\mathbf{i}} = \prod_{d=1}^{D}\left[i_d - \frac{h}{2}, i_d + \frac{h}{2}\right]$$



$\mathbf{X} \equiv \mathbf{X}(\xi), \quad \mathbf{X} : [0,1]^D \to \Omega \subset \mathbf{R}^D$

Mapped coordinates:

Mapping from abstract Cartesian coordinates into physical space

$$\mathbf{X} = \mathbf{X}(\boldsymbol{\xi}), \qquad \mathbf{X} : [0,1]^D \to \mathbb{R}^D$$

Fourth-order flux divergence average from fourth-order cell face averages

$$\int_{\mathbf{X}(V_{\mathbf{i}})} \nabla_{\mathbf{X}} \cdot \mathbf{F} d\mathbf{x} = \sum_{\pm=+,-} \sum_{d=1}^{D} \pm \int_{A_d^{\pm}} \left(\mathbf{N}^T \mathbf{F}\right)_d d\mathbf{A}_{\boldsymbol{\xi}} = h^{D-1} \sum_{\pm=+,-} \sum_{d=1}^{D} \pm F^d_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} + O\left(h^4\right)$$

where

$$\left(\mathbf{N}^T\right)_{p,q} = \det\left(\mathbf{R}_p\left(\frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}}, \mathbf{e}^q\right)\right)$$

$\mathbf{R}_p\left(\mathbf{A}, \mathbf{v}\right)$**: replace** ***p*-th row of** $\mathbf{A}$ **with** $\mathbf{v}$

$$F^d_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} = \sum_{s=1}^{D} \langle N^s_d \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} \langle F^s \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{12} \sum_{s=1}^{D} \left(\mathbf{G}_0^{\perp,d}\left(\langle N^s_d \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d}\right)\right) \cdot \left(\mathbf{G}_0^{\perp,d}\left(\langle F^s \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d}\right)\right)$$

$\mathbf{G}_0^{\perp,d} =$ **second-order accurate centered difference of** $\nabla_{\boldsymbol{\xi}} - \mathbf{e}^d \frac{\partial}{\partial \xi_d}$

$$\langle q \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} \equiv \frac{1}{h^{D-1}} \int_{A_d} q(\boldsymbol{\xi}) d\mathbf{A}_{\boldsymbol{\xi}} + O\left(h^4\right)$$