Including electromagnetic effects into COGENT simulations of edge plasmas

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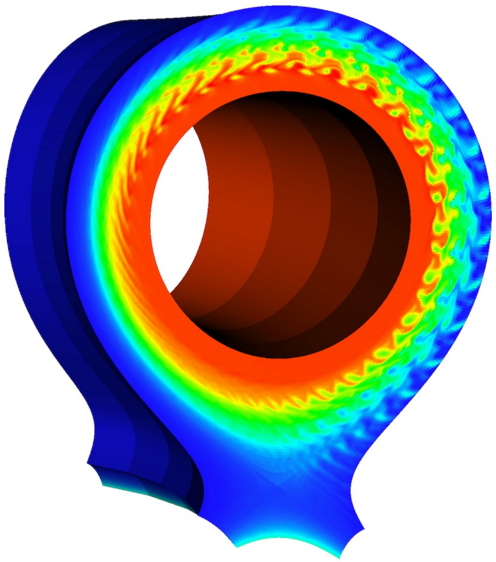

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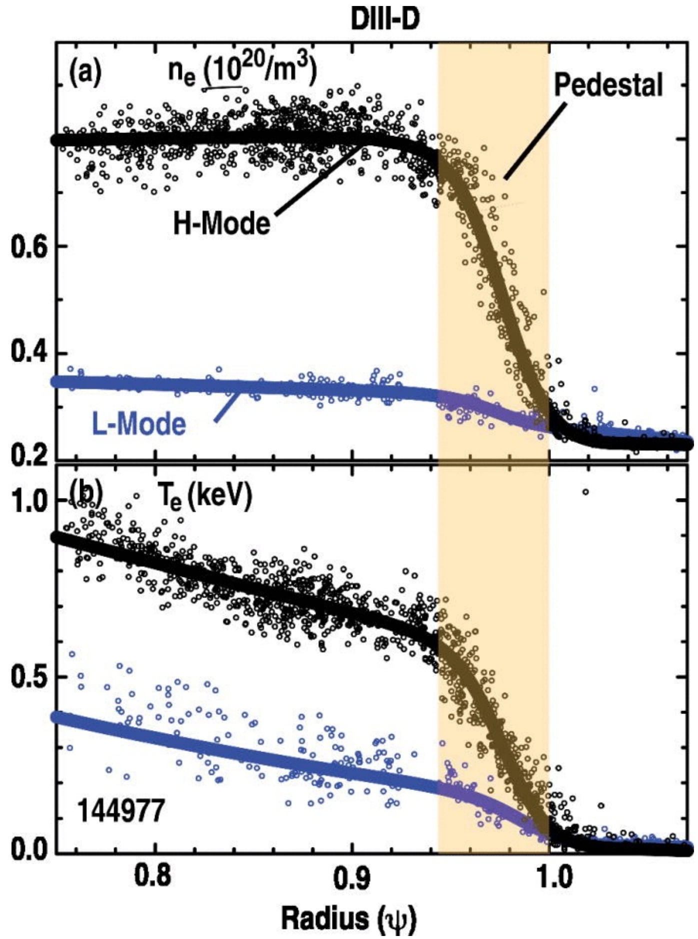
LLNL-PRES-***

OUTLINE

- *Overview of the COGENT code*
- *Hybrid (GK-ion – fluid electron) electrostatic vorticity model*
  - *Overview of electrostatic model results*
- *Extending the hybrid vorticity model to include EM effects*
  - *Verification, uniform slab*
  - *IMEX time integration (physics-based preconditioner)*
  - *Preliminary toroidal results*
- *Development of an MHD module*
- *Conclusions*

Tokamak edge plasma simulations can benefit from the use of high-order continuum methods

Radial scales are comparable to ion drift orbit excursions



- *H-mode is distinguished by strong edge plasma gradients*
- *F_0 strongly deviates from Maxwellian*
- Requires solving the full-F problem:
  - Low-amplitude turbulence (f_1) & quasi-equilibrium dynamics (F_0)
- *Motivates the use of continuum methods:*
  - *Free of particle noise (cf. PIC)*
  - *Can take advantage of high-order methods*

Successful applications of continuum methods to cross-separatrix modeling is demonstrated with the COGENT code

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

Continuum gyrokinetic code COGENT has been developed as part of the Edge Simulation Laboratory (ESL) collaboration

High-order (4th-order) finite-volume Eulerian gyrokinetic code

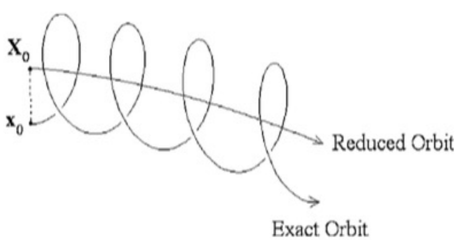
COGENT

Physics models (LLNL/UCSD)

- Multispecies full-F gyrokinetic equations
- Self-consistent electrostatic potential
- Collisions (including full Fokker-Planck)
- Anomalous transport models (in 4D)

Math algorithms (LLNL/LBNL)

- High-order mapped-multiblock technology to handle X-point
- Advanced multigrid solvers
- Advanced time integrators (ImEx)



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

Tokamak applications (AToM, ESL, PSI)

⇩

Low-Temp ⟷ **COGENT** ⟷ Z-pinch

New collaborations welcome!

https://github.com/LLNL/COGENT/

First-principles and reduced models in core gyrokinetics

Gyrokinetic Poisson equation (adopt long-wavelength limit)

$$\nabla_\perp \left(\frac{c^2 m_i n_{i,gc}}{B^2} \nabla_\perp \Phi \right) = e n_e - e \left(n_{i,gc} + \cancel{\frac{1}{m_i \omega_{ci}^2} \nabla_\perp^2 \frac{p_{i,\perp}}{2}} \right)$$

- Gyrokinetic ions and electrons
  - Most detailed approach
  - Computationally challenging due to stiff electron dynamics

- Gyrokinetic ions and adiabatic electrons, $n_e = n_{i,gc}^0 \left(1 + \frac{e\phi}{T_e} - \frac{e\langle\phi\rangle}{T_e} \right)$
  - Often used in core codes for ITG turbulence, neoclassical transport, etc
  - Cannot be straightforwardly extended across the separatrix
  - Does not capture resistive effects important in the cooler edge region

Need a computationally efficient (reduced) model for simulations of ion scale turbulence in single-null geometries

Hybrid GK ion – fluid electron vorticity model ($\nabla \cdot \boldsymbol{j} = 0$)

$$\frac{\partial}{\partial t}\varpi + \nabla_\perp\left(c\frac{-\nabla_\perp \Phi \times \boldsymbol{B}}{B^2}\varpi\right) + \nabla_\parallel\left(\cancel{V_{i,\parallel}\varpi}\right) = \boldsymbol{\nabla}_\perp \cdot \int \frac{2\pi}{m_i} e B_\parallel^* f_{i,gc} \boldsymbol{v_{mag}} dv_\parallel d\mu + \boldsymbol{\nabla}_\perp \cdot \left\{ec\frac{n_{i,gc}T_e}{B}\left(\nabla\times\boldsymbol{b} + \frac{\boldsymbol{b}\times\nabla B}{B}\right)\right\} + \boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel$$

Reynolds stress term — *Kinetic $\nabla \cdot \boldsymbol{j}_{i,\perp}$* — *Fluid $\nabla \cdot \boldsymbol{j}_{e,\perp}$*

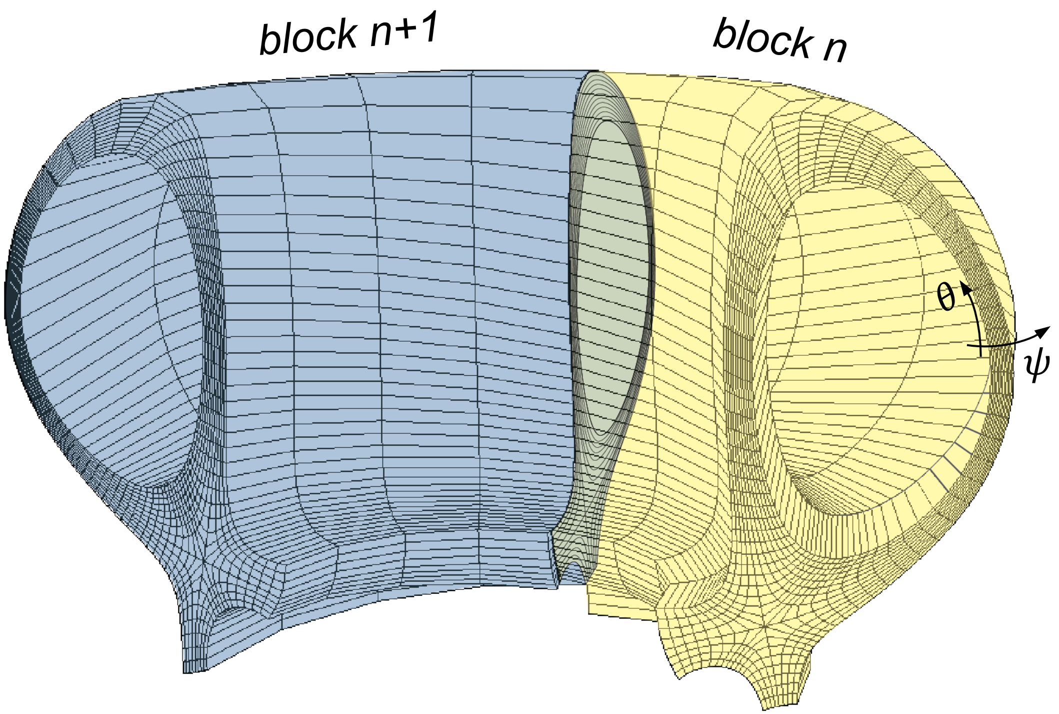
Vorticity	$\varpi = \nabla_\perp\left(\frac{c^2 m_i n_{i,gc}}{B^2}\nabla_\perp\Phi\right) + \cancel{\frac{e}{m_i\omega_{ci}^2}\nabla_\perp^2\frac{p_{i,\perp}}{2}}$	*Neglect the pressure corrections term*
Parallel current	$j_\parallel = \frac{e n_e}{0.51 m_e \nu_e}\left(\frac{1}{n_{i,gc}}\nabla_\parallel(n_e T_e) - e\nabla_\parallel\Phi + 0.71\nabla_\parallel T_e\right)$	*Stiff term (due to the large parallel conductivity) – treat implicitly*
Electron density	$n_e = n_{i,gc} + \nabla_\perp\left(\frac{c^2 m_i n_{i,gc}}{eB^2}\nabla_\perp\phi\right)$	*Include polarization corrections (required for high-k stabilization)*
Electron temperature	$T_e = const$	*Consider a simple isothermal electron model*

- **Captures ITG and resistive drift and ballooning modes**
- **Includes neoclassical ion physics effects**
- **Allows for efficient cross-separatrix simulations**

Discretization: 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



EDGE (COGENT)

(ψ, θ) - fine ⊥ coordinates

ϕ - coarse ∥ coordinate

Efficient for X-point modeling

CORE (GYRO, BOUT)

(ψ, ϕ) - fine ⊥ coordinates

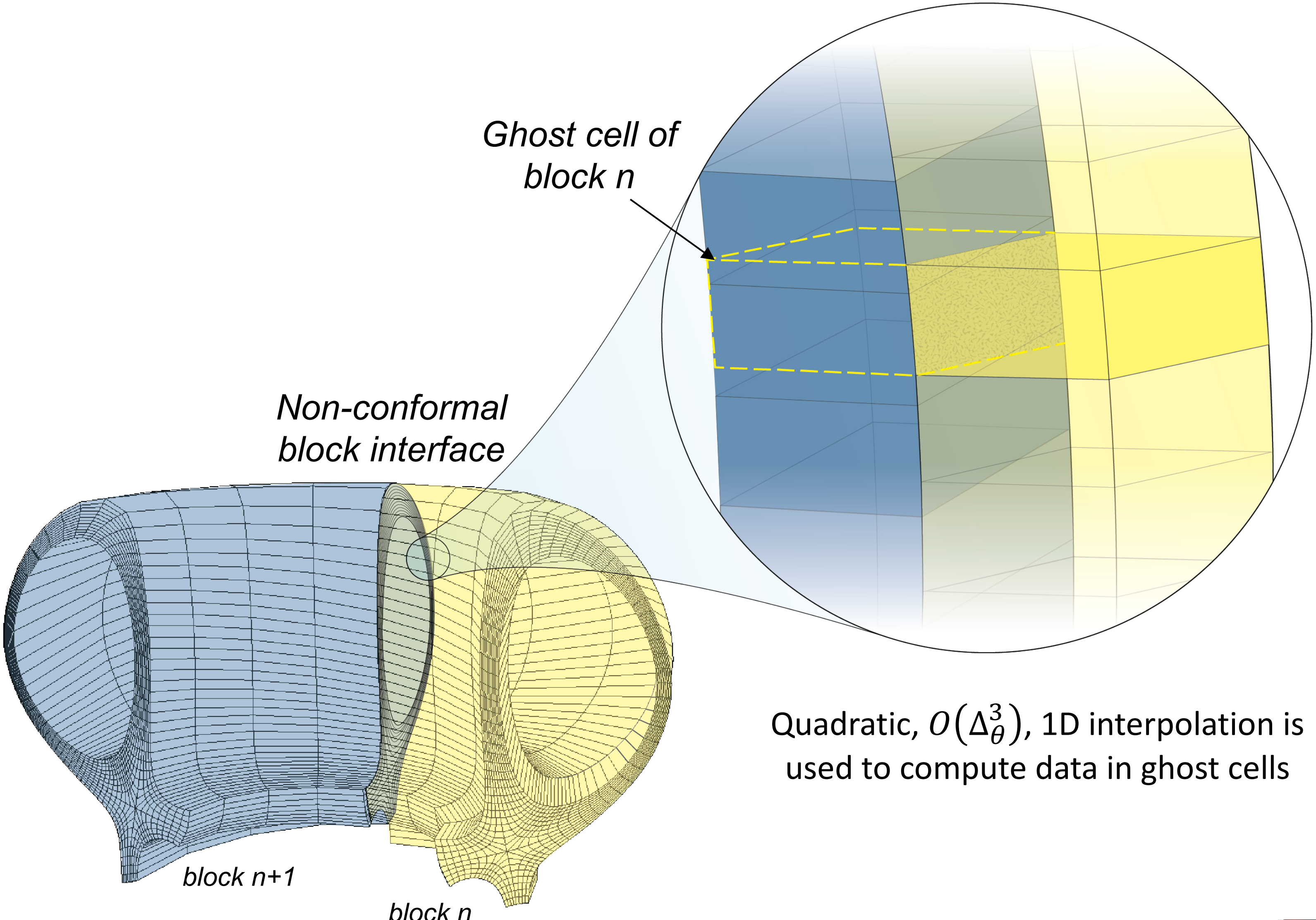
θ - coarse ∥ coordinate

Efficient for high-n wedge modeling

The approach is conceptually similar to the FCI approach*, but maintains flux surfaces (presently, including the X-point region)

*Hariri et al, Comp. Phys. Comm. (2013)

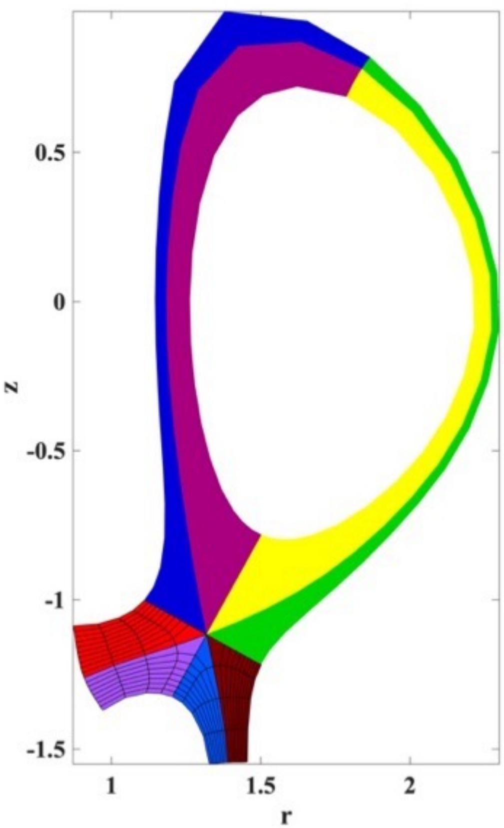
Interpolation is employed at a block interface



Quadratic, $O\left(\Delta_\theta^3\right)$, 1D interpolation is used to compute data in ghost cells

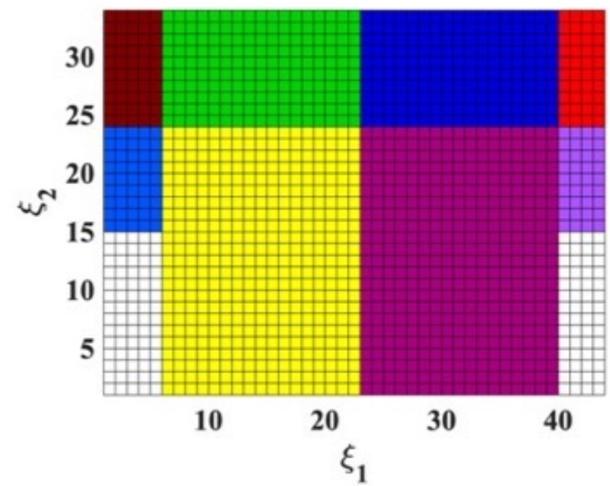
X-point geometry is handled by using poloidal sub-blocks

Physical domain (DIII-D)



Mapping

Computational multiblock domain



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

Problem: *X point → singular topology*

COGENT approach: *use multiblock grid technology*

Dorr et al., JCP (2018);

5D full-F simulations of plasma transport in a 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)

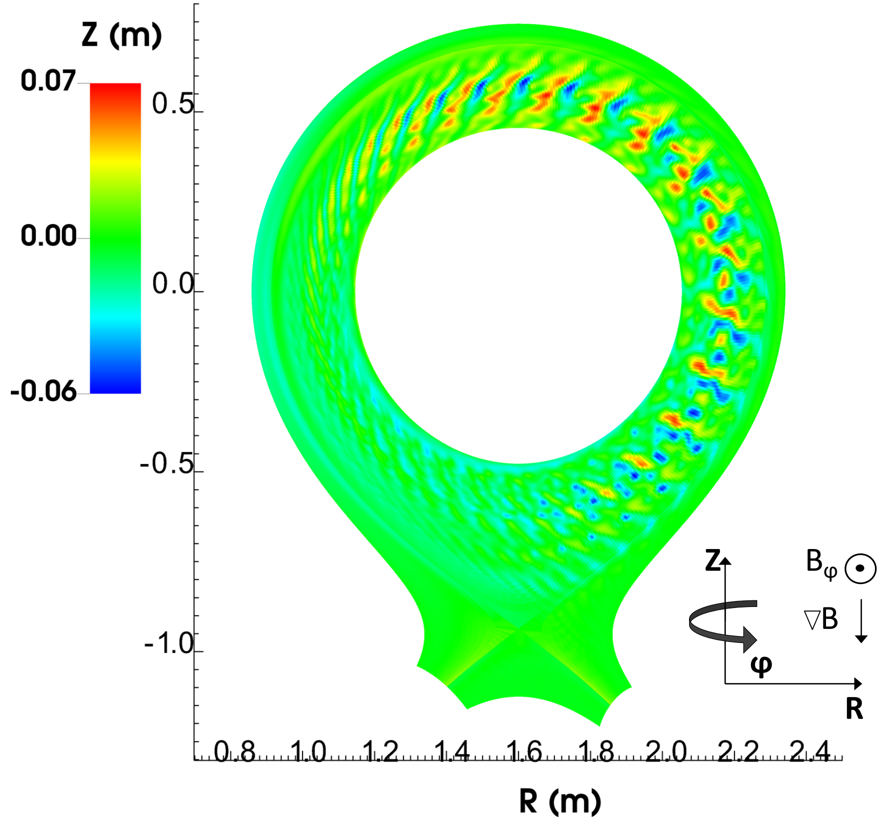
Resolution $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$ $(76,4,576,32,24)$

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

Performance 1 step ↔ 6s
Cori 1408 cores

Field-aligned multiblock version

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

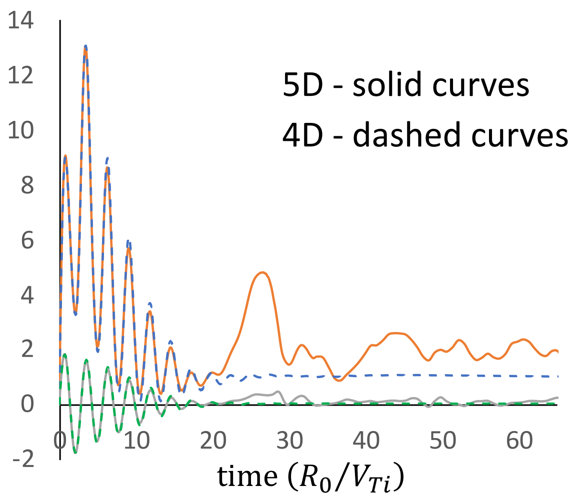


Model geometry

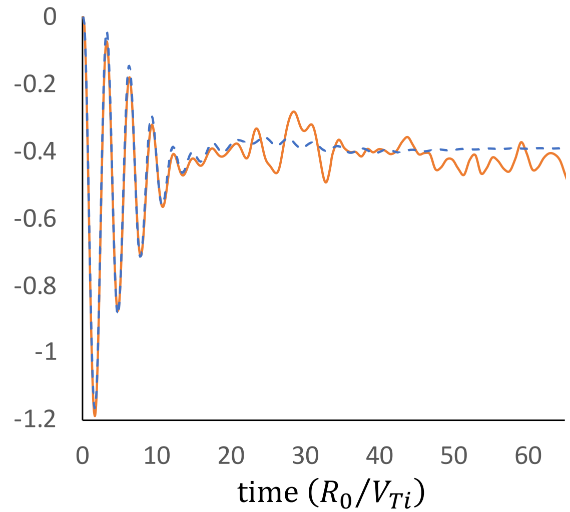
$R_0 = 1.6\, m, q \sim 2.5, RB_\phi = 3.5\, T \cdot m, \Delta\phi_{wedge} = 2\pi/8$

4D axisymmetric simulations can be used to provide insights into neoclassical transport and initial relaxation

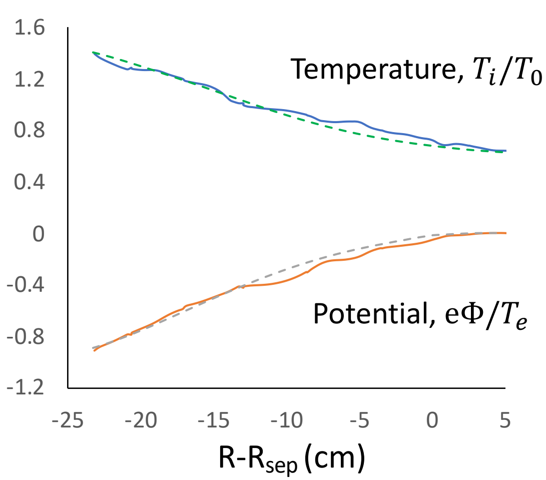
Transport power and particle flow



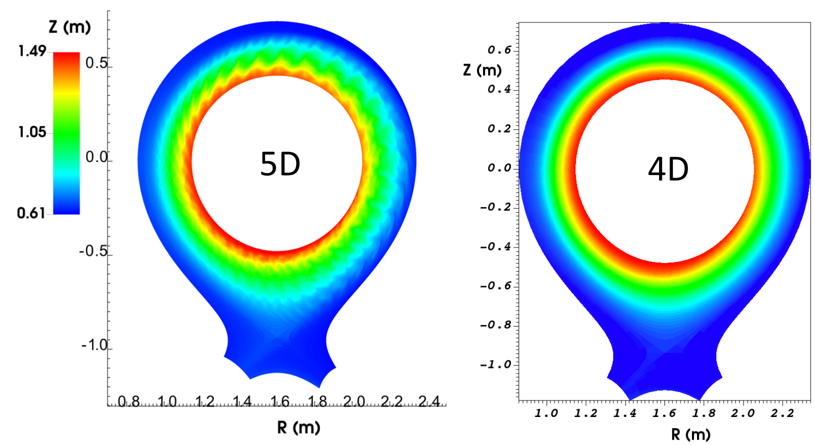
Electrostatic Potential



Outer midplane lineouts @ 59.7 R_0/V_{Ti}



Temperature profiles @ 59.7 R_0/V_{Ti}

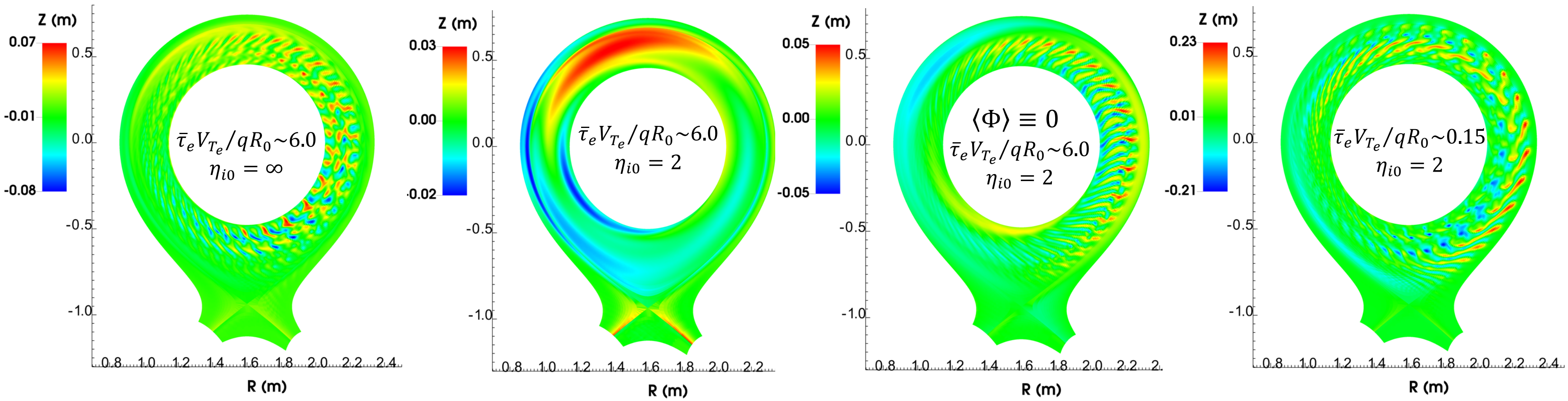


Poloidal background variations due to FOW effects

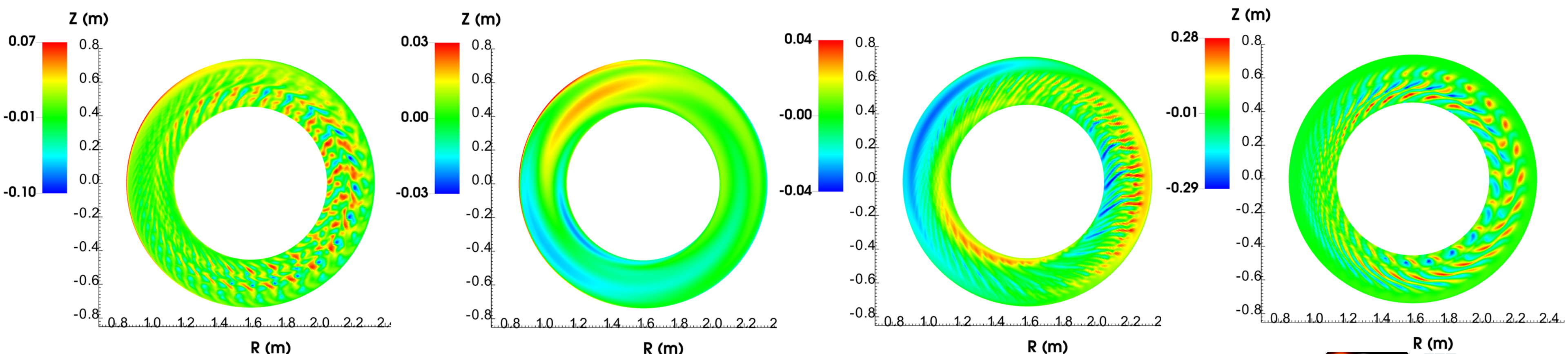
edge simulation laboratory

The role of X-point geometry can be explored by comparing with the counterpart toroidal annulus simulations

Increase conductivity to suppress resistive effects (ITG dominant case)	Increase density gradient to observe ITG stabilization ("H-mode-like" behavior)	Suppress self-consistent $\langle\Phi\rangle$ to observe ITG reemergence → demonstrates the role of E_r	Decrease conductivity to observe resistive drift and ballooning modes



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



Dorf and Dorr, Contrib. Plasma Phys. (2022)

Increased Er-well and pedestal build-up is consistent with turbulence suppression

Plasma parameters

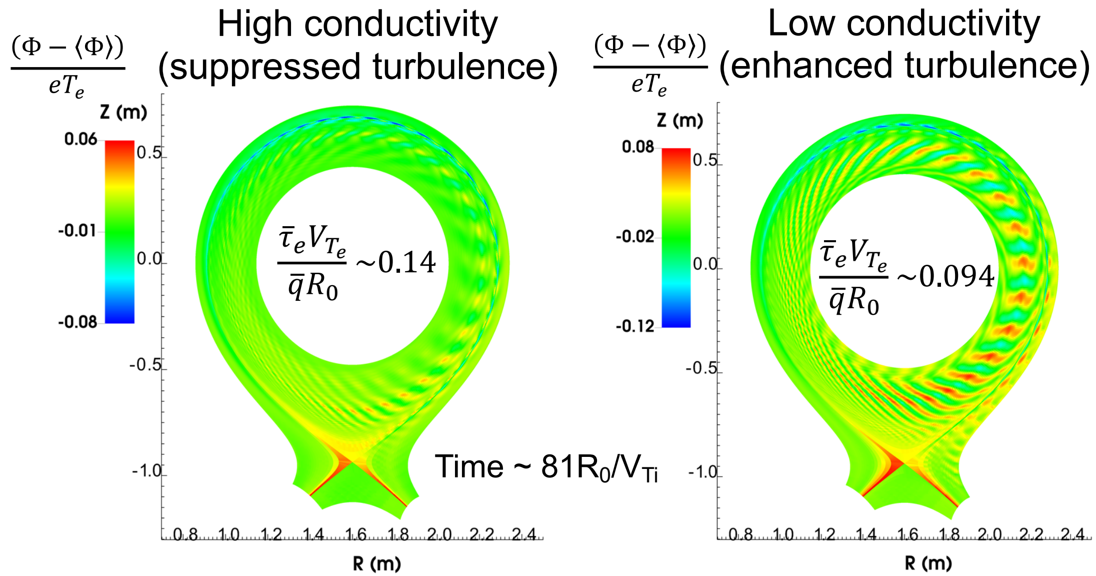
$T_0 = T_{i0} = 4$ keV, T_e=400eV

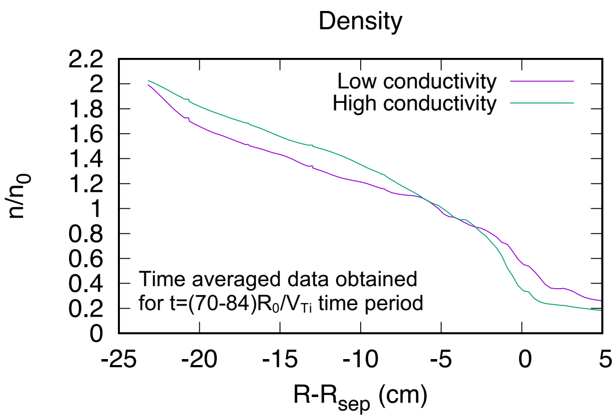
Ion-ion collisions $\nu_{ii} \sim 0.01 V_{Ti}/qR_0$

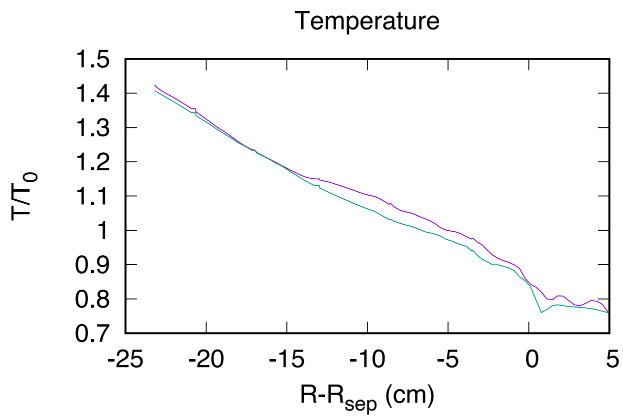
Model geometry parameters

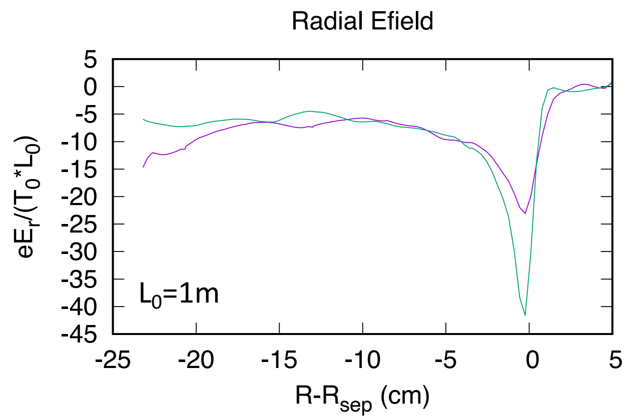
$R_0 = 1.6\ m, q \sim 2.5,$

$RB_\phi = 3.5\ T \cdot m, \Delta\phi_{wedge} = 2\pi/8$





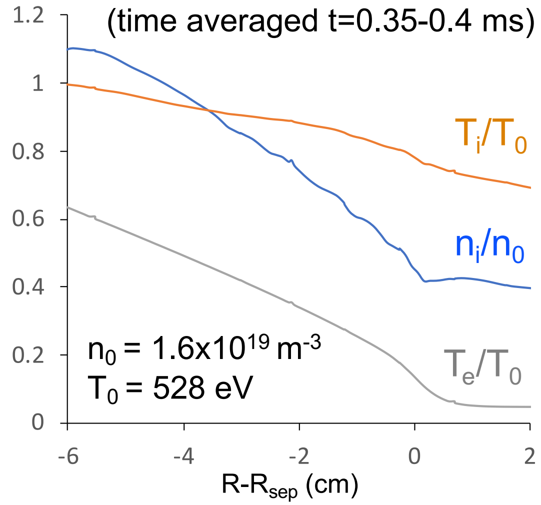




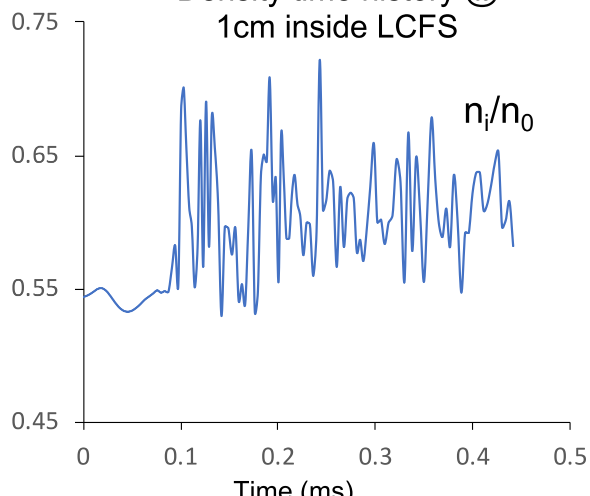
COGENT hybrid (reduced) model includes ion-scale resistive and ITG turbulence, background Er, NC and ion-orbit loss effects and can be used to study L-H transition and other edge-relevant phenomena while providing substantial speed-up over fully kinetic models

COGENT hybrid model has been used to simulate edge turbulence for realistic DIII-D discharge parameters*

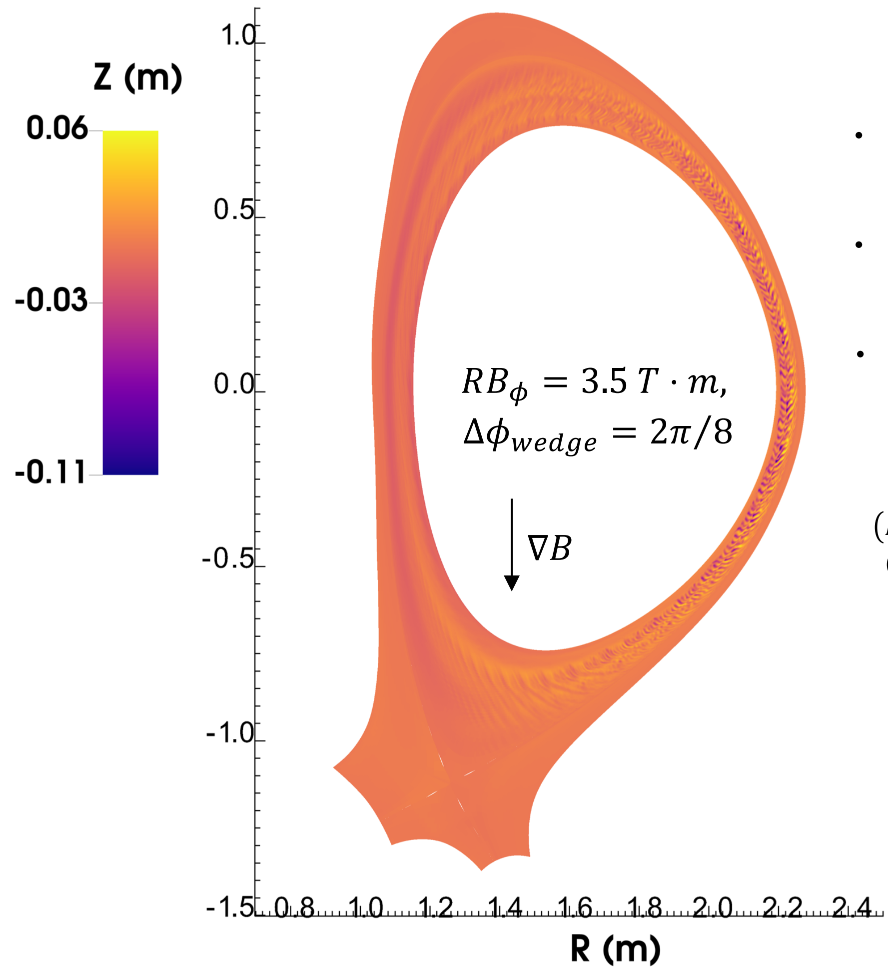
Outboard radial profiles
(time averaged t=0.35-0.4 ms)



Density time history @
1cm inside LCFS



$(\Phi - \langle\Phi\rangle)/eT_0 \; @ \; t = 0.28ms$



- BC: fixed n_i and T_i at radial boundaries
- Prescribed electron temperature
- Ion collisions and RS terms are turned OFF for simplicity

Resolution
$(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$
(80,4,2144,32,12)

Time step
$dt = 0.14\ \mu s$

Performance
1 step ↔ 9s
Cori 1728 cores

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

Simulation model [presently does not include peeling-drive (δB) terms[

$$\begin{cases} \dfrac{\partial}{\partial t}\varpi + \nabla_\perp \left(c\dfrac{-\nabla_\perp \phi \times \boldsymbol{B}}{B^2}\varpi \right) = \nabla_\perp \cdot \left(e\displaystyle\int \dfrac{2\pi}{m_i} B_\parallel^* f_{i,gc} \boldsymbol{v_{mag}} dv_\parallel d\mu - c\dfrac{\nabla_\perp p_e \times \mathbf{b}}{B} \right) + \nabla\cdot(\boldsymbol{b} j_\parallel) & \text{Quasi-neutrality} \\ \left[1 - \dfrac{c^2}{\omega_{pe}^2}\Delta_\perp\right]\dfrac{1}{c}\dfrac{\partial A_\parallel}{\partial t} = -\nabla_\parallel \Phi + \dfrac{\nabla_\parallel p_e}{e n_e} + 0.51\dfrac{\nu_e}{\omega_{pe}^2} c\Delta_\perp A_\parallel + \dfrac{0.71}{e}\nabla_\parallel T_e & \text{Electron parallel force balance} \\ -\Delta_\perp A_\parallel = \dfrac{4\pi}{c} j_\parallel & \text{Ampere's law} \end{cases}$$

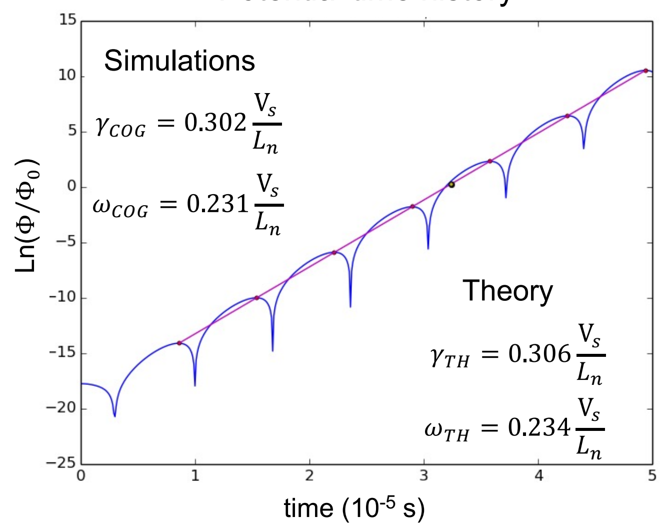
Simplified slab case verification

Adopting $\dfrac{\partial n_i}{\partial t} = c\nabla\Phi \times \dfrac{\boldsymbol{b}}{B}\cdot\nabla n_0$ we obtain

Dispersion for resistive drift instability with EM effects

$$\underbrace{\omega}_{\text{Electromagnetic induction}} + \underbrace{\frac{c^2 k_\perp^2}{\omega_{pe}^2}}_{\text{Electron inertia}}\underbrace{(\omega - 0.51 i\nu_e)}_{\text{Electron friction}} = \frac{k_\parallel^2 V_A^2}{\omega^2}\left(\omega - \underbrace{\frac{V_s}{|L_n|}k_\perp \rho_s}_{\text{Drift effects}}\right)$$

Potential time history



Simulation parameters:

$T_e = T_i = 100$eV
B = 2 T
$n_0 = 10^{13}$ cm^{-3}
$m_i = m_p$
$L_n = 5$ cm
$k_\perp \rho_s = 2$
$2\pi/k_\parallel = 30$ m
$V_{T_e} k_\parallel/\nu_e = 1$

edge simulation laboratory

Fusion Energy Sciences

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

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

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

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

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

Not valid in toroidal geometry, working on improvements

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

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

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

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

- Approximate solution of Eq. (1) as

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

- Substitute (3) into (2) and solve the second-order elliptic equation for $A_\parallel$
- Elliptic equations are efficiently solved by AMG methods (from Hypre)

*Similar ideas are expressed in B. Dudson et al, arXiv 1209.2054 (2012)

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

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

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

$$\frac{\partial}{\partial t}\nabla_\perp\left(\frac{c^2 m_i n}{B^2}\nabla_\perp\Phi\right) = \frac{2cT_e}{B}\boldsymbol{b}\times\boldsymbol{\kappa}\cdot\nabla(n-n_0) - \frac{\mathrm{c}}{4\pi}\nabla\cdot(\boldsymbol{b}\Delta_\perp A_\parallel)$$

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

Simulation parameters

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

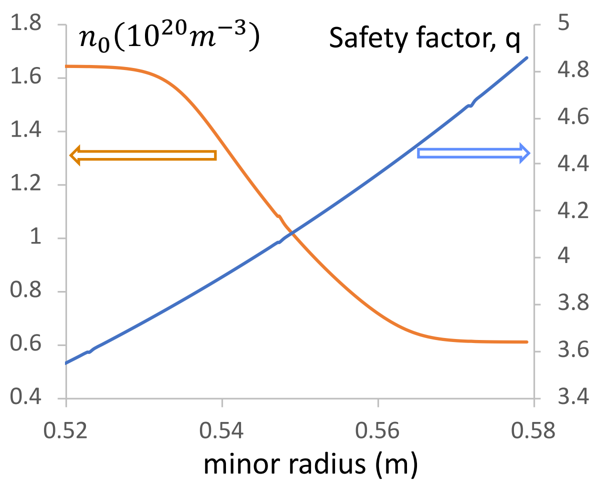
R_0=1.6 m, RB_ϕ=3.5Tm, wedge = $\pi/10$

Increased resistivity $\sigma_\parallel \leftrightarrow \nu_e^{-1}V_{T_e}/qR_0 \sim 0.15$

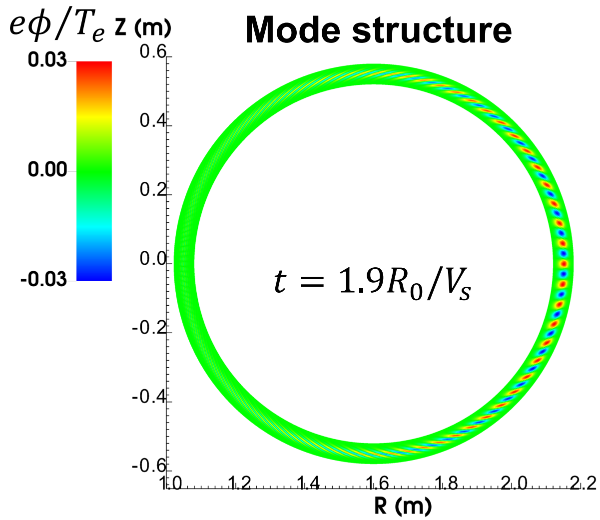
Taking q~4, L_n~3 cm, $k_\parallel \sim 1/qR_0$

$$\omega_A = V_A k_\parallel = 5.6\frac{V_s}{R_0},\quad \gamma_b = \frac{\sqrt{2}V_s}{\sqrt{R_0 L_n}} = 10.3\frac{V_s}{R_0}$$

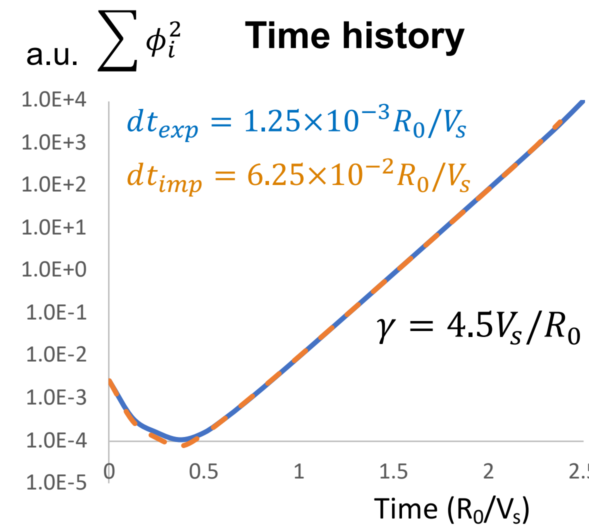
Background profiles



Mode structure



Time history



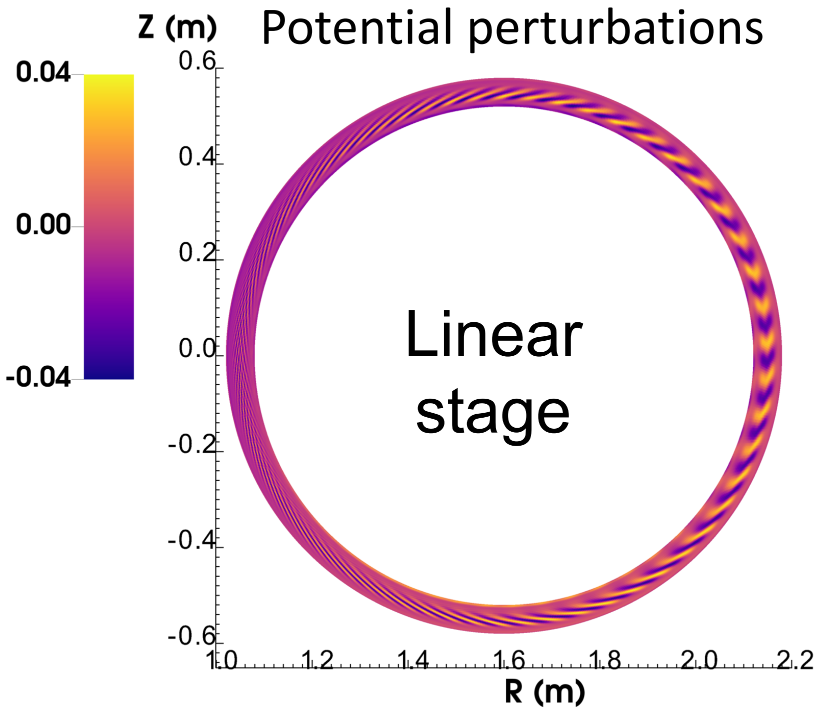
edge simulation laboratory

Fusion Energy Sciences

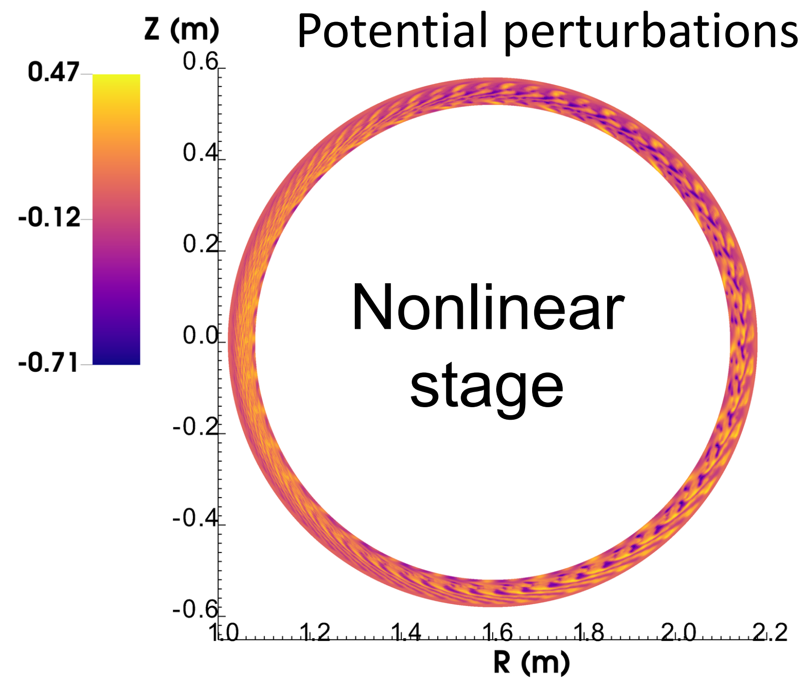
Preliminary results from the implicit hybrid GK-ions -- fluid electrons EM model (work in progress)

- DIII-D edge parameters, $N_0=2\text{x}10^{19}$ m^{-3}, $T_i=T_e=100$ eV, $m_i=2m_p$, $\sigma_{\|} \leftrightarrow \nu_e^{-1} V_{T_e}/qR_0 \sim 0.75$
- Include drift terms (DRBI mode is captured), and background Er, ion-ion collisions -- OFF
- Profiles shape $[n_0(\psi), q(\psi)]$ same as for the 3field fluid RBI test

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



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

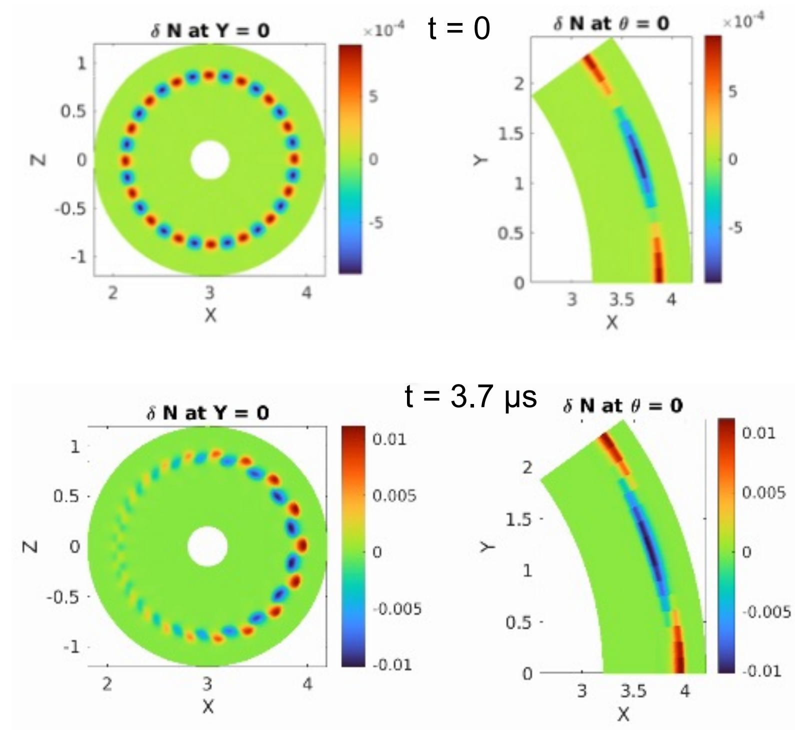


MHD fluid module is added to COGENT framework

Simulation model

- Ideal MHD equations with viscosity
- Finite volume scheme for conservative fluid variables implemented for general non-orthogonal coordinates.
- Constrained transport method for B (div**B**=0 to machine precision)
- ImEx time integration with option to treat stiff viscosity term in equation of motion implicitly
- Multiple flux computing methods
  - Characteristic-based upwinding (TVD,QUICK,WENO5) via Lax Flux splitting – diffusive, good for β~1 systems like Z-pinches where shocks are typical
  - ZIP upwinding – nondiffusive, stable to linear red-black modes and nonlinear antidiffusion modes. Good for long timescale tokamak simulations

3D simulation of peeling-ballooning mode in a toroidal annular geometry



- 3D toroidal wedge geometry
- ZIP upwinding for fluxes
- Linearized JxB force & isothermal model
- Equilibrium parameters: RB_T = 6 T-m, q=1.6
- initial Perturbation scales with cos(10ϕ - 16θ)

Conclusions

- **5D continuum** full-F gyrokinetic **cross-separatrix** simulations of edge plasma transport are being extended to include **EM effects**

- COGENT discretization is distinguished by
  - High-order finite-volume discretization
  - Mapped multiblock grid technology and locally field-aligned grids

- Present capabilities include
  - Gyrokinetic Poisson and vorticity model (extended to include EM effects)
  - Various collision models (including nonlinear Fokker-Planck)
  - Implicit-Explicit (ImEx) time integration capabilities
  - Fluid models for electron and neutral species

- In progress/future work:
  - Applications: L-mode turbulence, L-H transition, divertor heat-flux width
  - Capabilities: electromagnetics, kinetic electrons, FLR effects