A hybrid gyrokinetic ion – fluid electron model for edge plasma simulations

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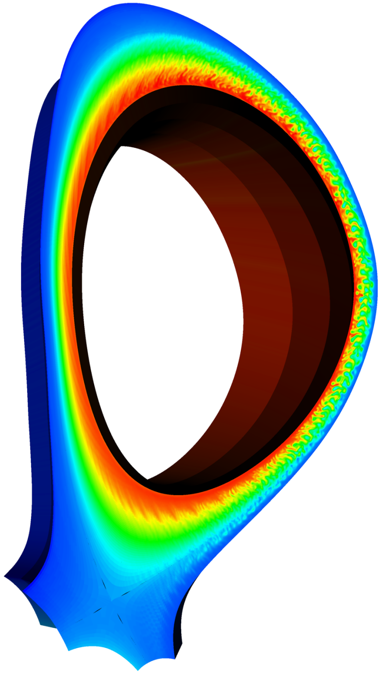

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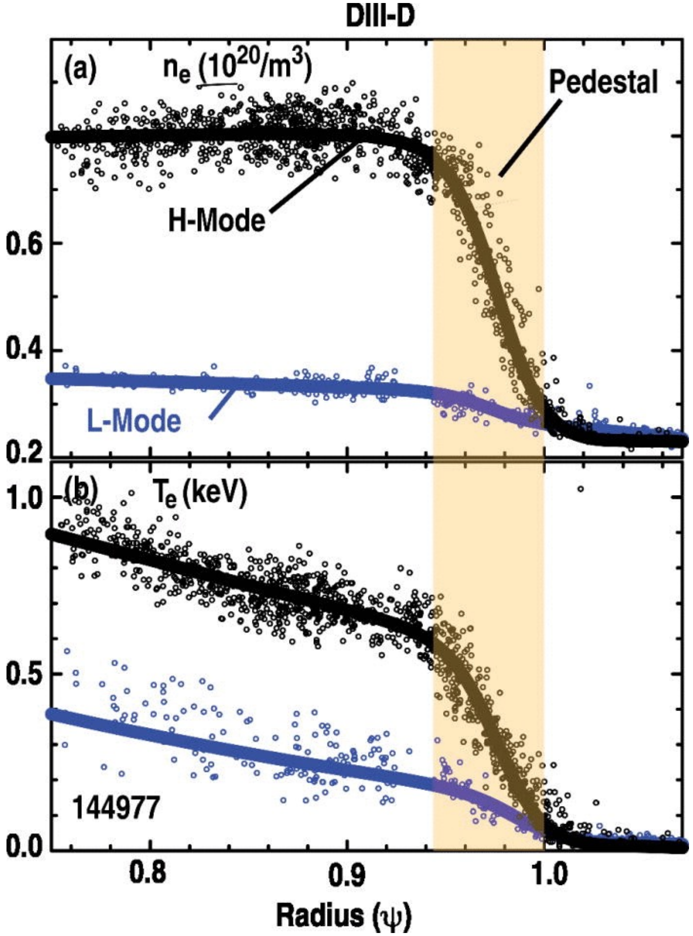
OUTLINE

- *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



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

- *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

edge simulation laboratory

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

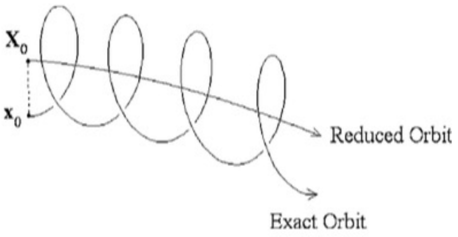
COGENT

Physics models (LLNL/UCSD)

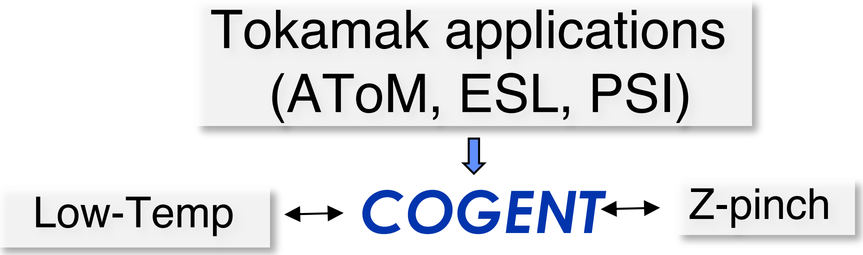
- Multispecies full-F gyrokinetic equations
- Self-consistent electrostatic potential
- Collisions (including full Fokker-Planck)
- Anomalous transport models (in 4D)

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)

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

- 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 ($\nabla \cdot \boldsymbol{j} = 0$)

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

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

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

$$j_\parallel = \frac{en_e}{0.51m_e\nu_e}\left(\frac{1}{n_{i,gc}}\nabla_\parallel(n_eT_e) - e\nabla_\parallel\Phi + 0.71\nabla_\parallel T_e\right)$$

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

$$T_e = const$$

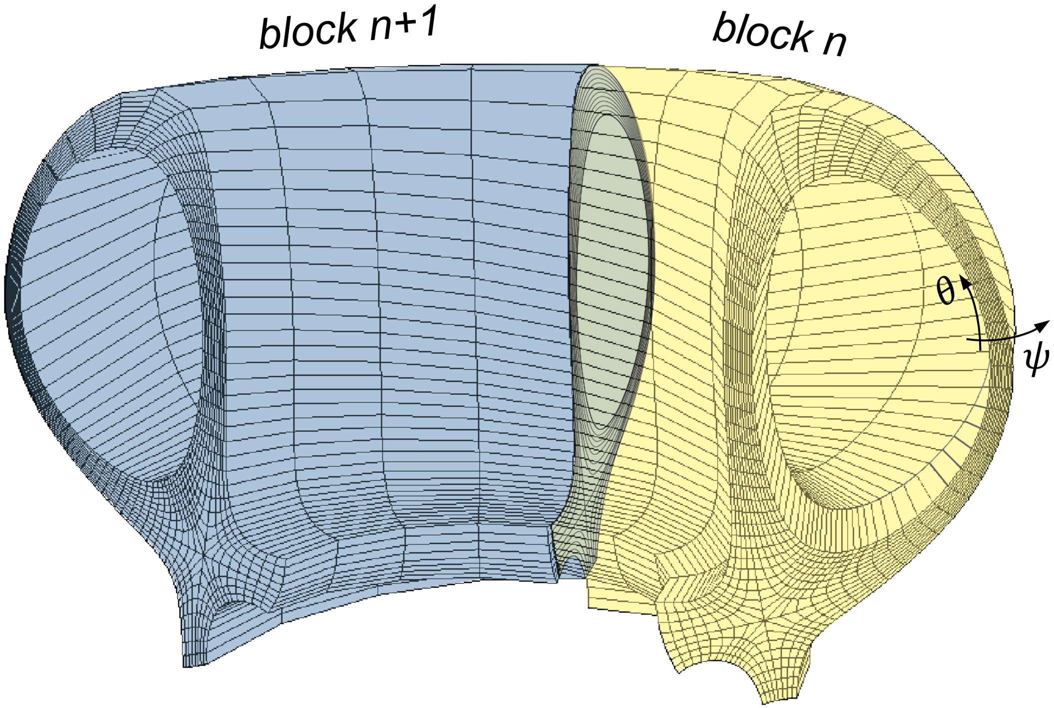
Consider a simple isothermal electron model

- **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)

edge simulation laboratory

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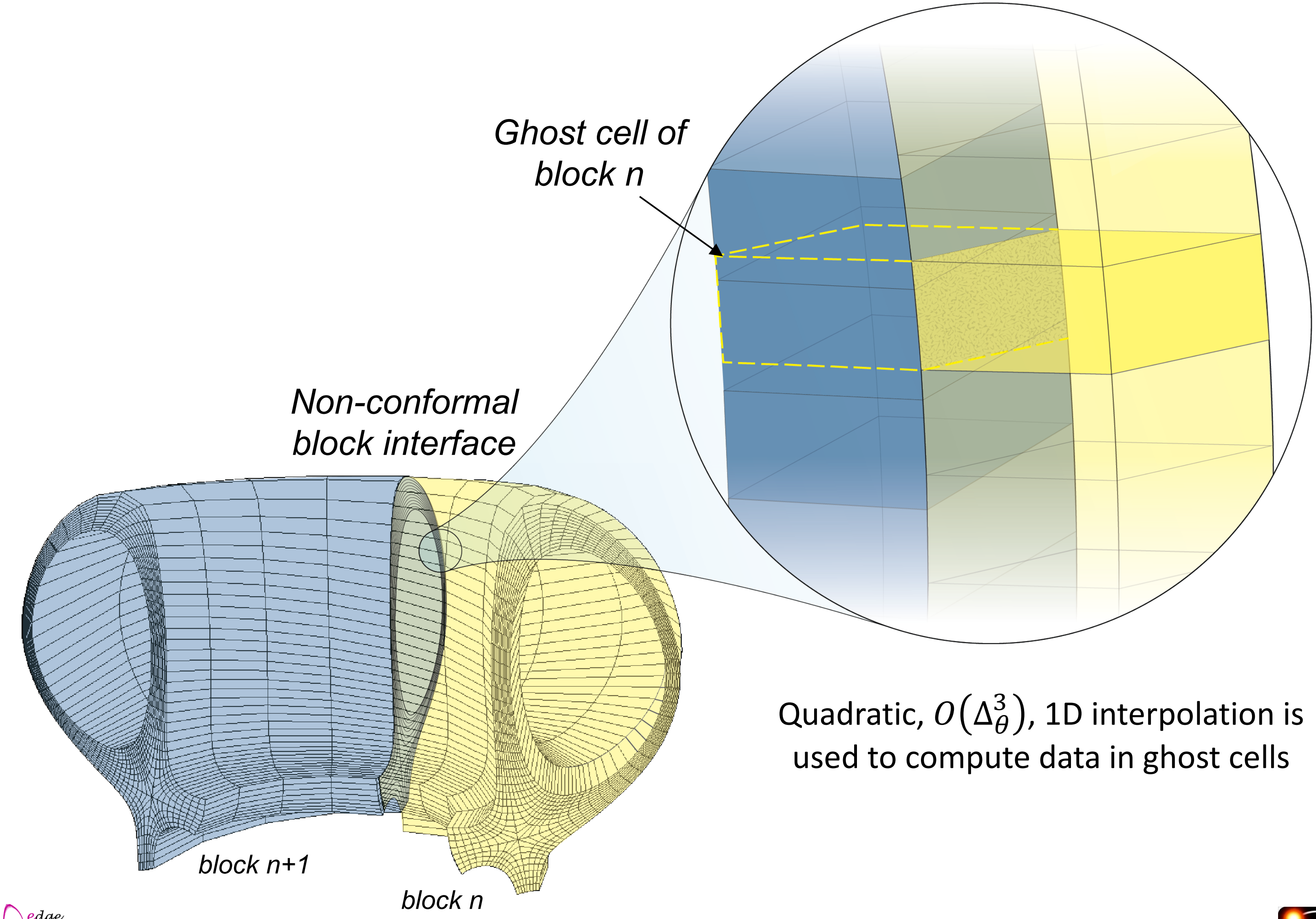
*Hariri et al, Comp. Phys. Comm. (2013)

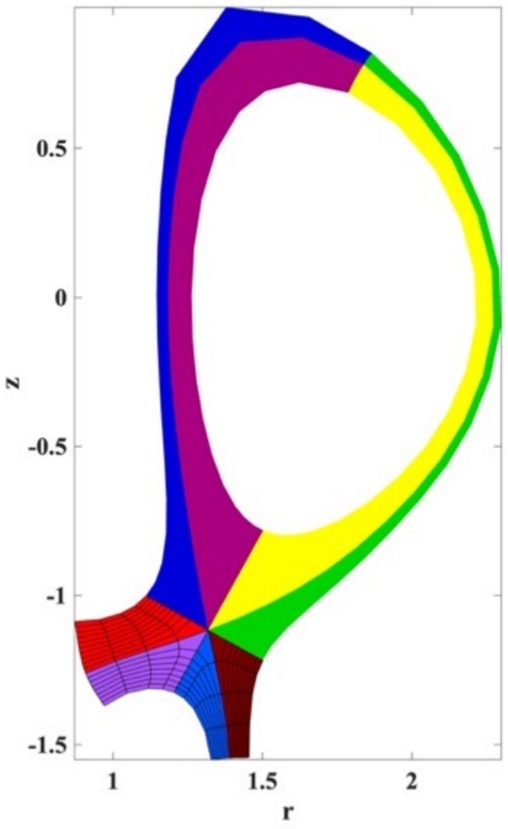
Interpolation is employed at a block interface



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

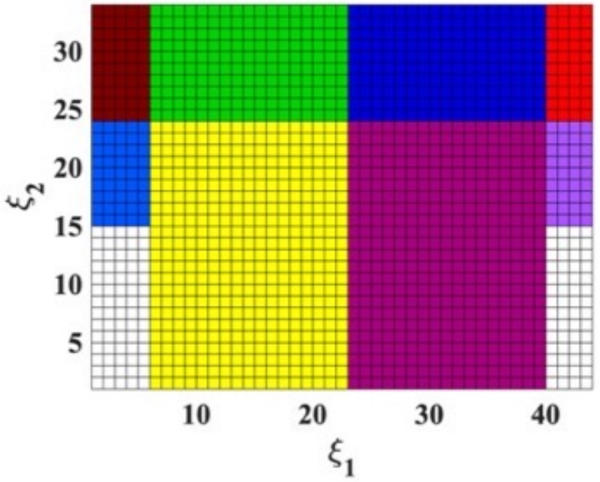
X-point geometry is handled by using poloidal sub-blocks

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)

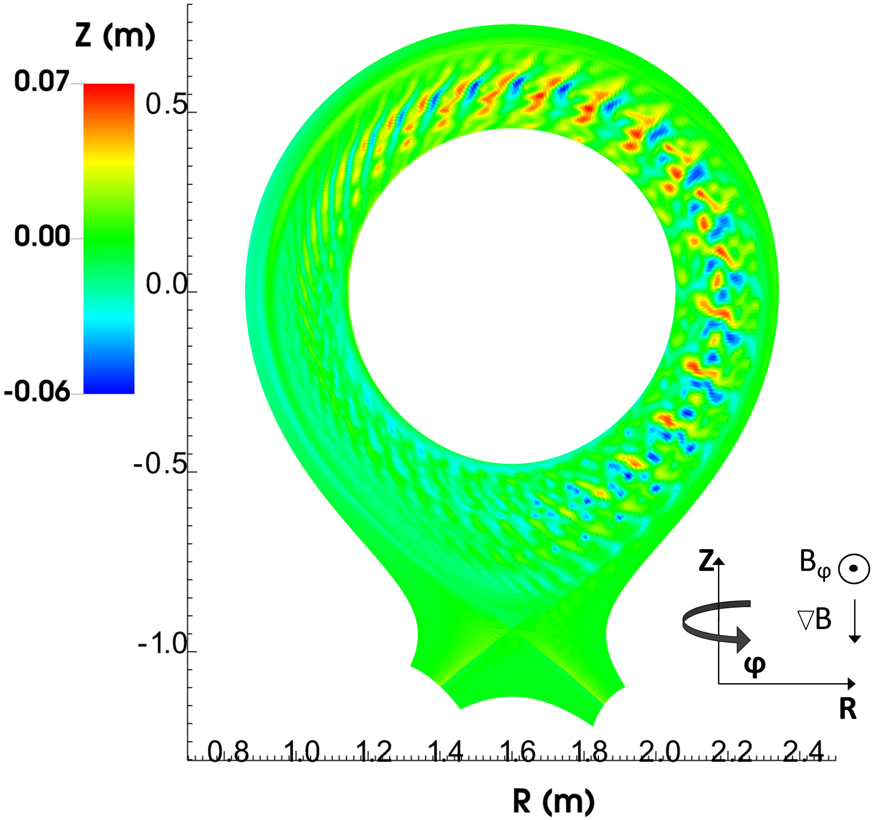
Resolution $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$ $(76,4,576,32,24)$

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

Performance 1 step ↔ 6s
Cori 1408 cores

Field-aligned multiblock version

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



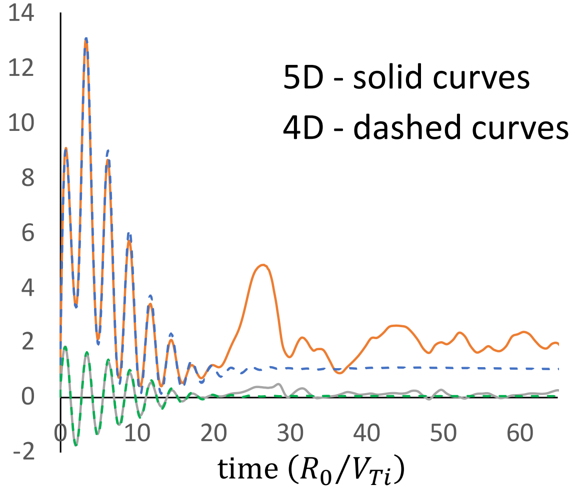
Model geometry

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

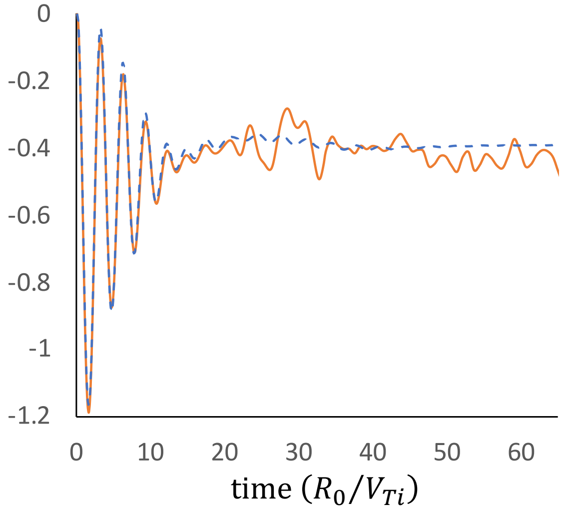
Dorf and Dorr, Contrib. Plasma Phys. (2022)

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

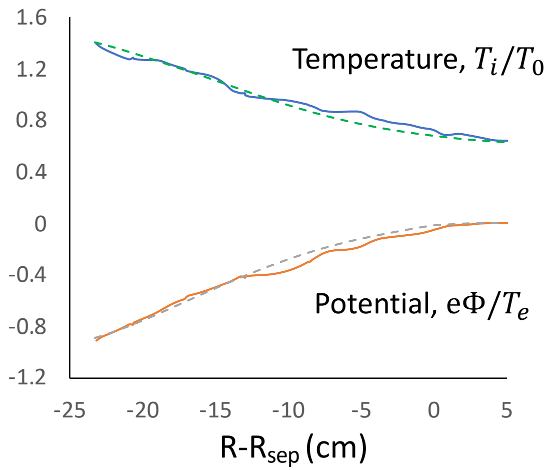
Transport power and particle flow



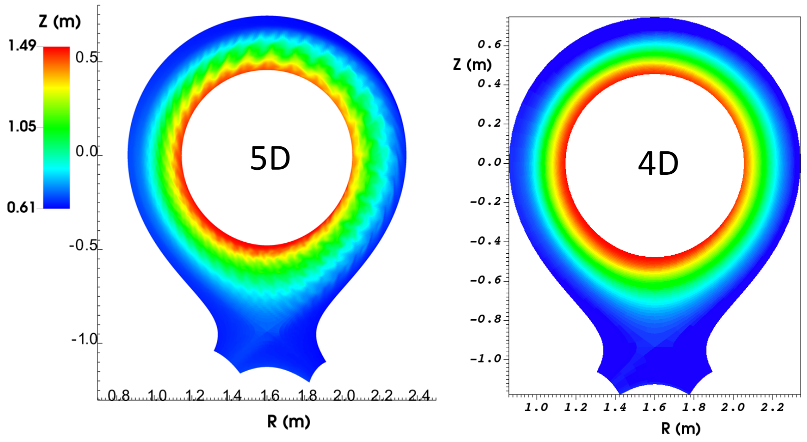
Electrostatic Potential



Outer midplane lineouts @ 59.7 R_0/V_{Ti}



Temperature profiles @ 59.7 R_0/V_{Ti}



Poloidal background variations due to FOW effects

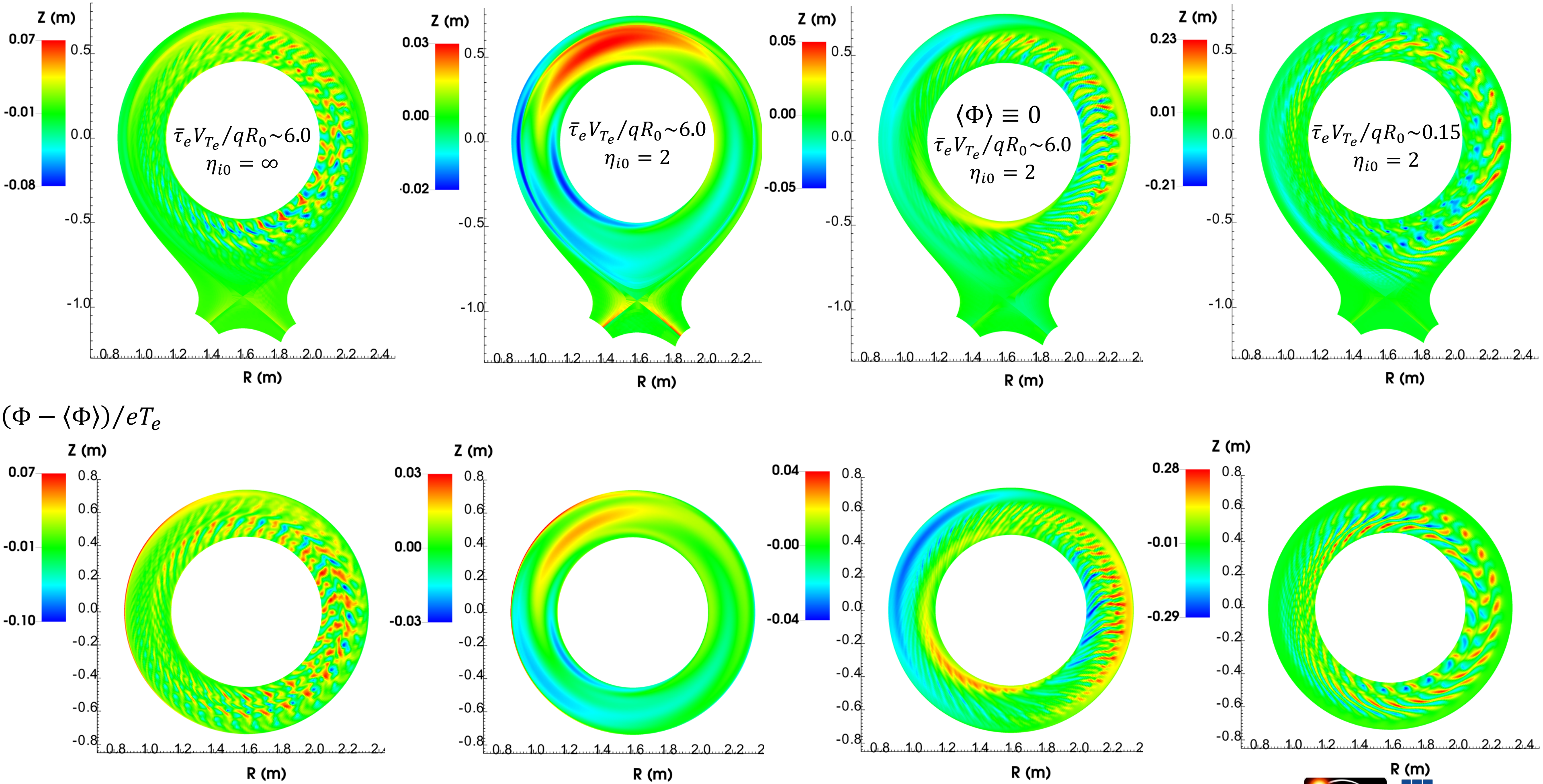
The role of X-point geometry can be explored by comparing with the counterpart toroidal annulus simulations

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



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

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

Plasma parameters

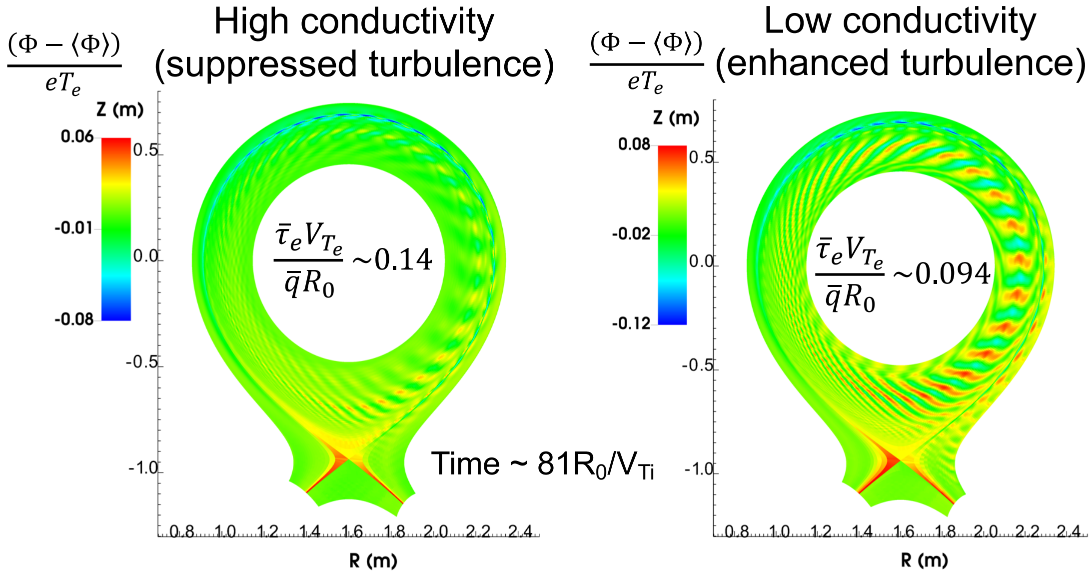
$T_0 = T_{i0} = 4\ \mathrm{keV},\ T_e = 400\mathrm{eV}$

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

Model geometry parameters

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

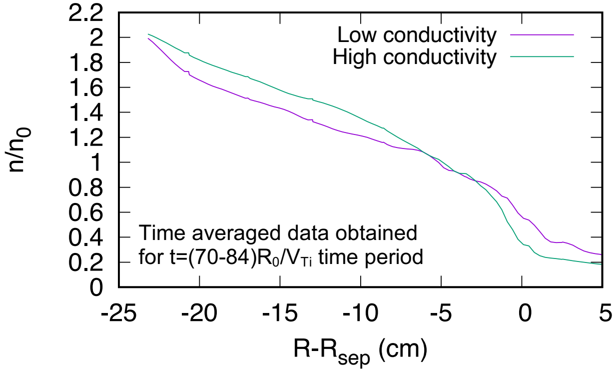
$RB_\phi = 3.5\ T \cdot m, \Delta\phi_{wedge} = 2\pi/8$



High conductivity (suppressed turbulence)

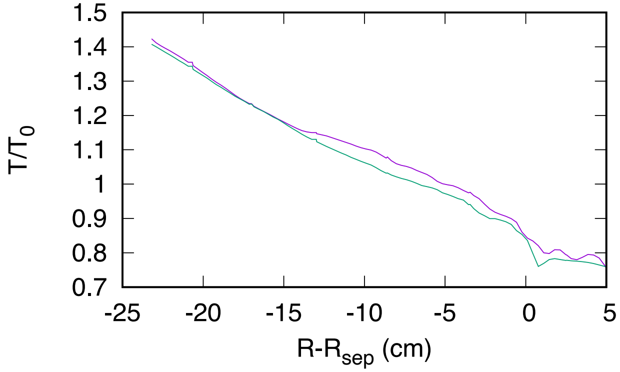
Low conductivity (enhanced turbulence)

Density

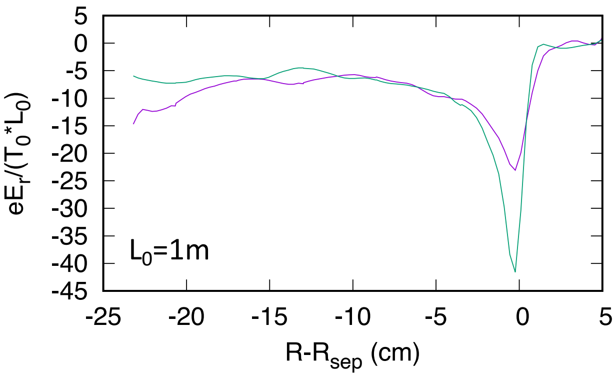


Time averaged data obtained for t=(70-84)R_0/V_{Ti} time period

Temperature

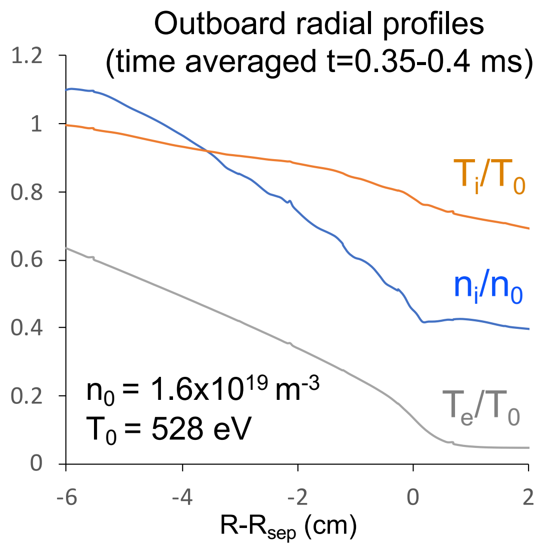


Radial Efield

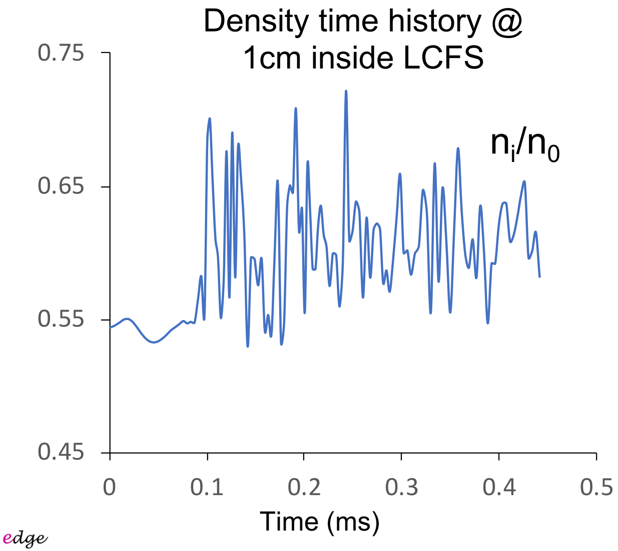


COGENT hybrid (reduced) model includes ion-scale resistive and ITG turbulence, background Er, NC and ion-orbit loss effects and can be used to study L-H transition and other edge-relevant phenomena while providing substantial speed-up over fully kinetic models

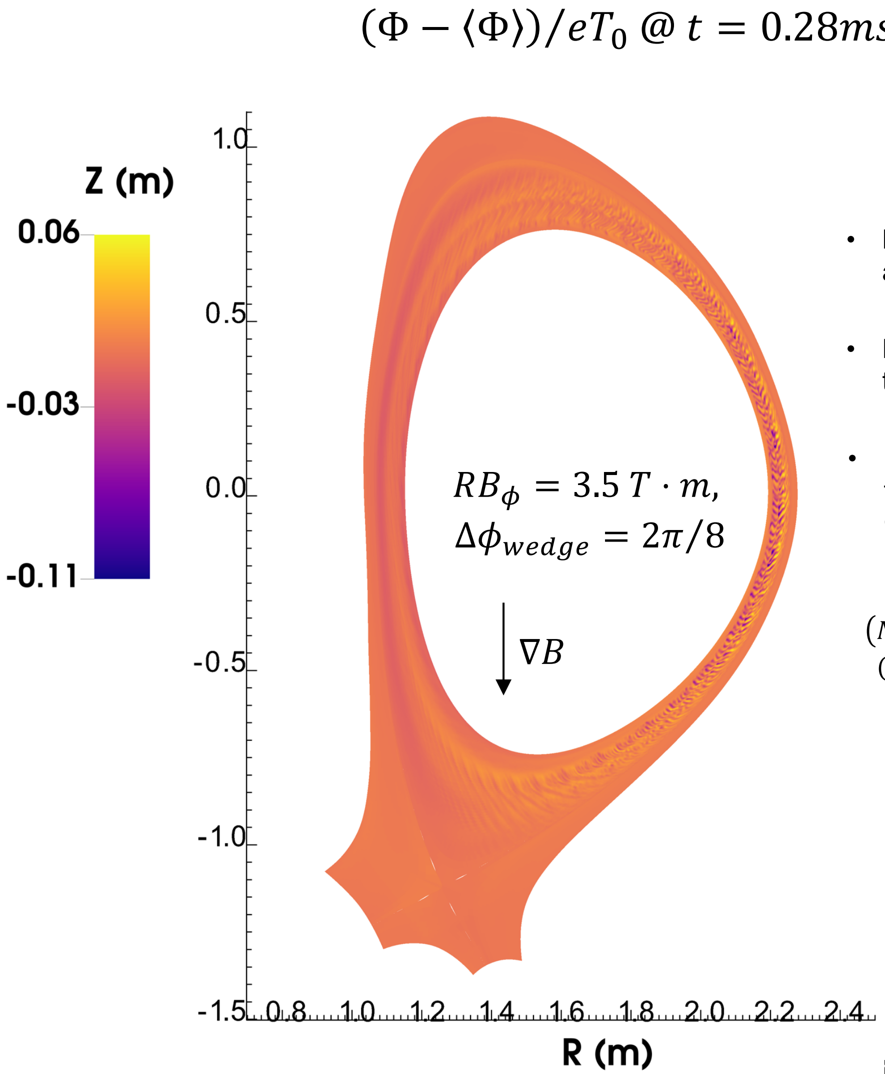
COGENT hybrid model has been used to simulate edge turbulence for realistic DIII-D discharge parameters*



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



Density time history @ 1cm inside LCFS



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

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

- 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

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*AToM SciDAC use case DIII-D 150142, with artificially increased density gradient

https://atom.scidac.io/usecase.html

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

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

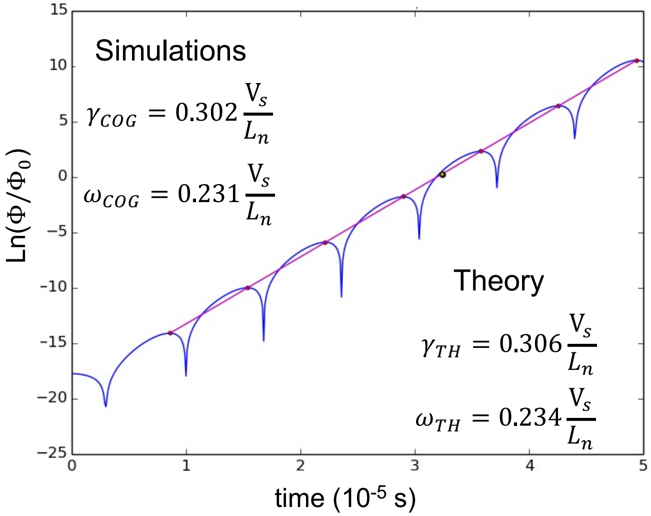
$$\left\{\begin{array}{ll}
\frac{\partial}{\partial t}\varpi + \nabla_\perp\left(c\frac{-\nabla_\perp\phi\times\boldsymbol{B}}{B^2}\varpi\right) = \nabla_\perp\cdot\left(e\int\frac{2\pi}{m_i}B_\parallel^* f_{i,gc}\boldsymbol{v_{mag}}dv_\parallel d\mu - c\frac{\nabla_\perp p_e\times\mathbf{b}}{B}\right)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

Simplified slab case verification

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

Dispersion for resistive drift instability with EM effects

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


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
$V_{T_e}k_\parallel/\nu_e = 1$

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

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

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

To further simplify adopt the following ad-hoc approximations

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

Valid for slow variations of background profiles

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

Not valid in toroidal geometry, working on improvements

⇩

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

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

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

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

➡

- 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 second-order elliptic equation for $A_\parallel$
- Elliptic equations are efficiently solved by AMG methods (from Hypre)

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*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

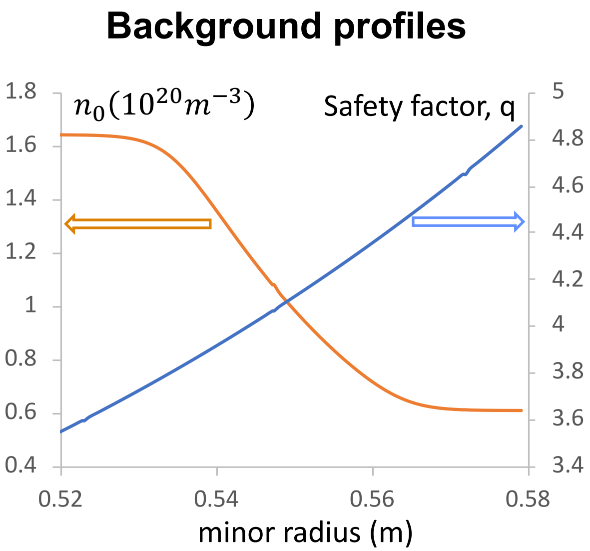
$N_0 = 10^{20}$ m^{-3}, $T_e = 400$ eV, $m_i = m_p$

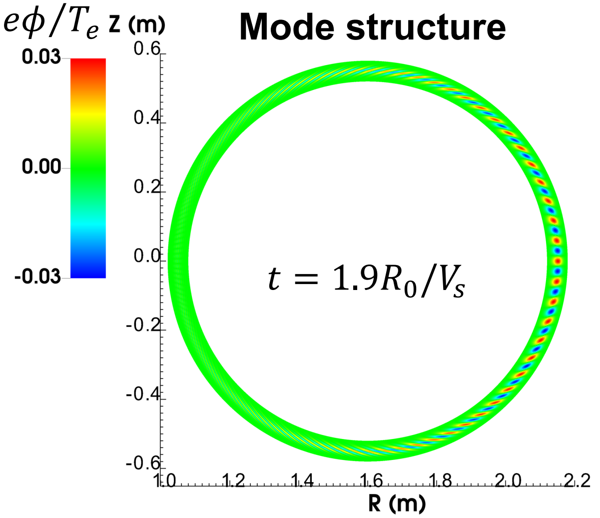
$R_0 = 1.6$ m, $RB_\phi = 3.5$Tm, wedge = $\pi/10$

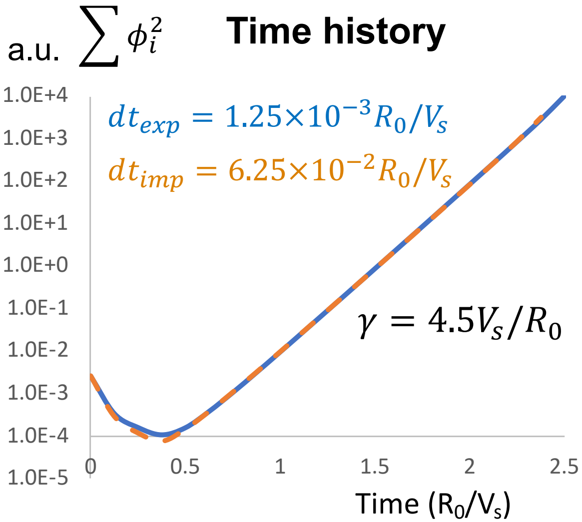
Increased resistivity $\sigma_\parallel \leftrightarrow \nu_e^{-1} V_{T_e}/qR_0 \sim 0.15$

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

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





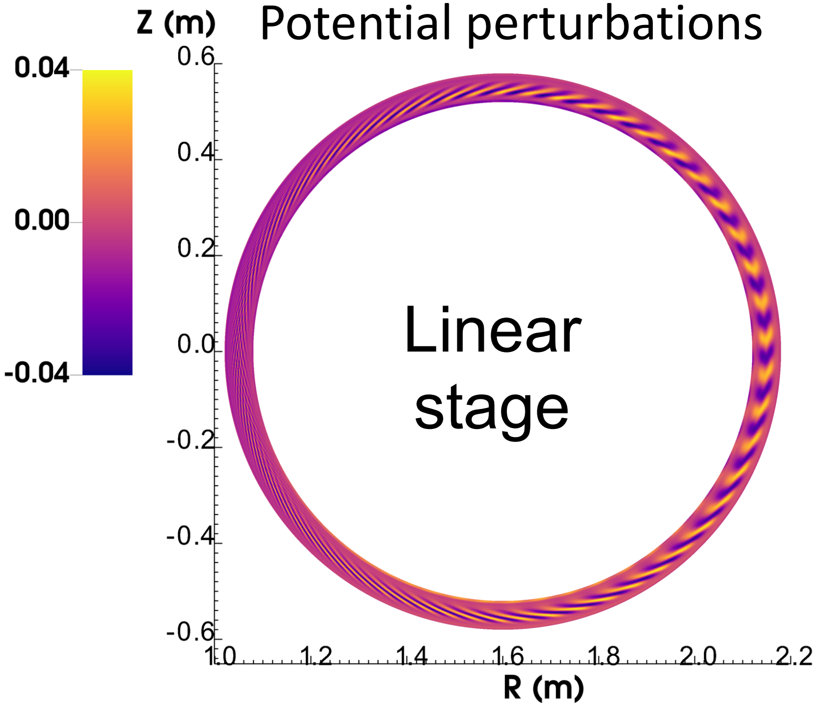


Preliminary results from the implicit hybrid GK-ions -- fluid electrons EM model (work in progress)

- DIII-D edge parameters, N_0=2x10^{19} m^{-3}, T_i=T_e=100 eV, m_i=2m_p , $\sigma_\parallel \leftrightarrow \nu_e^{-1} V_{T_e}/qR_0 \sim 0.75$
- 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 3-field fluid RBI test

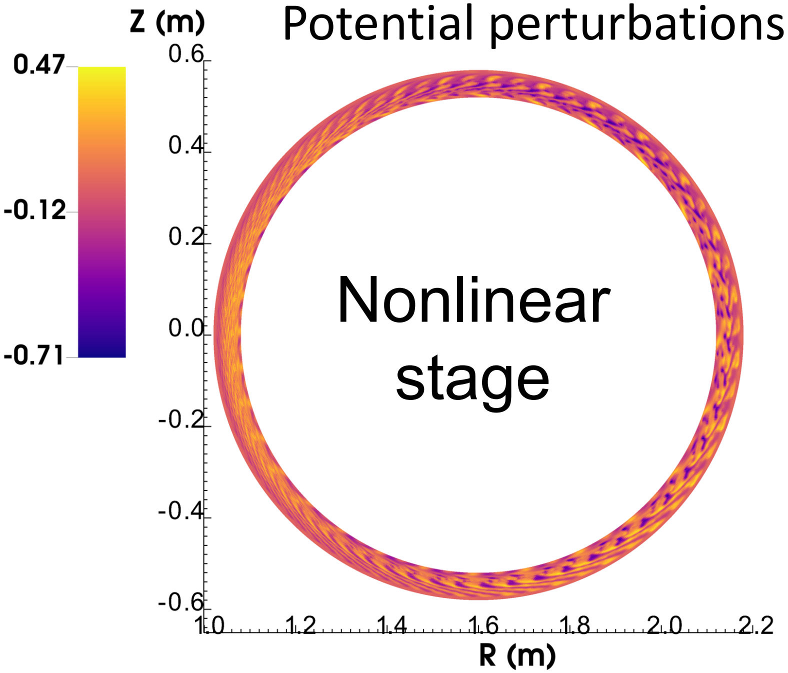
$(\Phi - \langle\Phi\rangle)/eT_e$

Potential perturbations



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

Potential perturbations

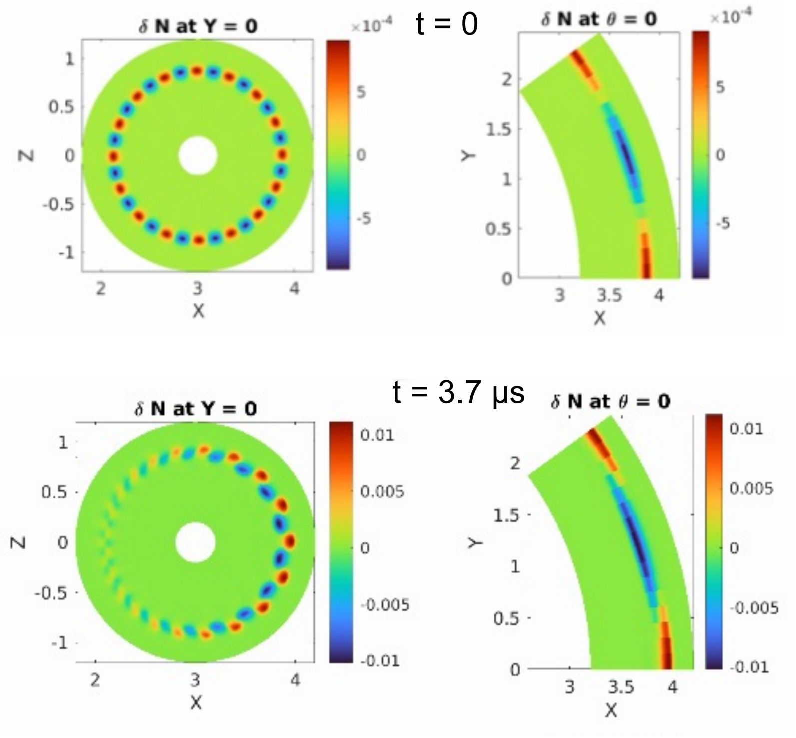


MHD fluid module is added to COGENT framework*

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)

*Courtesy of J. Angus

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