A BOUT++ Extension for Full Annular Tokamak Edge MHD and Turbulence Simulations

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In collaboration with

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Outline

• Introduction

• BOUT++ coordinate systems and hybrid field solver developed for full annular tokamak edge simulation

• Pedestal collapse with resistive drift-ballooning mode (RDBM) turbulence in shifted circular domain
  ➢ Scan of the maximum toroidal mode number solved by 2D field solver against pedestal collapse
  ➢ Impact of truncated toroidal domain on energy loss process
  ➢ Nonlinear generation on=1 global mode during pedestal collapse

• Summary
Low-n is an issue for full torus nonlinear simulation in BOUT++ as a tokamak edge simulation code [Dudson+ CPC'09]

- Moderate- \((O(n) > 1)\) and high-n \((O(n) \gg 1)\) modes can be with high accuracy by dual coordinate system (field-aligned coordinates & flux-surface coordinates)
  
  - Field solver for flow potential is reduced to 1D problem with flute-ordering

- Low-n \((O(n) \sim 1)\) modes sometimes suffer numerical instability due to the usage of flute-ordering \(k/\phi = 0\) in the field solver calculating flow potential

  - Computational domain can be limited to wedge torus for numerical instability as well as for saving computational cost
Low-n is an issue for full torus nonlinear simulation in BOUT++

BOUT++ as a tokamak edge simulation code [Dudson+ CPC'09]

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Improving low-n modes (taking full annular torus domain) is a key for more reliable tokamak edge simulations

- Convergence of core ITG turbulence against wedge number [K. Kim PoP2017]
- Nonlinear stabilization of ELM by multi-mode interaction [P.W. Xi PRL2014]
Large wedge number \( N \) can result in “false convergence” in core ITG turbulence [by XGC1, K. Kim PoP2017]

Full-f core ITG turbulence simulations with different wedge numbers \( N \) (1/\( N \) wedge tori)

- non-negligible heat transport reduction between \( N=2 \) and \( N=3 \)
- Convergence study in wedge number is needed to avoid “false convergence”

Convergence study in wedge number can be also important for edge turbulence
Nonlinear stabilization effect by mode-mode coupling can change ELM crash criteria [by BOUT++, P.W. Xi PRL2014]

Fig. 1 in P.W. Xi et al, Phys. Rev. Lett 112 (2014) 085001

Simulation with multi-mode initial perturbations and with single mode perturbation in 1/5th annular wedge torus captures the bifurcation between ELM and turbulence

- Full torus run is needed to handle complete set of nonlinear mode-mode couplings
Objective of this work

BOUT++ framework is extended with a hybrid field solver to address to full annular tokamak edge simulations, which is a key for

• Current-driven (low-n) giant ELMs
• ELM control by RMPs, edge turbulence with RMPs
• Convergence study against the wedge number for edge turbulence
• ELM crash with interplay between n=0 flow, low-n MHD and high-n turbulence
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Low-n field solver is discretized in flux surface coordinates

2D Helmholtz Eq. for toroidal mode $n$ defined in flux surface coords. $(\psi, \theta, \zeta)$

\[
\left( d \nabla^2 + \frac{1}{c} \nabla c \cdot \nabla_{\perp} + a \right) f(x, y, z) = h(x, y, z)
\]

\[
\left( L_{fs}^{10} \frac{\partial}{\partial \psi} + L_{fs}^{11} \frac{\partial^2}{\partial \psi^2} + \left( L_{fs}^{20} + inL_{fs}^{23} \right) \frac{\partial}{\partial \theta} + L_{fs}^{22} \frac{\partial}{\partial \theta^2} + inL_{fs}^{30} - n^2 L_{fs}^{33} \right) F(\psi, \theta|n) + aF(\psi, \theta|n) = H(\psi, \theta|n)
\]
Low-n field solver is discretized in flux surface coordinates

2D Helmholtz Eq. for toroidal mode $n$ defined in flux surface coords. $(\psi, \theta, \zeta)$

\[
\left( d \nabla^2_{\perp} + \frac{1}{c} \nabla \cdot \nabla_{\perp} + a \right) f(x, y, z) = h(x, y, z)
\]

coordinate transform in Fourier space

\[
d \left[ L_{fs}^{10} \frac{\partial}{\partial \psi} + L_{fs}^{11} \frac{\partial^2}{\partial \psi^2} + \left( L_{fs}^{20} + i n L_{fs}^{23} \right) \frac{\partial}{\partial \theta} + L_{fs}^{22} \frac{\partial^2}{\partial \theta^2} + i n L_{fs}^{30} - n^2 L_{fs}^{33} \right] F(\psi, \theta | n) \\
+ \frac{1}{c} \left( G_{fs}^{1} \frac{\partial c}{\partial \psi} \frac{\partial}{\partial \psi} + G_{fs}^{2} \frac{\partial c}{\partial \theta} \frac{\partial}{\partial \theta} + i n G_{fs}^{3} \frac{\partial c}{\partial \theta} \right) F(\psi, \theta | n) + a F(\psi, \theta | n) = H(\psi, \theta | n)
\]

- Discretized with 4th order central differences on $(\psi, \theta)$-plane and solved iteratively by GMRES + AMG precondition with PETSc and Hypre libraries

- Problem size: one matrix of $O(N_\psi N_\theta)$ rather than $N_y$ matrices of $O(N_\psi)$

- Slower than the flute-ordered solver but more stable for low-$n$ modes
Low-n field solver is discretized in flux surface coordinates

\[\left( d\nabla^2 + \frac{1}{c} \nabla c \cdot \nabla + a \right) f(x, y, z) = h(x, y, z) \quad \text{(x,y,z): field-aligned coordinates}
\]

\[\left( d L^{10}_{\text{fs}} \frac{\partial}{\partial \psi} + L^{11}_{\text{fs}} \frac{\partial^2}{\partial \psi^2} + \left( L^{20}_{\text{fs}} + i n L^{23}_{\text{fs}} \right) \frac{\partial}{\partial \theta} + L^{22}_{\text{fs}} \frac{\partial}{\partial \theta^2} + i n L^{30}_{\text{fs}} - n^2 L^{33}_{\text{fs}} \right) F(\psi, \theta | n) \]

coordinate transform in Fourier space

\[+ \frac{1}{c} \left( G^{1}_{\text{fs}} \frac{\partial c}{\partial \psi} \frac{\partial}{\partial \psi} + G^{2}_{\text{fs}} \frac{\partial c}{\partial \theta} \frac{\partial}{\partial \theta} + i n G^{3}_{\text{fs}} \frac{\partial c}{\partial \theta} \right) F(\psi, \theta | n) + a F(\psi, \theta | n) = H(\psi, \theta | n) \]

- Discretized with 4th order central differences on (ψ,θ)-plane and solved iteratively by GMRES + AMG precondition with PETSc and Hypre libraries
  - Problem size: one matrix of O(N_ψ*N_θ) rather than N_y matrices of O(N_ψ)
  - Slower than the flute-ordered solver but more stable for low-n modes

- The number of poloidal grids N_θ should be same as that of parallel grids N_y for transform between field-aligned (x,y,z) and flux surface (ψ,θ,ζ) coordinates
  - Poloidal resolution be fine enough for resonant poloidal modes m_{res}=nq
  - Hybrid field solver (low-n: 2D solver + high-n: 1D solver) is reasonable from the viewpoint of computational cost
A hybrid field solver for full annular tokamak edge simulation

The maximum toroidal mode number solved by 2D field solver $n_{2D_{\text{max}}}$ is a free parameter and should be chosen carefully not to affect simulation result.
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- Summary
Simulation setup for pedestal collapse simulation

- **IBM marginally unstable shifted circular equilibrium** \( (R_{ax}=3.5\text{m}, B_{ax}=2\text{T}) \)

  \[ \Delta W_{ped}/W_{ped} = -\int_{V_{ped}} P_1 dV/\int_{V_{ped}} P_0 dV, \]

  \( V_{ped} \) is the volume inside the \( \nabla P_0 \) peak (shaded region)

  \[ W_{\text{kin}}(n') = -\frac{1}{V_{\text{all}}} \int_{V_{\text{all}}} F^{n=n'} \omega dV = \frac{1}{V_{\text{all}}} \int_{V_{\text{all}}} \frac{|\nabla F^{n=n'}|^2}{2B_0^2} dV, \]

  \( V_{\text{all}} \) is the whole simulated domain

- **Scale separated 4-field RDBM model** [Seto+ CPP'20]

  \[ \frac{\partial}{\partial t} \omega = -[F_1, \omega] - [F_0, \omega] + \mathcal{G}(p_1, F) + \mathcal{G}(p_0, F_1) - B_0 \partial_{\omega} \left( \frac{J_{||}}{B_0} \right) + B_0 \left[ A_{||}, J_{||}/B_0 \right] + \kappa(p_1) + \mu_0 \nabla^2 \omega_1 + \mu_\perp \nabla \omega_1, \]

  \[ \frac{\partial}{\partial t} p_1 = -[\phi, p_1] - [\phi_0, p_1] - 2\beta_s \left( \kappa(p_1) - B_0 \partial_{\omega_1} \left( \frac{\omega_{||} + d_{J_{||}}}{2B_0} \right) + B_0 \left[ A_{||}, \omega_{||} + d_{J_{||}}/2B_0 \right] \right) + \kappa_0 \nabla_{||}^2 p_1 + \chi_{||} \nabla_{\perp}^2 p_1, \]

  \[ \frac{\partial}{\partial t} A_{||} = -[\phi, A_{||}] - \partial_{||} \phi_1 + \delta_e (\partial_{\omega} p_1 - [A_{||}, p_1]) + \eta J_{||} - \lambda \nabla_{||}^2 J_{||}, \]

  \[ \frac{\partial}{\partial t} v_{||} = -[\phi, v_{||}] - \frac{1}{2} (\partial_{||} p_1 - [A_{||}, p_1]) + \nu_{||} \nabla_{\perp}^2 v_{||}. \]

  \( \omega = \nabla_{\perp}^2 F, \quad J_{||} = \nabla_{\perp}^2 A_{||}, \quad F = \phi + \delta_e, \quad \phi = \phi_0 + \phi_1, \quad p = p_0 + p_1, \quad B = B_0 + \nabla A_{||} \times b_0, \quad J_{||} = J_{||0} + J_{||1}, \)

  \( n_{i0} = 10^{19} \quad [m^{-3}], \quad \eta = 10^{-8}, \quad \lambda = 10^{-12}, \quad \mu_\perp = \chi_{\perp} = \nu_{\perp} = 10^{-7}, \quad \mu_{||} = \chi_{||} = 10^{-1} \)

- Initially most unstable toroidal mode: \( n=32 \)
Sensitivity scan of $n_{2D_{\text{max}}}$ against full annular torus pedestal collapse simulation

3 runs with different $n_{2D_{\text{max}}}=4, 8, 12$ with $N_x=516$, $N_y=256$, $N_z=256$, $n_{1D_{\text{max}}}=80$
Sensitivity scan of $n_{2Dmax}$ against full annular torus pedestal collapse simulation

3 runs with different $n_{2Dmax} = 4, 8, 12$ ($N_x=516$, $N_y=256$, $N_z=256$, $n_{1Dmax}=80$)

$n_{2Dmax} = 4$ is high enough in this simulation setup
Toroidal domain length qualitatively changes energy loss process during pedestal collapse

- Resultant energy loss and $n=0$ and $n\neq 0$ amplitude of kinetic energy saturate to similar levels

![Graphs showing energy loss and perpendicular kinetic energy](image)

**quarter** and **full** torus run with $Nx=1028$, $Ny=128$, $Nz=64$ or **256**, $n_{2D_{\text{max}}}=4$, $n_{1D_{\text{max}}}=80$
Toroidal domain length qualitatively changes energy loss process during pedestal collapse.

- Resultant energy loss and $n=0$ and $n\neq 0$ amplitude of kinetic energy saturate to similar levels.
- There are qualitative difference during pedestal collapse.

**Figure:**

(a) Energy loss level $\Delta W_{\text{ped}}/W_{\text{ped}}$ during pedestal collapse.

- Quarter and full torus run with $N_x=1028$, $N_y=128$, $N_z=64$ or $256$, $n_{2D_{\text{max}}}=4$, $n_{1D_{\text{max}}}=80$.

(b) Perpendicular kinetic energy $W_{\text{kin}}$.
Initially unstable modes directly trigger the pedestal collapse, and then $n=0$ & low-$n$ modes are excited in quarter torus.

(a): energy loss level $\Delta W_{\text{ped}}/W_{\text{ped}}$

(b): perpendicular kinetic energy $W_{\text{kin}}$

(c): $W_{\text{kin}}$ spectra in quarter torus ($n = 0, 4, \ldots, 80$)
n=0 and low-n modes are excited before the collapse and the collapse is triggered by downshifted modes in full torus.
n=0 and low-n modes are excited before the collapse and the collapse is triggered by down-shifted modes in full torus.

The observation of collapse delay in full torus is qualitatively consistent with the stabilization by nonlinear mode couplings [Xi+ PRL’14].
n=1 global mode is nonlinearly excited and coexists with fine-scale turbulence during the pedestal collapse in full torus case.
Global $n=1$ structure has m/n=2/1 tearing parity
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Summary

- **BOUT++** has been extended for full annular tokamak edge simulations by hybrid field solver, which covers n=0, low-n, moderate-n and high-n modes
  - A key improvement for more self-consistent simulations of low-n mode relevant edge MHD and turbulence physics (type-I ELM, ELM control by RMPs, turbulence with RMPs, etc..)

- Full annular pedestal collapse simulation has been carried out and has been compared with that with the quarter torus domain
  - The truncated toroidal domain can qualitatively change the energy loss process during the pedestal collapse
  - Interplay between m/n=2/1 tearing like global structure and high-n fine-scale turbulence is observed during the pedestal collapse in the full torus case

- **On-going works**
  - Benchmark of 2D field solver against low-n modes
  - Full annular pedestal collapse simulation in single-null diverted geometry
Spatiotemporal structure of n=0 flow shear, low-n and high-n fluctuations

- Fine-scale zonal flow is generated by nonlinear couplings between high-n modes (t~200tₐ)
- Meso-scale zonal flow is then generated when low-n fluctuations are excited by nonlinear couplings between high-n modes (t=200tₐ~300tₐ)
- Large-scale mean flow is generated during pedestal collapse (t >330tₐ)
- Low-n fluctuations has radially elongated structure compared with high-n fluctuations

Details of generation mechanism of n=0 flow, those of interplay between n=0, low-n, and high-n modes are under investigation
Simulation setup for verification test of 2D field solver against IBM instability

### Linearized 3-field IBM model

\[
\frac{\partial U_1}{\partial t} = -B_0 \partial_t \left( \frac{J_{||}}{B_0} \right) + B_0 \left[ A_{||}, \frac{J_{||}}{B_0} \right] + \kappa (P_1), \\
\frac{\partial A_1}{\partial t} = -\partial_\parallel \phi_1, \\
\frac{\partial P_1}{\partial t} = -[\phi_1, P_0] \\
U_1 = \nabla \cdot \left( \frac{n_{i0}}{B_0^2} \nabla_\perp \phi_1 \right) = \frac{n_{i0}}{B_0^2} \nabla_\perp^2 \phi_1 + \nabla \left( \frac{n_{i0}}{B_0^2} \right) \cdot \nabla_\perp \phi_1, \\
J_{||1} = \nabla_\perp^2 A_{||1}, \\
\partial_\parallel f = b_0 \cdot \nabla f, \quad [f, g] = \frac{b_0 \times \nabla_\perp f \cdot \nabla_\perp g}{B_0}, \quad \kappa (f) = \frac{b_0 \times \kappa_0 \cdot \nabla f}{B_0}
\]

- Normalized with poloidal Alfvén units with \( R=3 \text{[m]}, B=2 \text{[T]}, n_i=10^{19} \text{[m}^{-3}] \), deuterium mass [Dudson CPC’09]

- Original BOUT++ employs flute-ordering in
  - Field solver for electrostatic potential \( (\nabla_\perp^2 + B_0^2 \nabla_\perp \frac{1}{B_0} \cdot \nabla_\perp) \phi_1 = B_0^2 U_1 \)
  - Laplacian operator for parallel current density \( J_1 = \nabla_\perp^2 A_{||1} \)

### IBM strongly unstable shifted circular equilibrium [Snyder PoP’02, Wilson PoP’02]

- Equilibrium used in cross-code benchmarks [Dudson CPC’09, PPCF’11, Ferraro PoP’10 etc...]

- IBM growth rates are calculated with 1D & 2D solver in \( 1/N \)-th annular wedge domains for \( n=N \) mode

<table>
<thead>
<tr>
<th></th>
<th>Nx</th>
<th>Ny</th>
<th>Nz</th>
<th>z-length</th>
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<tr>
<td>1D field solver &amp; Laplacian</td>
<td>512</td>
<td>64</td>
<td>32</td>
<td>2\pi/N</td>
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<tr>
<td>2D field solver &amp; Laplacian</td>
<td>512</td>
<td>512</td>
<td>32</td>
<td>2\pi/N</td>
</tr>
</tbody>
</table>
n=20 IBM growth rate by 2D field solver shows good agreement with the previous work [Ref. [14] Dudson CPC’09]

- The difference between growth rates by 2D solver and those by 1D solver becomes larger for lower-n modes
  - Qualitatively consistent with the expected flute-ordering correction of $O(1/n)$ [Connor PRSA’79]
**flux-surface & field-aligned** coords. are used with shifted metric

**quarter torus domain:** \((\psi, \theta, \zeta)\)

- Need fine pol.(\(\theta\)) grids for parallel difference \(m_{\text{res}} = nq\)
- No cell deformation by magnetic shear

**Used for** \((\zeta, \psi)\)-difference
**flux-surface & field-aligned** coords. are used with shifted metric

- **Need fine pol.**($\theta$) grids for parallel difference $m_{res} = nq$
- **No cell deformation by magnetic shear**

**Used for**($\zeta, \psi$)-difference

- shift: $z = \zeta - \alpha$

**Quarter torus domain:** ($\psi, \theta, \zeta$)

- **Quarter torus domain:** ($x, y, z$)

- Need only coarse para.($y$) grids for parallel difference
- Radial difference is degraded by cell-deformation

**Used for**($y, z$)-difference

- shift: $\zeta = z + \alpha$
**flux-surface & field-aligned coords.** are used with shifted metric

- **Quarter torus domain:** $(\psi, \theta, \zeta)$

  - Need fine pol.($\theta$) grids for parallel difference $m_{res} = nq$
  - No cell deformation by magnetic shear

  Used for $(\zeta,\psi)$-difference

  - Shift: $z = \zeta - \alpha$

- **Quarter torus domain:** $(x, y, z)$

  - Need only coarse para.($y$) grids for parallel difference
  - Radial difference is degraded by cell-deformation

  Used for $(y,z)$-difference

  - Shift: $\zeta = z + \alpha$

**Helmholtz Eq. of flow potential:**

$$\left( dV_\perp^2 + \frac{1}{c} \nabla c \cdot \nabla_\perp + a \right) f(x, y, z) = h(x, y, z)$$

Eq. for toroidal mode $n$ in quasi-ballooning coords. has $\psi$- and $y$- derivatives

$$d \left[ L_{q\theta}^{10} \frac{\partial}{\partial \psi} + L_{q\theta}^{11} \frac{\partial^2}{\partial \psi^2} + \left( L_{q\psi}^{20} + inL_{q\psi}^{23} \right) \frac{\partial}{\partial y} + L_{q\psi}^{22} \frac{\partial^2}{\partial y^2} + inL_{q\psi}^{30} - n^2 L_{q\psi}^{33} \right] F + \frac{1}{c} \left( G_{q\theta}^{1} \frac{\partial c}{\partial \psi} \frac{\partial}{\partial \psi} + G_{q\psi}^{2} \frac{\partial c}{\partial y} \frac{\partial}{\partial y} + inG_{q\psi}^{3} \frac{\partial c}{\partial y} \right) F + aF = H$$

$$d \left( L_{q\theta}^{10} \frac{\partial}{\partial \psi} + L_{q\theta}^{11} \frac{\partial^2}{\partial \psi^2} + inL_{q\theta}^{30} - n^2 L_{q\psi}^{33} \right) F(\psi \mid \theta, n) + \frac{1}{c} \left( G_{q\theta}^{1} \frac{\partial c}{\partial \psi} \frac{\partial}{\partial \psi} + inG_{q\psi}^{3} \frac{\partial c}{\partial y} \right) F(\psi \mid \theta, n) + aF(\psi \mid \theta, n) = H(\psi \mid \theta, n)$$

Flute-ordering reduces Eq. to 1D ($\psi$-dir) but can give numerical instability on low-$n$