Magnetized Plasma Simulations with High-Order Implicit-Explicit Time Integrators

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Debojyoti Ghosh, Mikhail Dorf, and Milo Dorr

CASC
Center for Applied Scientific Computing

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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

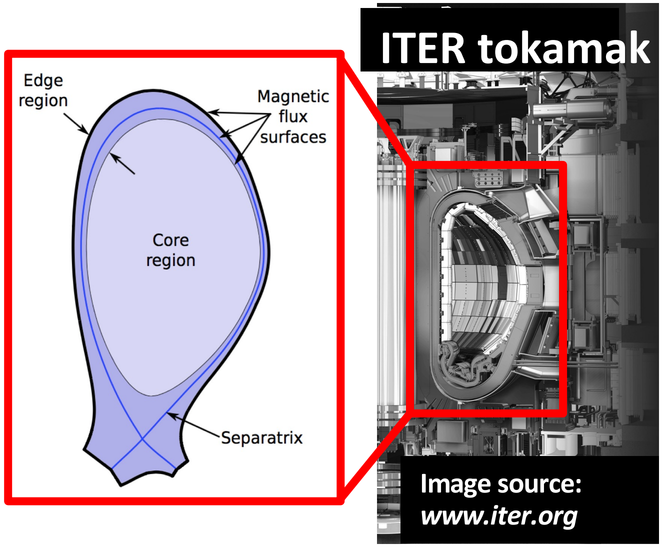


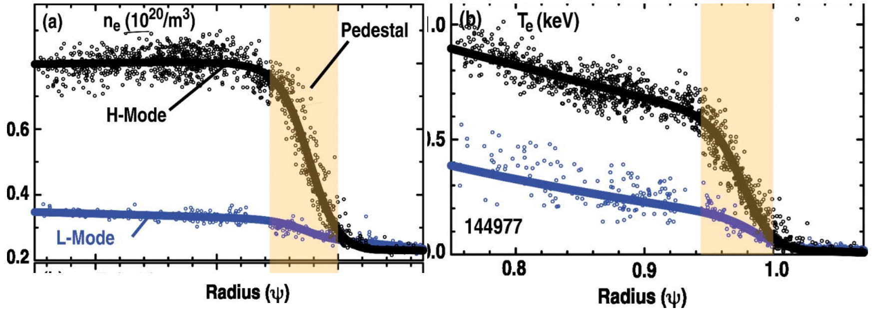
Image source: *www.iter.org*

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

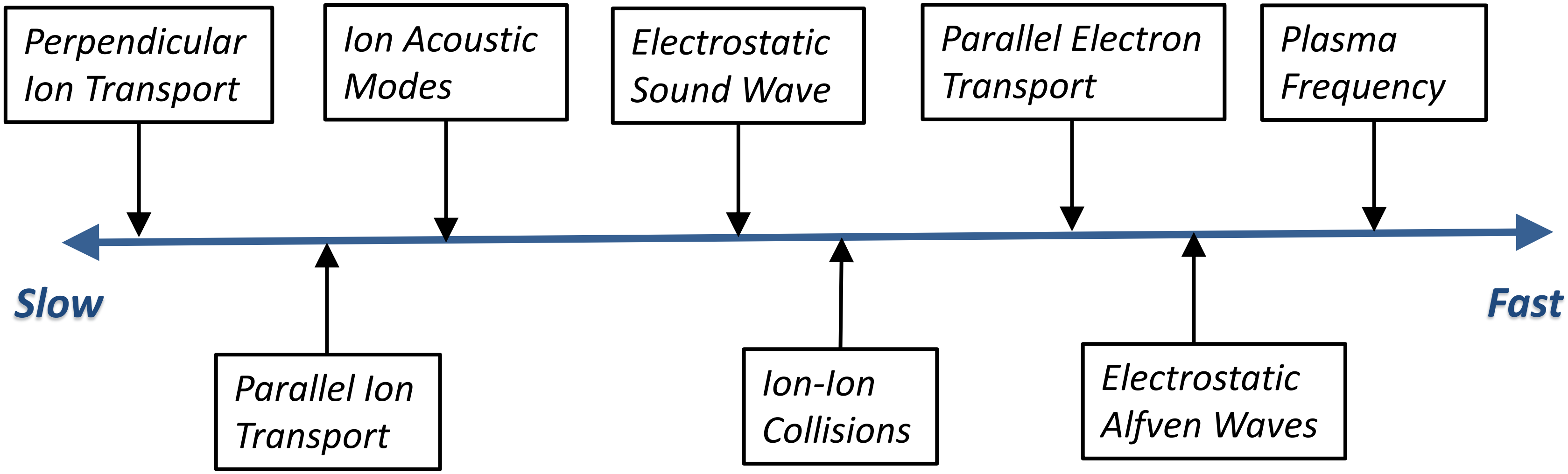
- Weakly-collisional in the hot core
- Strongly-collisional in the cold edge



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**



Slow

Perpendicular Ion Transport

Parallel Ion Transport

Ion Acoustic Modes

Electrostatic Sound Wave

Ion-Ion Collisions

Parallel Electron Transport

Electrostatic Alfven Waves

Plasma Frequency

Fast

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)*

Hierarchy of Edge Simulation Models

- **Kinetic Approach (5D) - GENE-X, XGC, GKEYLL**
    - 5D GK Vlasov equation with collision model + 3D field equations
    - High-fidelity description of important physics processes
        - Collisional ion transport, ion orbit losses, parallel electron heat flux
        - Microturbulence including trapped electron modes (TEMs)
- **Fluid Approach (3D) - BOUT++/HERMES, GRILLIX, GBS**
    - Moment equations for each plasma species + Vorticity & Ohm's Law for fields
    - Assumes strong collisionality → omits prompt ion orbit losses and TEMs
- **Kinetic/Fluid (5D/3D) Hybrid Approach - COGENT**
    - 5D GK Vlasov for ions + 3D fluid model for electrons and fields
    - Retains ion kinetic effects (weakly-collisional transport, orbit losses, ITG, etc.)
    - Omits electron kinetic effects in heat fluxes; does not capture TEMs.

Hybrid Schemes and Time Integration

- **5D Kinetic Approach: time integration is expensive**
  - *Time scales of interest arise from* ***ion dynamics****:* ion streaming, drift wave
  - Explicit time integration: *time step constrained by* ***electron dynamics*****:**
    - Electron streaming
    - Alfven waves
  - Implicit time integration: *expensive to solve* ***5D nonlinear system of equations***
- **5D/3D Hybrid Approach** ***can be potentially faster***

5D ion kinetic system

$$\frac{\partial f_i}{\partial t} + L[f_i, u_f] = C[f_i, u_f]$$

Only contains time scale of interest
→ **often treated explicitly**

3D fluid/field system

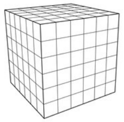
$$\frac{\partial u_f}{\partial t} = M[f_i, u_f]$$

Contains fast time scales →
treated implicitly (3D, not 5D!)

For edge simulations 3D implicit and 5D explicit steps can be comparable in terms of computational intensity

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

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



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

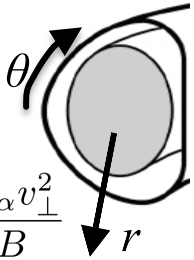
Fokker-Planck collision model

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

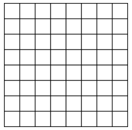


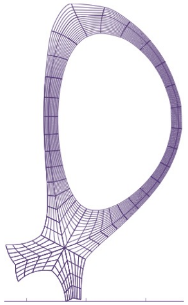
$$\mathbf{X} \equiv \{r, \theta\}$$

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

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

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

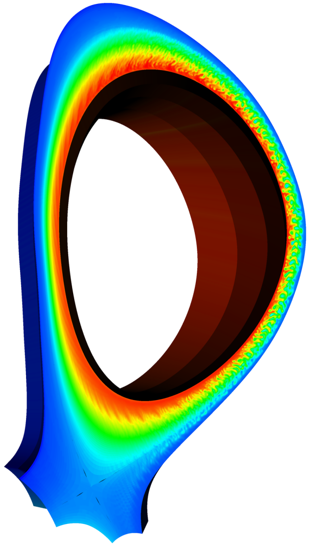




Solved on a mapped, multi-block mesh representing the tokamak edge

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

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

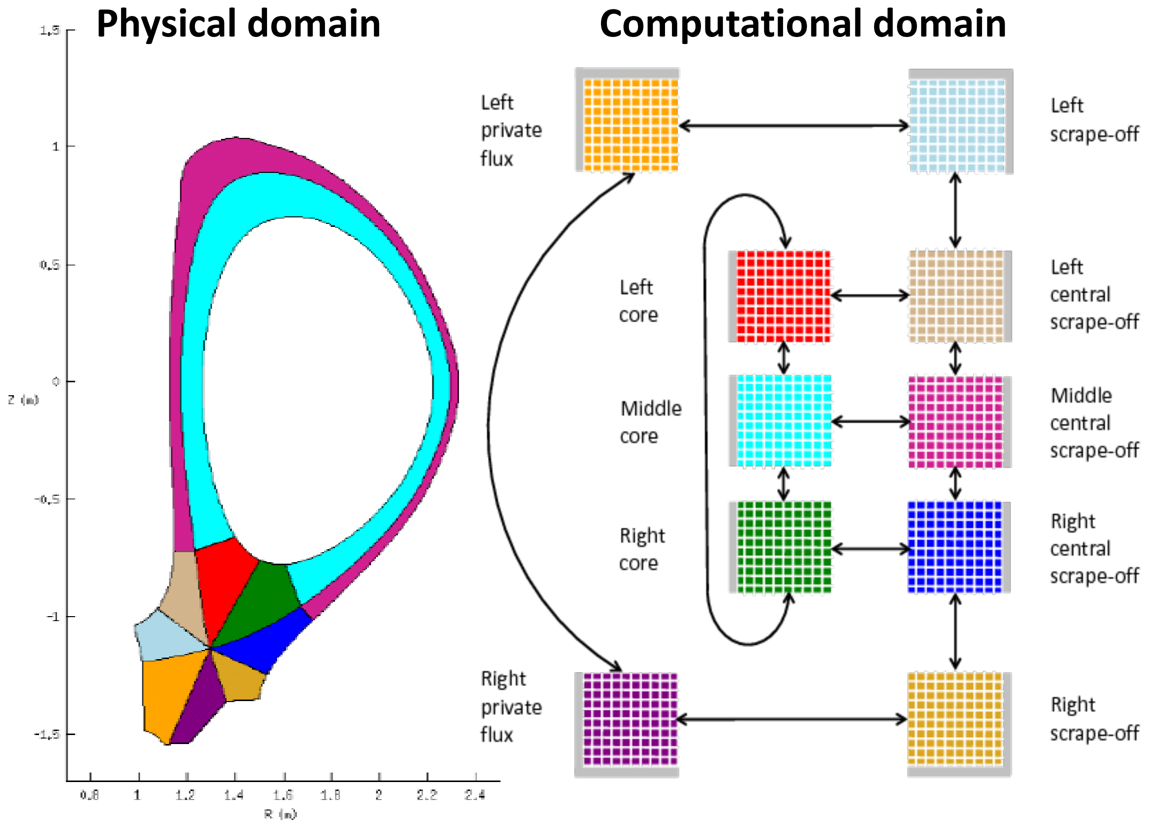


Physics/Mathematical characteristics	**Algorithm choice**
High dimensionality (kinetic modelling)	High-order (4th-order) spatial discretization
Numerical Conservation	Finite volume discretization; Conservative semi-implicit time integration
Complex geometry and anisotropy (tokamak edge, Z-pinch)	Mapped, multiblock, field-aligned grids
Multiple time scales	**Implicit-explicit (IMEX) time integration** (high-order additive Runge-Kutta methods)

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)

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



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

Implicit-Explicit (IMEX) Time Integration

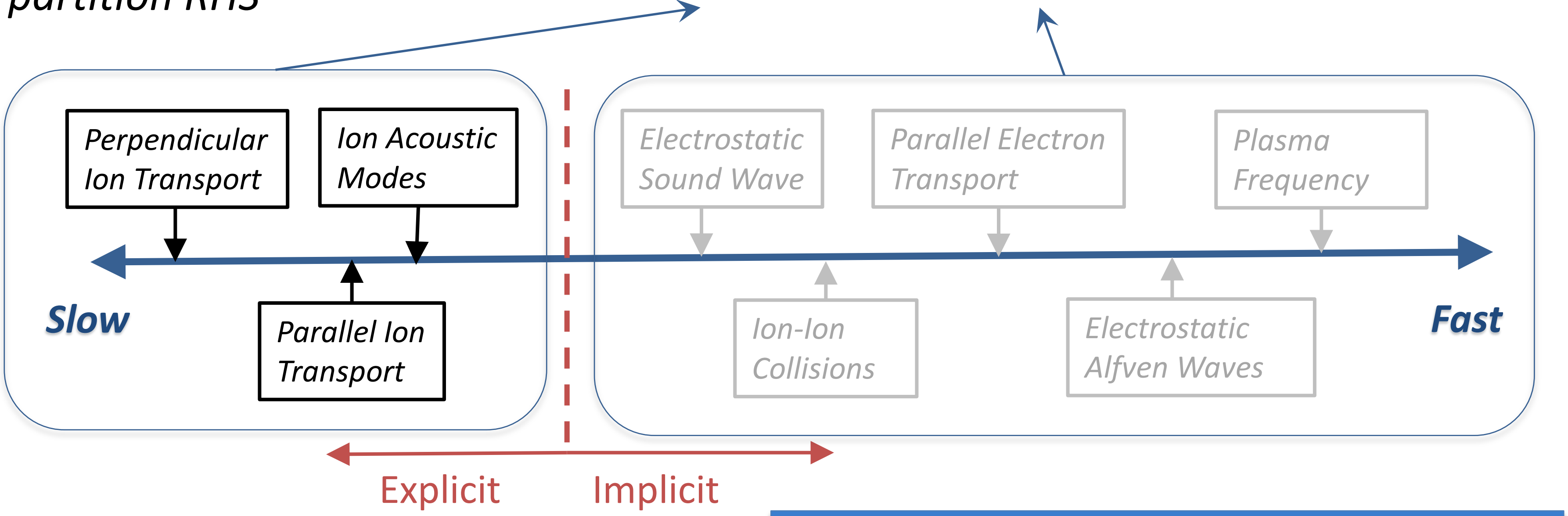
Resolve scales of interest; Treat implicitly faster scales

ODE in time Resulting from spatial discretization of PDE

$$\frac{d\mathbf{y}}{dt} = \mathcal{R}\left(\mathbf{y}\right)$$

IMEX time integration:
partition RHS

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



Time step constrained by
fastest explicit time scale

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

Semi-Discretized ODE and Stiff Terms

Semi-discrete ODE for the kinetic ions

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

Semi-discrete ODE for the electrostatic potential

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

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

ODE with nonlinear LHS operator

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

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

(vectors of solution at grid points)

Partitioned system of ODEs for IMEX time integration

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

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

$$\mathcal{R}_{\text{stiff}} \equiv \begin{bmatrix} \mathcal{C}\left(\mathbf{f}\right) \\ \mathcal{R}_{\parallel}\left(\mathbf{f}, \mathbf{\Phi}\right) \end{bmatrix}$$

***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

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

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**

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

Jacobian

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

Approximation for Preconditioner

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

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

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

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

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

- 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

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

$\mathcal{C}\left(\tilde{f}\right)$ 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

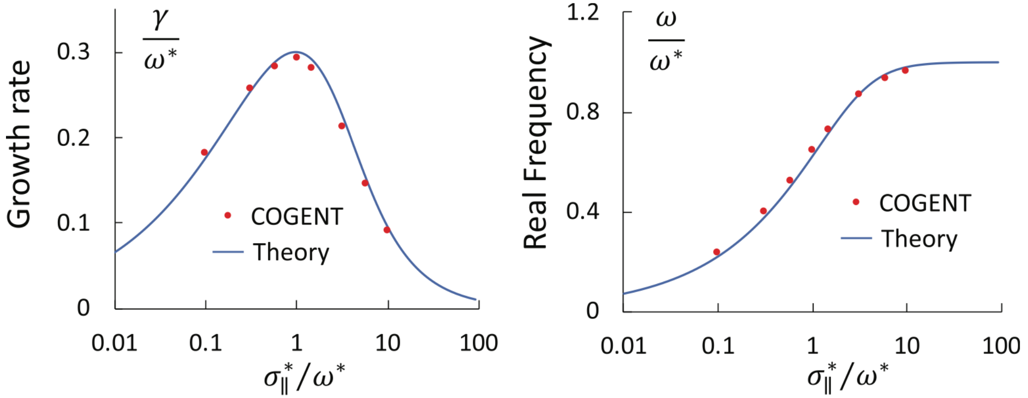
Solved with the **Algebraic Multigrid (AMG) method** implemented in the *hypre* library

Simple Test Case: Resistive Drift Instability

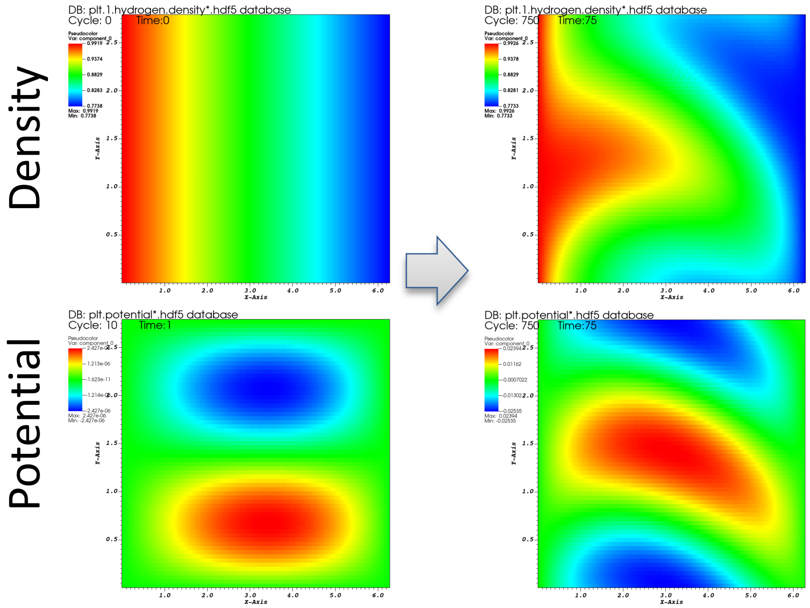
Kinetic Ion Species with Fokker-Plank Collisions and Fluid Potential Model

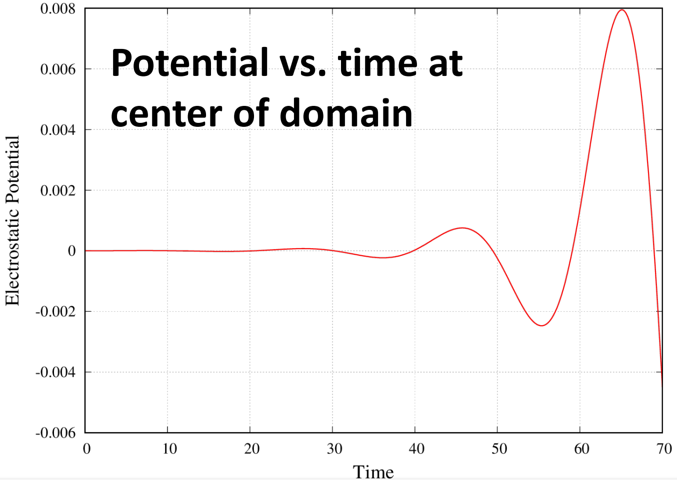
Resistive drift mode in a 2D slab:

- **Collisionless**: kinetic equation is explicit; fluid equation is semi-implicit
- **Collisional:** both kinetic and fluid equations are semi-implicit
- **Stiffness** of fluid equation ***proportional to parallel conductivity***



Dorf & Dorr, Phys. Plasmas, 2021: *Growth rate and real frequency vs. parallel conductivity*





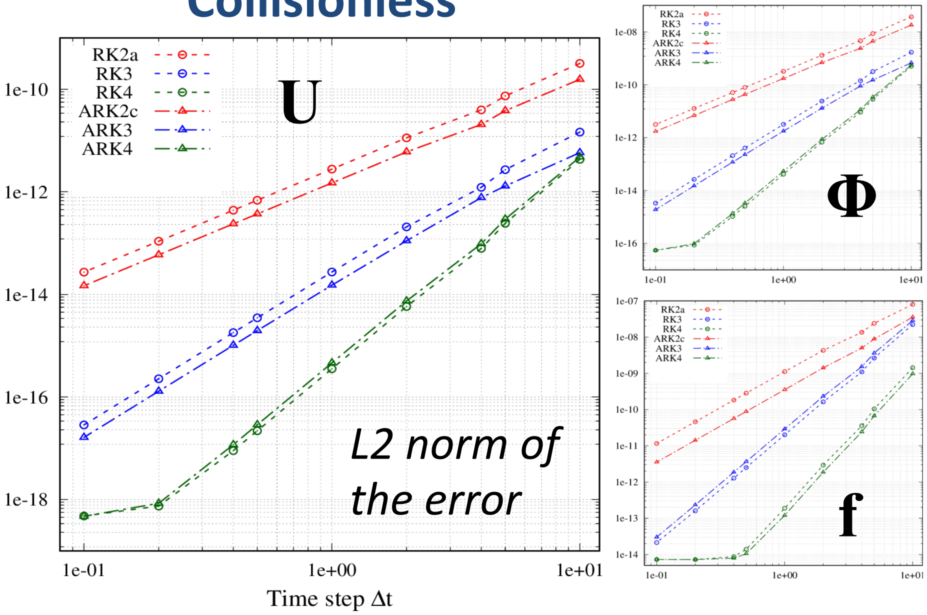
Potential vs. time at center of domain

Convergence: *Non-Stiff Case*

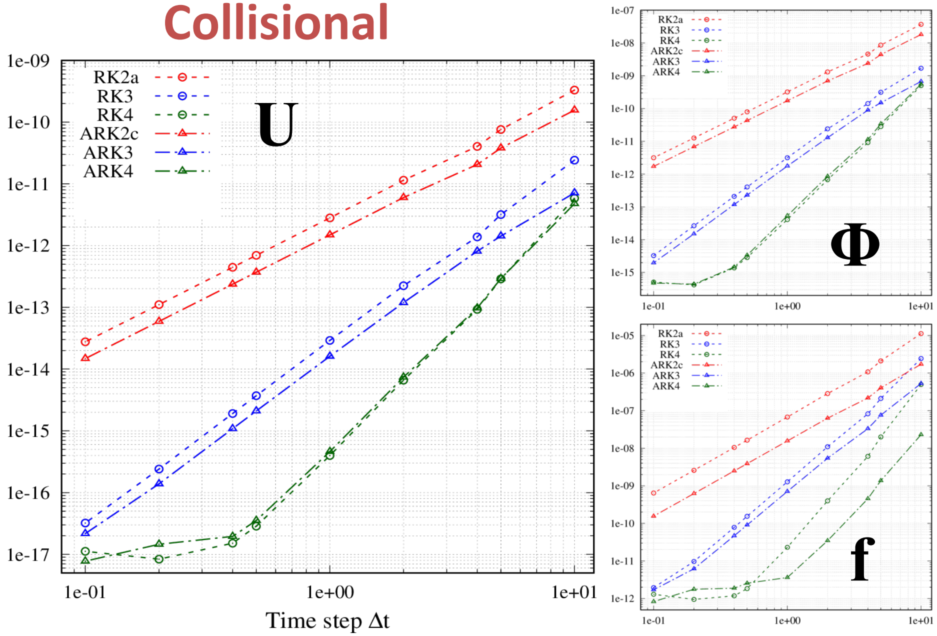
ARK2c: 2nd order, 3-stage
ARK3: 3rd order, 4-stage
ARK4: 4th order, 6-stage

Low parallel conductivity results in a non-stiff fluid equation: *Both **explicit** and **semi-implicit time integrators** can be used with ion-dynamics-scale time steps.*

Collisionless



Collisional



Final time $t_f = 10.0$ (normalized units)

Reference solution generated with *fifth-order Dormand-Prince RK (RKDP)* at $\Delta t_{ref} = 0.02 \Delta t_{min}$ in convergence study

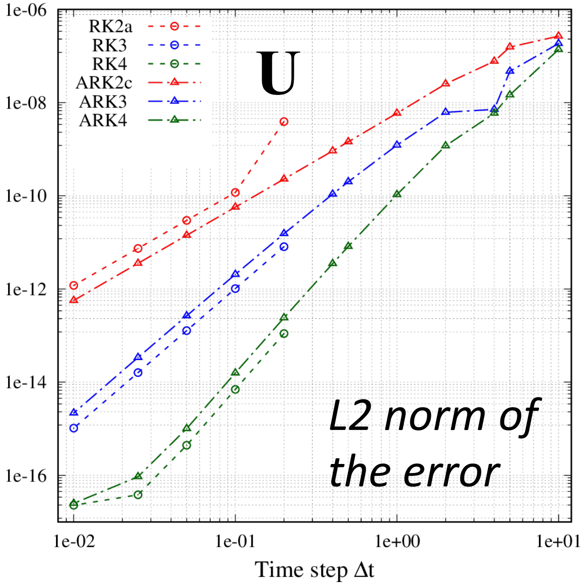
***Theoretical orders of convergence observed** for all ARK methods*
→ verifies implementation of nonlinear left-hand-side operator

Convergence: *Stiff Case*

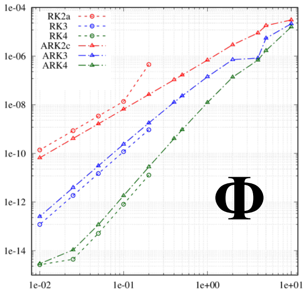
ARK2c: 2nd order, 3-stage
ARK3: 3rd order, 4-stage
ARK4: 4th order, 6-stage

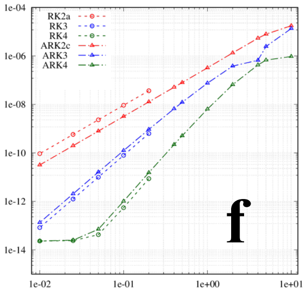
Higher parallel conductivity results in a stiff fluid equation: ***Explicit time integration*** *can be used with small steps;* ***semi-implicit time integrators*** *can be used with ion-scale time steps.*

Collisionless

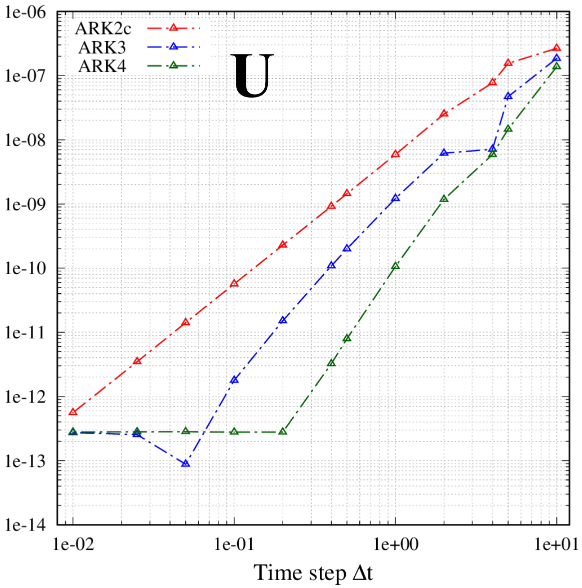


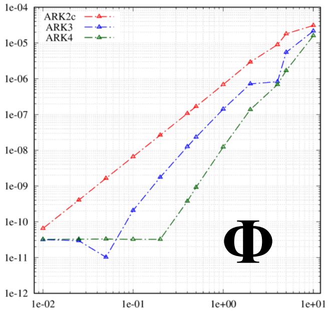
L2 norm of the error

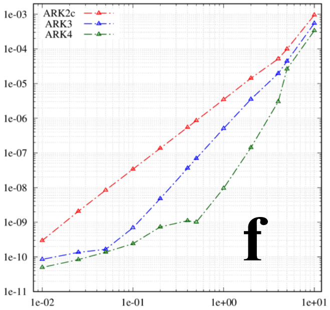




Collisional







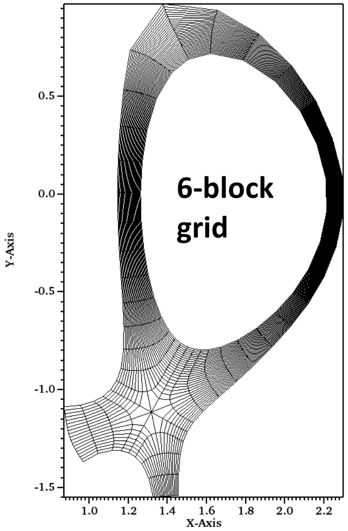
Final time $t_f = 10.0$ (normalized units)

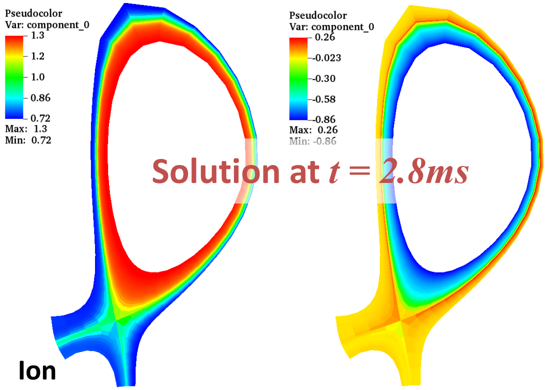
Reference solution generated with *fifth-order Dormand-Prince RK (RKDP)* at $\Delta t_{ref} = 0.02\Delta t_{min}$ in convergence study

Theoretical orders of convergence observed *for all ARK methods*
→ verifies convergence in stiff regime where RK unstable

Tokamak Edge Simulations

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





Solution at $t = 2.8ms$

Ion Temperature

Potential

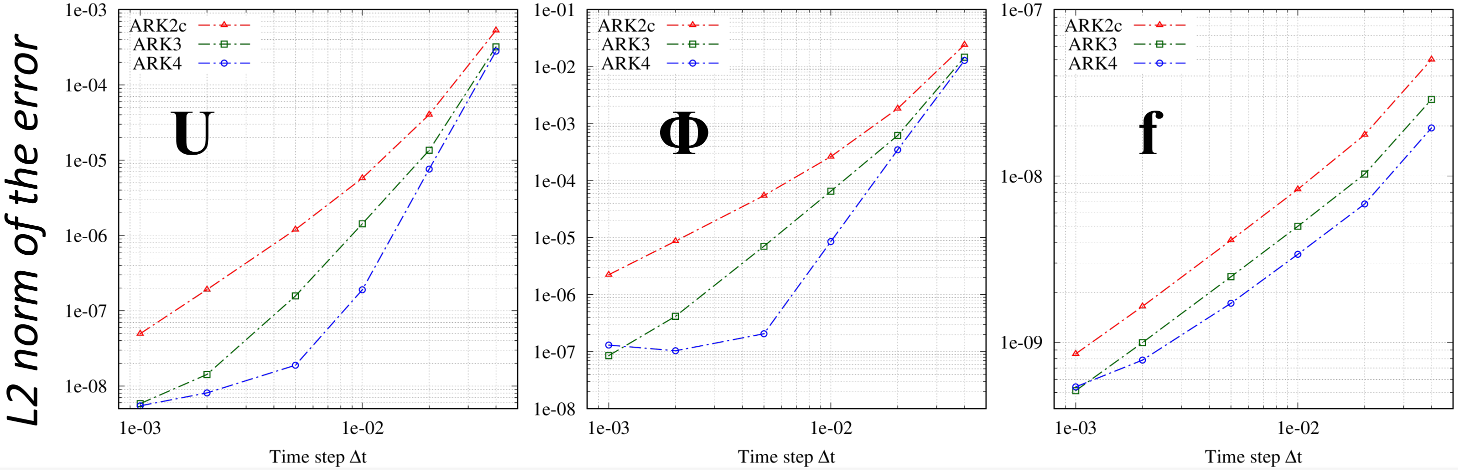
Reference: Dorf & Dorr, 2018, Contrib. Plasma Phys.

- ***Characterized by very high stiffness of the fluid equation***
- **Electrostatic potential** (Φ) converges at the theoretical orders (*semi-implicit in time*, with ***nonlinear LHS operator***)
- **Distribution function** ($\mathbf{f}$) converges at ~***1st order***

Final time $t_f = 0.040$

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 simple cases with varying stiffness.
  - Currently investigating cause of sub-optimal convergence for more realistic simulations

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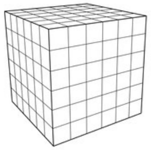
Thank you.
Questions?

“Multiple-Dimensioned” Governing Equations

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

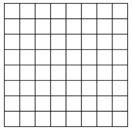
Phase-space kinetic equations (4D/5D) – *ions, electron*

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

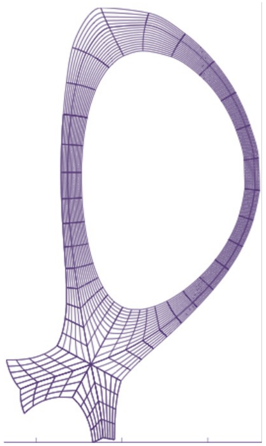


Configuration space fluid/field equations (2D/3D)
– *ions, electron, vorticity, neutrals*

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



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 Center for Applied Scientific Computing

L. Ricketson
M. Dorr
D. Ghosh
P. Tranquilli

Berkeley Lab

D. Martin
P. Colella
P. Schwartz

Physics (FES)

Fusion Energy Sciences

M. Dorf
V. Geyko
J. Angus

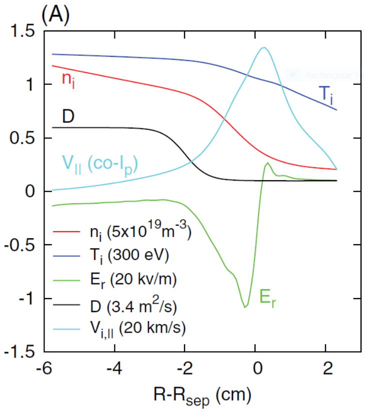
General Atomics and Affiliated Companies

P. Snyder
J. Candy
E. Belli

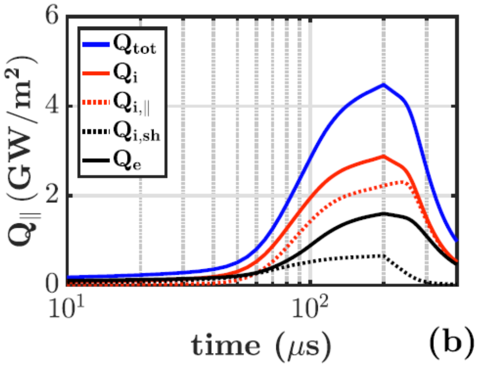
UC San Diego

S. Krasheninnikov

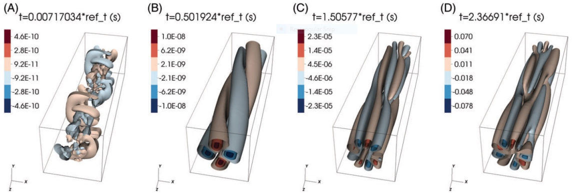
Cross separatrix transport (Dorf et al., Contrib. Plasma Phys.,58, 434-444, 2018)



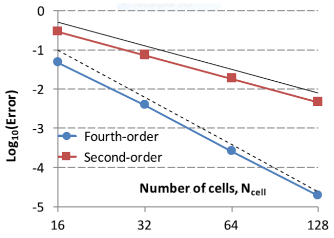
ELM heat pulse (Joseph et al., Nucl. Mater. Energy, 19, 330-334, 2019)



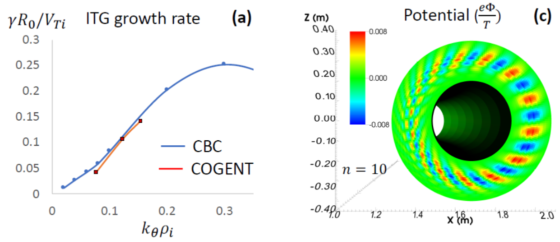
Kinetic drift-wave instability (Lee et al., Contrib. Plasma Phys., 58, 445-450, 2018)



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



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

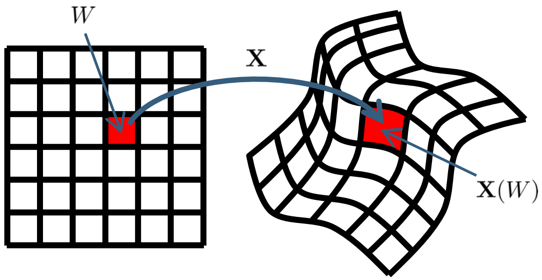


4th Order Mapped Finite-Volume Discretization

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** $\nabla_{\boldsymbol{\xi}} - \mathbf{e}^d \dfrac{\partial}{\partial \xi_d}$

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