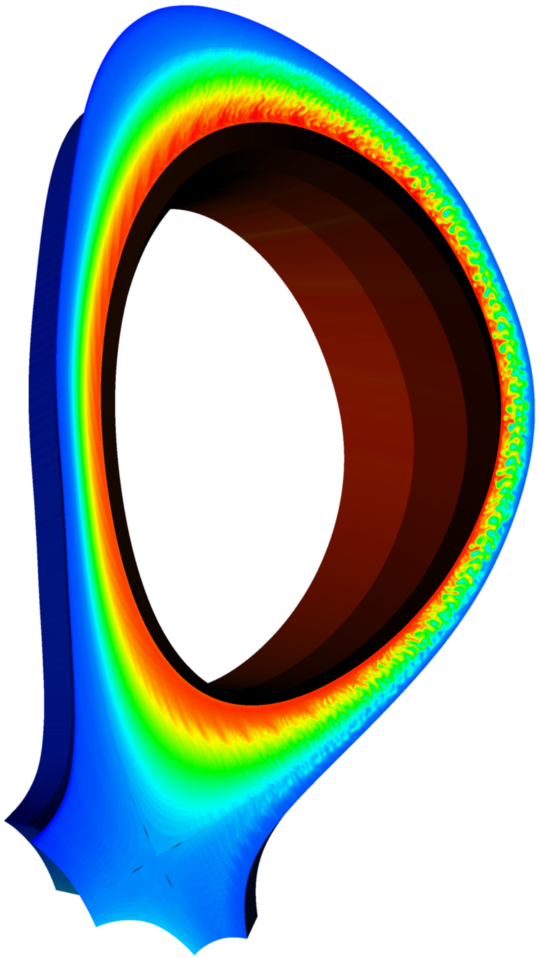
A semi-implicit gyrokinetc ion – fluid electron hybrid model for edge plasma simulations

M. Dorf, M. Dorr, and D. Ghosh

Lawrence Livermore National Laboratory



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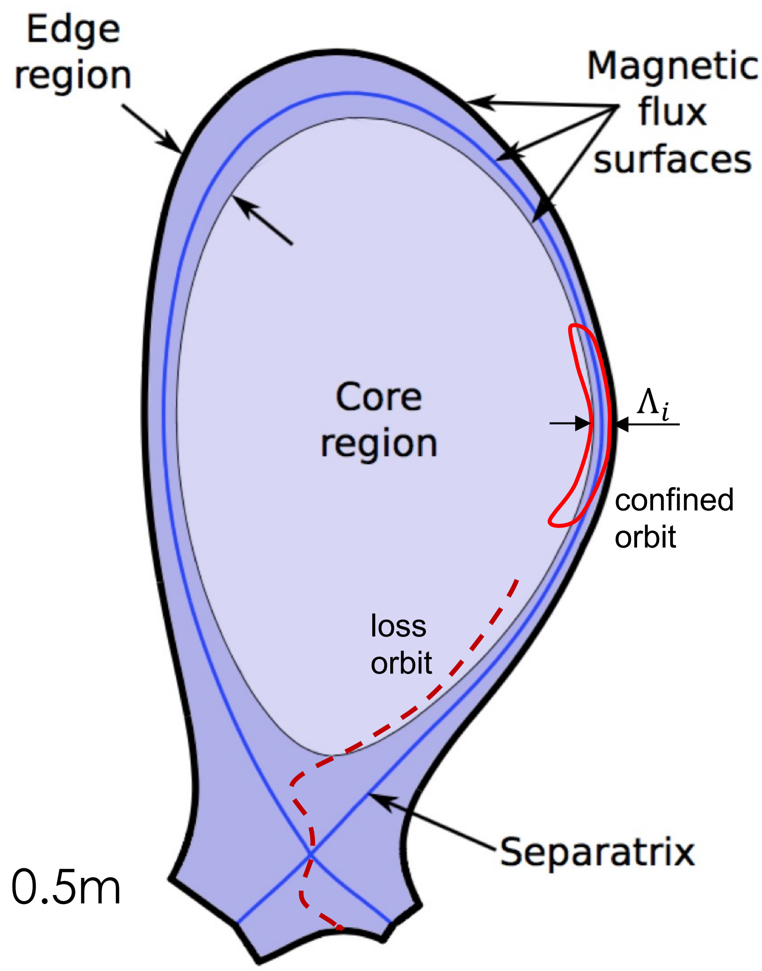
Tokamak edge is challenging to model numerically

- **Essential kinetic effects**
  - wide drift orbits $\Lambda_i \sim L_T$, prompt losses
  - weakly collisional near-separatrix region
- **Complicated geometry**
  - magnetic separatrix / device boundaries
- **Strongly anisotropic transport**
  - $k_\perp^{-1} \sim \rho_s \sim 1\text{mm}$ / $k_\parallel^{-1} \sim qR_0 \sim 6\text{m}$
- **Multiple spatial and time scales**
  - turbulence scale $\rho_s \sim 1\text{mm}$ / device size a ~ 0.5m
  - electron streaming 1μs / transport time ~ 1 ms



Hierarchy of edge simulation models

5D kinetic approach (GENE-X, XGC, GKEYLL)

- 5D GK Vlasov equation with collision model + 3D field (elliptic) equations
- High fidelity description of important physics processes
  - Collisional ion transport, ion orbit losses, parallel electron heat flux
  - Microturbulence including trapped electron modes (TEMs)

3D fluid approach (BOUT++/HERMES, GRILLIX, GBS, …)

- Moment equations for plasma species + Vorticity & Ohm's Law for fields
- Assumes strong collisionality ⟶ omits prompt ion orbit losses & TEMs;

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, …)
- Omits electron kinetic effects in heat fluxes; does not capture TEMs

*A hybrid approach was previously used for core (e.g., in the GEM code)

Why use hybrid schemes?

5D kinetic approach is slow due to expensive time integration

- Time scales of interest (ion physics): $\omega_{tr,i} \sim k_\parallel V_{Ti}$ (streaming), $\omega_{dr} \sim k_\perp \rho_s \frac{V_s}{L}$ (drift wave)
- Time step limitations for explicit models are strenuous:

  electron streaming $\omega_{tr,e} \sim k_\parallel V_{Te}$, Alfven wave $\omega_H \sim \frac{k_\parallel V_{Te}}{k_\perp \rho_s}$ (ES case), $\omega_A \sim k_\parallel V_A$ (EM case)
- Implicit approach for a 5D system is expensive

5D/3D hybrid approach can be much faster

5D ion kinetic system

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

Only contains time scales of interest → treated explicitly

3D fluid/field system

$$\frac{\partial u_f}{\partial t} = M[f_i, u_f] \qquad u_f = [\Phi, A_\parallel, T_e]$$

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

5D/3D GK ion – fluid electron hybrid scheme is implemented in the COGENT code

High-order (4^{th}-order) finite-volume Eulerian code

COGENT

Physics models (LLNL)

- Multispecies full-F gyrokinetic equations
- Collisions (including full Fokker-Planck)
- Gyro-Poisson eq. (for fully kinetic models)
- Hybrid/Fluid models (electrons, neutrals)
- Ideal/Extended MHD models

Math algorithms (LLNL/LBNL)

- High-order mapped-multiblock technology to handle X-point
- Solvers (multigrid, GMRES)
- Advanced time integrators (ImEx)
- Sparse grids

Tokamak applications

⇓

Low-Temp ↔ COGENT ↔ Z-pinch, mirrors

New collaborations welcome!

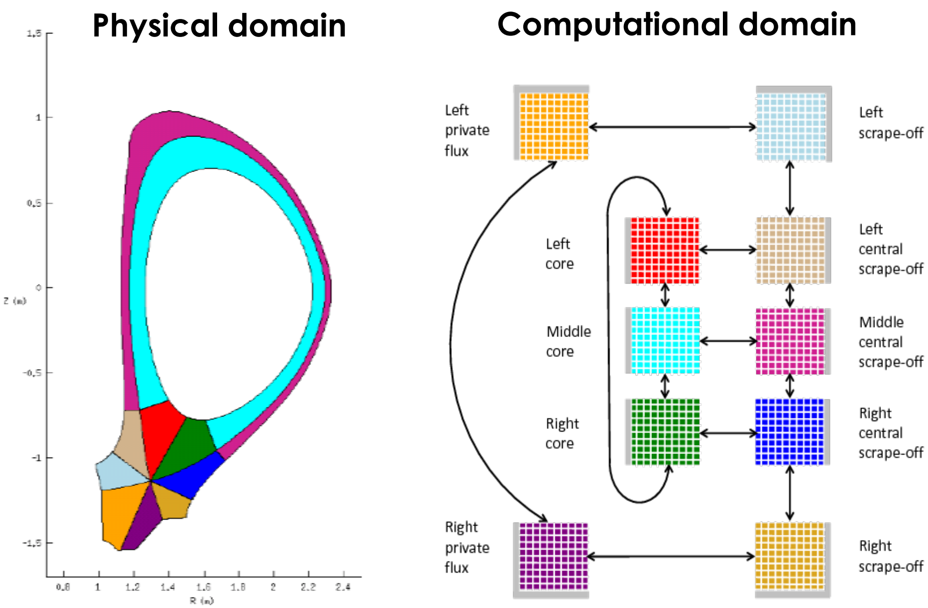
Use multiblock grid technology to discretize the edge domain

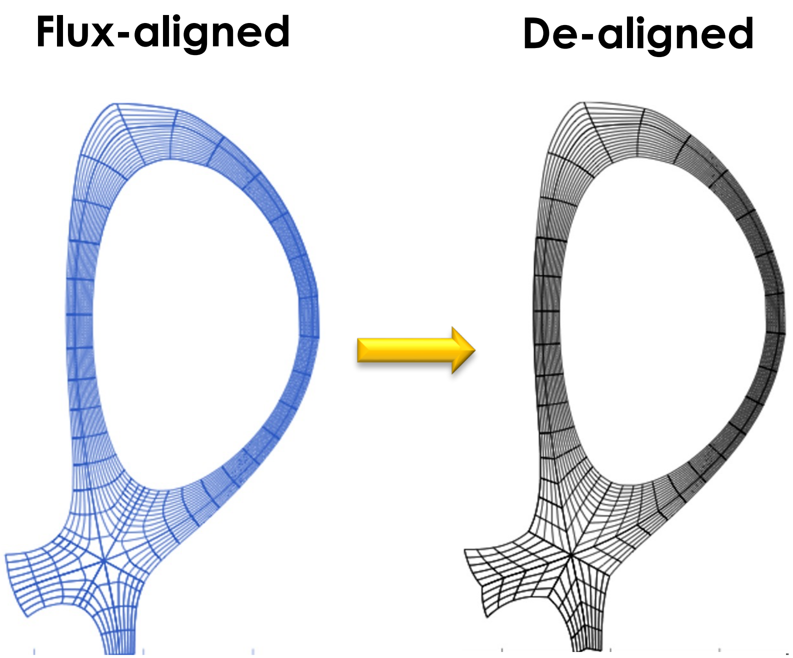
Strong anisotropy of plasma transport motivates the use of flux-aligned grids

Problem: X point → singular topology

Approach:

- decompose domain into blocks with smooth grids
- use high-order interpolation for block communication





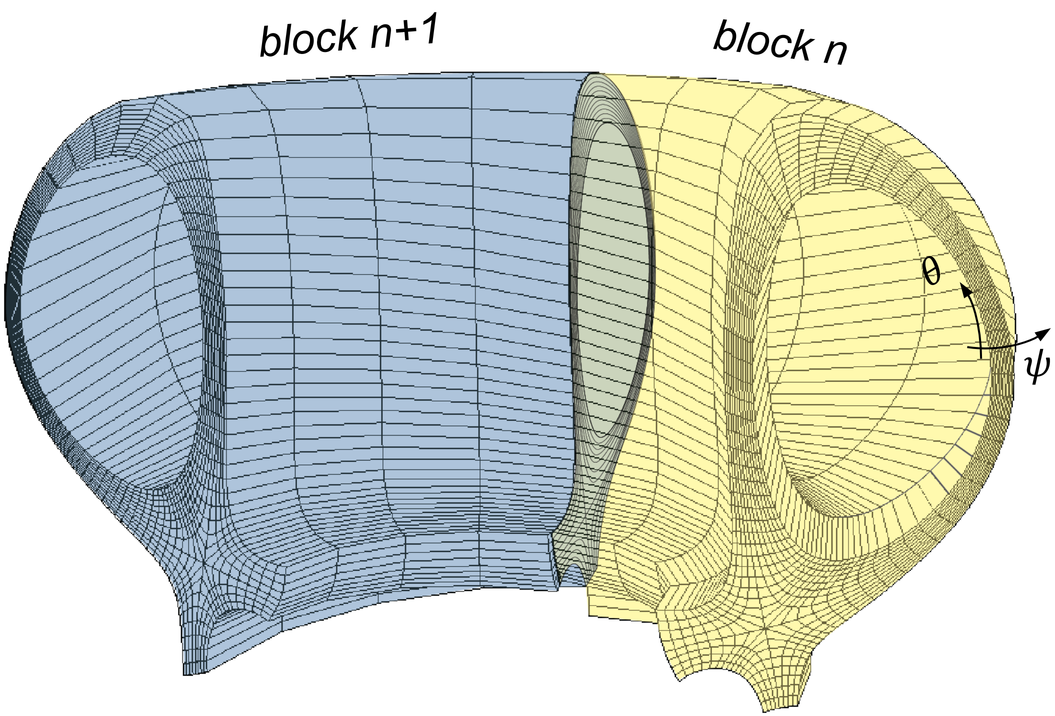
- Transport is less anisotropic near the X-point
- Flux-surface alignment can be abandoned near the X-point to avoid singular metrics
- High-order convergence demonstrated for ion advection in X-point geometry*
- *In this work, use fully flux-aligned grids*

*Dorr et al., JCP (2018);

3D extension: locally field-aligned multiblock approach

To exploit strong anisotropy of microturbulence

- Toroidal direction is divided into block (wedges)
- Control cells are field-aligned (F-A) within each block



COGENT: maintains flux alignment

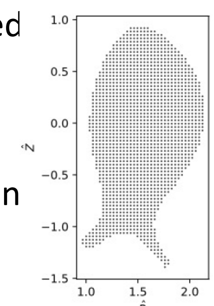
(ψ, θ) - finely gridded poloidal plane
ϕ - coarse parallel coordinate

(+) Minimizes numerical pollution
(+) Same poloidal grid for 5D and 4D
(-) Loss of accuracy due to X-point
(unless we de-align – in progress)

GENE-X: FCI approach

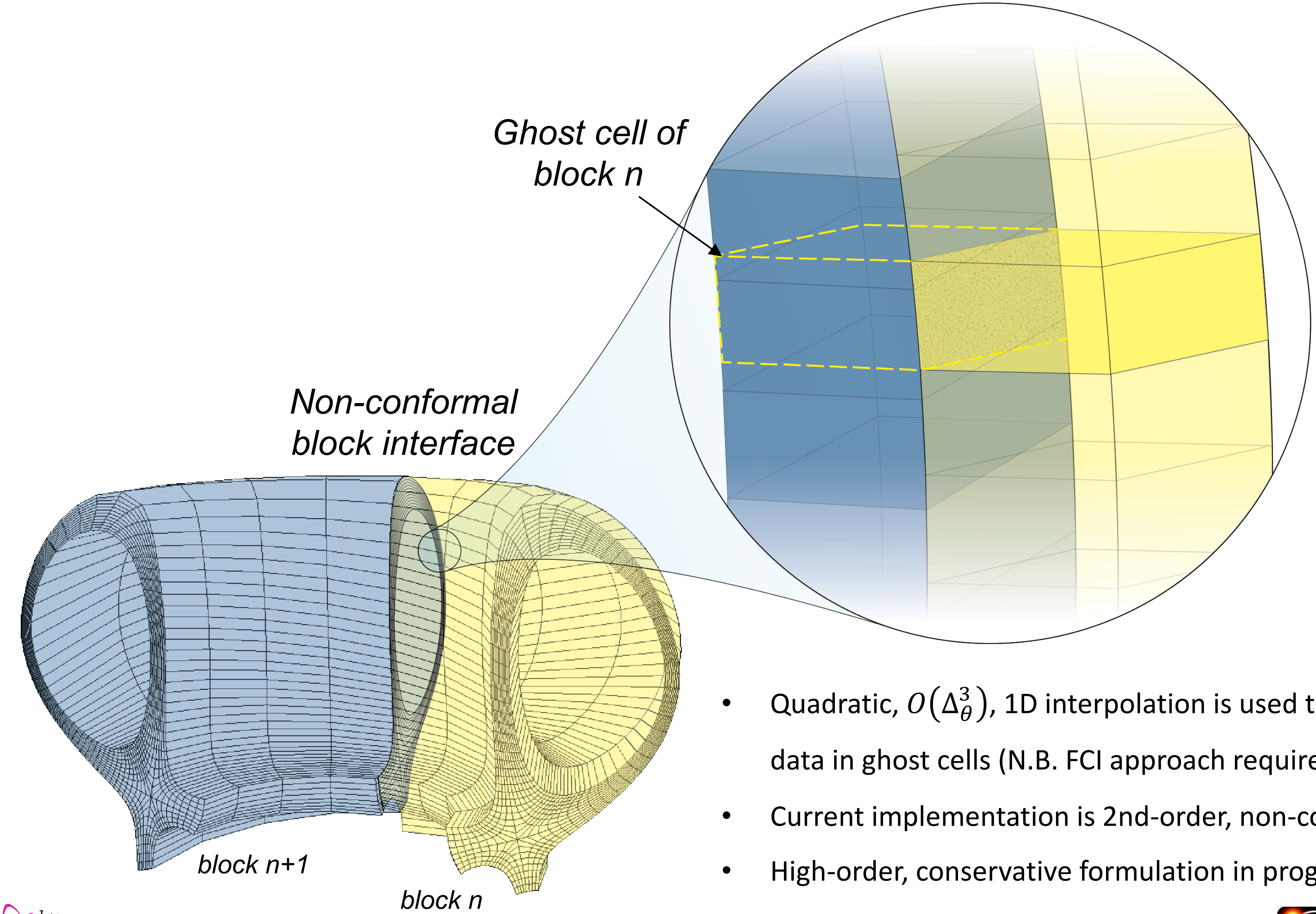
Poloidal plane: fine unstructured grid, not flux aligned

(+) No X-point/O-point issues
(-) Potential numerical pollution
(-) Not efficient for 4D



* D. Michels (2020)

Interpolation is employed at a toroidal block interface



- Quadratic, $O\left(\Delta_\theta^3\right)$, 1D interpolation is used to compute data in ghost cells (N.B. FCI approach requires 2D interp.)
- Current implementation is 2nd-order, non-conservative
- High-order, conservative formulation in progress

Electrostatic hybrid GK ion – drift fluid electron model

5D ion gyrokinetic eq.

$$\frac{\partial B_\parallel^* f_i}{\partial t} + \nabla_{\boldsymbol{R}}\left(\dot{\boldsymbol{R}}_{gc} B_\parallel^* f_i\right) + \frac{\partial}{\partial v_\parallel}\left(\dot{v}_\parallel B_\parallel^* f_i\right) = C\left[B_\parallel^* f_i\right]$$

Gyrokinetic advection *Collisions*

3D quasi-neutrality

$$\frac{\partial}{\partial t}\varpi + \nabla_\perp\left(c\frac{-\nabla_\perp \Phi \times \boldsymbol{B}}{B^2}\varpi\right) = \boldsymbol{\nabla}\cdot\int \frac{2\pi}{m_i} e B_\parallel^* f_i \boldsymbol{v}_\perp^{\boldsymbol{mag}} dv_\parallel d\mu - \boldsymbol{\nabla}\cdot\left\{c\frac{\boldsymbol{\nabla}_\perp(n_i T_e)\times\boldsymbol{b}}{B}\right\} + \boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel$$

Pol. current *Reynolds stress* *Kinetic* $\nabla \cdot j_{i,\perp}$ *Fluid* $\nabla \cdot j_{e,\perp}$ *Fluid* $\nabla \cdot j_\parallel$

Vorticity

$$\varpi = \nabla_\perp\left(\frac{c^2 m_i n_i}{B^2}\nabla_\perp \Phi\right)$$

Neglect the diamagnetic pressure corrections term

Parallel current

$$j_\parallel = \sigma_\parallel\left(\frac{\nabla_\parallel(n_e T_e)}{n_i} - \nabla_\parallel \Phi + \frac{0.71}{e}\nabla_\parallel T_e\right)$$

Stiff term (due to the large parallel conductivity $\sigma_\parallel = \frac{e^2 n_e}{0.51 m_e \nu_e}$*) – treat implicitly*

Electron density

$$n_e = n_i + \nabla_\perp\left(\frac{c^2 m_i n_i}{e B^2}\nabla_\perp \Phi\right)$$

Include polarization corrections (required for high-k stabilization)

Electron temperature

$$T_e = const$$

Consider a simple isothermal electron model

4D: Captures ion neoclassical and orbit loss effects

5D: Includes ITG and resistive drift and ballooning modes

IMEX (ARK) approach is employed for time integration

- **Semi-implicit ARK scheme with Newton-Krylov (JFNK) approach is developed for**

$$\frac{d}{dt}M[\mathrm{u}] = F_i[\mathrm{u}] + F_e[\mathrm{u}]$$

u - is the state vector including 5D&3D quantities

- **COGENT ES hybrid vorticity model**, $\mathrm{u} = [\mathrm{f_i}, \Phi]$

$$\frac{\partial B_\parallel^* f_i}{\partial t} + \nabla_{\boldsymbol{R}}\left(\dot{\boldsymbol{R}}_{gc} B_\parallel^* f_i\right) + \frac{\partial}{\partial v_\parallel}\left(\dot{v}_\parallel B_\parallel^* f_i\right) = C\left[B_\parallel^* f_i\right]$$

$$\frac{\partial}{\partial t}\varpi[\Phi] + \underbrace{B\nabla_\parallel\left(\frac{\sigma_\parallel}{B}\nabla_\parallel\Phi\right)} - \underbrace{B\nabla_\parallel\left(\frac{\sigma_\parallel}{B}\frac{T_e}{n_i}\nabla_\parallel\varpi[\Phi]\right)} = \boldsymbol{\nabla}\cdot\boldsymbol{j}_{\boldsymbol{i},\perp} + \boldsymbol{\nabla}\cdot\boldsymbol{j}_{\boldsymbol{e},\perp} + B\nabla_\parallel\left(\frac{\sigma_\parallel}{B}\frac{T_e}{n_i}\nabla_\parallel \mathrm{n_e}\right) + \nabla_\perp\left(c\frac{\nabla_\perp\Phi\times\boldsymbol{B}}{B^2}\varpi\right)$$

Stiff and anisotropic 2nd order elliptic problem, $\omega_e \sim \nu_e \frac{k_\parallel^2 v_{Te}^2}{k_\perp^2 \rho_s^2}$

4th order correction (polarization density term)

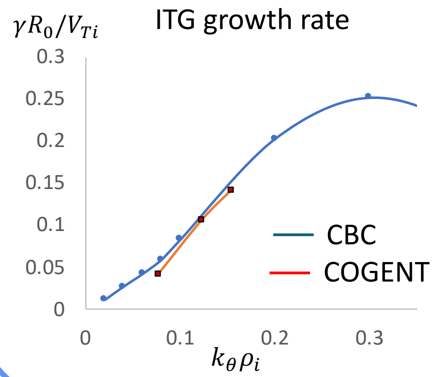
- **Multigrid solvers are employed for preconditioning Krylov solvers (GMRES)**

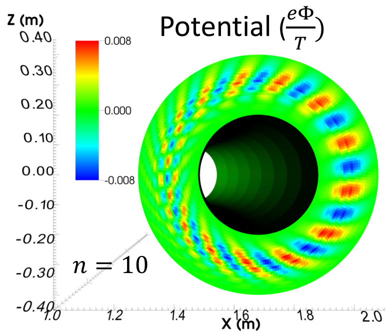
$$P[\Phi] = -\alpha^2\nabla_\perp^2\Phi - \beta^2\nabla_\parallel^2\Phi + \gamma^2\nabla_\perp^2\nabla_\parallel^2\Phi$$

  - Use AMG solvers from Hypre (can stall due to Xpt, but a few iterations is good enough for PC)
  - Hypre's semi-structured interface is well-suited for multiblock discretization

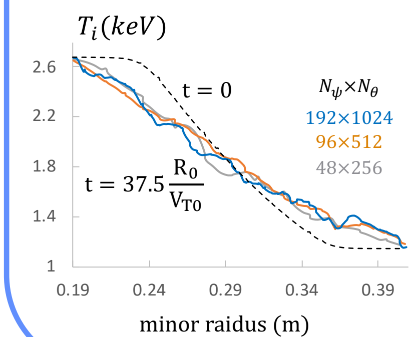
Verification

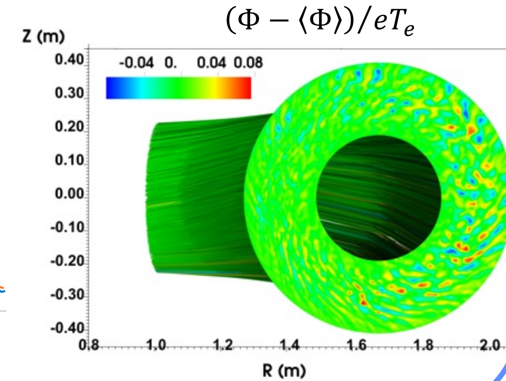
ITG instability with adiabatic electrons →recover the cyclone base case results



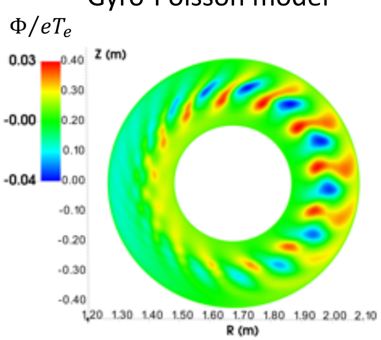


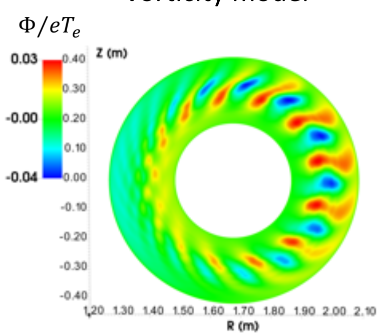
Full-F ITG-driven transport →demonstrate convergence



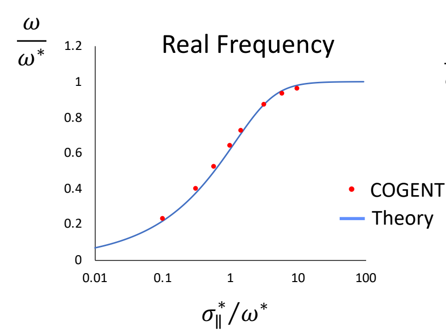


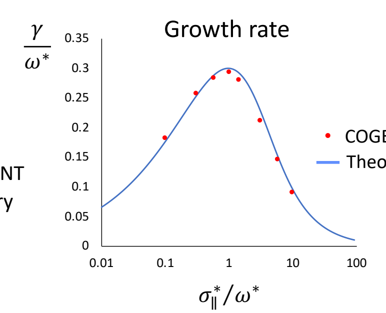
Hybrid model: high-conductivity limit →recover adiabatic electron results





Hybrid model: low-conductivity limit →recover drift resistive mode





Proof-of-principle 5D full-F simulations of plasma transport in a model SN geometry

Vorticity model $\sigma_{\parallel} \leftrightarrow V_{T_e}/qR_0\nu_e \sim 0.6$

Ion-ion collisions $\nu_{ii} \sim 0.01 V_{Ti}/qR_0$

IC: Local Maxwellian, T_0 = 4 keV

Boundary conditions (Φ):

- Self-consistent BC @ core boundary
- Zero-Dirichlet @ all other boundaries

Boundary conditions (f):

- Thermal Maxwellian baths (consistent with initial conditions)

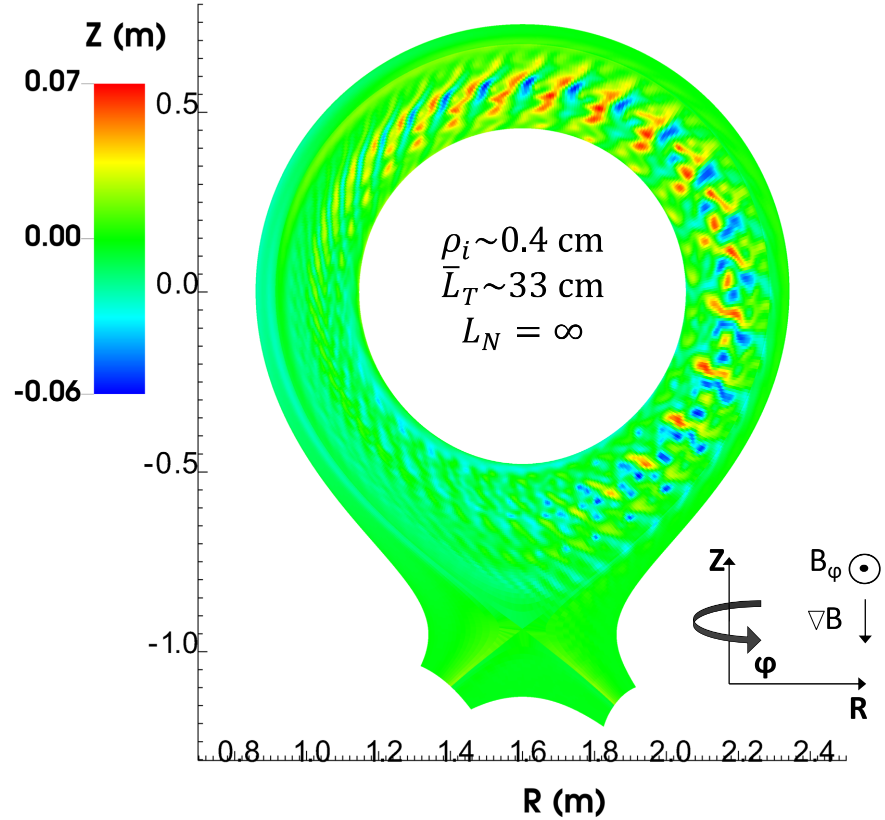
Resolution $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$ $(76,4,576,32,24)$

Time step $dt = 0.016\, R_0/V_{Ti}$

Performance 1 step ↔ 6s
Cori 1408 cores

Field-aligned multiblock version

$(\Phi - \langle\Phi\rangle)/eT_e$

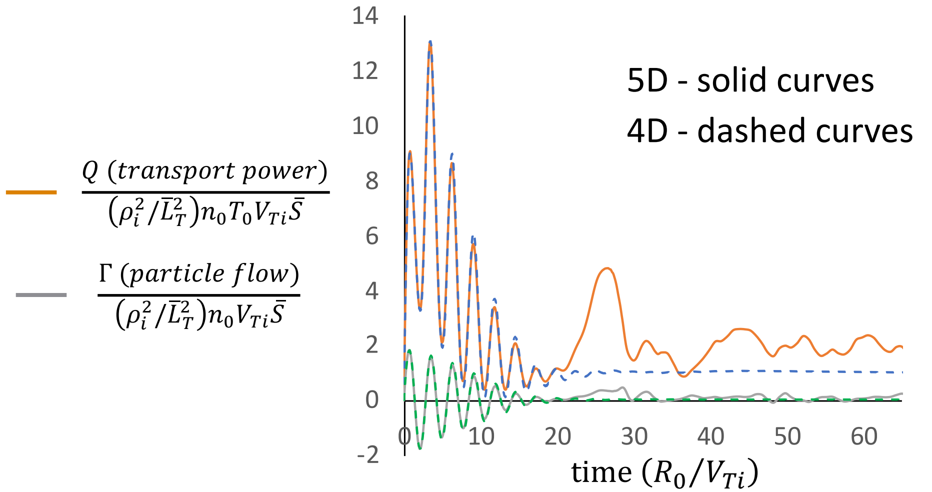


Model geometry

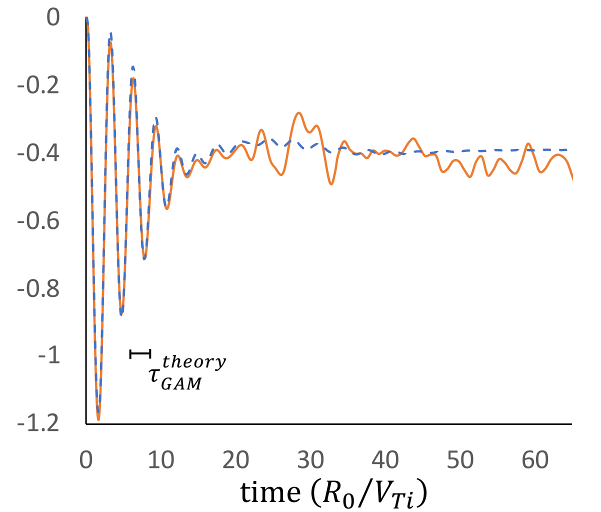
$R_0 = 1.6\, m, q \sim 2.5, RB_\phi = 3.5\, T \cdot m, \Delta\phi_{wedge} = 2\pi/8$

Flux-aligned discretization enables straightforward comparison between 5D and 4D simulations

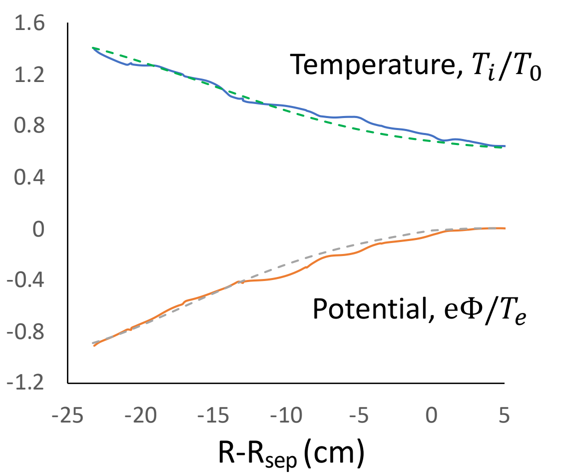
Transport power and particle flow



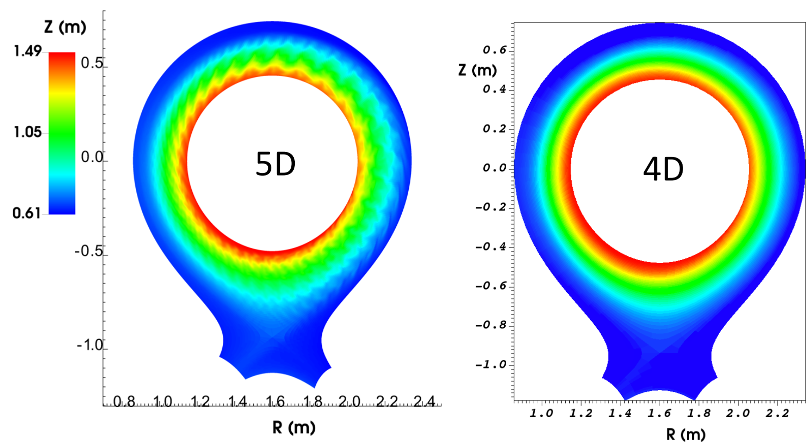
Electrostatic potential, Φ/eT_e



Outer midplane lineouts @ 59.7 R_0/V_{Ti}

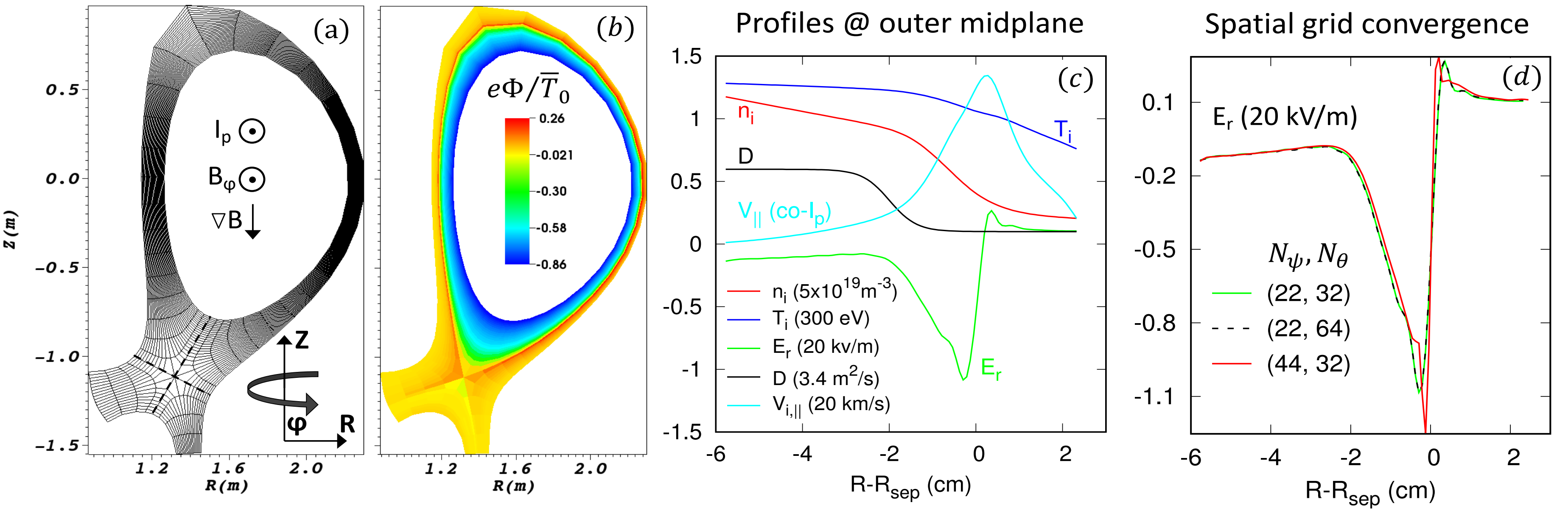


Temperature profiles @ 59.7 R_0/V_{Ti}



Poloidal background variations due to FOW effects

Modeling realistic geometries: 4D COGENT



- Hybrid vorticity model with isothermal $T_e = 300\ eV$
- Full ion-ion Fokker-Planck collisions
- 1 ms ⟷ 64 CPU hours (0.5 h x 128 cores)
- Grid resolution (core: $N_\psi = 22, N_\theta = 32, N_{v_\parallel} = 36, N_\mu = 24$)

Near-separatrix DIII-D

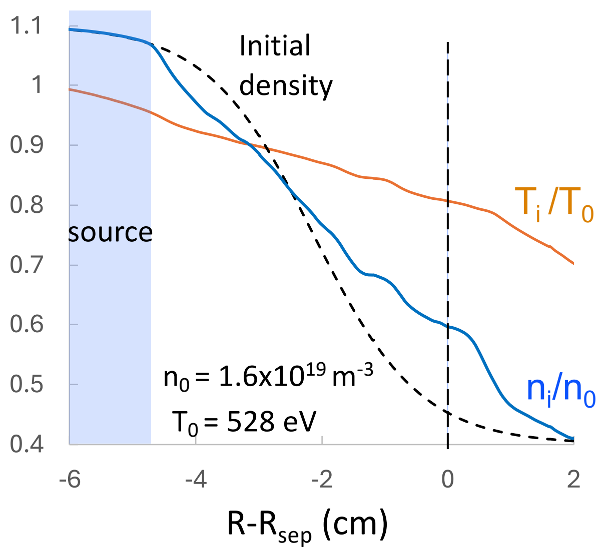
$$E_r \sim 20\frac{\text{kV}}{\text{m}} \quad V_\parallel \sim 40\frac{\text{km}}{\text{s}}$$

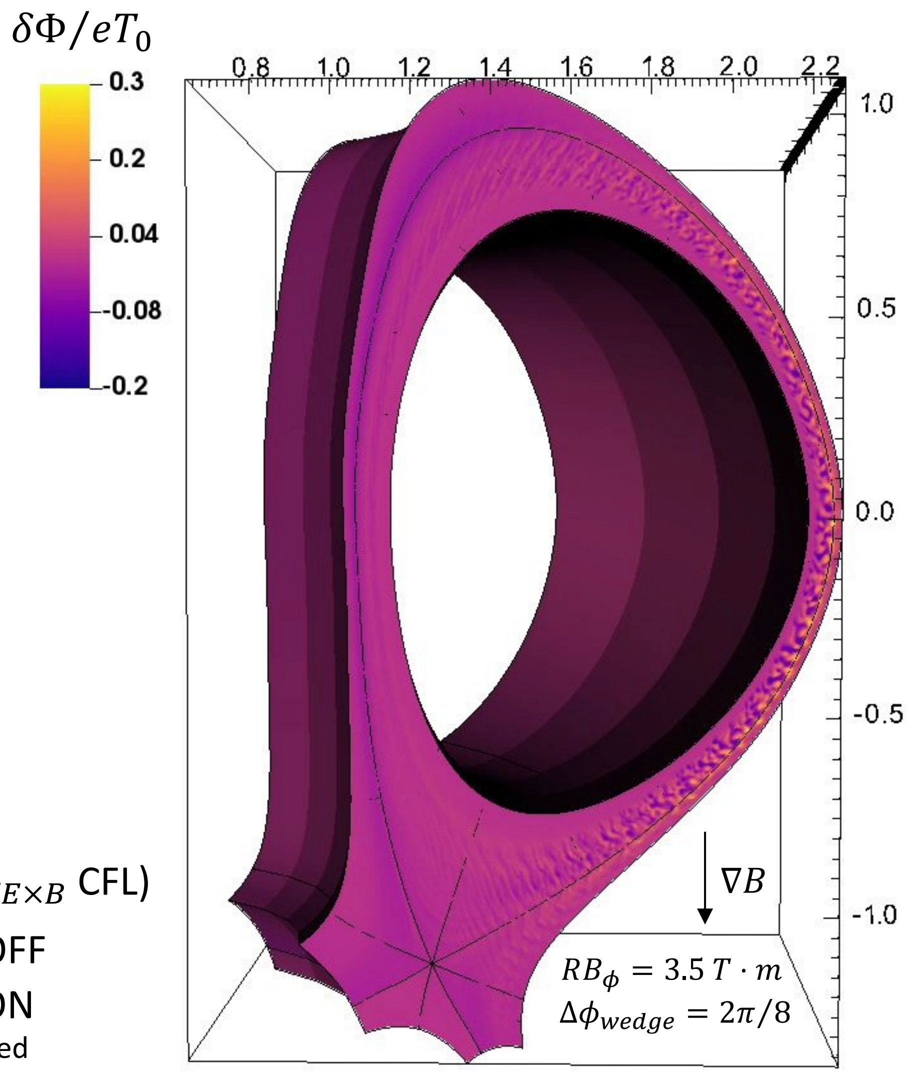
Boedo et al., PoP 2016

Qualitative agreement with DIII-D H-mode co-I_p rotation and E_r is observed

Modeling realistic (DIII-D) geometry: 5D COGENT

Outboard radial profiles
(time averaged t=0.2-0.3 ms)





- BC: fixed n_i and T_i at radial boundaries
- Fixed $T_e = 320$ eV
- Enhanced resistivity
  $\sigma_\parallel \leftrightarrow \tau_e V_{T_e}/qR_0 \sim 0.25$
- Ion collisions and RS term are turned OFF
- Resolution
  $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$
  $(80, 4, 2144, 32, 12)$
- Wall clock time (dominated by 3D implicit solve)
  1 step ↔ 30s
  Nersc 1152 cores

Linear stage ($V_{\nabla B}$ CFL)

$\Delta t = 0.2\ \mu s$

Nonlinear stage ($V_{\delta E\times B}$ CFL)

$\Delta t = 0.07\ \mu s$ RS – OFF

$\Delta t = 0.13\ \mu s$ RS – ON (mitigated turbulence)

Hybrid GK ions – fluid electron model is extended to include electromagnetic (EM) effects

- EM effects are important in a steep edge region under H-mode conditions, $\omega_{\mathrm{A}} \sim \omega_{dr}$

$$\omega_A = k_{\parallel} V_A \,, \qquad \omega_{dr} = k_{\perp} \rho_s V_s / L_n$$

- Implicit treatment is needed to avoid CFL constraints for $\omega_{\mathrm{A}} > \omega_{dr}$
  - In low-density or high-B regions → large $V_A = B/\sqrt{4\pi n_i m_i}$
  - Under L-mode conditions (shallow gradients)

- 5D ion GK equation is modified to include inductive field*: $E_{\parallel} = -\nabla_{\parallel}\Phi - \frac{1}{\mathrm{c}}\frac{\partial A_{\parallel}}{\partial t}$

- 3D field part of the semi-implicit EM hybrid system*:

$$\begin{cases} \frac{\partial}{\partial t}\varpi + \nabla_{\perp}\left(c\frac{-\nabla_{\perp}\phi\times\boldsymbol{B}}{B^2}\varpi\right) = \nabla_{\perp}\cdot\left(e\int\frac{2\pi}{m_i}B_{\parallel}^{*} f_{i,gc}\boldsymbol{v_{mag}}\,dv_{\parallel}d\mu - c\frac{\nabla_{\perp}(n_i T_e)\times\mathbf{b}}{B}\right) + \nabla\cdot(\boldsymbol{b}j_{\parallel}) & \text{Quasi-neutrality} \\ \frac{1}{c}\frac{\partial}{\partial t}\left[\left(1 - \frac{c^2}{\omega_{pe}^2}\Delta_{\perp}\right)A_{\parallel}\right] = -\nabla_{\parallel}\Phi + \frac{\nabla(n_e T_e)}{e n_i} + \frac{c}{4\pi\sigma_{\parallel}}\Delta_{\perp}A_{\parallel} & \text{Electron parallel force balance} \\ -\Delta_{\perp}A_{\parallel} = \frac{4\pi}{c}j_{\parallel} & \text{Ampere's law} \end{cases}$$

*Presently, omit magnetic flutter terms

ImEx framework with physics-based preconditioner is used to handle fast Alfven-wave time scale

Physics-based preconditioner* (PC) includes Alfven-wave, electron inertia and resistive terms

$$\frac{\partial}{\partial t}\nabla_\perp\left(\frac{c^2 m_i n}{B^2}\nabla_\perp\Phi\right) = -\frac{c}{4\pi}\nabla\cdot(\boldsymbol{b}\Delta_\perp A_\parallel)$$

$$\frac{1}{c}\frac{\partial}{\partial t}\left[\left(1-\frac{c^2}{\omega_{pe}^2}\Delta_\perp\right)A_\parallel\right] = -\nabla_\parallel\Phi + 0.51\frac{\nu_e}{\omega_{pe}^2}c\Delta_\perp A_\parallel$$

To further simplify adopt the following ad-hoc approximations

$$\nabla_\perp\left(\frac{c^2 m_i n}{B^2}\nabla_\perp\Phi\right) \to \Delta_\perp\frac{c^2 m_i n}{B^2}\Phi$$

Valid for slow variations of background profiles

$$\nabla\cdot(\boldsymbol{b}\Delta_\perp A_\parallel) \to \Delta_\perp\nabla\cdot(\boldsymbol{b}A_\parallel)$$

May be good enough for stiffest (k~1/h) scales in $A_\parallel$

When included into the ImEx Newton-Krylov framework, the PC system to be solved is

$$\alpha\nabla_\perp\left(\frac{c^2 m_i n}{B^2}\nabla_\perp\Phi\right) + \frac{c}{4\pi}\nabla\cdot(\boldsymbol{b}\Delta_\perp A_\parallel) = r_\phi \quad (1)$$

$$\frac{1}{c}\left[\alpha - (\alpha + 0.51\nu_e)\frac{c^2}{\omega_{pe}^2}\Delta_\perp\right]A_\parallel + \nabla_\parallel\Phi = r_A \quad (2)$$

$\alpha \propto \Delta t^{-1}$ is a constant coefficient

- Now, approximate solution of Eq. (1) as

$$\Phi = \frac{B^2}{\alpha c^2 m_i n}\left(-\frac{c}{4\pi}\nabla\cdot(\boldsymbol{b}A_\parallel) + \Delta_\perp^{-1}r_\phi\right) \quad (3)$$

- Substitute (3) into (2) and solve the parabolic problem for $A_\parallel$
- Elliptic/parabolic equations are solved by AMG methods (from Hypre)

*Similar approach (but without radial coupling terms) is developed in B. Dudson et al, arXiv 1209.2054 (2012)

Efficiency of the physics–based PC is successfully demonstrated for the RBI mode

RBI 3-field simulation model [omits δB and drift terms]

$$\frac{\partial n}{\partial t} = \nabla \cdot \left(c\nabla\Phi \times \frac{\boldsymbol{b}}{B} n_0 \right)$$

$$\frac{\partial}{\partial t} \nabla_\perp \left(\frac{c^2 m_i n}{B^2} \nabla_\perp \Phi \right) = -\nabla \cdot \left(cT_e \frac{\nabla_\perp n \times \mathbf{b}}{B} \right) - \frac{\mathrm{c}}{4\pi} \nabla \cdot (\boldsymbol{b} \Delta_\perp A_\parallel)$$

$$\left[1 - \frac{c^2}{\omega_{pe}^2} \Delta_\perp \right] \frac{1}{c} \frac{\partial A_\parallel}{\partial t} = -\nabla_\parallel \Phi + \frac{c}{4\pi\sigma_\parallel} \Delta_\perp A_\parallel$$

Simulation parameters

$N_0 = 10^{20}$ m^{-3}, T_e=400 eV, $m_i = m_p$

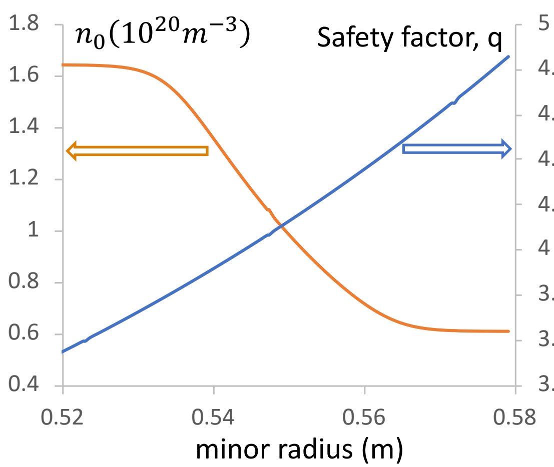
R_0=1.6 m, RB_ϕ=3.5Tm, wedge = $\pi/10$

Increased resistivity $\sigma_\parallel \leftrightarrow \tau_e V_{T_e}/qR_0 \sim 0.075$

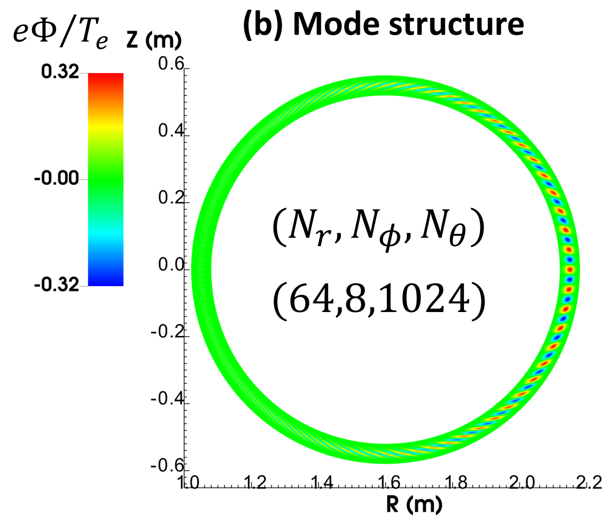
Taking q~4, L_n~3 cm, $k_\parallel \sim 1/qR_0$

$$\omega_A^{-1} = qR_0/V_A = 1.3\mu s \,, \;\; \gamma_b^{-1} = \frac{\sqrt{R_0 L_n}}{\sqrt{2} V_s} = 0.9\mu s$$

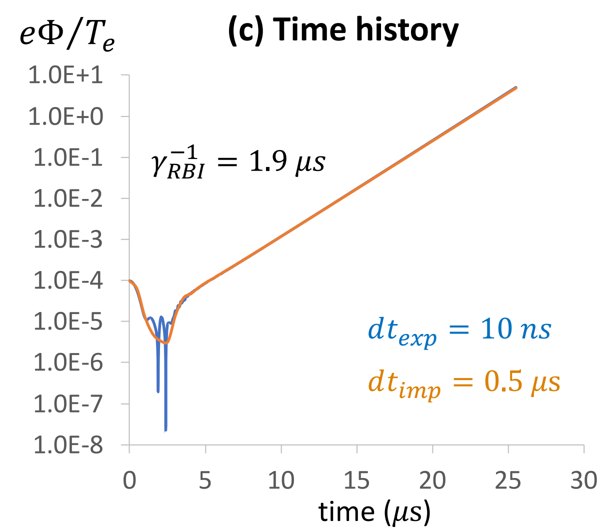
(a) Background profiles



(b) Mode structure



(c) Time history



50x increase in Δt, 10x decrease in wall time

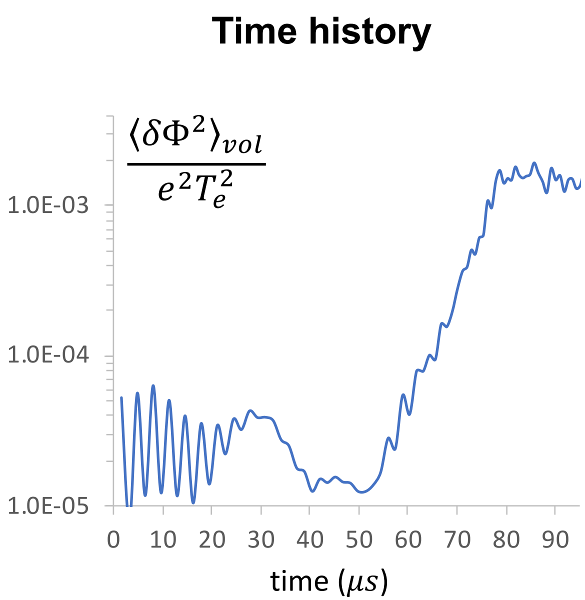
edge simulation laboratory

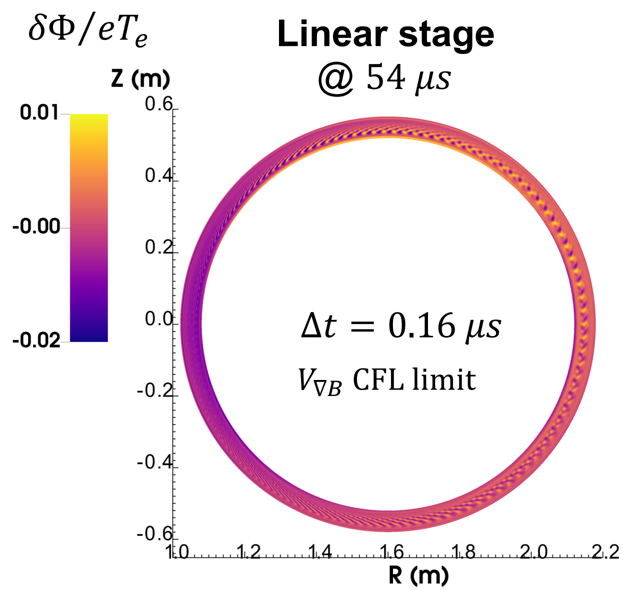
Dorf, Dorr and Ghosh, Contrib. Plasma Phys. (2024)

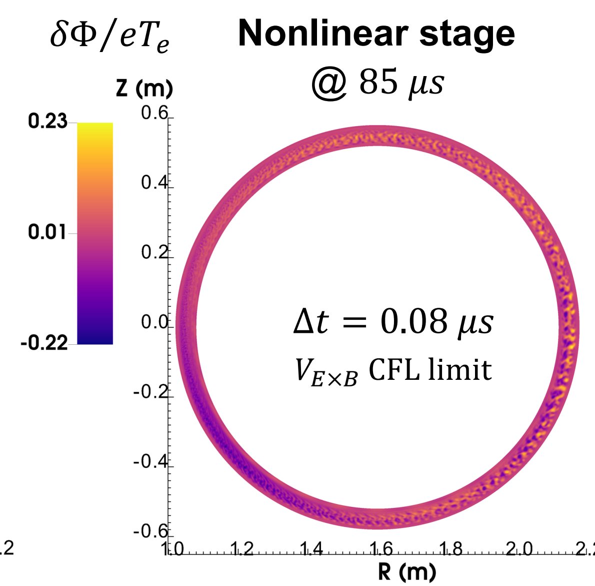
Fusion Energy Sciences

First results from from the semi-implicit hybrid EM model: DRBM turbulence

- Include drift terms (DRBM modes are captured) and background Er
- N_0~$2\text{x}10^{19}$ m^{-3}, T_i=T_e=400 eV, m_i=$2m_p$, L_n~3cm, q ~ 4, prescribed $\sigma_{\parallel} \leftrightarrow \tau_e V_{T_e}/qR_0 \sim 0.75$
- $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu) = (64,4,2048,32,24)$, wedge = $\pi/8$, 1 step ↔ 25s @ Cori 1024 cores







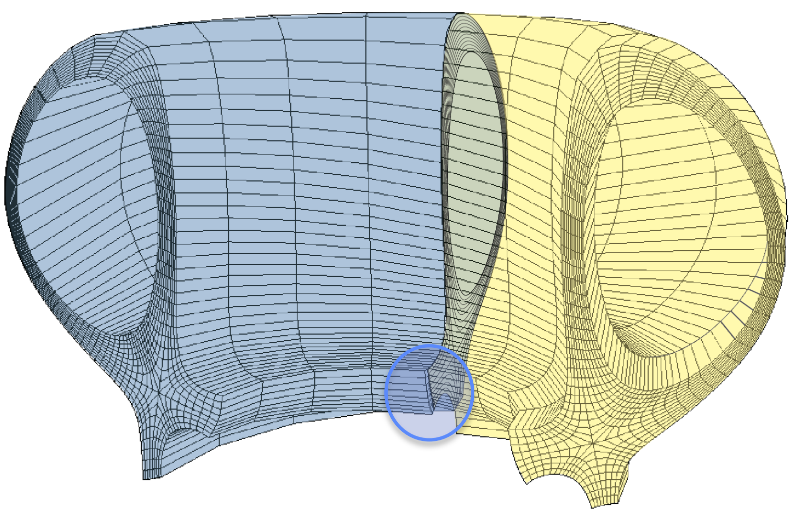
- IMEX Vs Explicit: 6x increase in Δt, 5x decrease in wall time
- Low-overhead from IMEX -> promise for stiffer (more realistic) applications

Conclusions

- **COGENT = framework for edge plasma simulations**
  - Physics models: kinetic, fluid, or hybrid
  - Computational capabilities:
    - High-order mapped multiblock to handle Xpoint
    - IMEX framework to handle stiff time scales
    - Solvers (multigrid, …)

- **A semi-implicit (IMEX) hybrid model is applied to (4D) axisymmetric and (5D) turbulence edge simulations in single-null geometries**
  - Includes ion kinetic effects and enables efficient time integration
  - Implicit time integration is facilitated by making use of
    - Physics based preconditioning (PC)
    - Multigrid solvers

Approximate divertor boundary condition is used

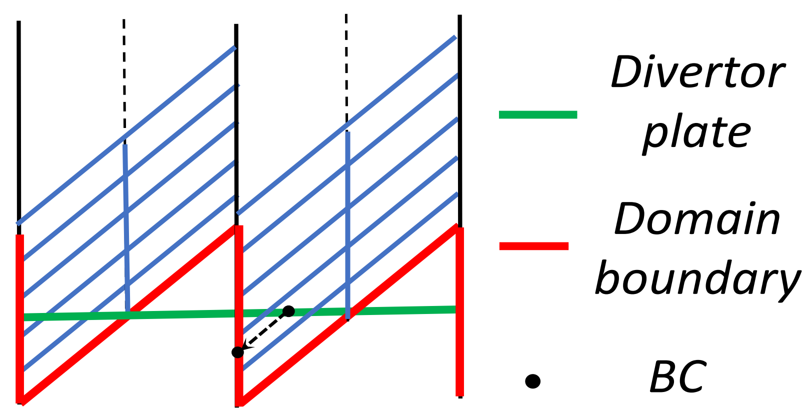


Toroidal angle measures a field-aligned coordinate

⇓

$\theta = const$ divertor plates are not aligned with the grid

Challenges with diverter BCs: divertor plates are not aligned with the computational grid



- *Present approximation* makes use of small parallel derivatives in f and Φ.

  Example: grounded plates – impose $\Phi = 0$ at the simulation domain boundary (shown in red)