Continuum Gyrokinetic Simulations of Edge Plasmas in Single-Null Geometries

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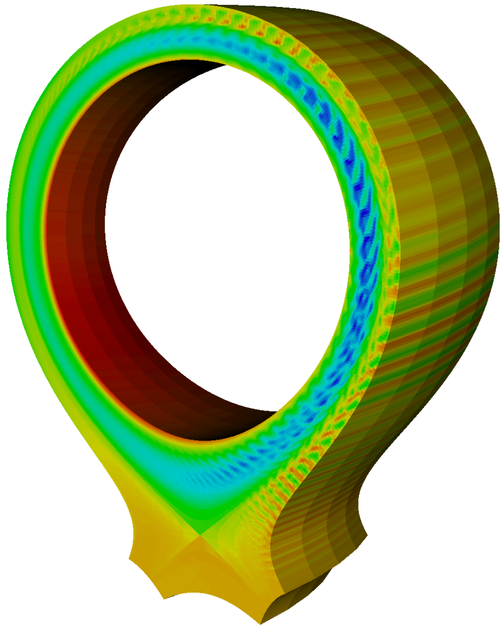

In collaboration with

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OUTLINE

- ***Distinguishing features of edge plasma modeling***

- ***Overview of the COGENT code***

- ***Cross-separatrix 4D (axisymmetric) transport***

  -- Verification studies

  -- Illustrative DIII-D simulations

- ***Cross-separatrix 5D turbulence***

  -- Locally field-aligned discretization

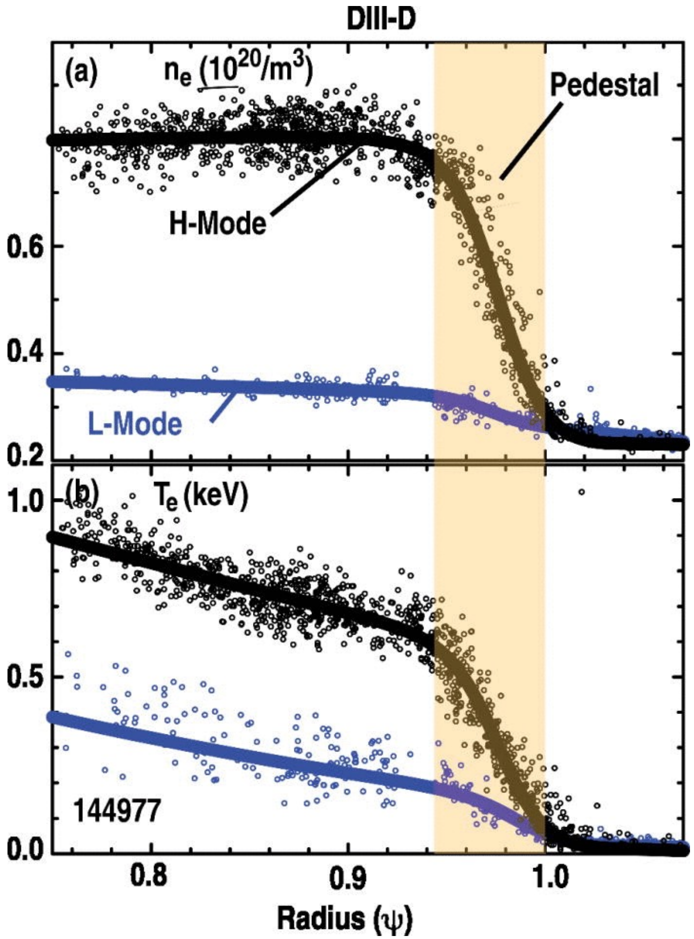
  -- Verification studies in a toroidal annulus (CBC test, etc)

  -- First ITG simulations in a single-null geometry

- ***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*

COGENT is the only <u>continuum</u> code for cross-separatrix gyrokinetic modeling

[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

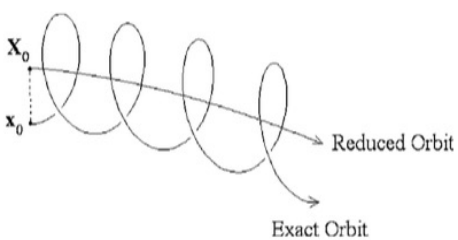
COGENT

Physics models (LLNL/UCSD)

- Multispecies full-F gyrokinetic equations
- Self-consistent electrostatic potential
- Collisions (including full Fokker-Plank)
- 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)



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

Tokamak applications (AToM, ESL, PSI)

⇓

Low-Temp ↔ **COGENT** ↔ Z-pinch

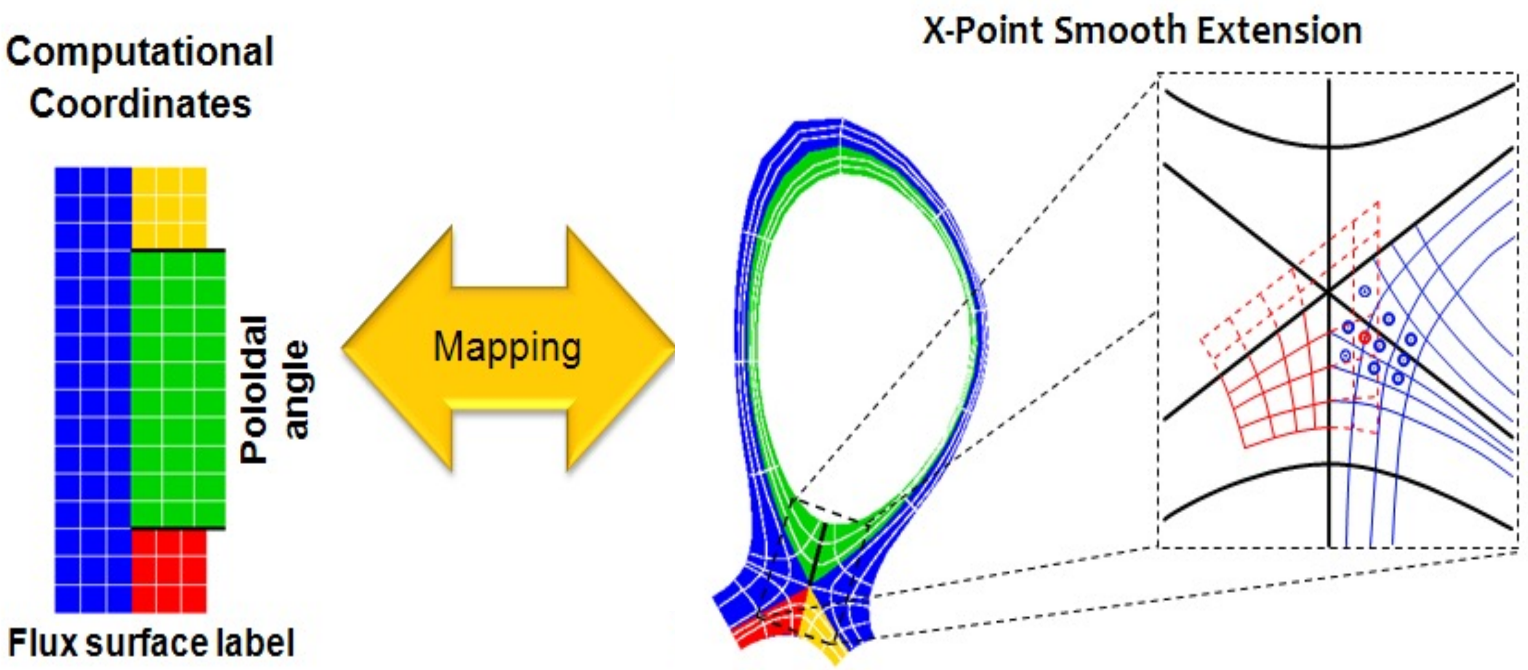
New collaborations welcome!

edge simulation laboratory

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

Fusion Energy Sciences

X-point geometry is handled by using a mapped multiblock technology



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

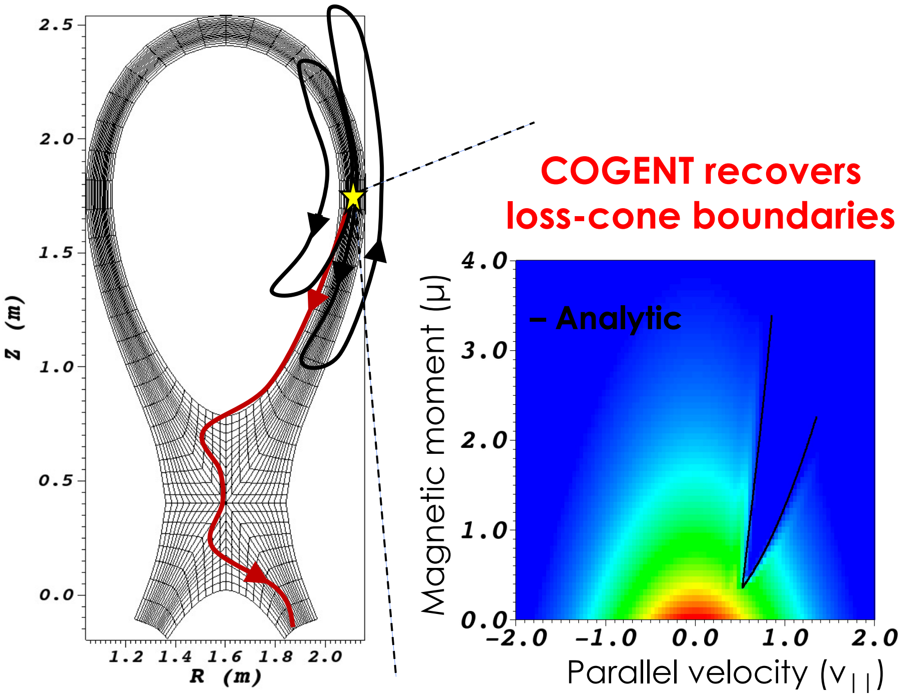
Problem: *the metric coefficients diverge at the x-point*

COGENT approach: *the use of a multiblock grid technology*

Colella et al. , JCP (2011); McCorquodale et al., JCP (2015)

X-point high-order discretization has been verified with 4D COGENT

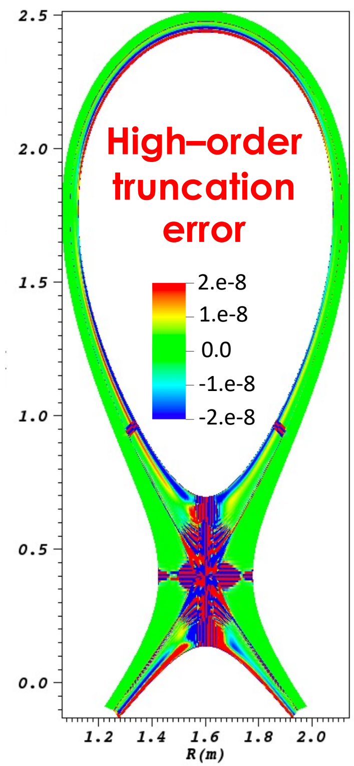
Collisionless ion losses

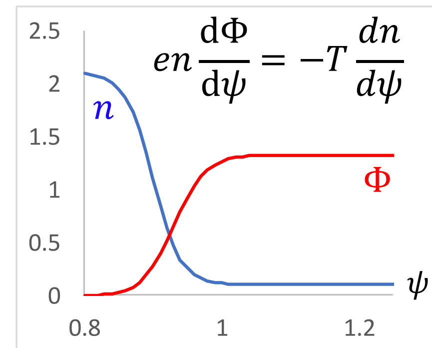


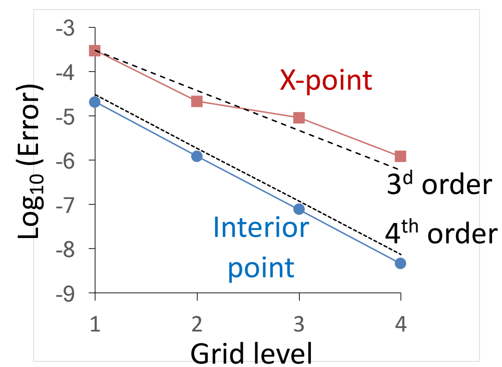
Dorf et al, PoP 2016

- Uniform n and T Maxwellian is initialized
- Particles are absorbed by divertor plates and outer radial boundaries / E-field is turned OFF

Boltzmann Equilibrium







Dorr et al, JCP 2017

- High-order convergence is demonstrated
- Maximum error is within de-aligned region

COGENT E-field models: Gyro-Poisson equation

Presently, adopt the long-wavelength electrostatic limit

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

- 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

Need a computationally efficient model for ion scale turbulence in single-null geometries

COGENT E-field models: Vorticity model

Hybrid gyrokinetic ion – fluid electron model $\nabla \cdot \boldsymbol{j} = 0$

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

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

Vorticity $\varpi = \nabla_\perp\left(\frac{c^2 m_i n_{i,gc}}{B^2}\nabla_\perp \Phi\right) + \frac{e}{m_i\omega_{ci}^2}\nabla_\perp^2\frac{p_{i,\perp}}{2}$ — *Neglect the pressure corrections term*

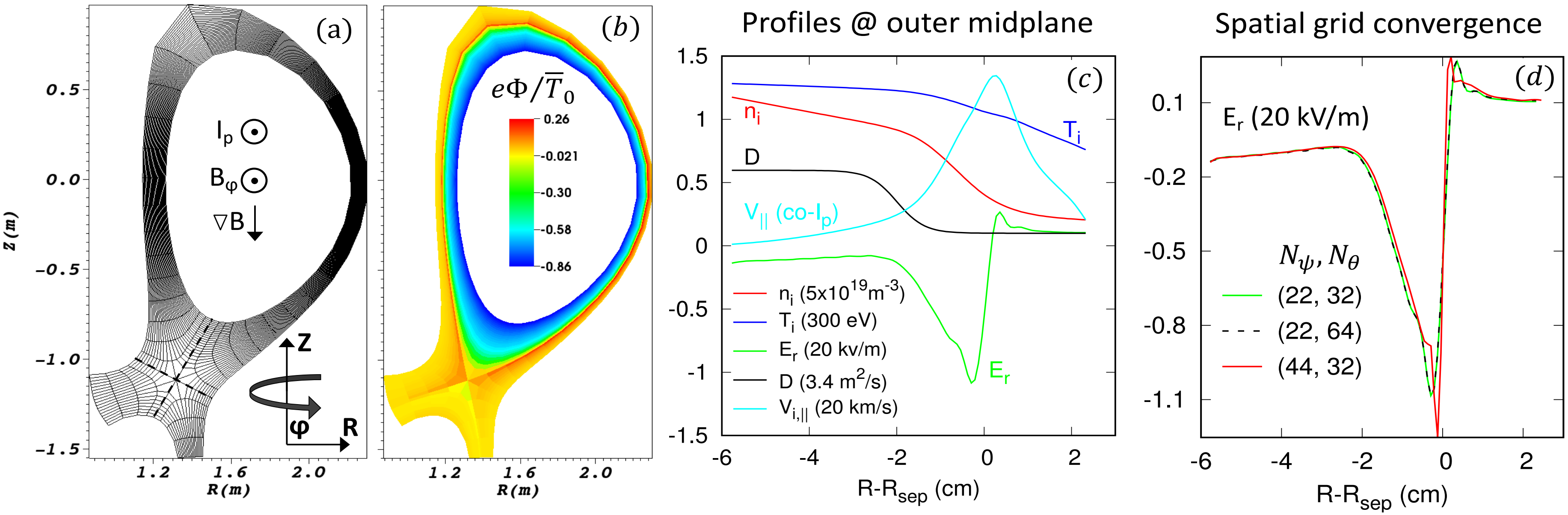
Parallel current $j_\parallel = \frac{e n_e}{0.51 m_e \nu_e}\left(\frac{1}{n_{i,gc}}\nabla_\parallel(n_e T_e) - e\nabla_\parallel \Phi + 0.71\nabla_\parallel T_e\right)$ — *Stiff term (due to the large parallel conductivity) – treat implicitly*

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*

Hybrid vorticity model allows for computationally efficient cross-separatrix simulations with self-consistent E-fields

4D COGENT: qualitative agreement with DIII-D H-mode co-I_p rotation and E_r is observed



- 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

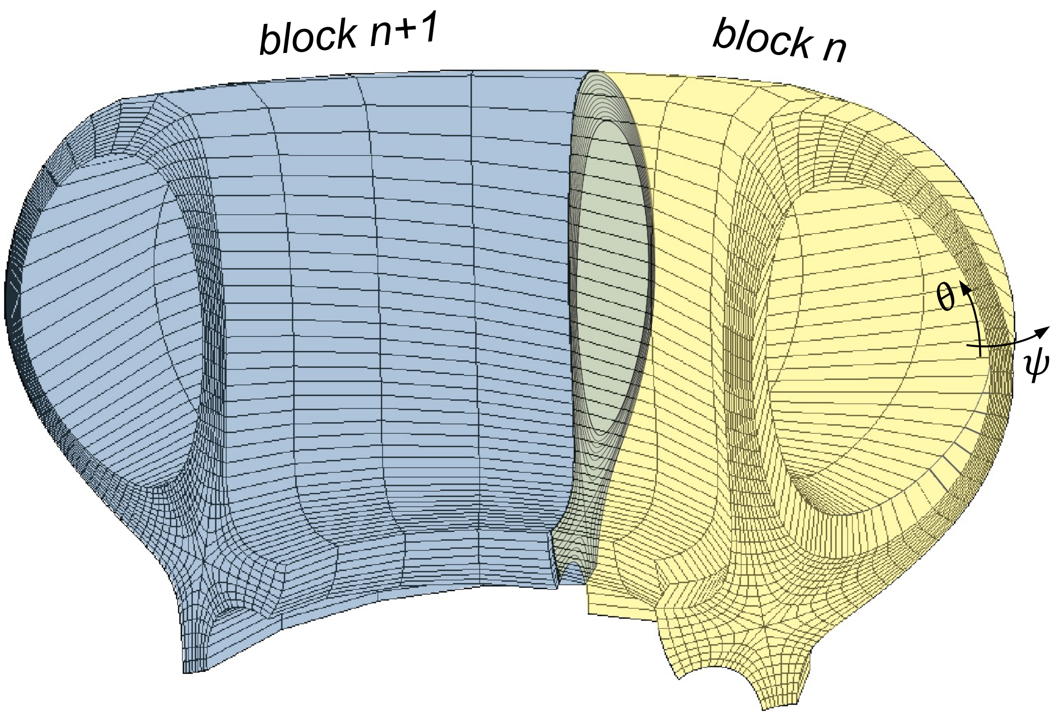
$$E_r \sim 20\,\frac{\text{kV}}{\text{m}} \quad V_\parallel \sim 40\,\frac{\text{km}}{\text{s}}$$

Boedo et al., PoP 2016

5D COGENT: locally field-aligned multiblock approach

To exploit strong anisotropy of microturbulence

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



EDGE (COGENT)

(ψ, θ) - fine ⊥ coordinates
ϕ - coarse ‖ coordinate

Efficient for X-point modeling

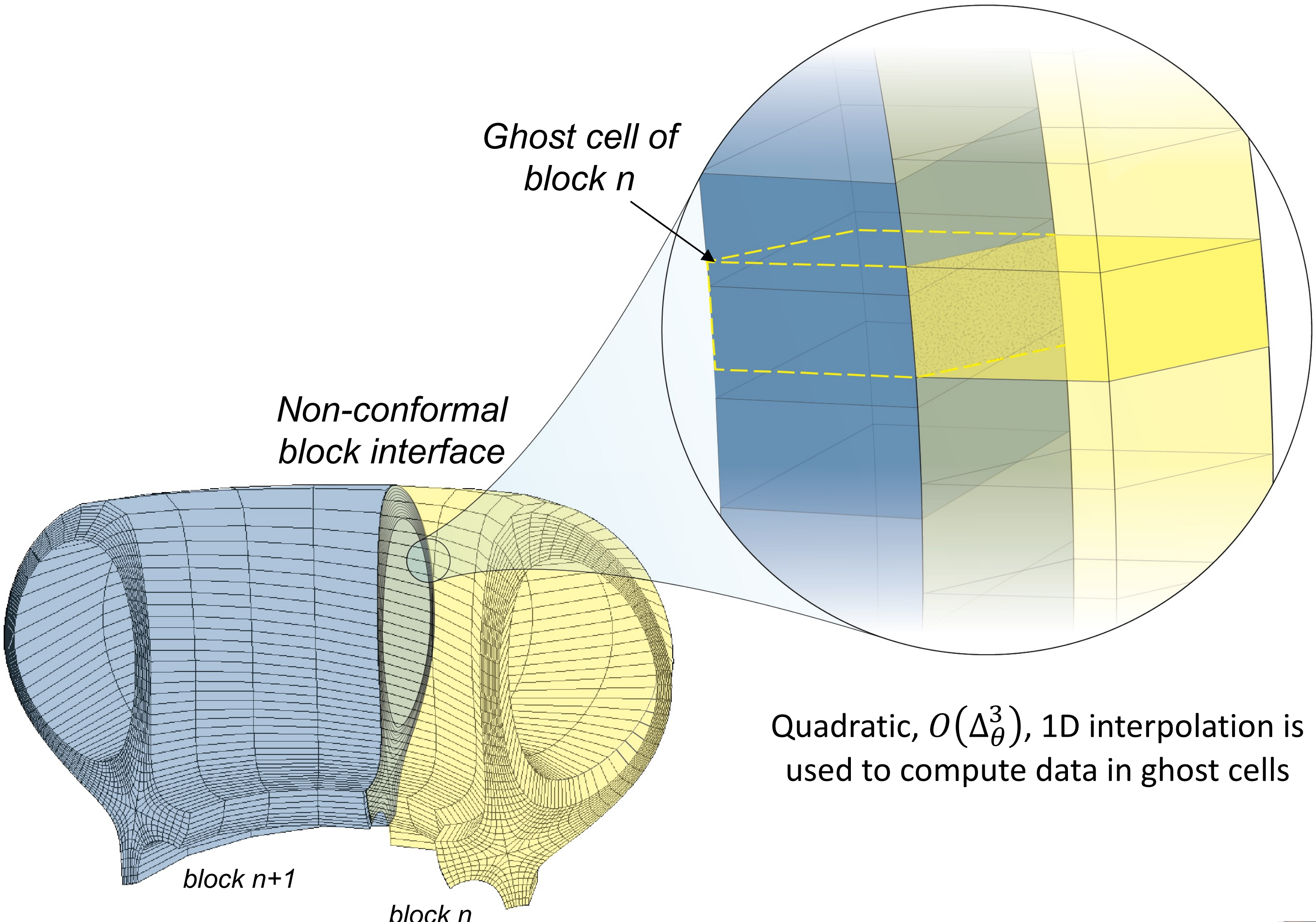
CORE (GYRO, BOUT)

(ψ, ϕ) - fine ⊥ coordinates
θ - coarse ‖ coordinate

Efficient for high-n wedge modeling

The approach is conceptually similar to the FCI approach (Hariri, CPC 2013), but maintains flux surfaces (presently, including the X-point region)

Interpolation is employed at a block interface

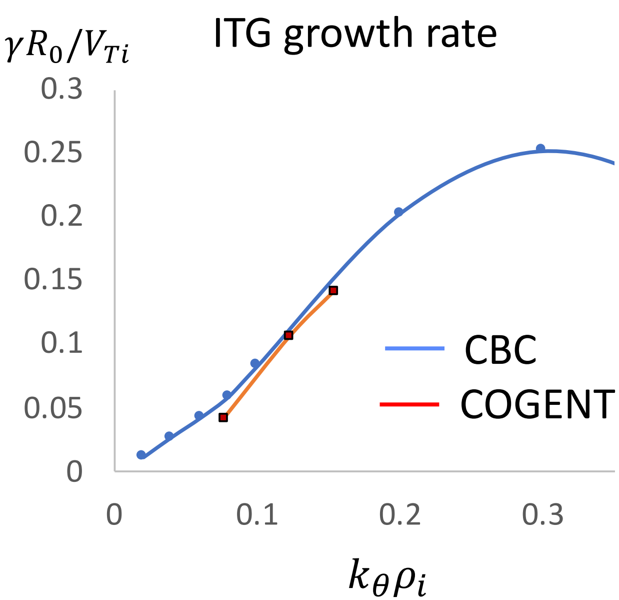


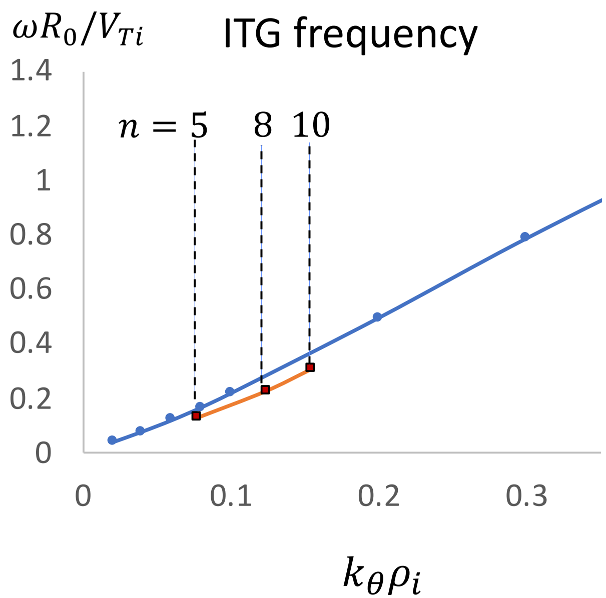
Quadratic, $O\left(\Delta_\theta^3\right)$, 1D interpolation is used to compute data in ghost cells

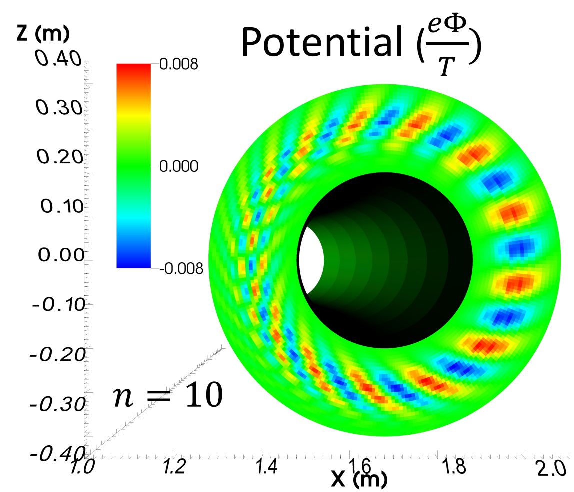
Cyclone Base Case verification

- Full-F toroidal (r, θ, ϕ) version of the code is used; filtering of toroidal harmonics is applied
- Gyro-Poisson (GP) model with adiabatic electron response is used

Long-wavelength part of CBC spectrum is recovered







Simulation parameters

$\rho_i/a=1/181$, $q=1.4$, $s=0.78$, $R_0/L_T=6.9$, $R_0/L_n=2.3$, $m_i=2m_p$

Grid resolution

$$\left(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu\right) = (24, 8, 256, 32, 24)$$

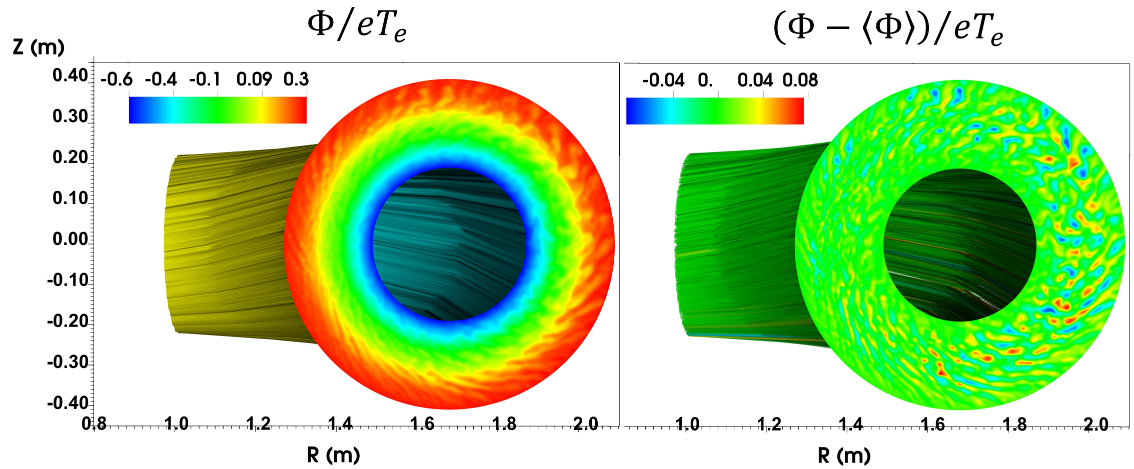
Dorf and Dorr, CPP, 2020

ITG-driven full-F transport simulation in toroidal annulus

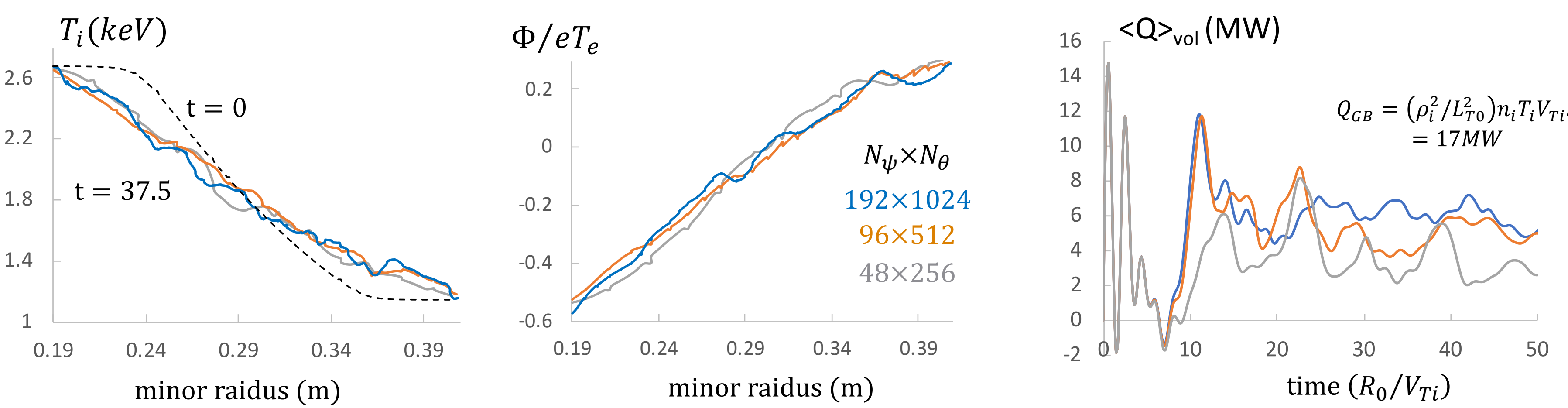
- F-A coordinates, $\Delta\phi_{wedge} = \pi/2$
- GP model with adiabatic electrons*
- Self-consistent BC is used
  no buffer zones required

$$\left\langle n_i m_i c^2 \frac{|\nabla\psi|^2}{B^2} \right\rangle \frac{\partial^2 \Phi}{\partial t \partial \psi} = \langle \boldsymbol{j}_i^{GC} \cdot \nabla\psi \rangle$$

- Linearized model collisions included



Spatial resolution studies demonstrate convergence at $\Delta_\perp \sim \rho_i$



n=10^{20} m^{-3}, RB_ϕ=3.5 Tm. Initialization: local Maxwellian R_0/L_{T0}=12, R_0/L_{n0}=2.2, Φ_0=0, T_e=T_i

edge simulation laboratory

*Limitations apply: Parra & Catto, PPCF (2009); Dorf et al, PoP (2013)

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Field-aligned mapping provides significant computational efficiency in full-torus simulations

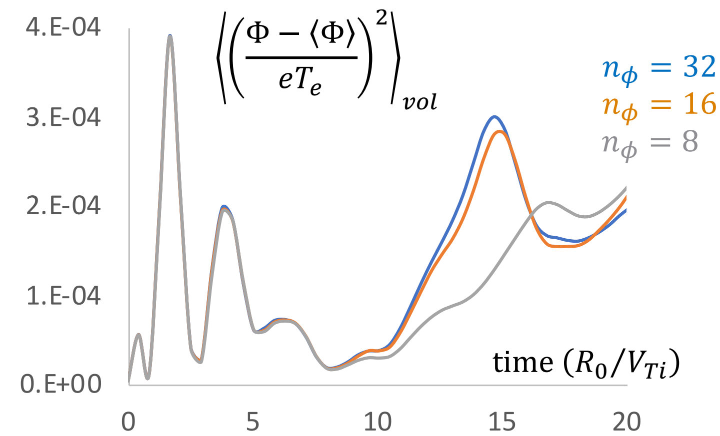
Microturbulence anisotropy

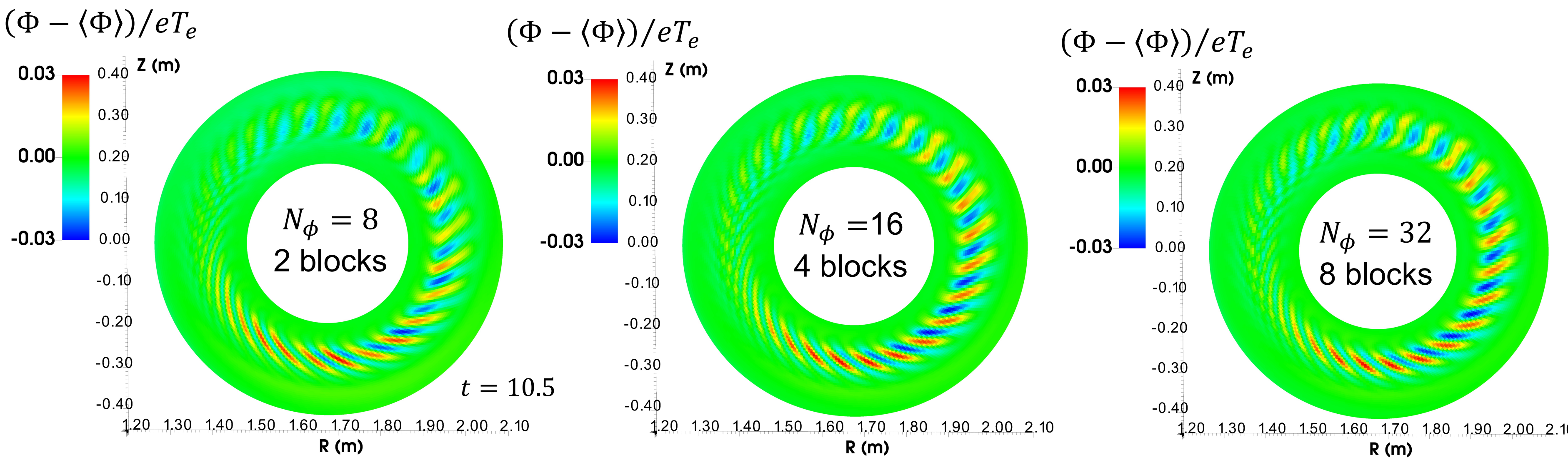
$$k_\perp \rho_i \sim 1,\ k_\parallel \sim 1/(qR_0) \qquad m \approx q \cdot n$$

Toroidal coordinates version would require $N_\phi \sim \frac{N_\theta}{q} = 365\ cells$

Field-aligned version requires only $N_\phi = 16\ cells$

Convergence in full-torus sims is achieved with only 16 toroidal cells





Domain $\Delta\phi = 2\pi$, resolution $(N_r, N_\theta, N_{v_\parallel}, N_\mu) = (48, 256, 48, 32)$

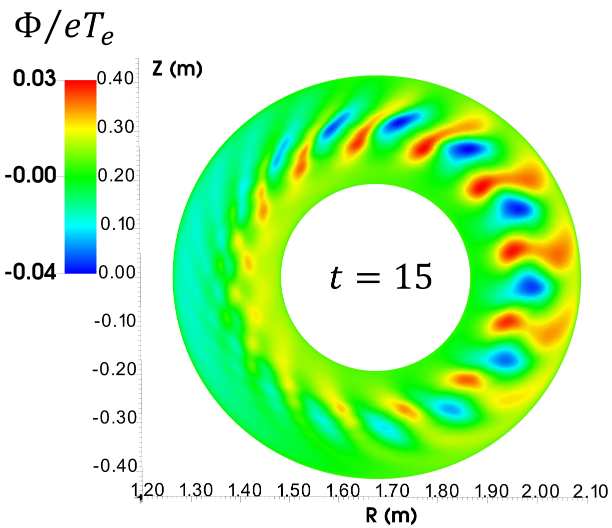
Vorticity model verification: consistency with gyro-Poisson model is confirmed in full-F ITG simulations

- $\sigma_{\|}$ corresponds to weakly-collisional electrons $qR_0\nu_e/V_{T_e}\sim 10$
- Initialization: Canonical Maxwellian
  - Provides equilibrium for full-F simulations

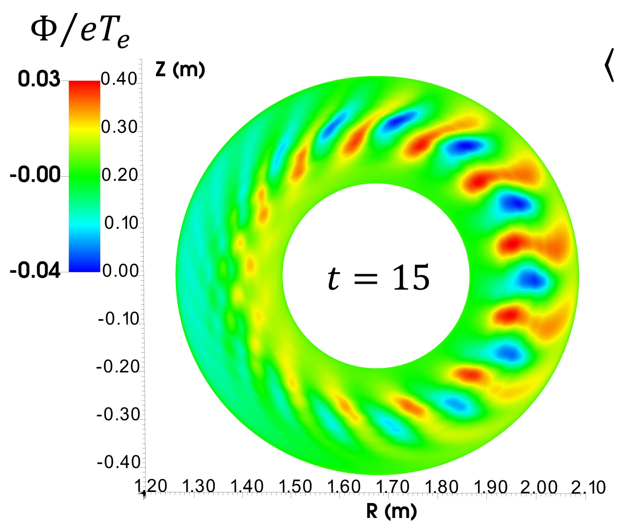
$$F_0 = n(\bar{\psi})\left[\frac{m_i}{2\pi T(\bar{\psi})}\right]^{\frac{3}{2}} \exp\left(-\frac{m_i v_{\|}^2}{2T(\bar{\psi})} - \frac{\mu B}{T(\bar{\psi})}\right), \qquad \bar{\psi} = \psi + \frac{m_i}{Z_i e}\frac{RB_\phi}{B}v_{\|}$$

Motion invariant

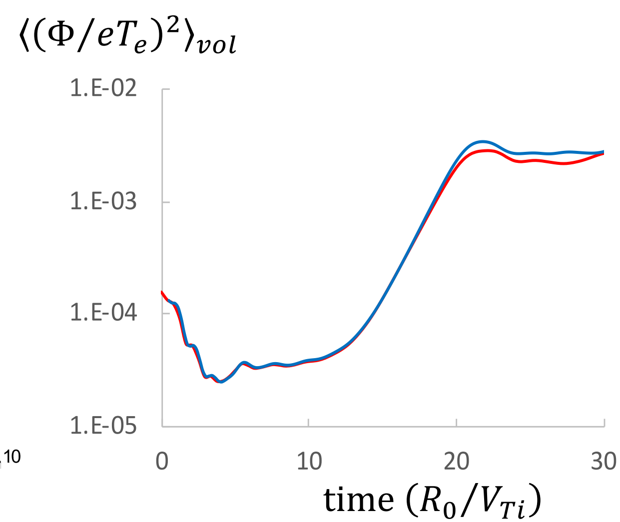
Gyro-Poisson model



Vorticity model



Effective electrostatic energy



F-A code, $\Delta\phi = 0.2\pi$, T_0=7 keV, R_0/L_{T0}=16, R_0/L_{n0}=5, collisions – OFF, grid res. $= (96, 4, 512, 48, 32)$

Vorticity model verification II: resistive-drift mode is recovered

Slab test model (**B**=const) is considered

$$\frac{\partial f}{\partial t} + \nabla\left\{c\frac{[\boldsymbol{E}\times\boldsymbol{B}]}{B^2}f\right\} = 0 \qquad \frac{\partial}{\partial t}\varpi = \nabla_\parallel j_\parallel$$

ExB drift motion **Quasineutrality**

Parallel current

$$j_\parallel = \frac{en_e}{0.51 m_e \nu_e}\left(\frac{\mathrm{T}_e}{n_{i,gc}}\nabla_\parallel n_e - e\nabla_\parallel \phi\right)$$

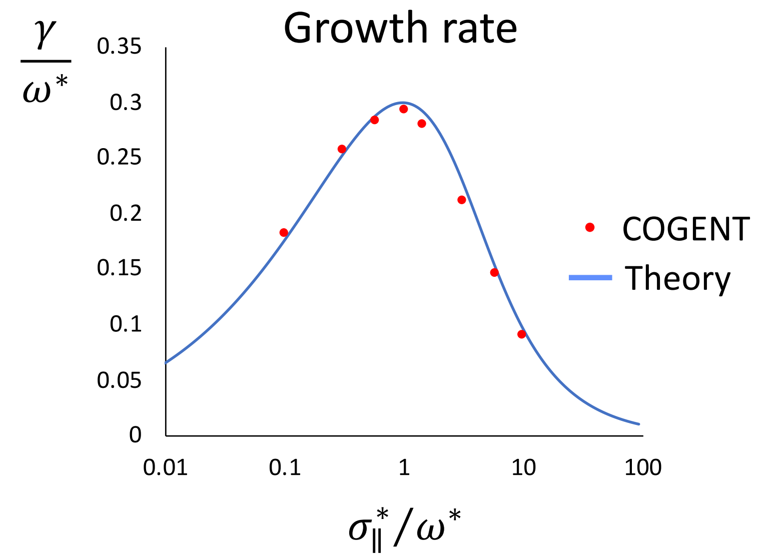
Electron density

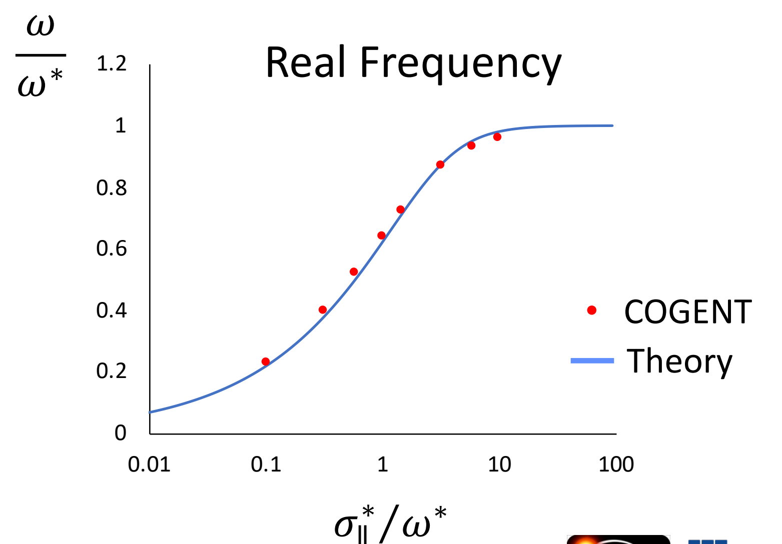
$$n_e = n_{i,gc} + \nabla_\perp\left(\frac{c^2 m_i n_{i,gc}}{eB^2}\nabla_\perp \phi\right)$$

Dispersion relation

$$\left(\frac{\omega}{\omega^*}\right)^2 - i\frac{\sigma_\parallel^*}{\omega^*}\left(\frac{\omega}{\omega^*} - 1\right) = 0$$

$$\sigma_\parallel^* = \left(\frac{k_\parallel}{k_\perp}\right)^2 \frac{\omega_{ci}\omega_{ce}}{0.51\nu_e}(1 + k_\perp^2\rho_s^2), \qquad \omega^* = \frac{k_\perp V_{Te}^2}{\omega_{ce}L_n}\frac{1}{(1 + k_\perp^2\rho_s^2)}$$





Vorticity model: numerical pollution issue

$$\frac{\partial}{\partial t}\varpi + \nabla_\perp\left(c\frac{-\nabla_\perp\Phi\times\boldsymbol{B}}{B^2}\varpi\right) = \boldsymbol{\nabla}_\perp\cdot\left(\boldsymbol{j}_{\perp,i}^{GC}+\boldsymbol{j}_{\perp,e}\right) + \boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel$$

Polarization current | ***Reynold-Stress term*** | ***Determines Er on closed field lines, where*** $\langle\nabla\cdot j_\parallel\rangle\equiv 0$ | ***Dominant term determines*** $E_{//}$

- Significant numerical pollution can occur if $\langle\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rangle\equiv 0$ is not discretely enforced on closed field lines
- Can be important for other codes involving remapping: e.g., BOUT, GBS, GRILLIX, GDB

Truncation errors in $\langle\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rangle\sim\langle\nabla_\parallel\sigma_e\nabla_\parallel p_e/en_e\rangle$ due remapping/interpolation of order *n*

$$\mathrm{Er}\{\langle\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rangle\}\sim\frac{eT_e}{\nu_e m_e}\frac{\delta n}{q^2R_0^2}(k_\perp\Delta_\theta)^n$$

Magnitude of RS term

$$\langle RS\rangle = \langle\nabla_\perp\left(c\frac{[\nabla_\perp\delta\Phi\times\boldsymbol{B}]}{B^2}\delta\varpi\right)\rangle\sim c^3\frac{n_i m_i}{B^3}k_\perp^4\delta\Phi^2$$

Adopt standard ordering for turbulence

$$\frac{\delta n_{tb}}{n_e}\sim\frac{e\delta\Phi_{tb}}{T_e}\sim\frac{\rho_i}{L_{eq}},\ k_\perp\rho_i\sim 1$$

$$\frac{Er\{\langle\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rangle\}}{\langle RS\rangle}\ll 1 \leftrightarrow \left(\frac{\Delta_\theta}{\rho_i}\right)^n\ll\frac{qR_0}{L_{eq}}\frac{\nu_e qR_0}{V_{Te}}\frac{T_e^2}{T_i^2}\frac{V_{Ti}}{V_{Te}}$$

Consider DIII-D edge ($qR_0\nu_e/V_{te}$~1)

q ~ 3, R_0 ~ 1.6 m, T_i~300 eV, T_e ~ 50 eV, B~1.6 T, B_p/B ~ 0.2

$$(\Delta_\theta/\rho_i)^n\ll 10^{-3}\,qR_0/L_{eq}$$

More strenuous condition than standard $\Delta_\theta\lesssim\rho_i$

COGENT approach: $\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rightarrow\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel-\langle\boldsymbol{\nabla}\cdot\boldsymbol{j}_\parallel\rangle_{COGENT}$

Deleterious effects of $\langle \nabla \cdot j_{\parallel} \rangle \neq 0$ numerical pollution are confirmed in ITG simulations

Consider ITG simulations with $\sigma_{\parallel}$ corresponding to moderately-collisional electrons $qR_0\nu_e/V_{T_e}\sim 1$

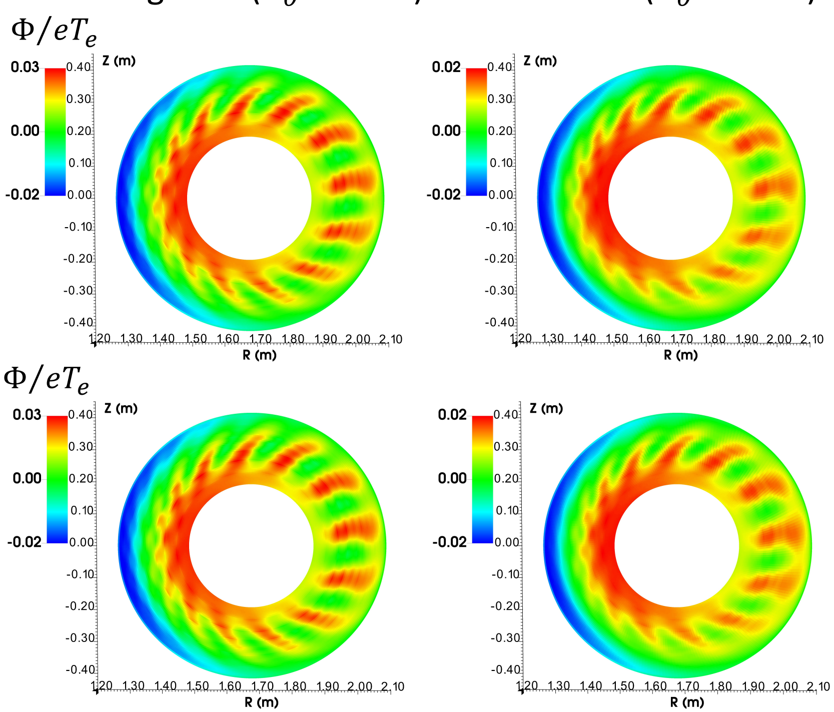
Linear stage
Pollution errors are insignificant

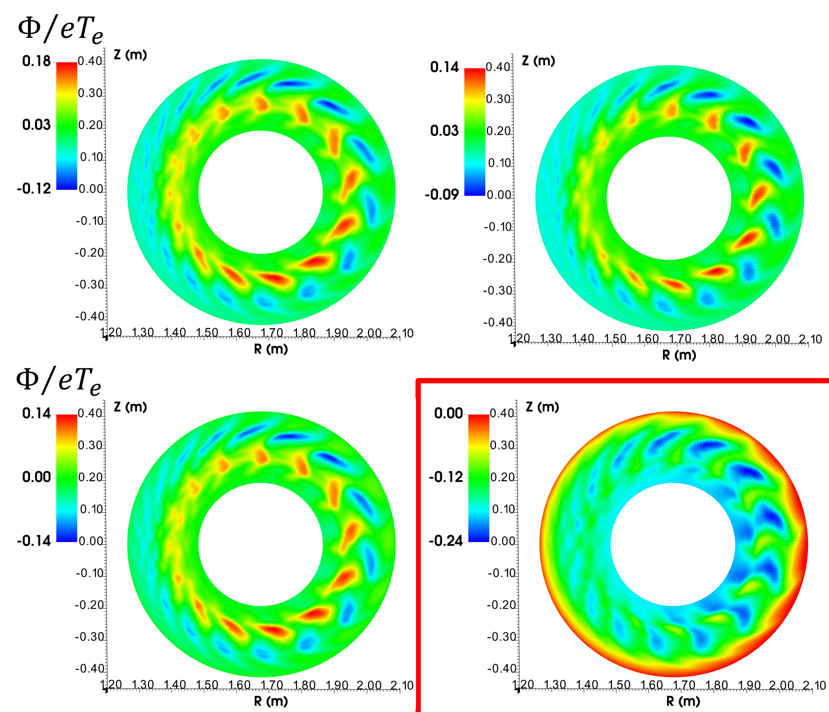
Nonlinear stage
Pollution errors can dominate $\langle \Phi \rangle$ solution

High-res ($n_\theta = 512$) | Low-res ($n_\theta = 256$) | High-res ($n_\theta = 512$) | Low-res ($n_\theta = 256$)

$\langle \nabla \cdot \boldsymbol{j}_{\parallel} \rangle$ *fix ON*

$\langle \nabla \cdot \boldsymbol{j}_{\parallel} \rangle$ *fix OFF*





Canonical Maxwellian, T_0=7 keV, R_0/L_{T0}=16, R_0/L_{n0}=5, collisions – OFF, $(N_r, N_\phi, N_{v_\parallel}, N_\mu) = (48,8,32,24)$

Proof-of-principle ITG simulation in a single-null geometry

Vorticity model $\sigma_{\parallel} \leftrightarrow V_{T_e}/qR_0\nu_e \sim 0.4$

Canonical Maxwellian, T_0=7 keV

Boundary conditions (Φ):

- Zero-Dirichlet @ diverter plates
- Zero Neumann @ radial boundaries

Boundary conditions (f):

- Inflow fluxes correspond to the initial distribution @ all boundaries

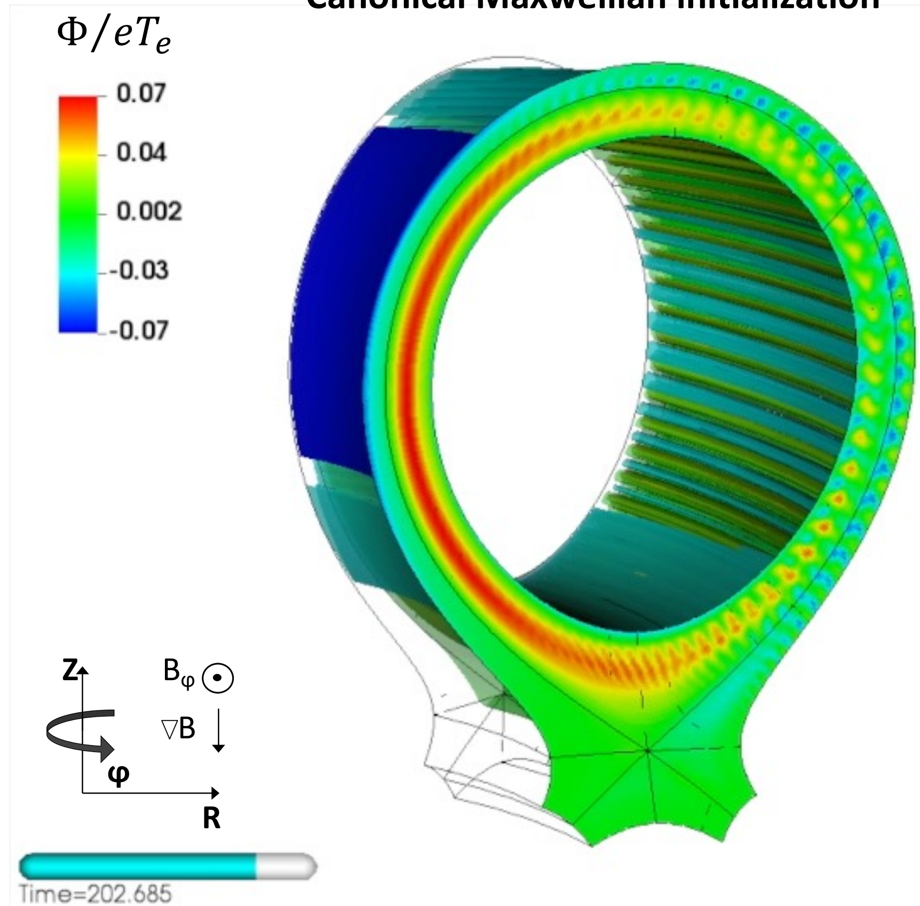
F-A version $\Delta\phi_{wedge} = 2\pi/16$

Resolution $(N_r, N_\phi, N_\theta, N_{v_\parallel}, N_\mu)$ (52,4,548,32,24)

Time step $dt = 0.01\ R_0/V_{Ti}$

Performance 1 step ↔ 4s, Cori 1344 cores

Canonical Maxwellian initialization



Model geometry

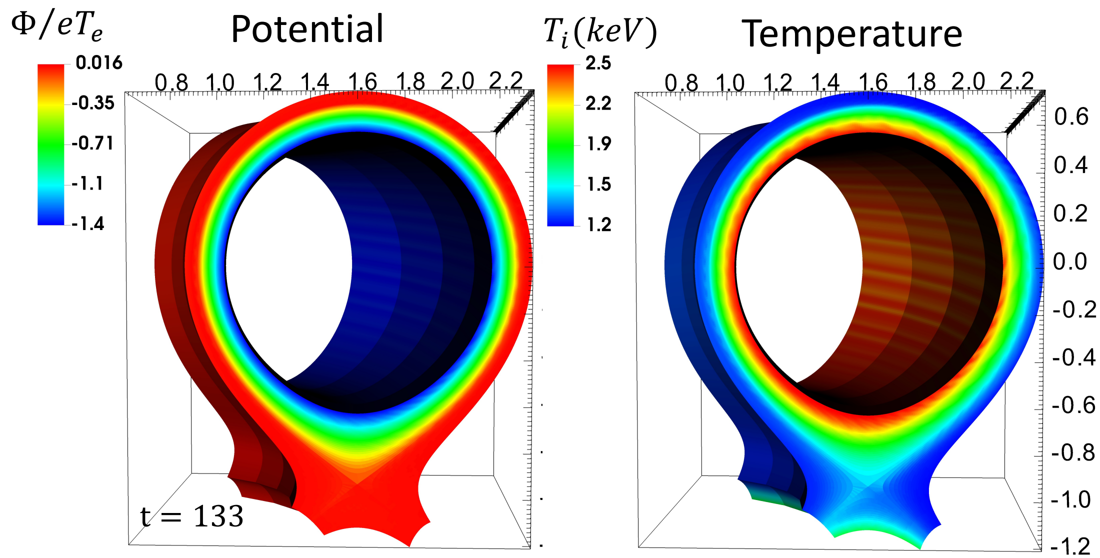
$R_0 = 1.6\ m, q{\sim}4, RB_\phi = 3.5\ T \cdot m$

ITG-driven full-F transport simulation in a SN geometry

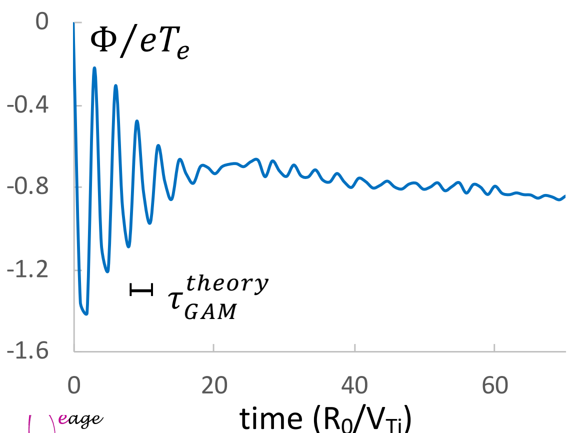
- F-A version, $\Delta\phi_{wedge} = 2\pi/8$
- Vorticity model, $\sigma_{\parallel} \leftrightarrow V_{T_e}/qR_0\nu_e \sim 0.4$
- Self-consistent BC is used
  no buffer zones required

$$\left\langle n_i m_i c^2 \frac{|\nabla\psi|^2}{B^2} \right\rangle \frac{\partial^2 \Phi}{\partial t \partial \psi} = \langle \boldsymbol{j}_i^{GC} \cdot \nabla\psi \rangle$$

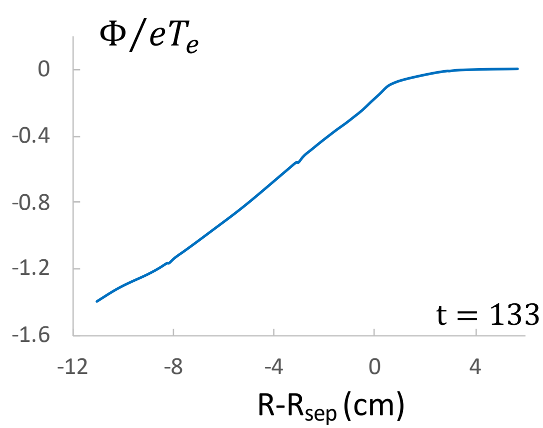
- Local Maxwellian is initialized
- Poloidal resolution, $\Delta_{\perp} \sim \rho_i$
- Collisions are not included



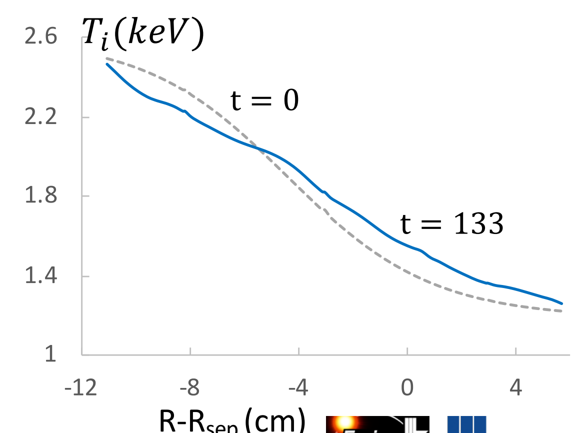
Potential relaxation exhibits GAMs



Potential barrier develops



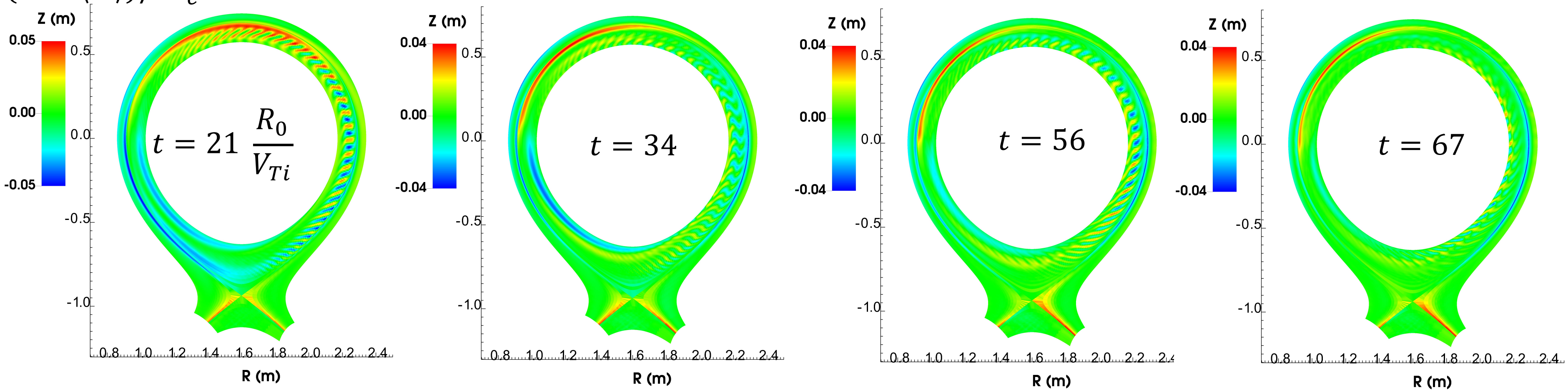
Temperature relaxation observed



Effects of a self-consistent Er on the ITG turbulence

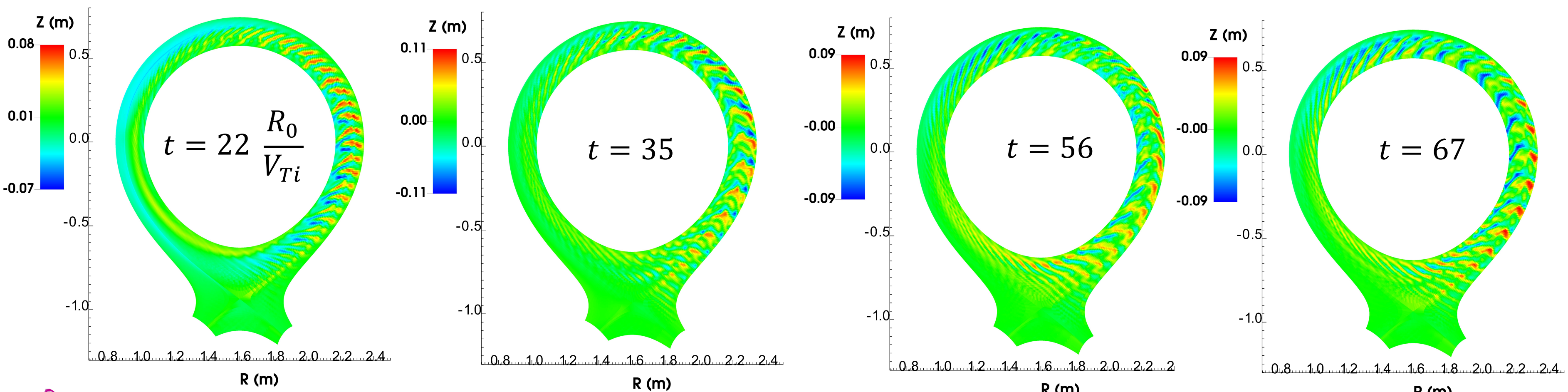
Self-consistent <Φ> is retained: intermittent turbulence behavior

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



<Φ> is artificially suppressed: stronger steady turbulence

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



edge simulation laboratory

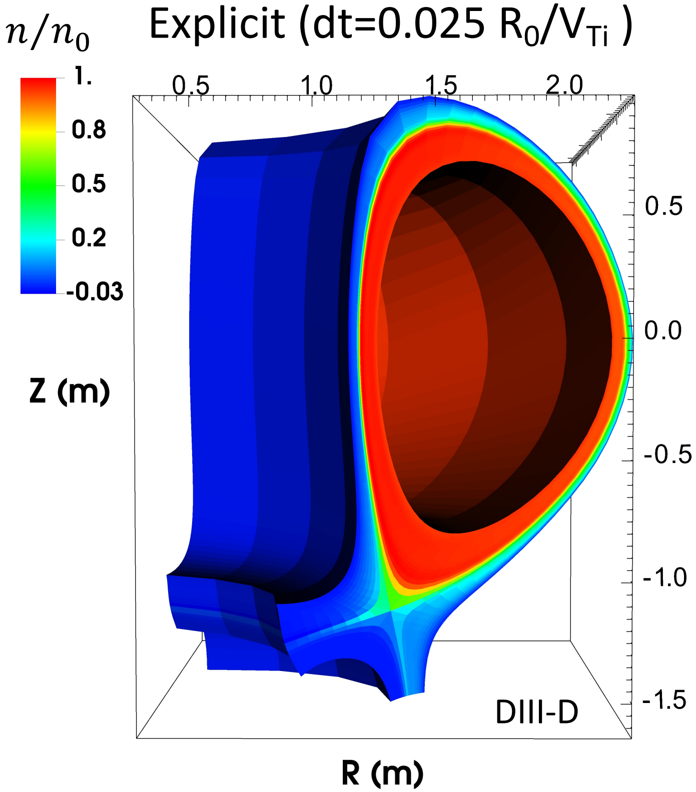
Fusion Energy Sciences

Moving toward implicit kinetic electrons: implicit advection capability has been implemented

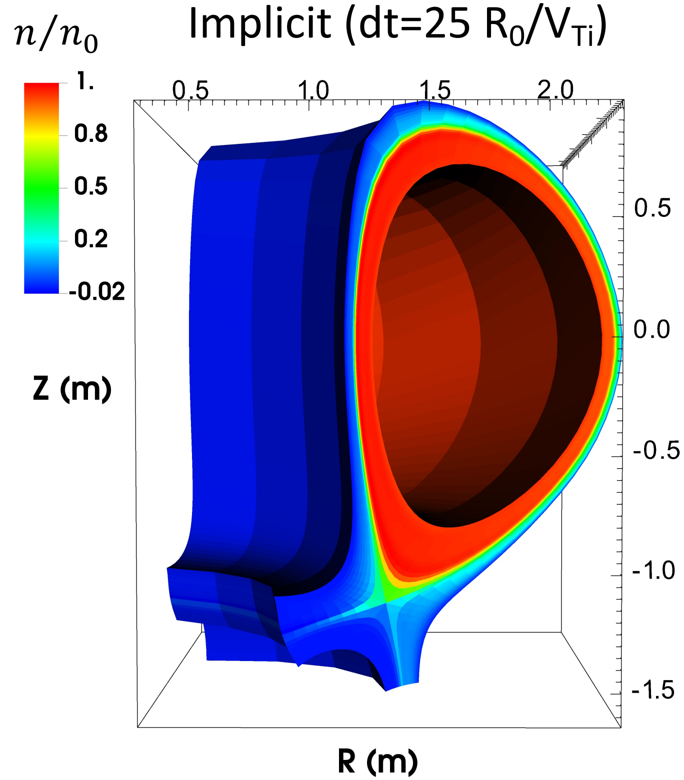
COGENT employs ImEx time integration capability

- allows implicit treatment of selected stiff terms
- makes use of the Newton-Krylov methods / requires preconditioning for efficiency
- here, use hypre's pAIR AMG solver for a low-order (UW1) passive advection preconditioner

Explicit (dt=0.025 R_0/V_{Ti})



Implicit (dt=25 R_0/V_{Ti})



- Passive advection test

  Initially uniform n and T plasma absorbed on the plates and outer radial boundaries

- DIII-D like parameters

x20 runtime speed-up is demonstrated

Conclusions

- The **first continuum** full-F gyrokinetic **cross-separatrix** simulations of
  - 4D axisymmetric transport
  - 5D ion-scale turbulence

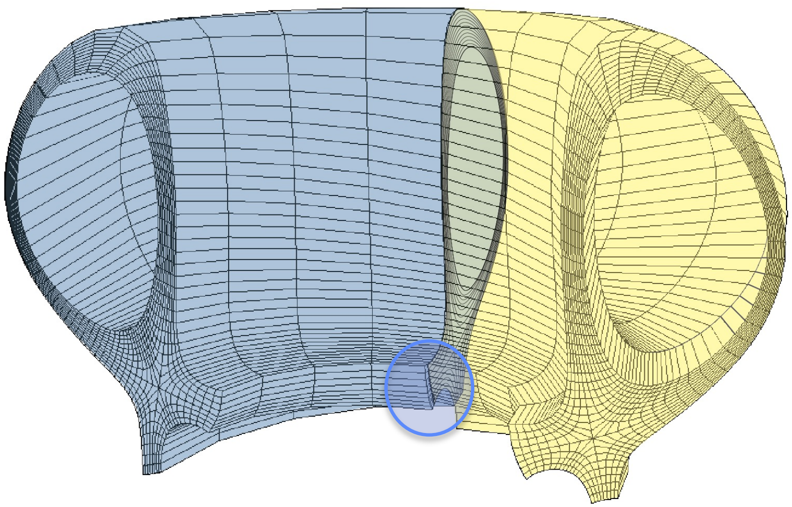
  are performed with the COGENT code

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

- Present capabilities include
  - 2D/3D gyro-Poisson and vorticity models for electrostatic potential
  - Various collision models (including nonlinear Fokker-Planck)
  - Implicit-Explicit (ImEx) time integration capabilities
  - Fluid models for electron and neutral species

- Future directions:
  - Applications: L-H transition, divertor heat-flux width
  - Capabilities: electromagnetics, kinetic electrons, FLRs

Approximate divertor boundary condition is used

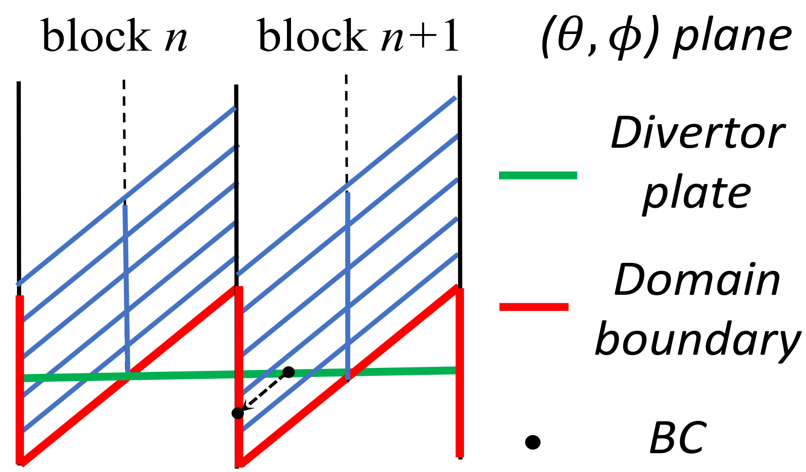


Toroidal angle measures a field-aligned coordinate

⇓

$\theta = const$ 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)