Project TOKDGE:
A hybrid Poisson solver for full annular tokamak edge turbulence simulation

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Outline

- Introduction: BOUT++ code and objectives of TOKEDGE project
- Numerical scheme of a hybrid Poisson solver for full annular tokamak edge simulations
- **[Erratum of CSC WS'21]** impact of flute-ordering assumption in low-n ideal ballooning mode
- Pedestal collapse simulation in full annular tours domain in shifted circular geometry
- Preliminary test of full annular torus turbulence simulation in single-null divertor geometry
- Summary

BOUT++ code and objectives of TOKEDGE project

BOUT++ framework as an edge tokamak simulation code [Dudson CPC2009]

- BOUT++ calculates middle-n (O(n)>1) and high-n (O(n)≫1) structure with high accuracy in complex boundary region in tokamak plasmas

- BOUT++ employs flute-ordering $k_{//}=0$ on Poisson solver for $n \neq 0$ modes calculating flow potential from vorticity

  ✓ Flute-ordering may not be accurate for low-n modes (O(n)~1) especially in diverted geometries

TOKEDGE is a ~~two~~ three years project to extend BOUT++ framework for tokamak edge simulation solving interplay between n=0, low-n, middle-n and high-n modes in diverted geometries

➡ improvement of current-driven ELMs, RMPs, full annular tours edge turbulence simulations, etc…

- FY2020: development of flute-ordering-free Poisson solver for low-n modes [CSC WS 2021]
- FY2021: production run of full annular tokamak edge simulation with circular cross section
- FY2021: preliminary test of full annular tokamak edge simulation with single-null divertor geometry

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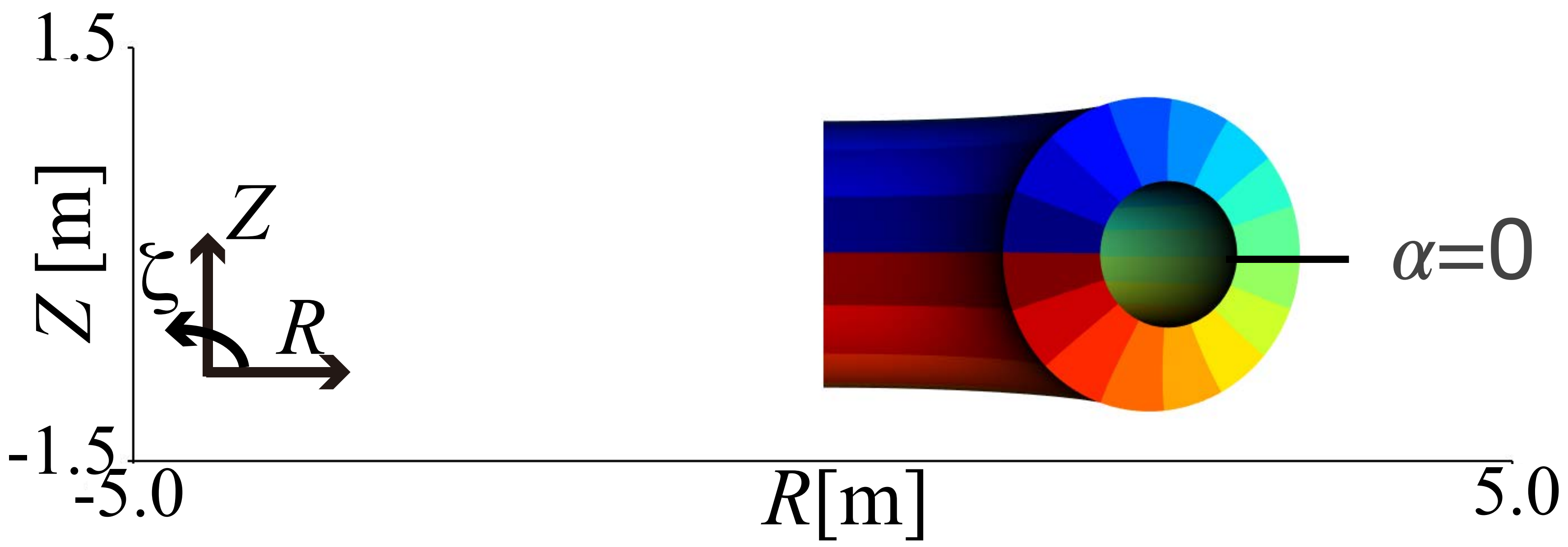
BOUT++ uses dual coordinate system but has problem in n=0 and low-n

BOUT++ calculates middle-n and high-n mode with high accuracy and cheap cost using both flux surface coords. (ψ,θ,ζ) and field-aligned coords. (x,y,z) with shifted metrics for tokamaks

1/4th annular torus domain by (ψ,θ,ζ)



- Need large poloidal (θ) resolution for parallel differencing for large q and n

❖ Differencing in radial (ψ) direction

➡ 1D Poisson solver for n in radial direction **with flute-ordering $k_{//}$=0** for calculating flow potential

coord. transform by FFT: $z=\zeta-\alpha$

field-aligned coords:

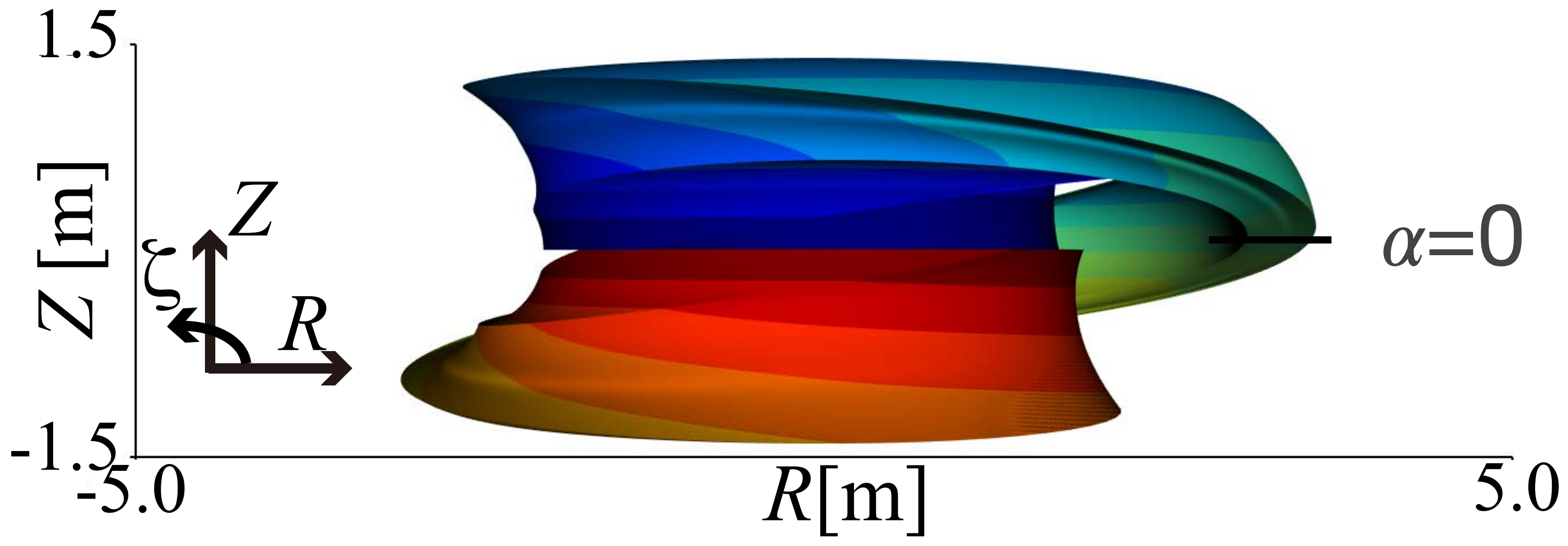
$$x = \psi - \psi_0$$
$$y = \theta$$
$$z = \zeta - \alpha$$

shift angle for aligning:

$$\alpha = \int_{\theta=\pi}^{\theta} \frac{\boldsymbol{B}\cdot\nabla\zeta}{\boldsymbol{B}\cdot\nabla\theta} d\theta$$

coord. transform by FFT: $\zeta=z+\alpha$

1/4th annular torus defined by (x,y,z)



- Need small parallel (y) resolution for parallel differencing
- Cell deformation by magnetic shear degrades radial (x) differencing

❖ Differencing in parallel (y) dir.

❖ Differencing in binormal (z) dir.

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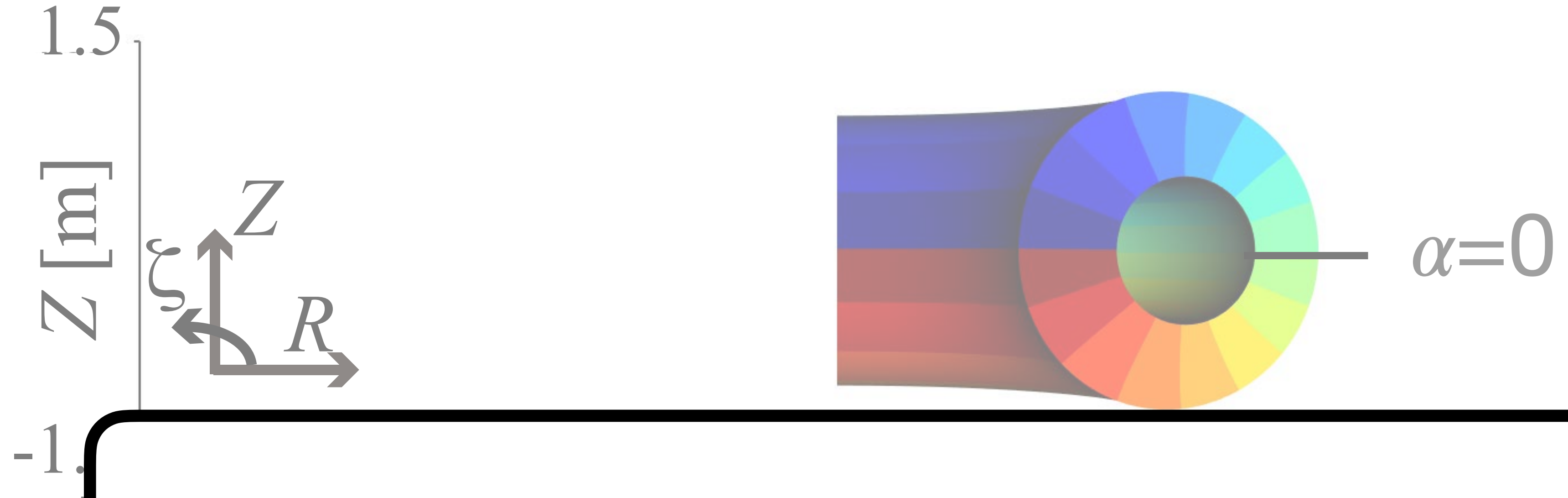
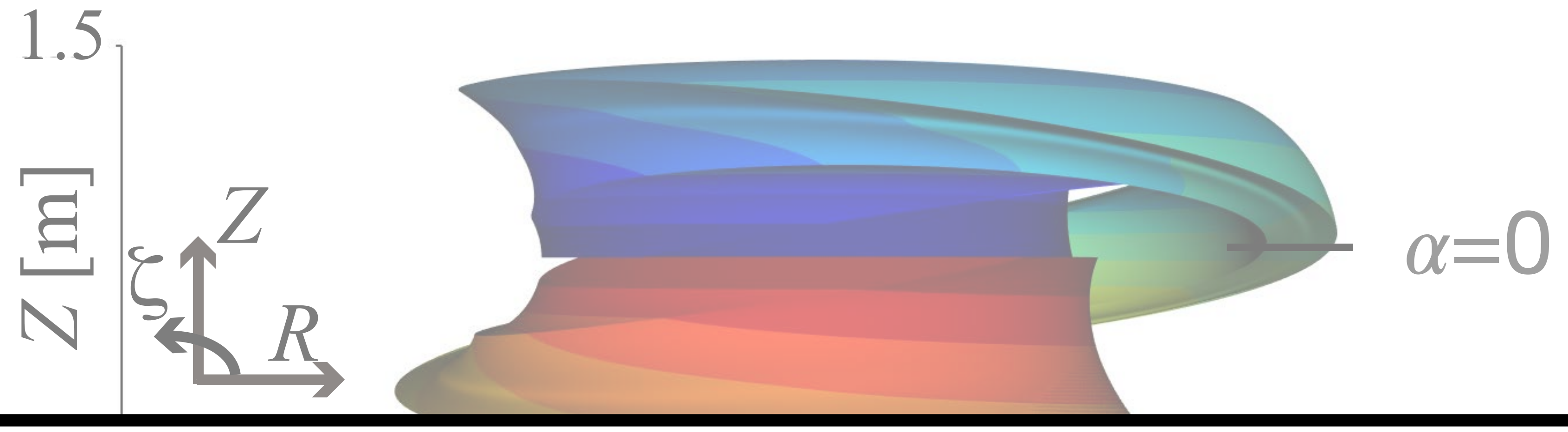
1/4th annular torus domain by (ψ,θ,ζ)



coord. transform by FFT: $z=\zeta-\alpha$

1/4th annular torus defined by (x,y,z)



field-aligned coords:

Flute-ordering $k_{//}=0$ may not be valid for n=0 and low-n modes especially in diverted geometries

➡**Cannot address to nonlinear tokamak edge simulation selfconsiestently including interplay between flow (n=0), (low-n) MHD, and turbulence**

• N
p

degrades radial (x) differencing

$$\alpha = \int_{\theta=\pi} \frac{\boldsymbol{B}\cdot\nabla\zeta}{\boldsymbol{B}\cdot\nabla\theta} d\theta$$

❖ Differencing in radial (ψ) direction

➡ 1D Poisson solver for n in radial direction **with flute-ordering $k_{//}=0$** for calculating flow potential

❖ Differencing in parallel (y) dir.

❖ Differencing in binormal (z) dir.

coord. transform by FFT: $\zeta=z+\alpha$

Numerical issue on Poisson solver in BOUT++ : flute ordering on low-n modes

Linearized Poisson solver for $n=n'$ mode vorticity ($n_{i1}/n_{i0} \ll O(1)$) in Fourier space

$$U_1(\cdot,\cdot,n') = \nabla\cdot\left(\frac{n_{i0}}{B_0}\nabla_\perp\phi_1\right) = \mathcal{L}_{\text{shifted}}(\partial_\psi, \partial_\psi^2, \partial_y, \partial_y^2, n)\phi_1(\cdot,\cdot,n') \longrightarrow \phi_1(\cdot,\cdot,n') = \mathcal{L}^{-1}_{\text{shifted}}(\partial_\psi, \partial_\psi^2, \partial_y, \partial_y^2, n')U_1(\cdot,\cdot,n') \quad ?$$

Poisson solver however cannot be defined as a boundary problem straightforwardly

- 1D Poisson solver in flux-surface coordinates for $n\neq0$ modes using flute-ordering approximation ($\partial_y=0$) [Dudson CPC2009]

$$\phi_1(\psi,\theta,n') = \mathcal{L}^{-1}_{\text{shifted}}(\partial_\psi, \partial_\psi^2, n')U_1(\psi,\theta,n')$$

- 2D Poisson solver in field-aligned coordinates for $n=0$ mode using toroidal symmetry ($\partial_x=\partial_\psi+I\partial_\zeta=\partial_\psi$) [Dudson PPCF2017]

$$\phi_1(x,y) = \mathcal{L}^{-1}_{\text{shifted}}(\partial_x, \partial_x^2, \partial_y, \partial_y^2)U_1(x,y)$$

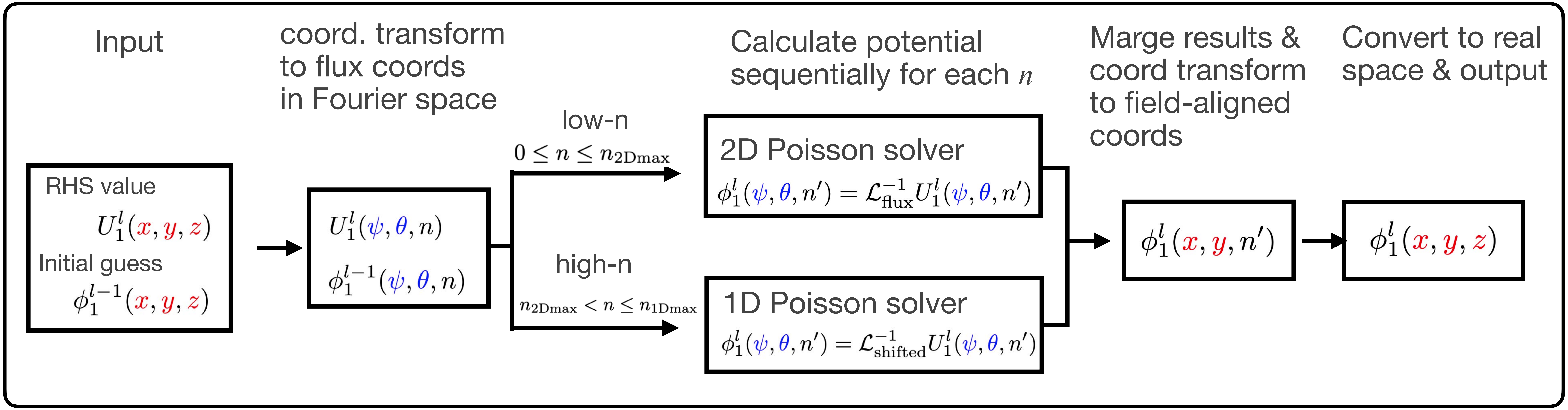
- 2D Poisson solver in flux-surface coordinates for low-n modes with flux-surface coordinates' metrics [TOKEDGE 2020-cycle]

$$\phi_1(\psi,\theta,n') = \mathcal{L}^{-1}_{\text{flux surface}}(\partial_\psi, \partial_\psi^2, \partial_\theta, \partial_\theta^2, n')U_1(\psi,\theta,n')$$

  - Poloidal grid resolution must be fine enough to describe poloidal structure of low-n modes
  - Iterative solver using GMRES for KSP solver and AMG for preconditioning via PETSc and Hypre

Flute-ordering-free 2D Poisson solver for low-n modes is developed

A hybrid linearized Poisson solver function consisting of flute-ordered 1D Poisson and flute-ordering-free 2D Poisson solver for full annular tokamak edge turbulence simulation



- The highest toroidal mode number solved by 2D Poisson solver n_{2Dmax} and that by 1D Poisson solver n_{1Dmax} are free parameters to be chosen carefully

- A hybrid Laplacian operator consistent with the hybrid Poisson solver is also important for numerically stable simulation

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Linearized IBM model and where the flute-ordering are used in original BOUT++

Linearized IBM model

$$\frac{\partial U_1}{\partial t} = -B_0\partial_{\|}\left(\frac{J_{\|1}}{B_0}\right) + B_0\left[A_{\|1}, \frac{J_{\|0}}{B_0}\right] + \mathcal{K}\left(P_1\right),$$

$$\frac{\partial A_1}{\partial t} = -\partial_{\|}\phi_1,$$

$$\frac{\partial P_1}{\partial t} = -\left[\phi_1, P_0\right]$$

$$U_1 = \nabla\cdot\left(\frac{n_{i0}}{B_0^2}\nabla_{\perp}\phi_1\right),$$

$$J_1 = \nabla_{\perp}^2 A_{\|1},$$

$$[f,g] = \frac{\boldsymbol{b}_0\times\nabla_{\perp}f\cdot\nabla_{\perp}g}{B_0}, \quad \mathcal{K}\left(f\right) = \frac{\boldsymbol{b}_0\times\boldsymbol{\kappa}_0\cdot\nabla f}{B_0},$$

- constant ion number density $n_{i0} = 10^{19}$ [m^{-3}]
- normalized with poloidal Alfven unit
- original BOUT++ employs flute-ordering in
  - ❖ Poisson solver for electrostatic potential

$$\left(\nabla_{\perp}^2 + B_0^2\nabla B_0^{-2}\cdot\nabla_{\perp}\right)\phi_{1,n} = B_0^2 U_{1,n}$$

  - ❖ Laplacian operator for parallel current (for consistency with Poisson solver)

$$J_1 = \nabla_{\perp}^2 A_{\|1}$$

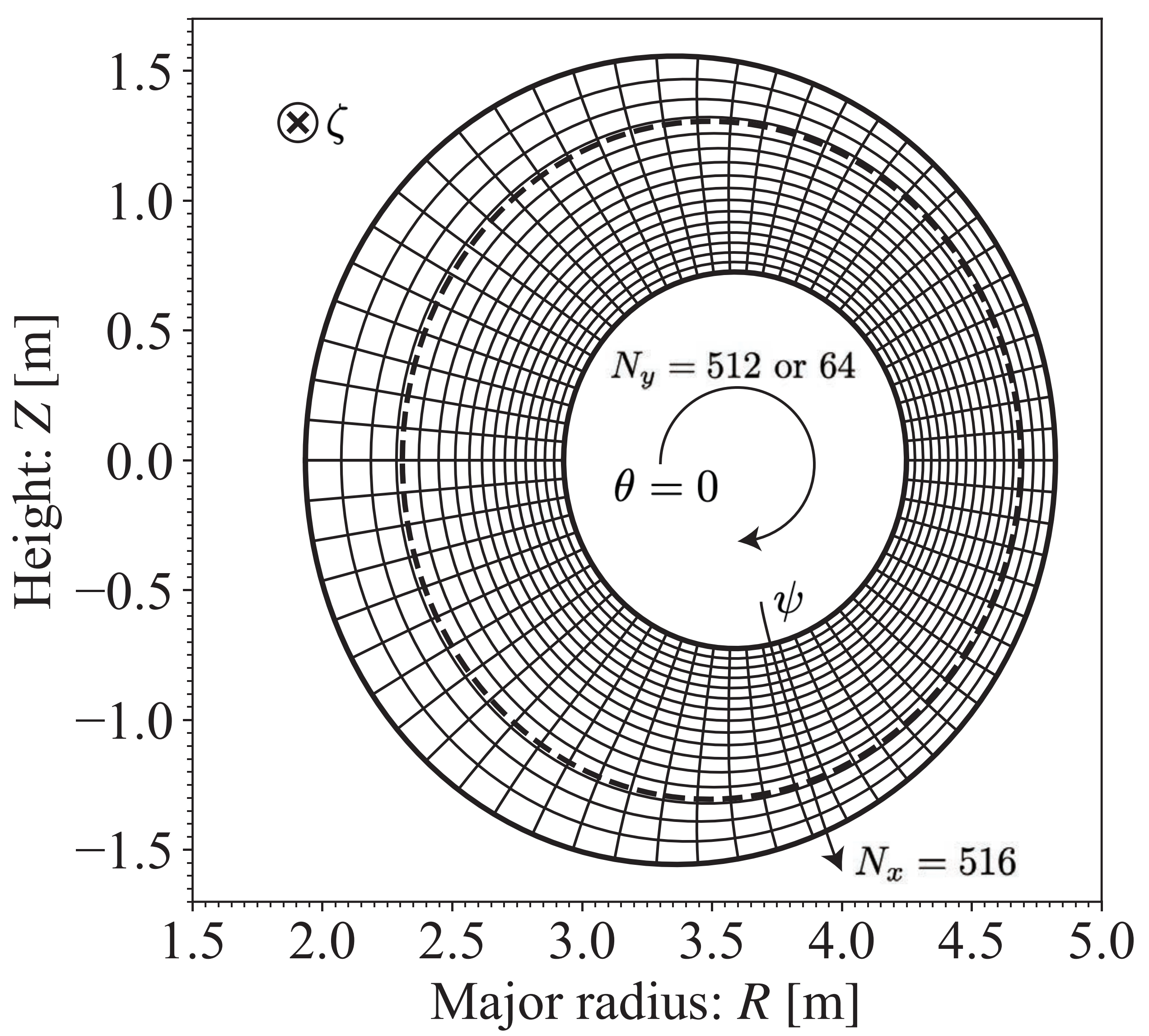
Benchmark of Poisson solvers & Laplacians against IBM unstable equilibrium

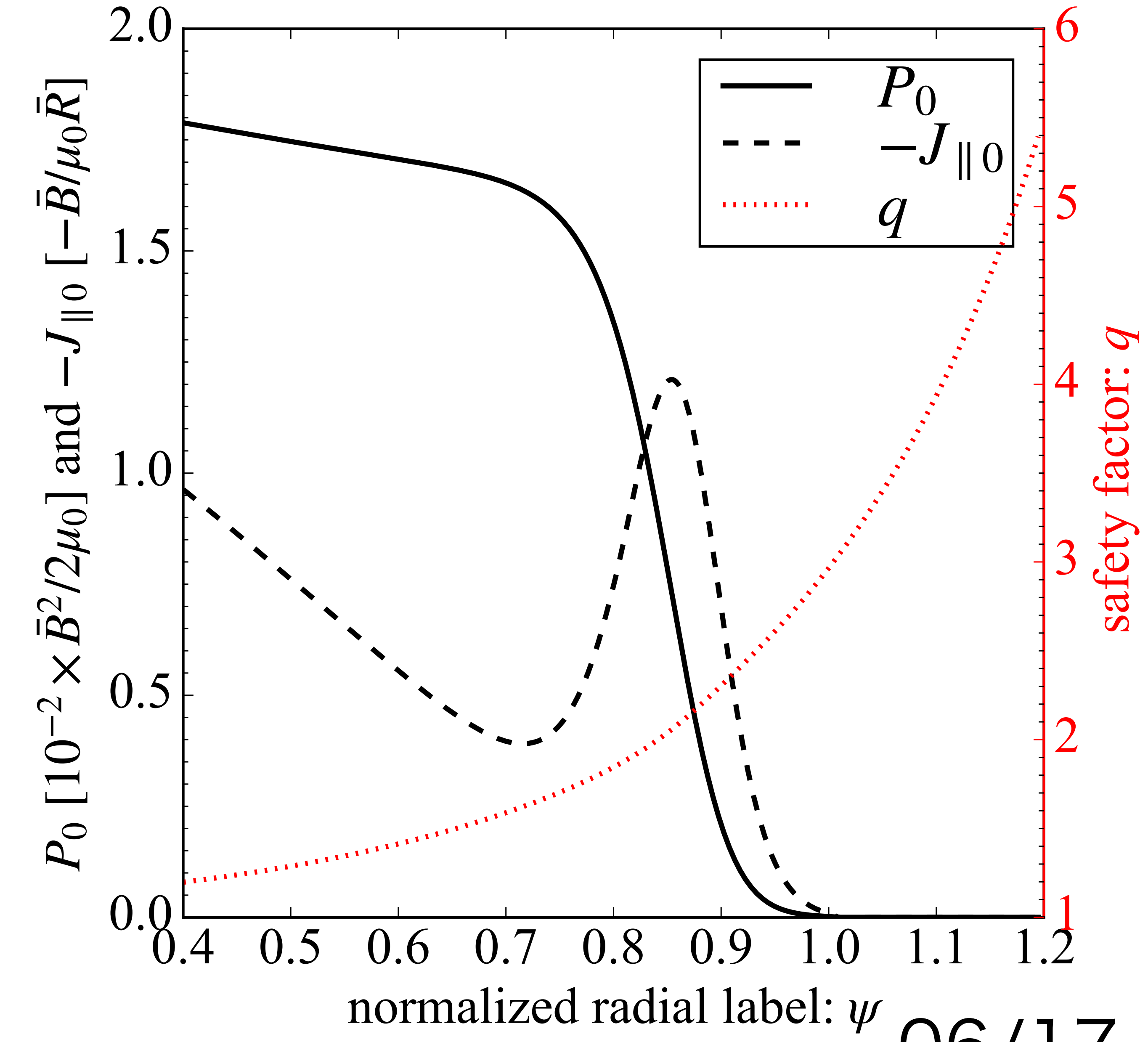
cbm18_dens8: a well-benchmarked equilibrium with circular cross section strongly unstable for ideal ballooning mode [Dudson CPC2009 PPCF2011]

- $1/n$-th annular wedge domain in z for n mode with following resolutions

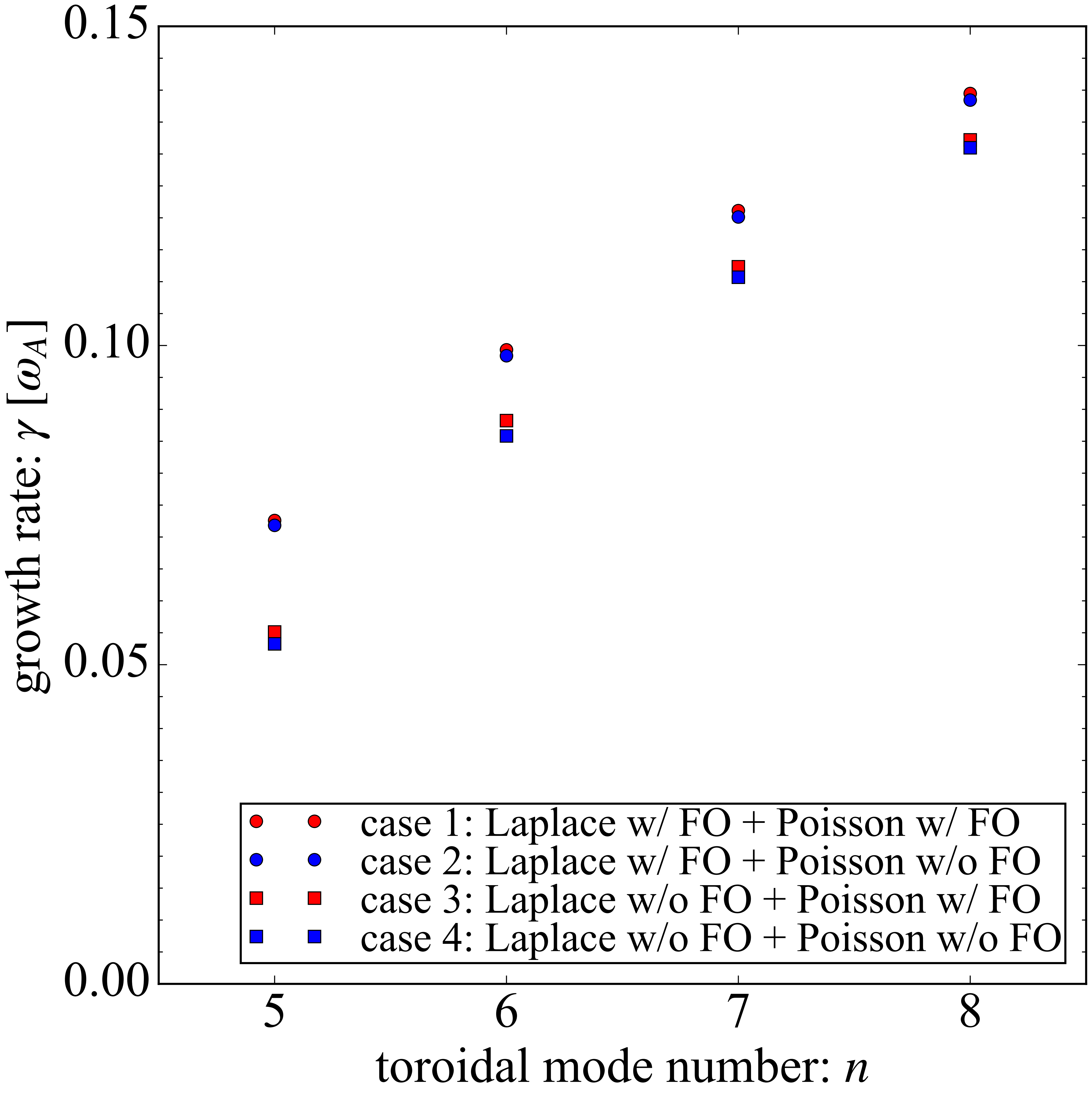
Grid Resolution	Nx	Ny	Nz
Case1: Laplace w/ FO + Poisson w/ FO (same flute-ordering rule used in original BOUT++)	512	64	32
Case 2: Laplace w/ FO + Poisson w/o FO	512	512	32
Case 3: Laplace w/o FO + Poisson w/FO (reported in CSC workshop 2021 as case1 by mistake)	512	64*	16
Case 4: Laplace w/ FO + Poisson w/ FO	512	512	32

- In CSC WS2021, case 3 was reported as case 1 by mistake and it was concluded that flute-ordering has little impact in this equilibrium





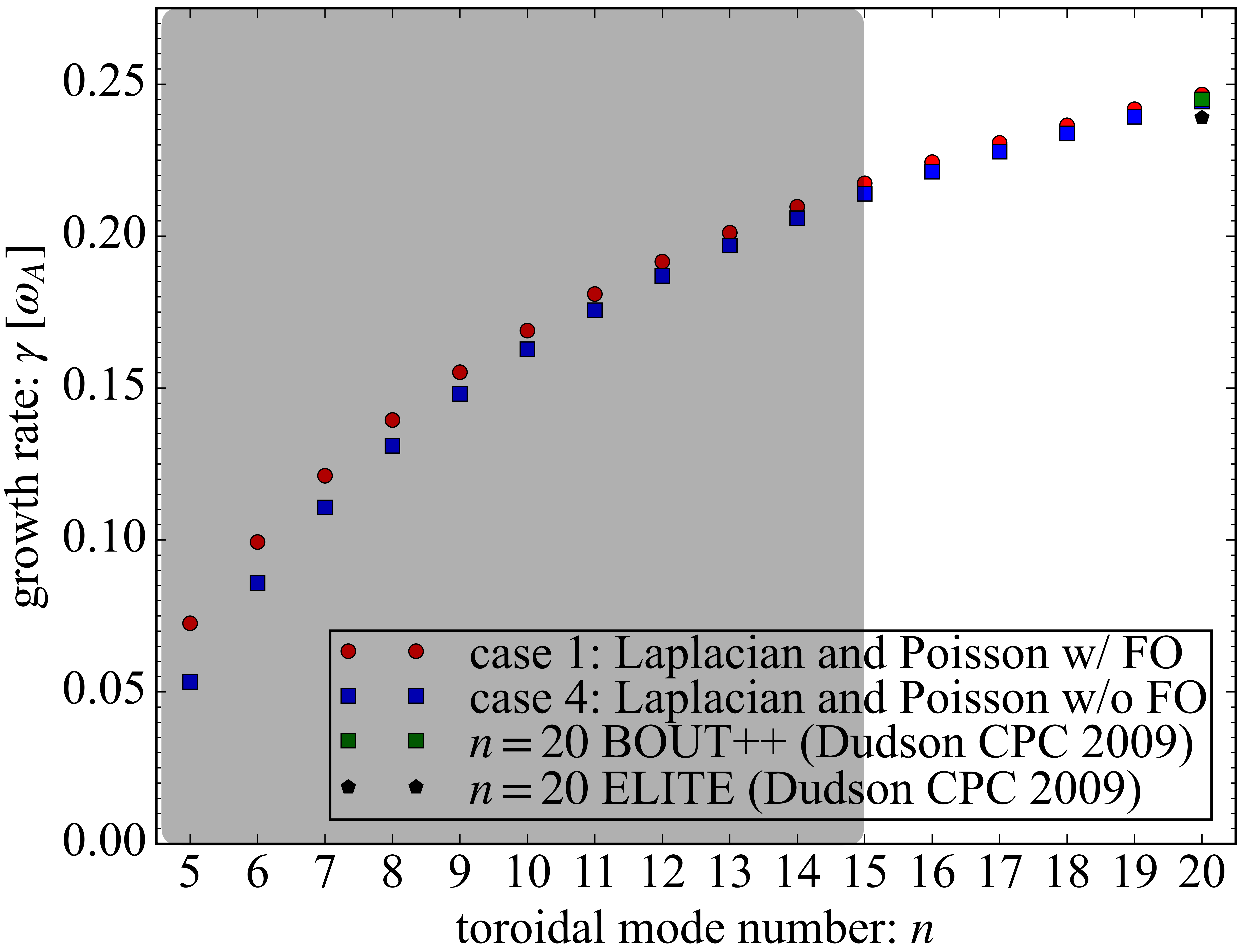
FO in Laplacian for $J_{//}$ has large impact while FO in Poisson solver for ϕ has little



- Flute-ordering in Laplacian for J// has large impact in low-n regime (difference between circles and squares)
- Flute-ordering in Poisson solver for ϕ has little impact in even low-n regime (difference between red symbols and blue ones)

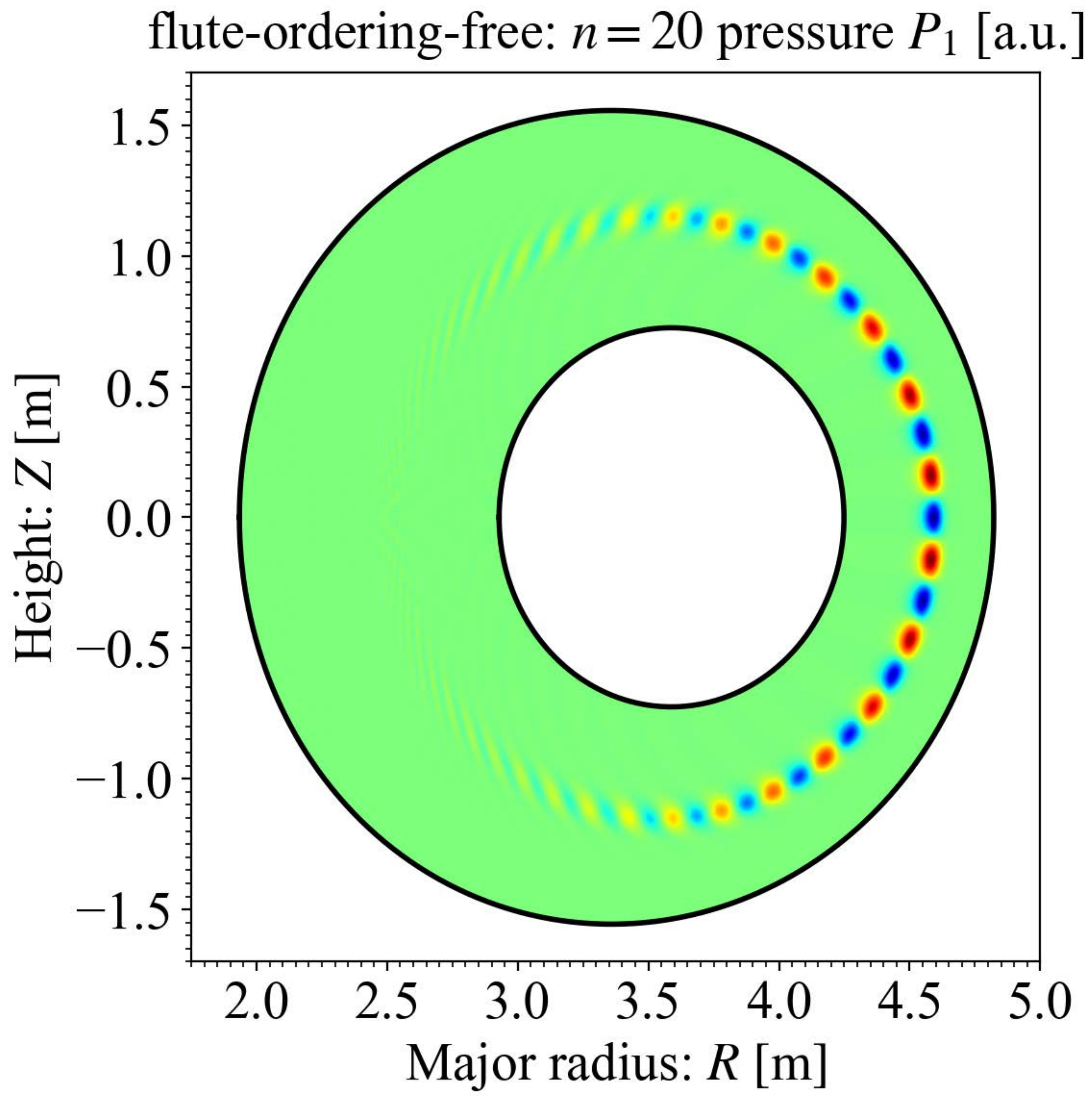
Asymmetric usage of flute-ordering (case 2 and 3) can give disruptive numerical instabilities

Flute-Ordering-free Laplacian and Poisson solver can reproduce high-n IBM



- Flute-ordering seems good for high-n regimes (~1% difference at n=20)

➡FO-free Laplacian and Poisson solver (case 4) can capture IBM eigenfunction for high-n (n=20)



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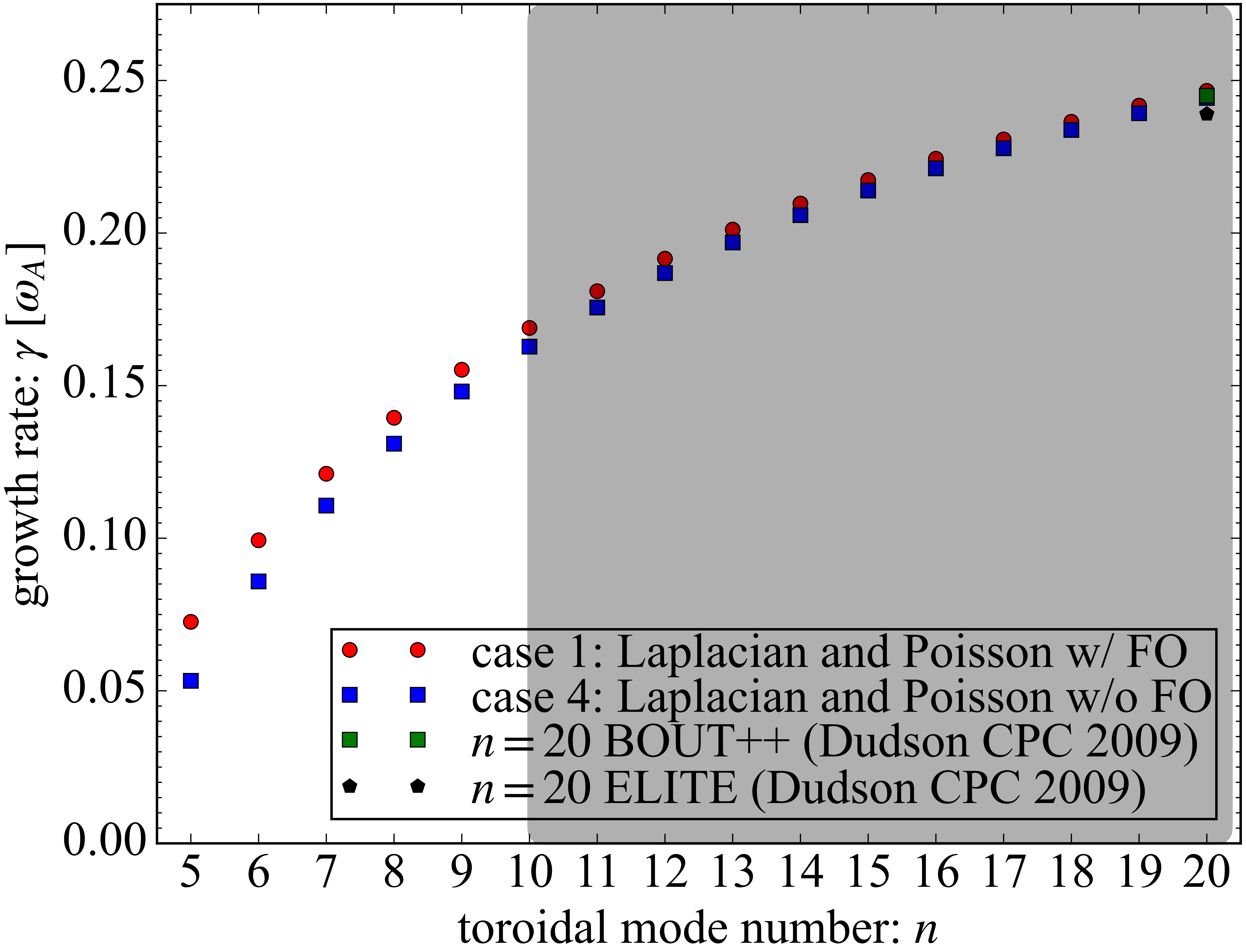

- Flute-ordering seems good for high-n regimes (~1% difference at n=20)

  ➡FO-free Laplacian and Poisson solver (case 4) can capture IBM eigenfunction for high-n (n=20)

- Flute-ordering gives large difference for low-n regimes (~36% at n=5)

  ➡BOUT++ overestimates growth rate in low-n regime [Dudson PPCF'11] and FO-free scheme can suppress this overestimation to some level

Test of FO-free Poisson solver and Laplacian against low-n linear RBM in a single-null diverted geometry was also finished [reported in CSC WS'21]

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Impact of binormal domain length in pedestal collapse simulations

- **Scale separated four-field RBM+DW model [Seto+ CPP'20]**

$$\frac{\partial}{\partial t}\varpi_1 = -[F_1,\varpi] - [F_0,\varpi_1] + \mathcal{G}(p_1,F) + \mathcal{G}(p_0,F_1) - B_0\partial_\parallel\left(\frac{J_{\parallel 1}}{B_0}\right) + B_0\left[A_{\parallel 1},\frac{J_\parallel}{B_0}\right] + \mathcal{K}(p_1) + \mu_\parallel\partial_\parallel^2\varpi_1 + \mu_\perp\nabla_\perp^2\varpi_1,$$

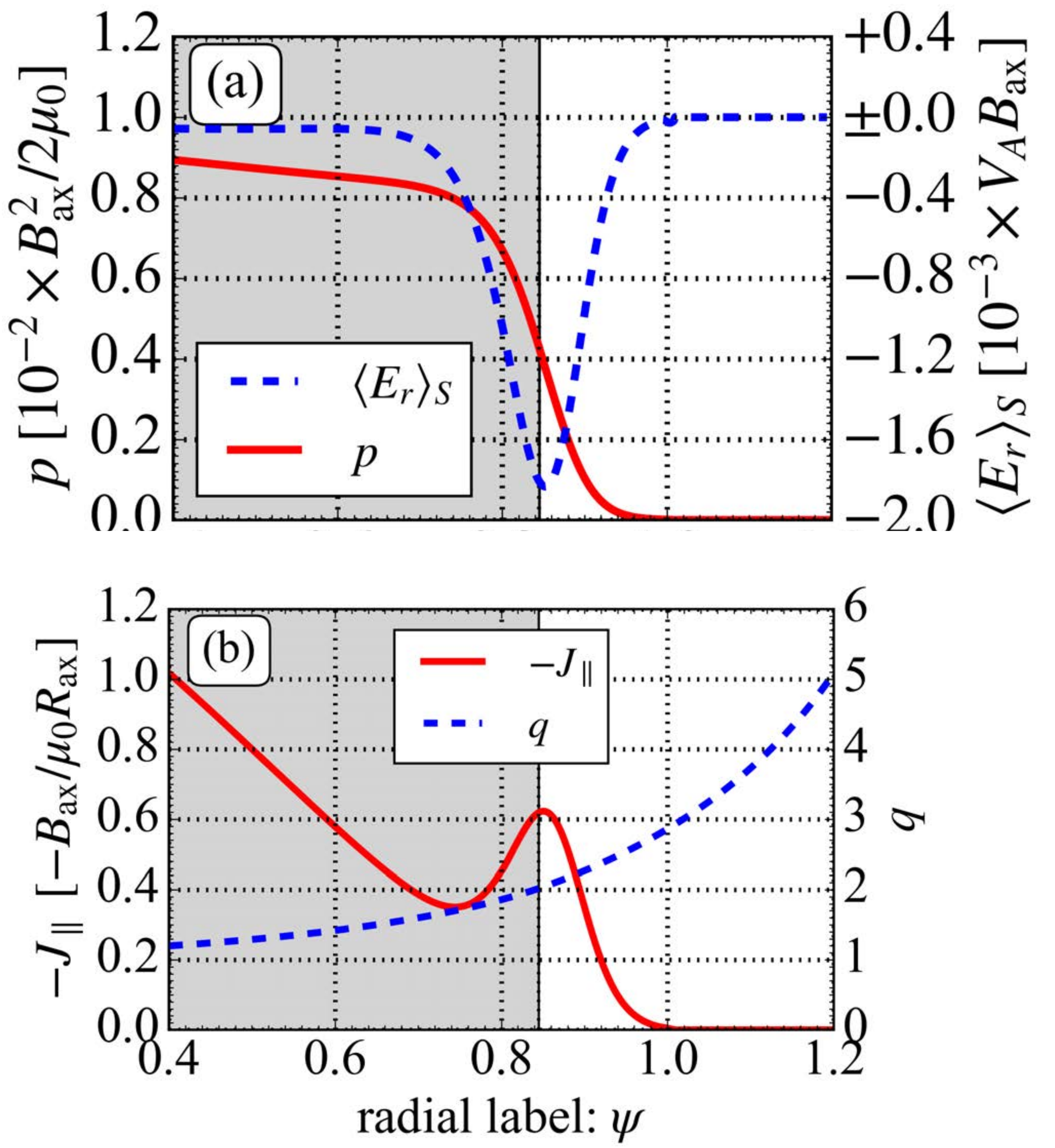
$$\frac{\partial}{\partial t}p_1 = -[\phi_1,p] - [\phi_0,p_1] - 2\beta_*\left(\mathcal{K}(p_1) - B_0\partial_\parallel\left(\frac{v_{\parallel 1}+d_iJ_{\parallel 1}}{2B_0}\right) + B_0\left[A_{\parallel 1},\frac{v_{\parallel 1}+d_iJ_{\parallel 1}}{2B_0}\right]\right) + \chi_\parallel\partial_\parallel^2 p_1 + \chi_\perp\nabla_\perp^2 p_1,$$

$$\frac{\partial}{\partial t}A_{\parallel 1} = -[\phi,A_{\parallel 1}] - \partial_\parallel\phi_1 + \delta_e\left(\partial_\parallel p_1 - [A_{\parallel 1},p]\right) + \eta J_{\parallel 1} - \lambda\nabla_\perp^2 J_{\parallel 1},$$

$$\frac{\partial}{\partial t}v_{\parallel 1} = -[\phi,v_{\parallel 1}] - \frac{1}{2}\left(\partial_\parallel p_1 - [A_{\parallel 1},p]\right) + \nu_\perp\nabla_\perp^2 v_{\parallel 1},$$

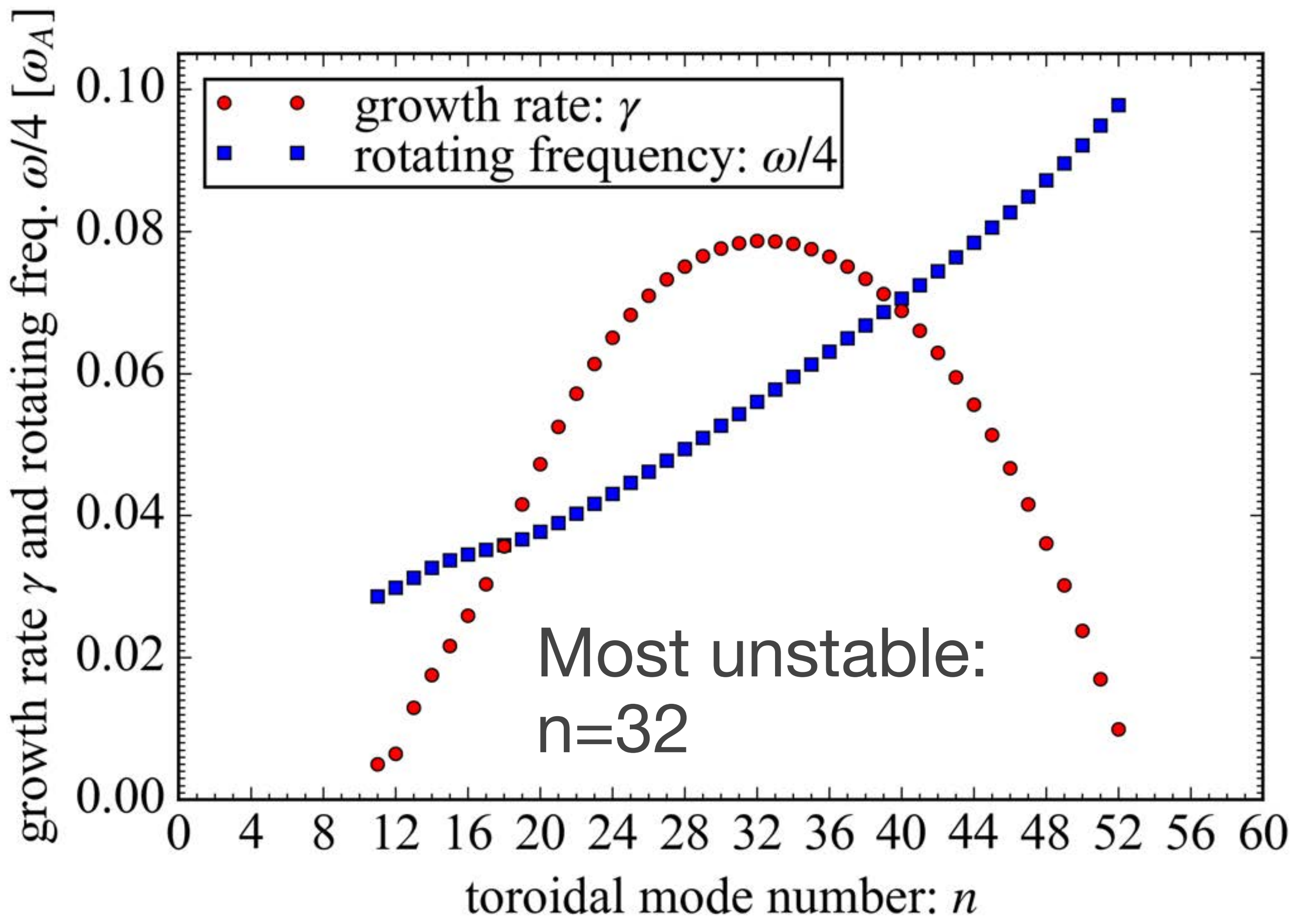
$$\varpi = \nabla_\perp^{*2}F,\quad J_1 = \nabla_\perp^2 A_\parallel,\quad F = \phi + \delta_i p,\quad \phi = \phi_0 + \phi_1,\quad p = p_0 + p_1,\quad \boldsymbol{B} = \boldsymbol{B}_0 + \nabla A_{\parallel 1}\times\boldsymbol{b}_0,\quad J_\parallel = J_{\parallel 0} + J_{\parallel 1},$$

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

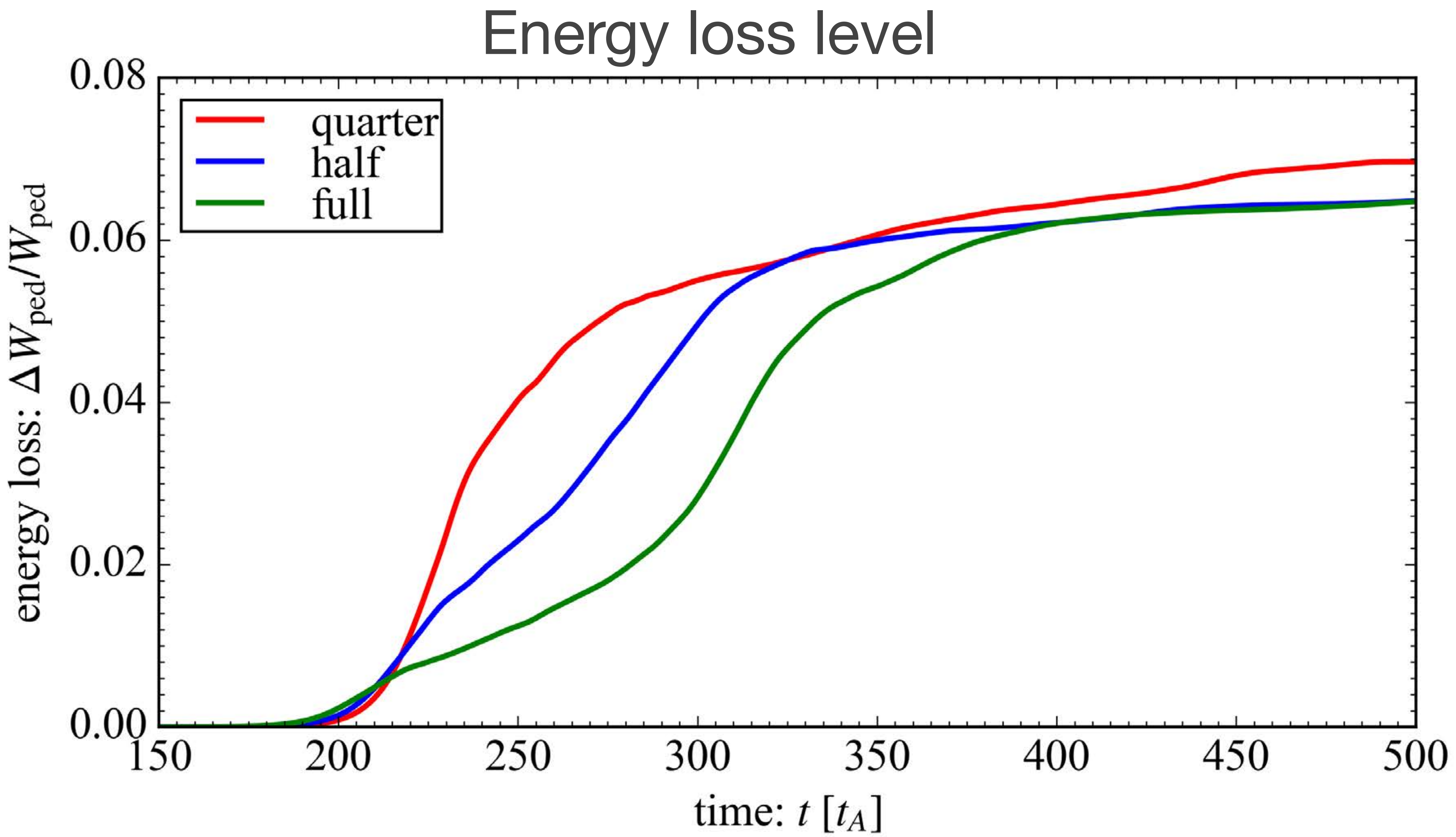


- **Gird resolution and toroidal mode numbers to be solved**

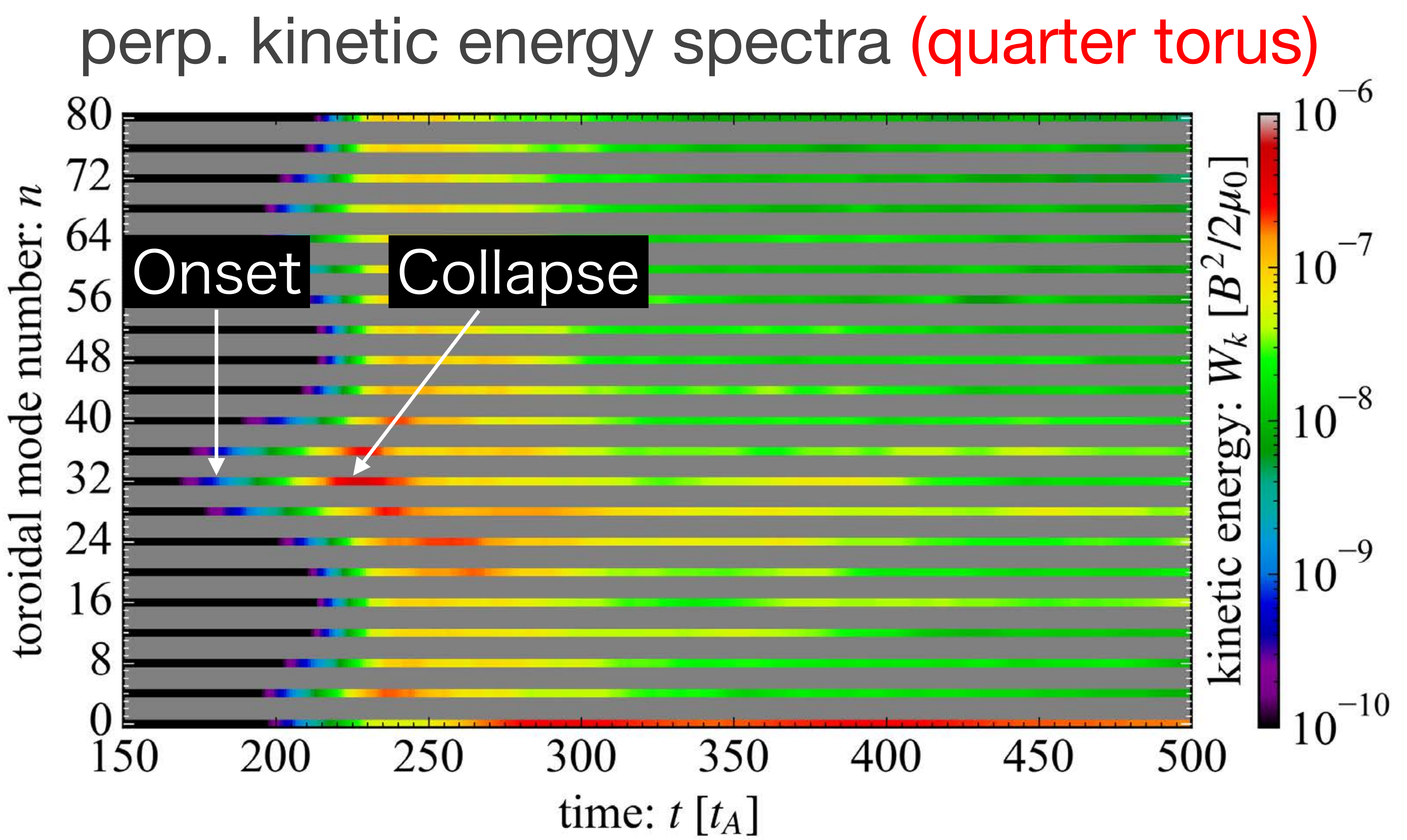
binormal domain length	Nx	Ny	Nz	tor. mode # to be solved	2D Poisson +2D Laplace	1D Poisson +1D Laplace
full torus ($0\leq z<2\pi/1$)	1028	128	256	n=0,1,…,80	n=0,1,2,3,4	n=5,6,…,80
half torus ($0\leq z<2\pi/2$)	1028	128	128	n=0,2,…,80	n=0,2,4	n=6,8,…,80
quarter torus ($0\leq z<2\pi/4$)	1028	128	64	n=0,4,…,80	n=0,4	n=8,12,…,80

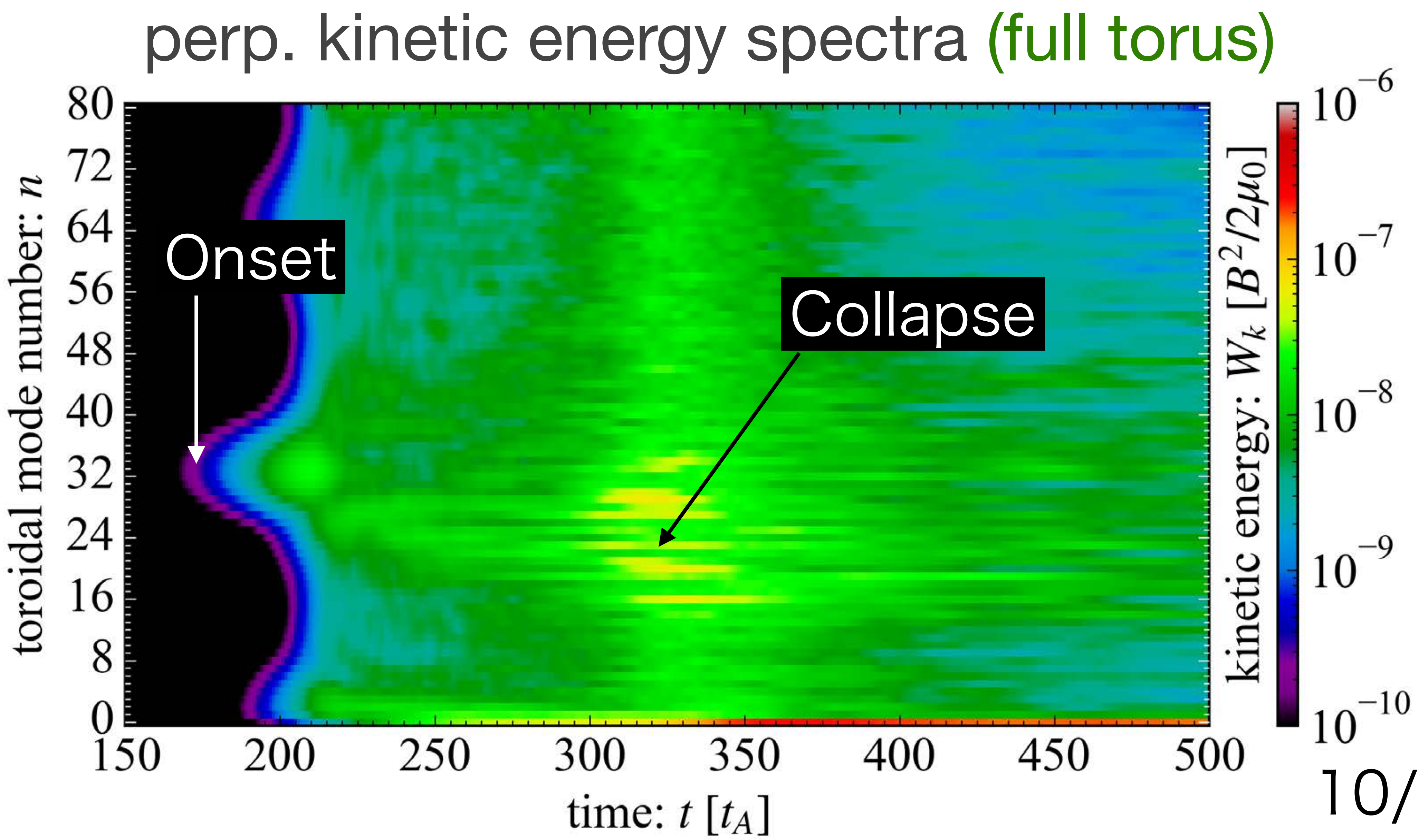


Impact of binormal domain length on energy loss during pedestal collapse



- **Initially unstable modes (IUMs) (n~32)** sets the pedestal collapse onset at t~200t_A
- IUMs are strongly excited and directly drive the collapse for quarter case
- Low-n (n~1) modes are generated via nonlinear coupling between IUMs and collapse is triggered by down-shifted modes (n=20~30) for full torus case (and half torus case)





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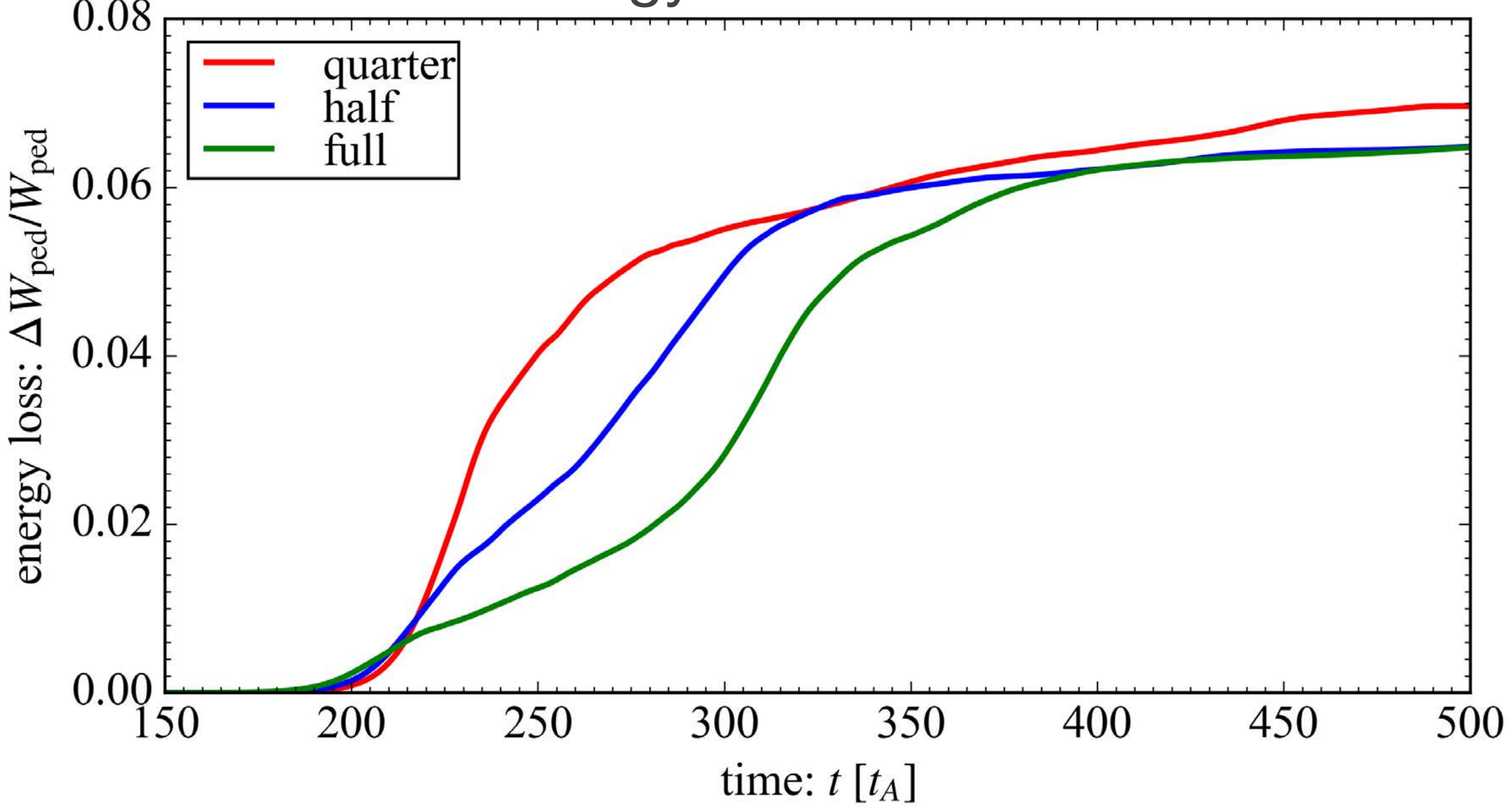
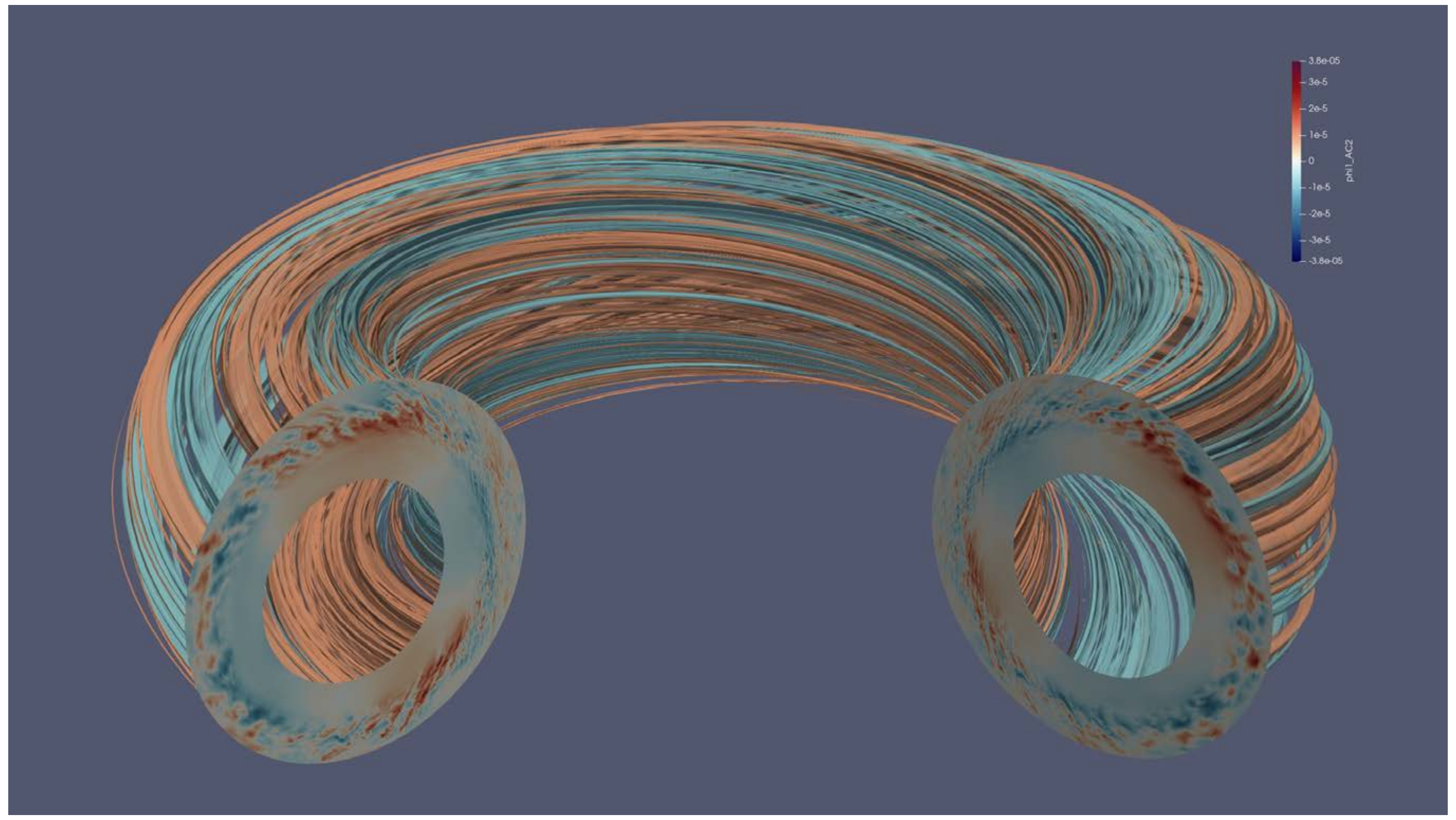
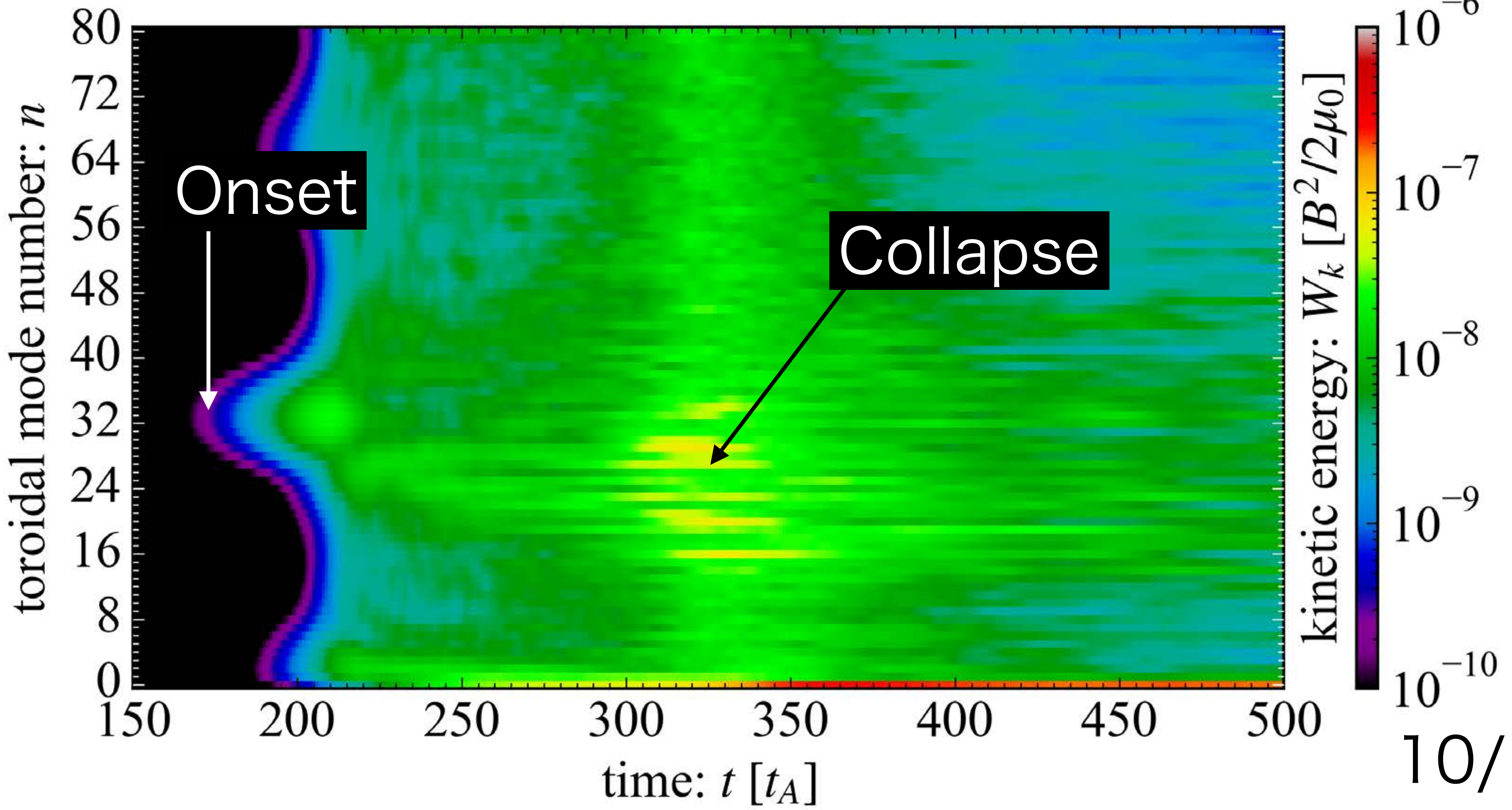
Energy loss level



ϕ w/o n=0 in full torus during collapse t=330



perp. kinetic energy spectra (full torus)



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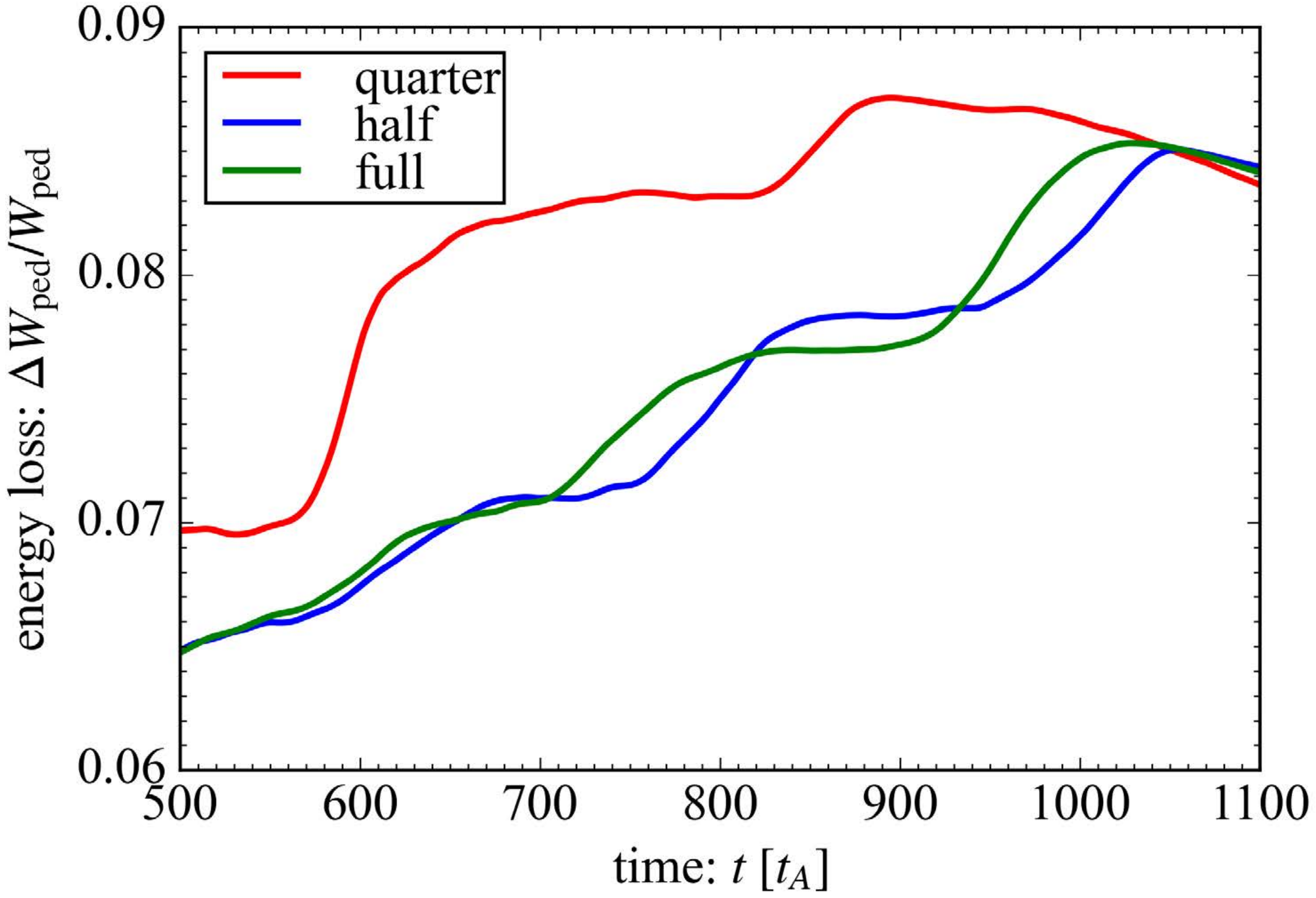
Impact of binormal domain length on energy loss after pedestal collapse



Energy loss enhancement by interplay between zonal flow (ZF) and turbulence [Seto PoP'19] is also observed in full torus case as well as half and quarter torus cases

- Similar energy loss level
- cf.) generation mechanism of ZF [Yagi PET2021]
  - ❖Reynolds stress cancels with Maxwell stress
  - ❖Pressure gradient drives ZF via geodesic curvature

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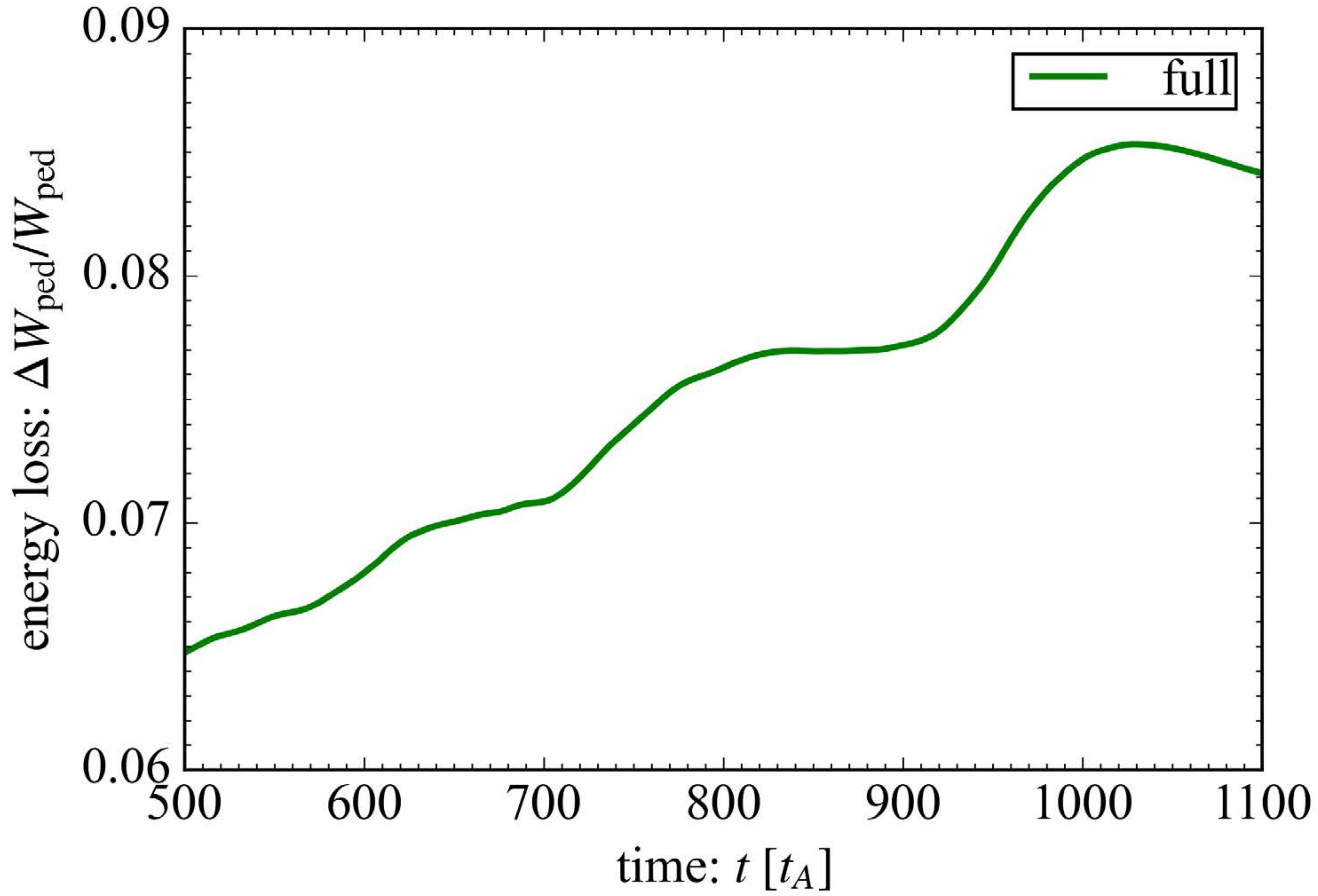

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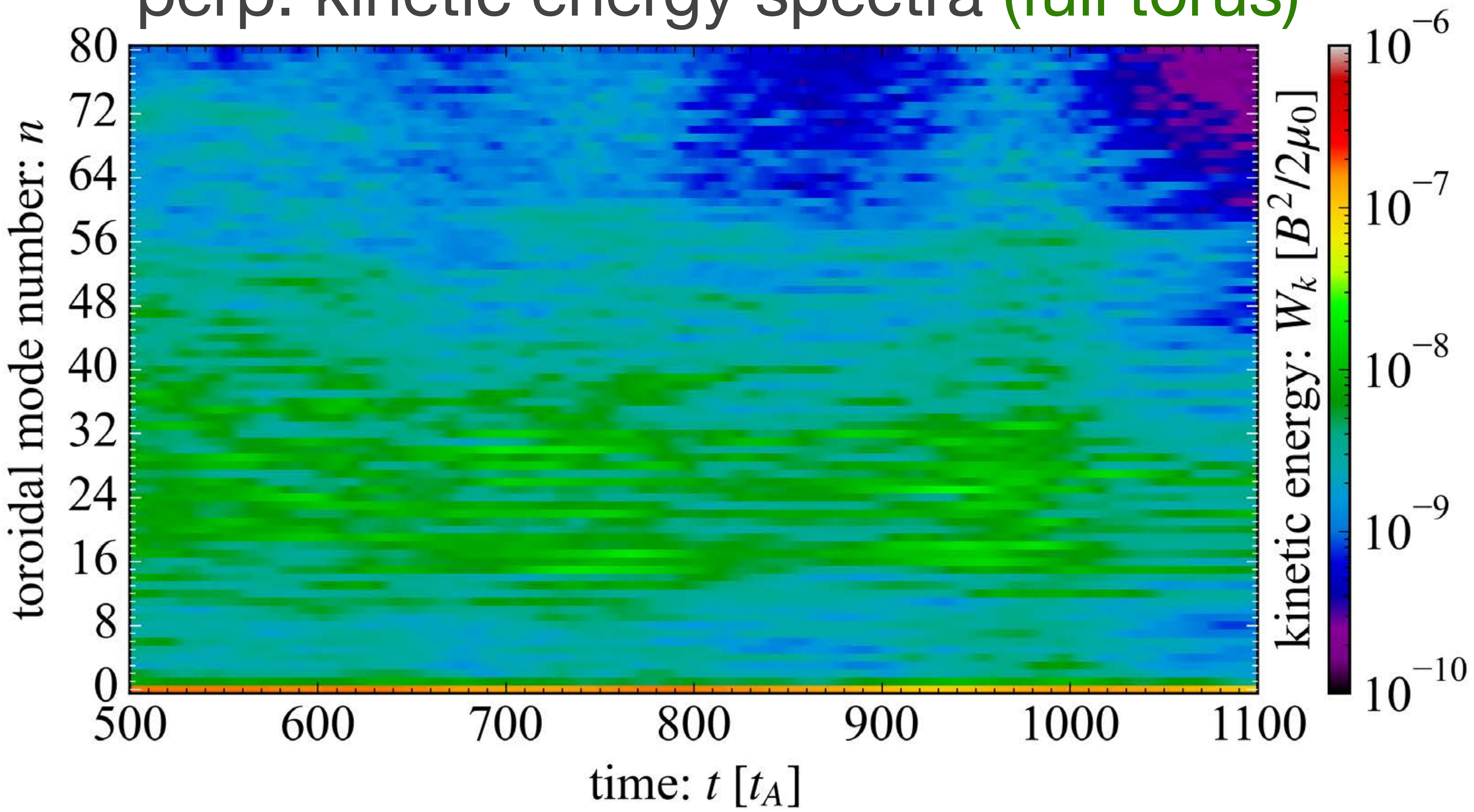

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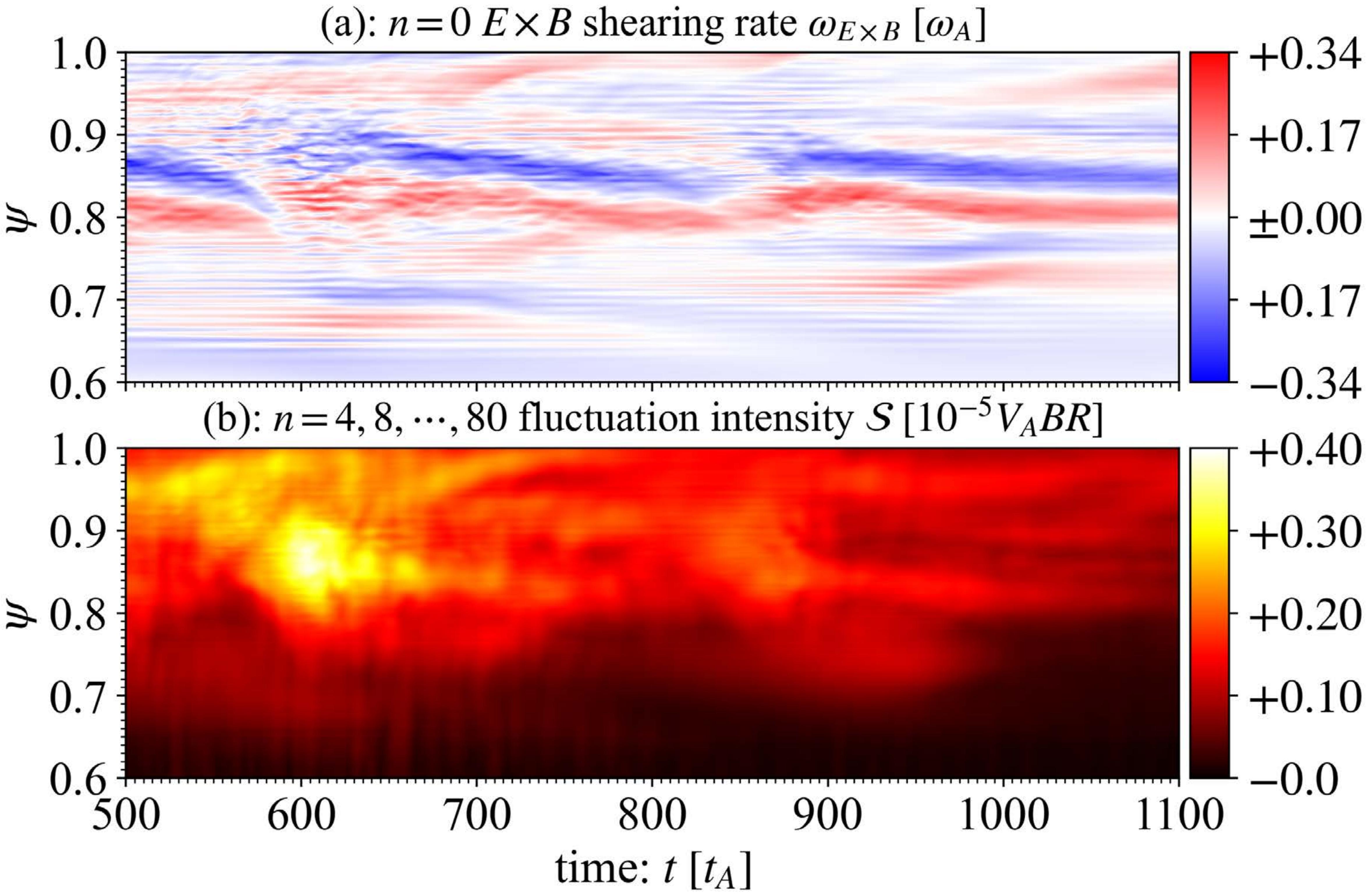
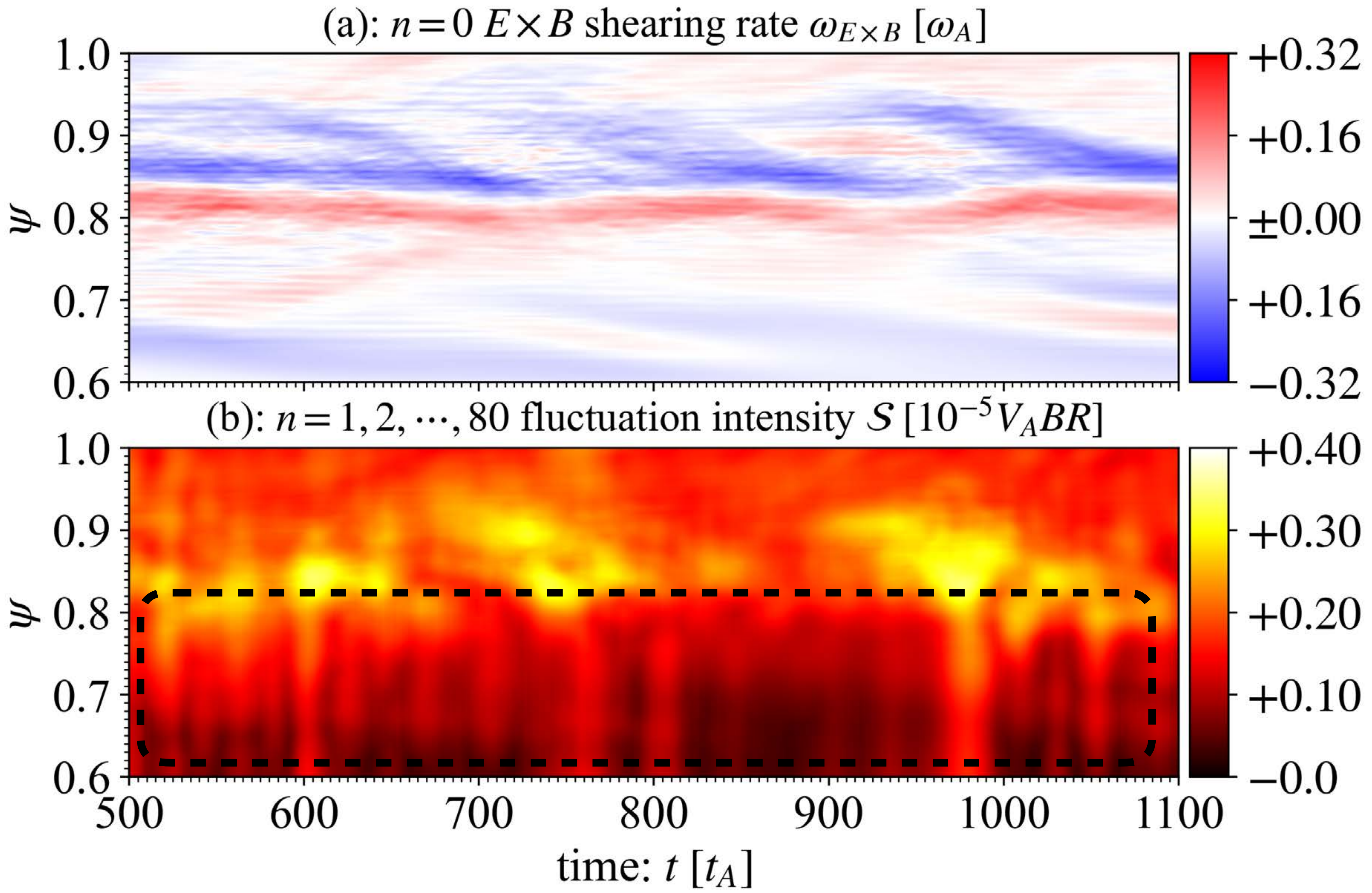
Turbulence burst occurs periodically after the pedestal collapse

Spatio-temporal structure of flow and turbulence after pedestal collapse

flow & turbulence structure: quarter torus



flow & turbulence structure: full torus



Fluctuation intensity: $\mathcal{S}(\psi) = \sqrt{\sum_{n\neq 0}\sum_{m} \phi(\psi, m, n)\phi(\psi, -m, -n)}$

- Turbulence bursts with cyclic oscillation between ZF and turbulence are observed in all cases
- n=1 fluctuation has global structure whose peak is located at turbulence bursts in full torus case

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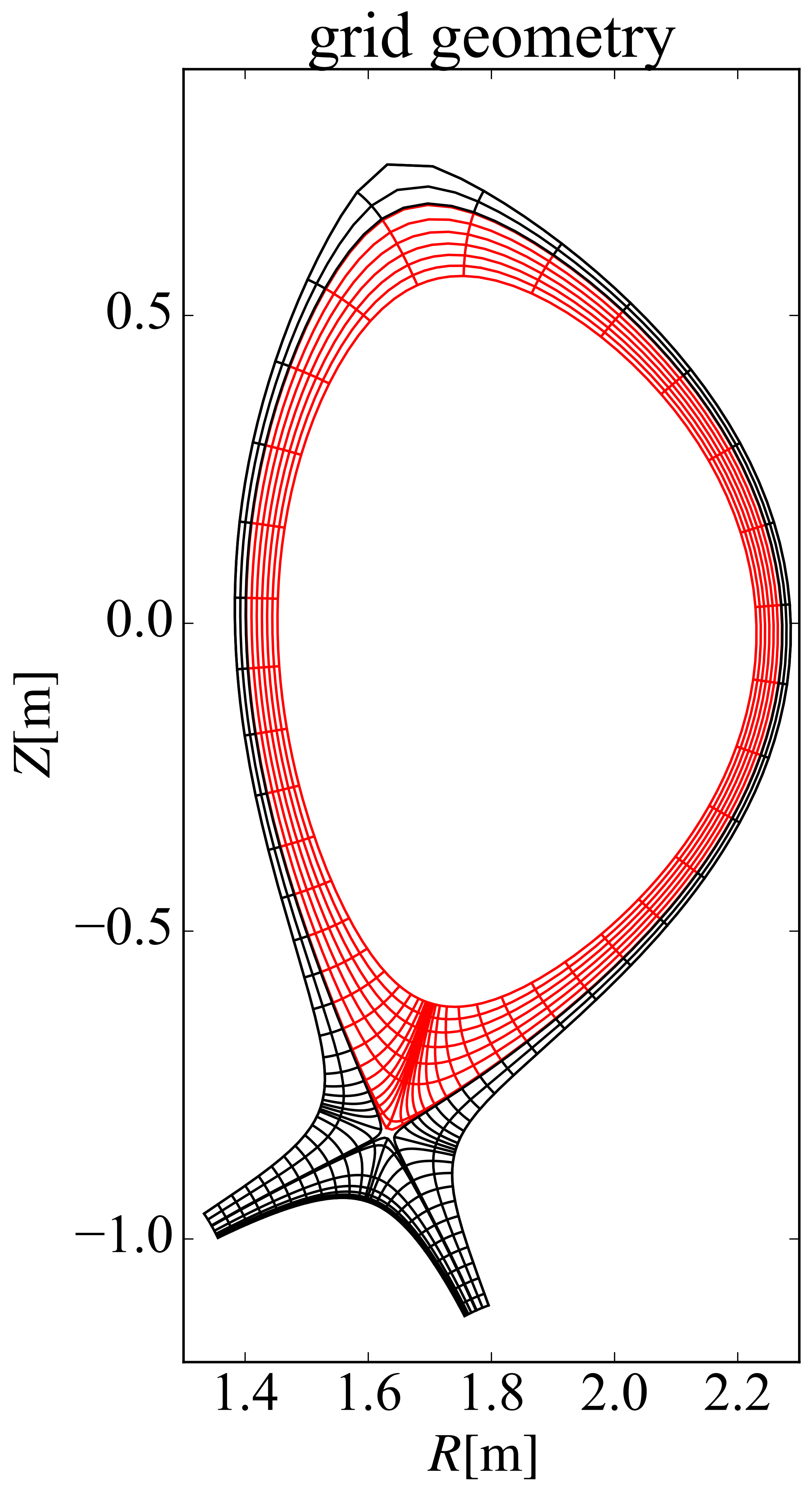
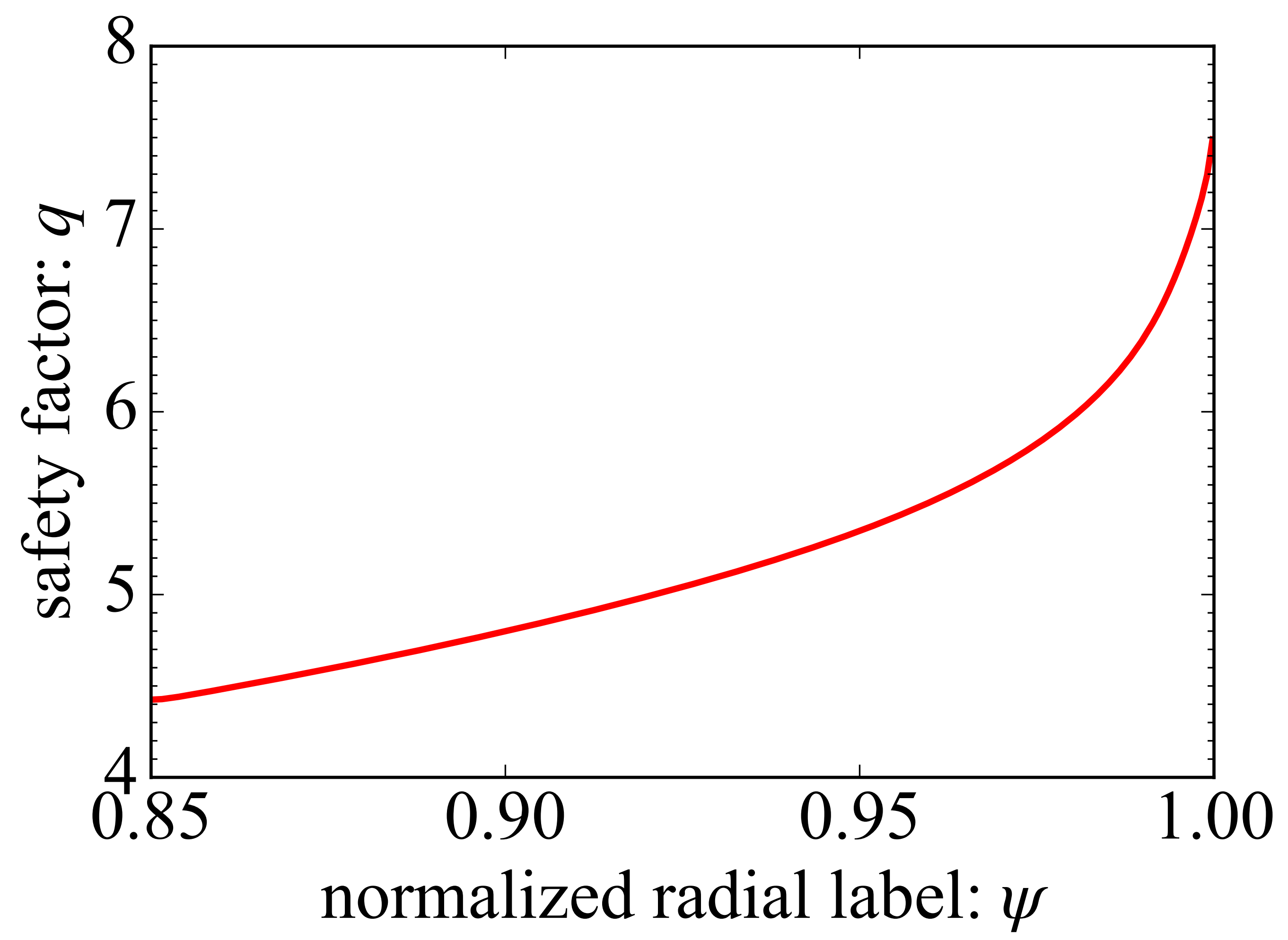
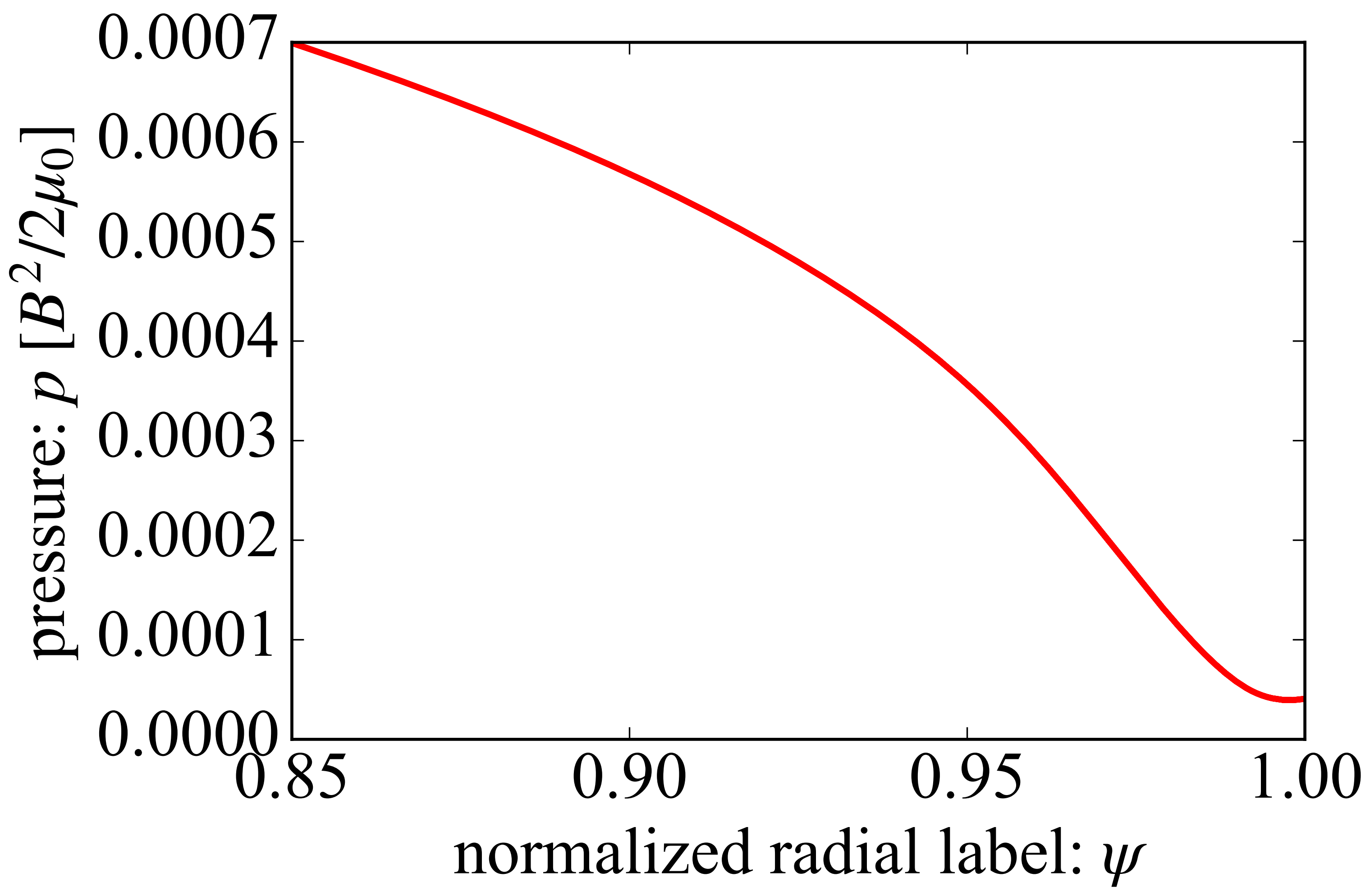
Numerical grid for full torus pedestal collapse in single-null configuration







Grid information

- Nx=260 (Ny_core=195) for $[0.85,1.05]$
- Ny=288 (Ny_core=192)
- Nz=256 for zperiod=1, $[0,2\pi]$
- lowpass=80, n=0,1,2,…,80 are taken
  - ✓ n=0, 1, …, 4: 2D Poisson solver
  - ✓ n=5, 6, …, 80: 1D Poisson solver

Governing equation and assumptions

Scale separated 3-field DW+RBM model (simplified ion diamagnetism + electron Hall effect)

$$\frac{\partial}{\partial t}\varpi_1 = -[\phi_1, \varpi] - B_0\partial_\parallel\left(\frac{J_{\parallel 1}}{B_0}\right) + B_0\left[A_{\parallel 1}, \frac{J_\parallel}{B_0}\right] + \mathcal{K}(p_1) + \mu_\parallel\partial_\parallel^2\varpi_1 + \mu_\perp\nabla_\perp^2\varpi_1,$$

$$\frac{\partial}{\partial t}p_1 = -[\phi_1, p] + \chi_\parallel\partial_\parallel^2 p_1 + \chi_\perp\nabla_\perp^2 p_1,$$

$$\frac{\partial}{\partial t}A_{\parallel 1} = -[\phi, A_{\parallel 1}] - \partial_\parallel\phi_1 + \delta_e\left(\partial_\parallel p_1 - [A_{\parallel 1}, p]\right) + \eta J_{\parallel 1}$$

$$\varpi = \nabla_\perp^{*2}F, \quad J_1 = \nabla_\perp^2 A_\parallel, \quad F = \phi + \delta_i p, \quad \phi = \phi_0 + \phi_1, \quad p = p_0 + p_1,$$

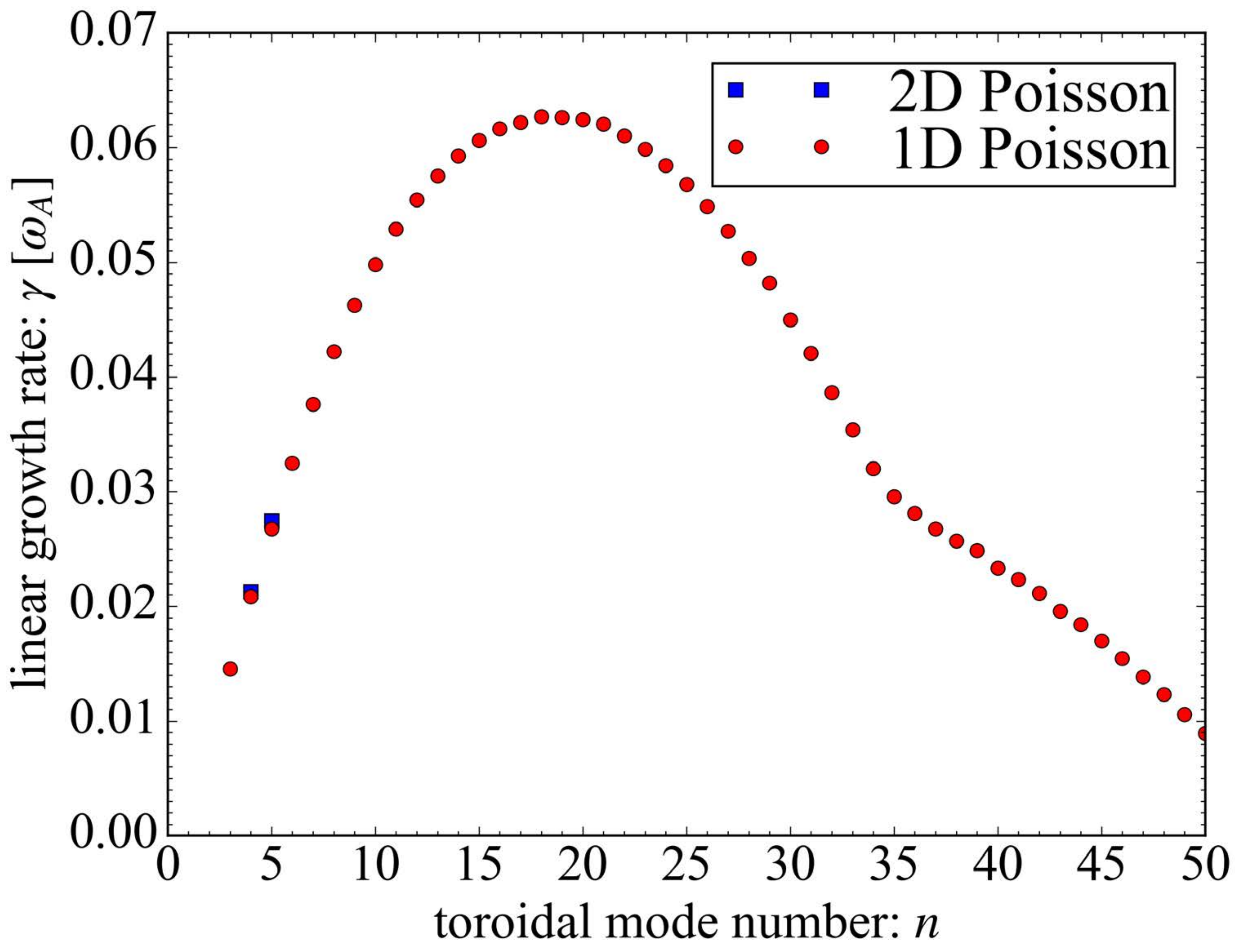
$$\boldsymbol{B} = \boldsymbol{B}_0 + \nabla A_{\parallel 1}\times\boldsymbol{b}_0, \quad J_\parallel = J_{\parallel 0} + J_{\parallel 1},$$

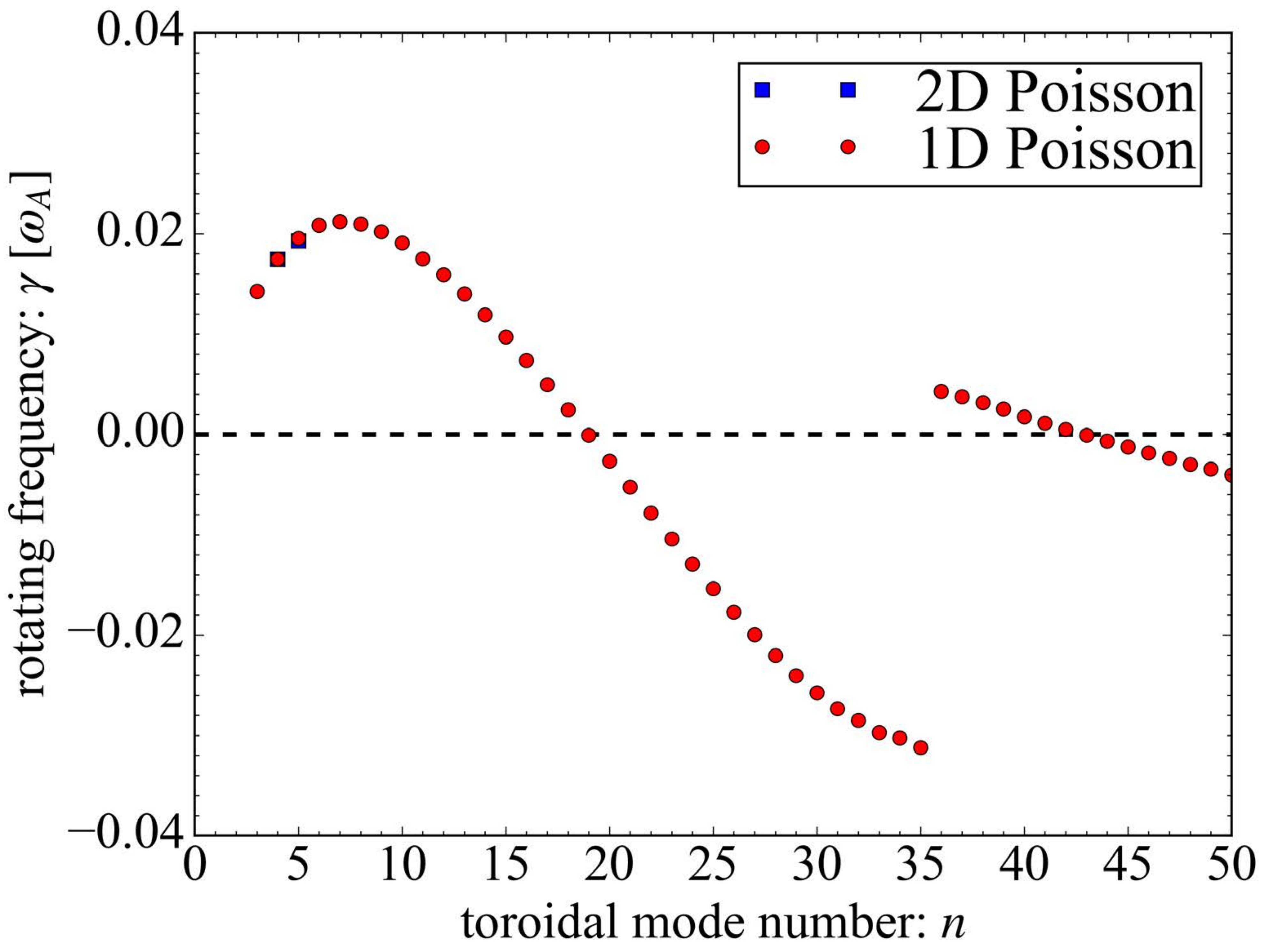
Bmag	3.129918 [T]
Rmag	2.286076 [m]
n_0	10^{19} [m^{-3}]
$\mu_{/\!/}$	1.0×10^{-1}
$\mu_\perp$	1.0×10^{-7}
$\chi_{/\!/}$	1.0×10^{-1}
$\chi_\perp$	1.0×10^{-7}
η	1.0×10^{-6}

- Normalized with poloidal Alfven unit
- Use equilibrium pressure and parallel current profiles
- Use modeled constant ion number density and dissipations (not based on equilibrium)
- No equilibrium radial electric field, SOL/DIV physics

Preliminary test only for checking whether the hybrid Poisson solver makes full annular torus simulation possible

Dispersion relation of preliminary pedestal collapse simulation





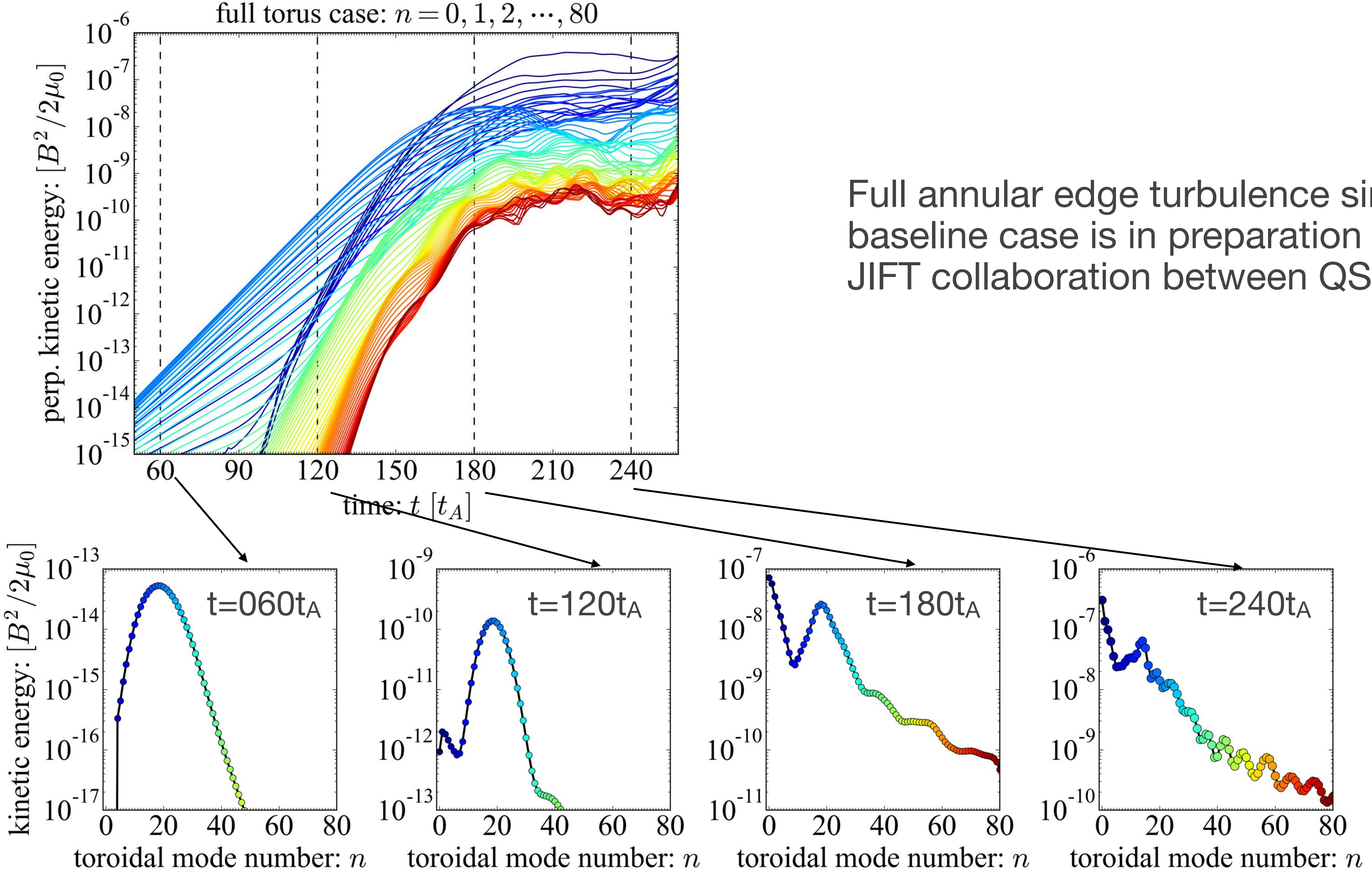
- n≥36 modes are no longer in ballooning branch, they have broad structures in radial direction

  ➡Pedestal collapse is triggered mainly by DWRBMs spectra whose peak is n=18

- n=3 is stable for DWRBM with 2D Poisson solver while n=3 is unstable for DWRBM with 1D solver
- Small (~3%) differences in n=4 and n=5 growth rate between 2D and 1D Poisson solver

  ➡Using 2D Poisson solver for n ≤4 seems to be appropriate

Kinetic energy grows in reasonable manner and low-n modes get excited



Full annular edge turbulence simulations in ITER baseline case is in preparation partially under JIFT collaboration between QST and LLNL

Outline

- Introduction: BOUT++ code and objectives of TOKEDGE project
- Numerical scheme of a hybrid Poisson solver for full annular tokamak edge simulations
- **[Erratum of CSC WS’21]** impact of flute-ordering assumption in low-n ideal ballooning mode
- Pedestal collapse simulation in full annular tours domain in shifted circular geometry
- Preliminary test of full annular torus turbulence simulation in single-null divertor geometry
- Summary

Summary

A hybrid Poisson solver for full annular tokamak edge turbulence simulation has been developed

- **[Erratum of CSC WS'21] impact of flute-ordering assumption in low-n ideal ballooning mode**
  ❖Flute-ordering (in Laplacian for J//) has large impact on IBM growth rate in the presented case

- **Pedestal collapse simulation in full annular tours domain in shifted circular geometry**
  ❖Low-n modes generated via nonlinear couplings among initially unstable modes before pedestal collapse for half and full tori

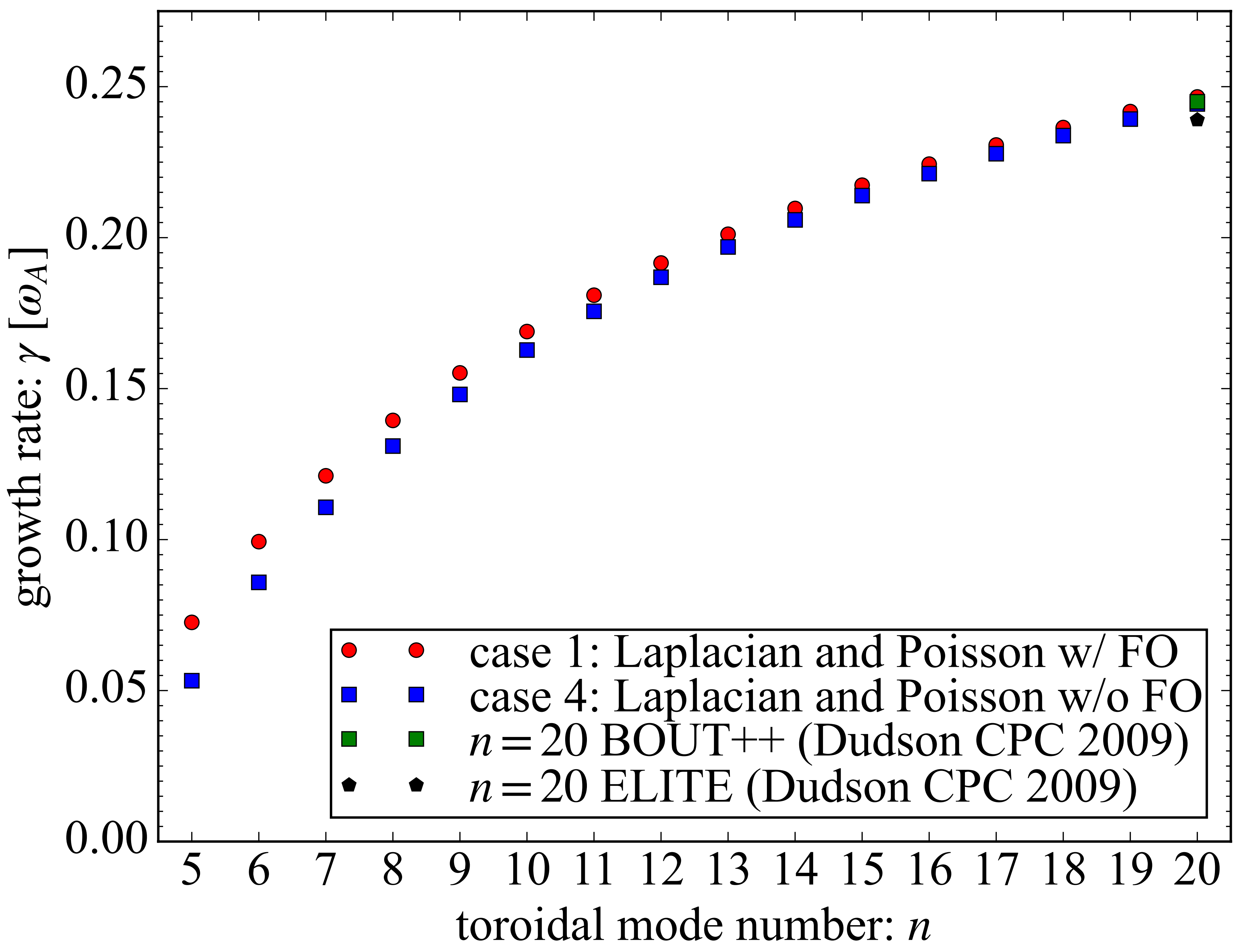
  ❖n=1 fluctuation has global radial structure during / after collapse in full torus case

  ❖Energy loss enhancement by interplay between flow and turbulence is observed after the pedestal collapse and energy loss levels are saturated to a similar level in all cases

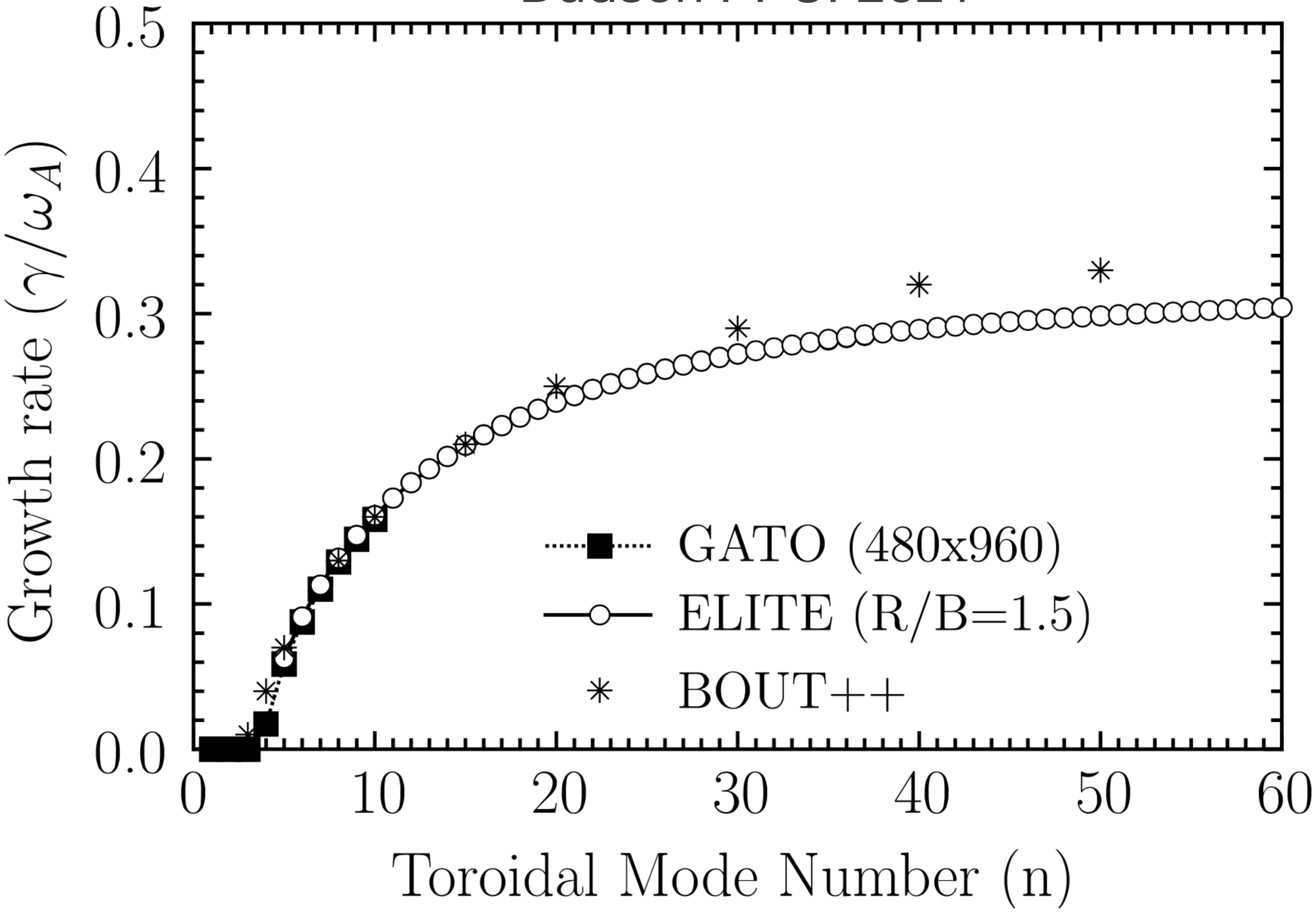
- **Preliminary test of full annular torus turbulence simulation in single-null divertor geometry**
  ❖Hybrid Poisson solver enables nonlinear full annular torus simulation in diverted geometry

  ❖Production run with ITER baseline equilibrium is in preparation

Backup Slide



Dudson PPCF2021



2D Poisson solver test 2: linear resistive ballooning mode in single null geometry

2D Poisson solver is tested in single-null geometry by comparing linear RBM growth rates by 2D Poisson solver and those by1D flute-ordered Poisson solver

Linearized RBM model with dissipation

$$\frac{\partial \varpi_1}{\partial t} = B_0 \partial_\parallel \left(\frac{J_\parallel}{B_0} \right) - B_0 \left[A_{1\parallel}, \frac{J_{\parallel 0}}{B_0} \right] + \frac{\boldsymbol{b}_0 \times \boldsymbol{\kappa}_0 \cdot \nabla P_1}{B_0} + \mu_\perp \nabla_\perp^2 \varpi_1 + \mu_\parallel \partial_\parallel^2 \varpi_1$$

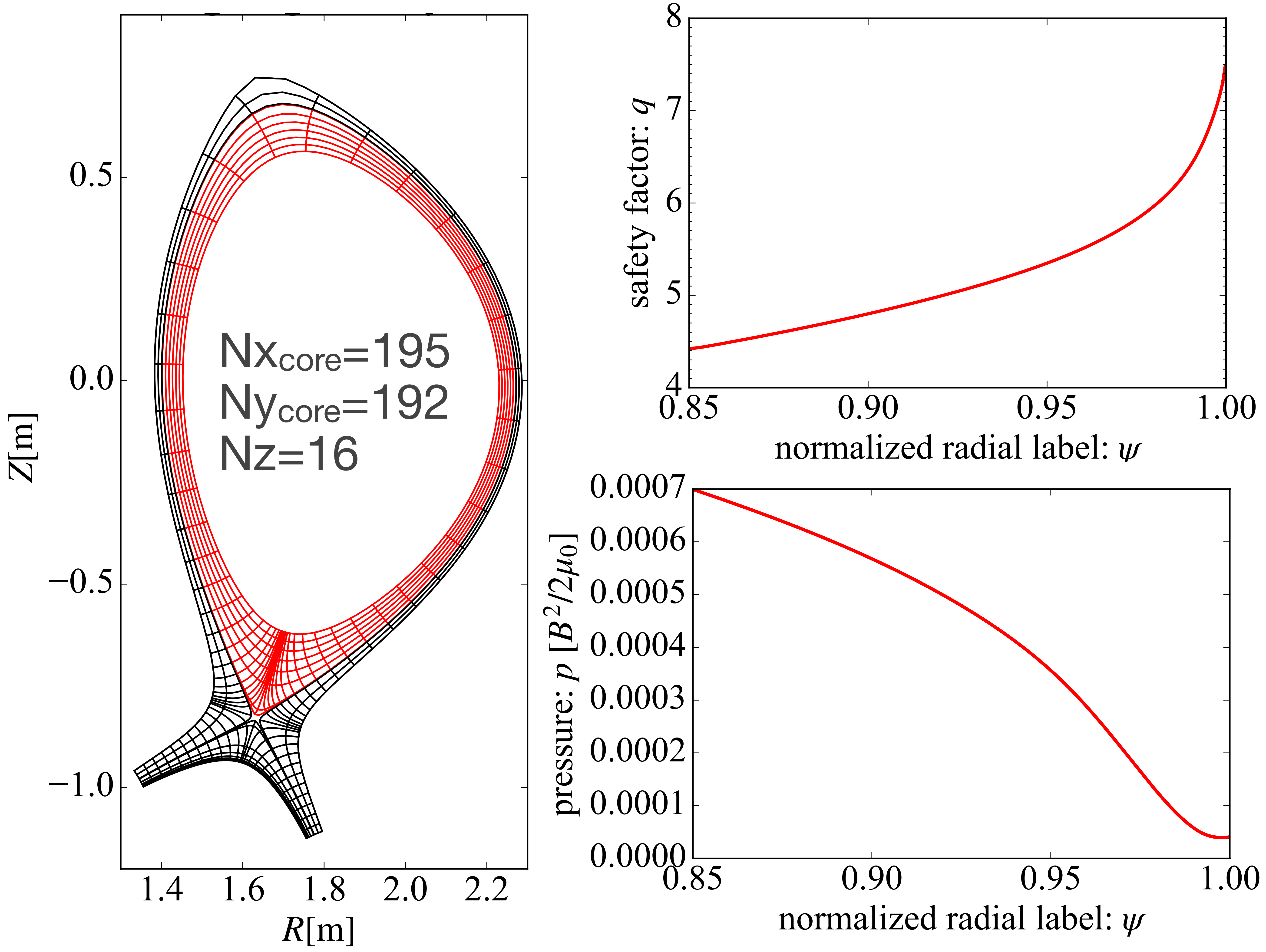
$$\frac{\partial P_1}{\partial t} = - [\phi_1, P_0]$$

$$\frac{\partial A_{\parallel 1}}{\partial t} = - \partial_\parallel \phi_1 + \eta J_{\parallel 1}$$

$$\varpi = \nabla \cdot \left(\frac{1}{B_0^2} \nabla_\perp \phi \right), \quad J_{\parallel 1} = \nabla_\perp^2 A_{\parallel 1}$$

$$\eta = 10^{-6}, \quad \mu_\perp = 10^{-7}, \quad \mu_\parallel = 10^{-1}$$

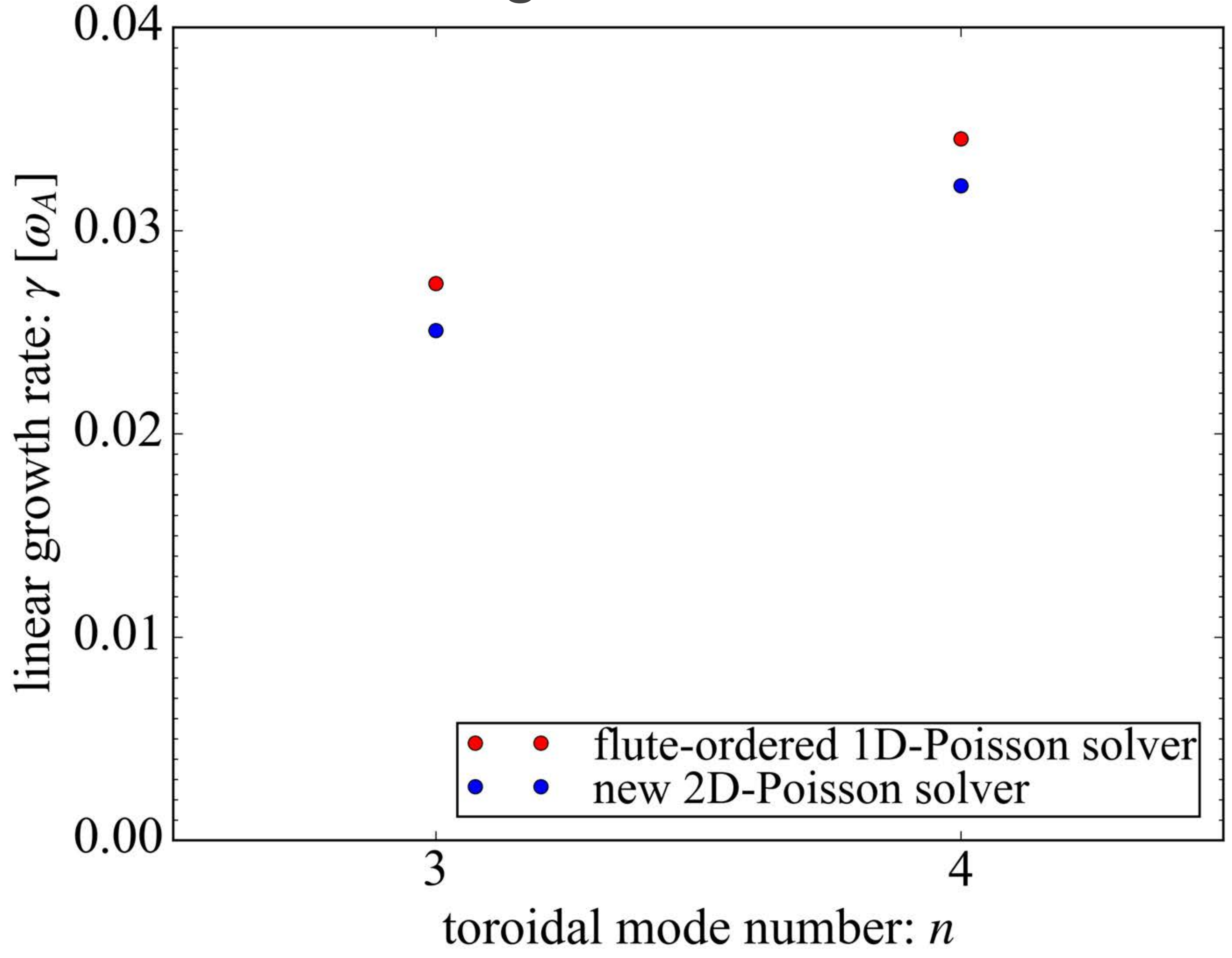
- constant ion density $n_{i0} = 10^{19}$ [m^{-3}]
- Dissipations in vorticity equation are required for numerical stability in both 2D and 1D Poison solver.



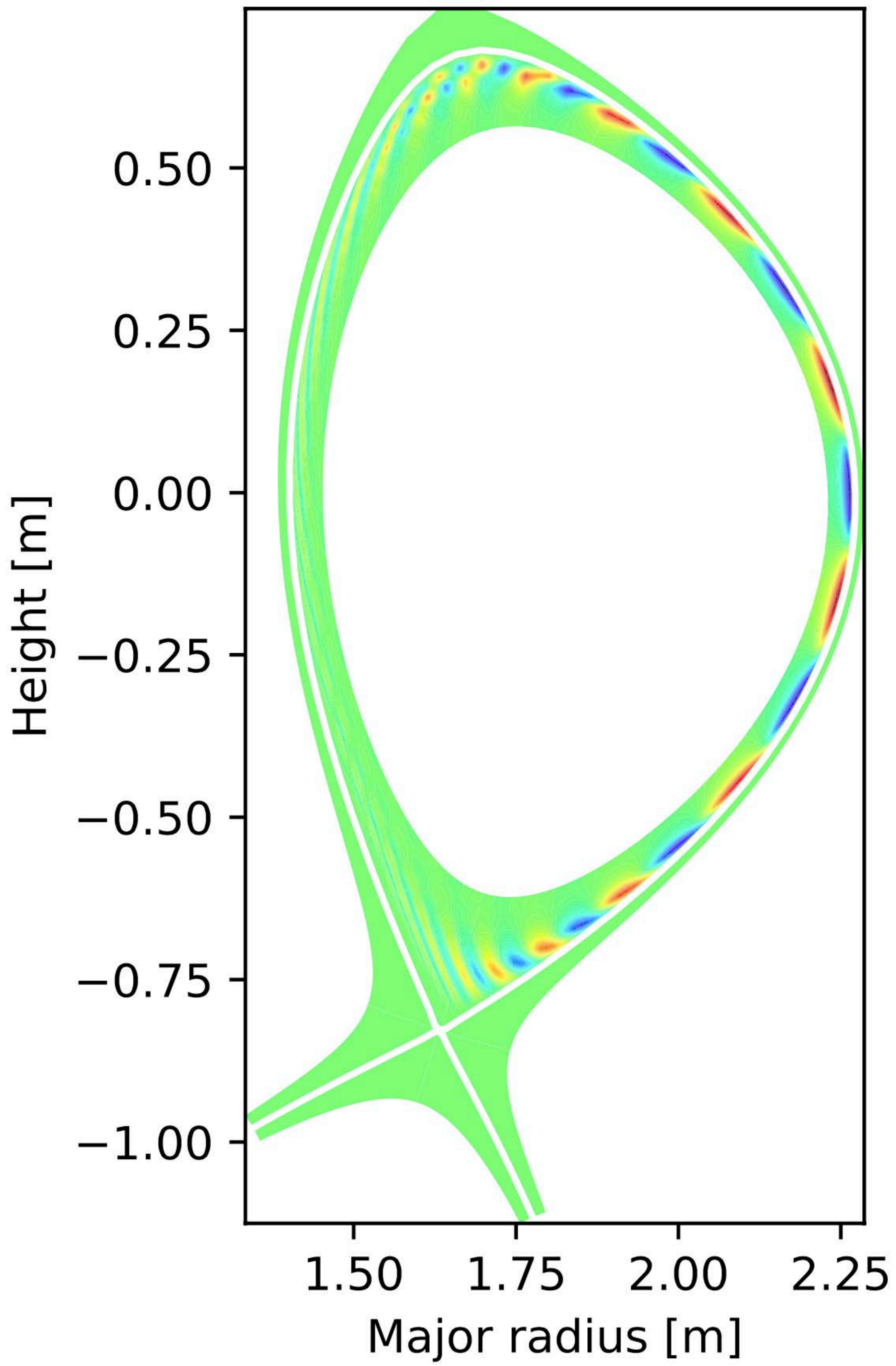
- $1/n$-th annular wedge domain for n=3,4
- z-derivatives are evaluated with FFT

2D Poisson solver captures RBM instability but growth rates are different

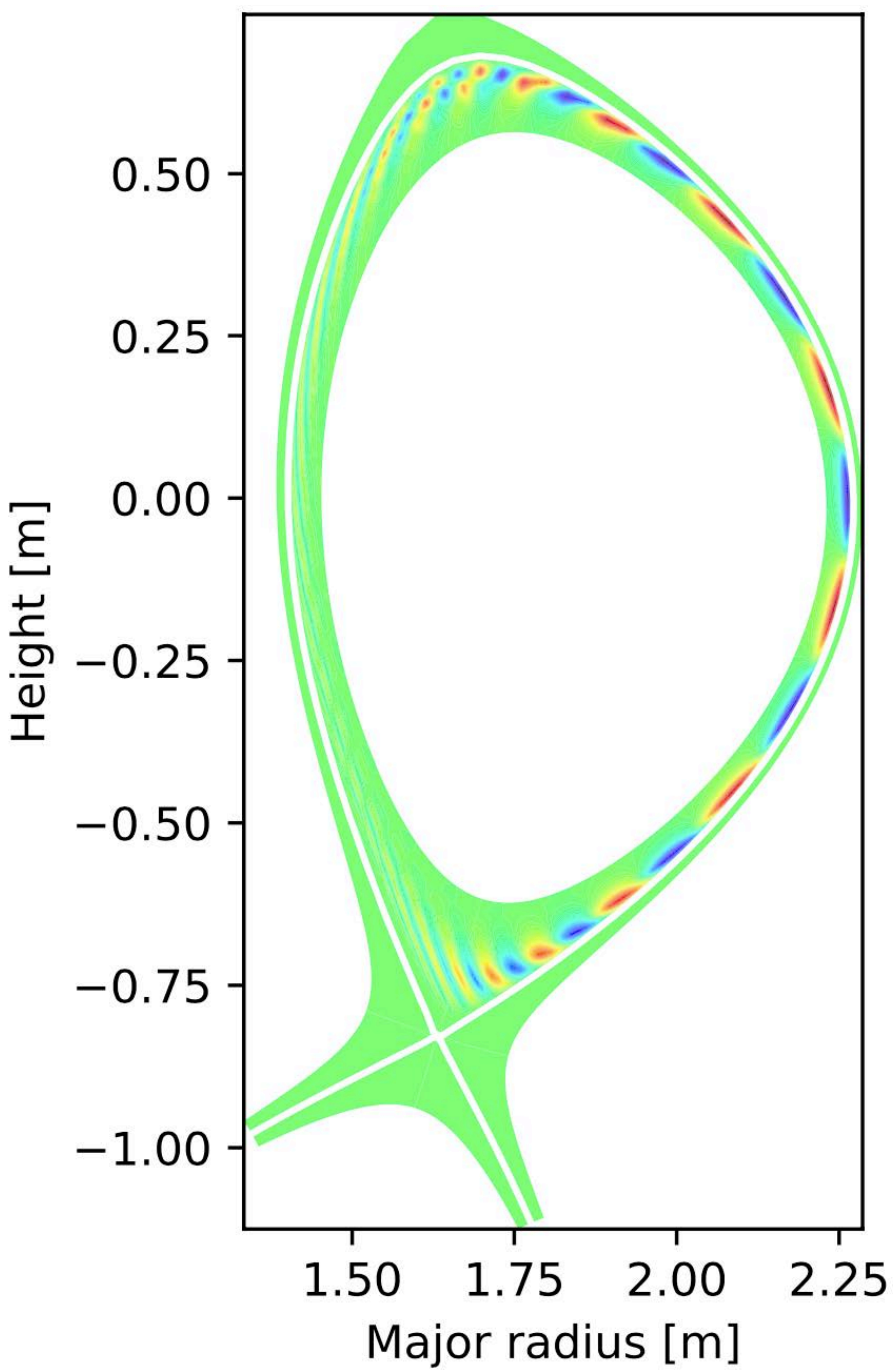
Linear growth rate of RBM



n=4 perturbed pressure by 1D Poisson solver



n=4 perturbed pressure by 2D Poisson solver

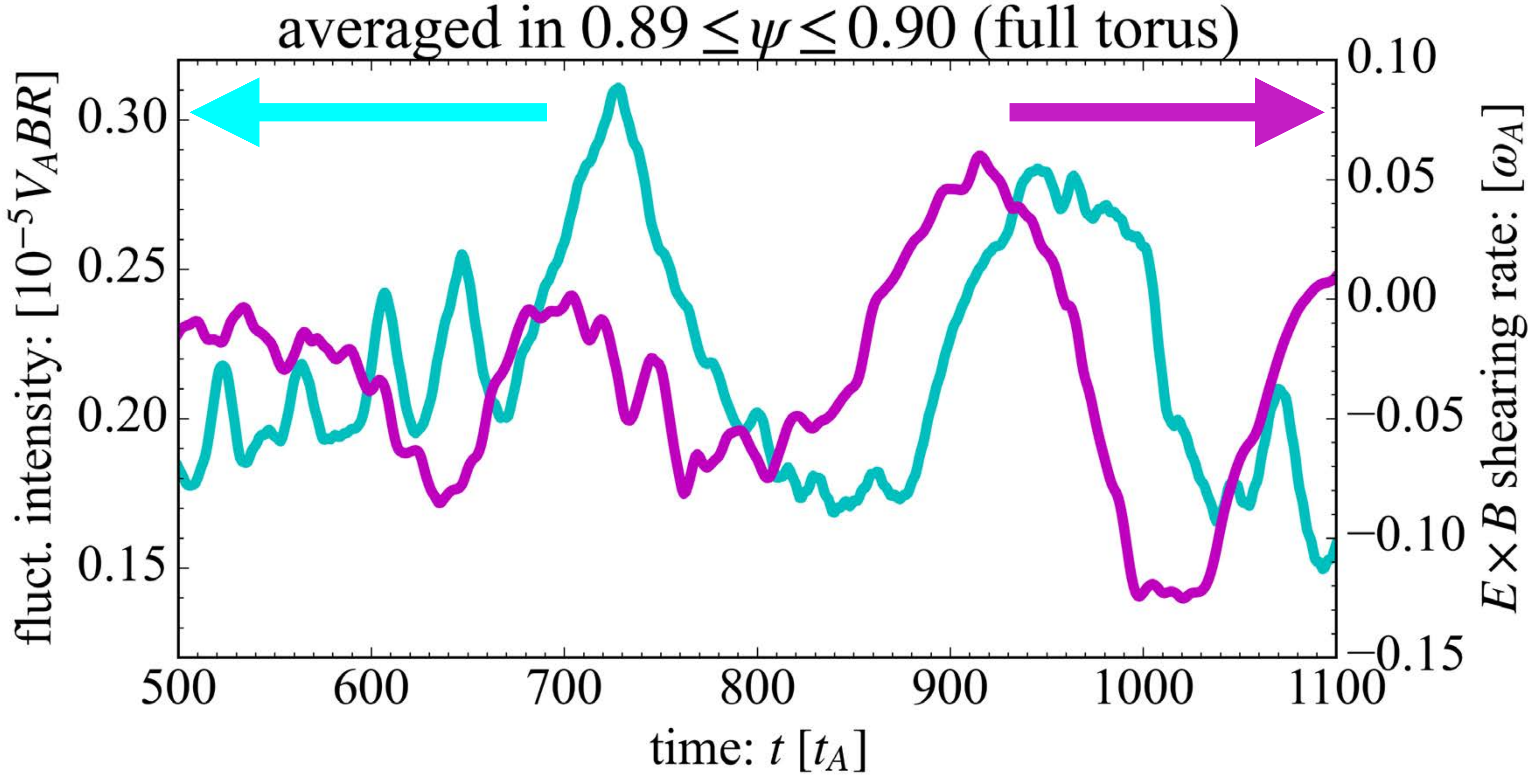


RBM eigen-functions are clearly obtained by both Poisson solvers but their growth rates are different by 6~8%

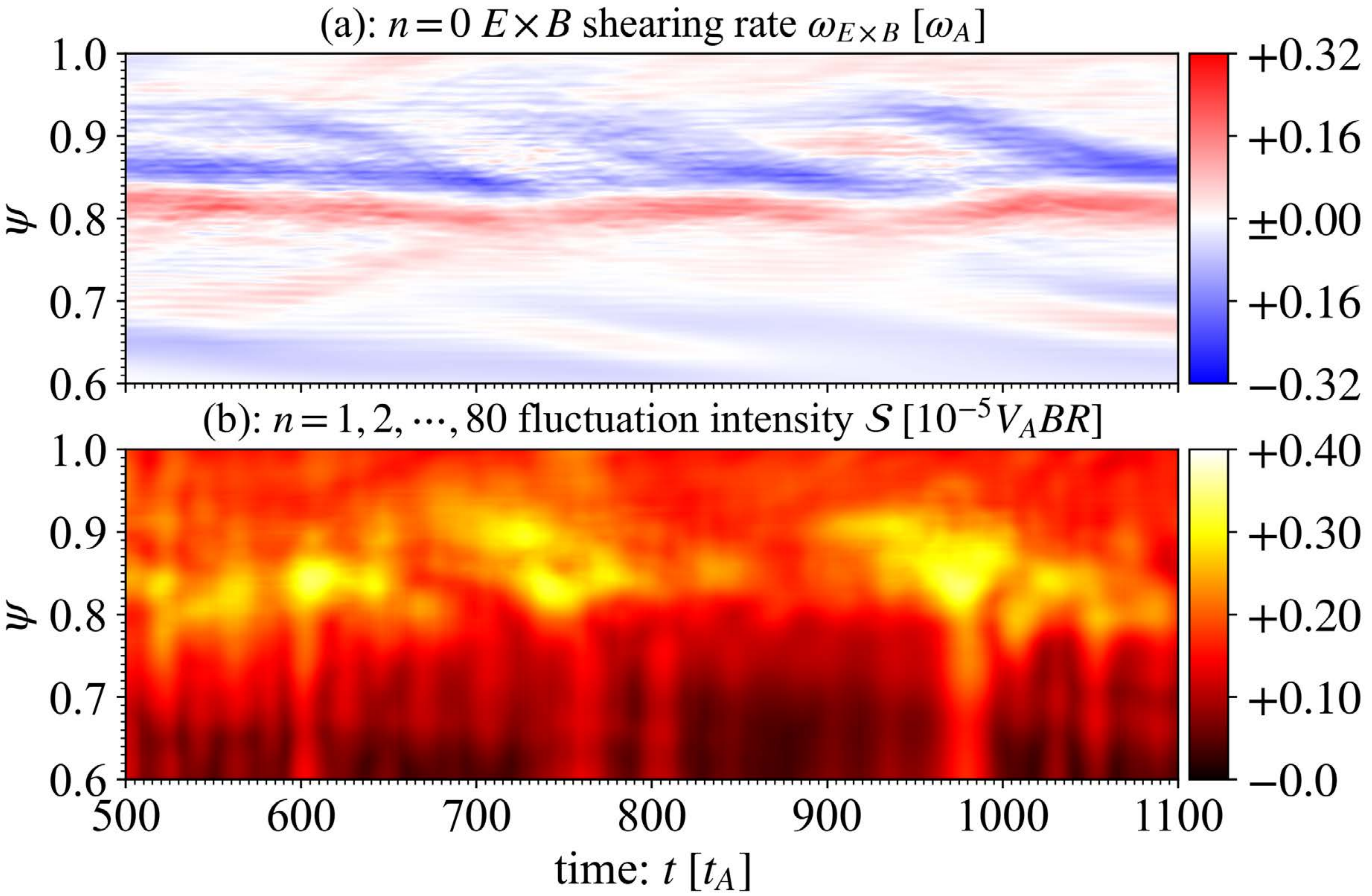
➡Further tests (mesh convergence etc…) are required to clarify impact of flute-ordering in complex geometries

Spatio-temporal structure of flow and turbulence after pedestal collapse

flow & turbulence phase: full torus



flow & turbulence structure: full torus

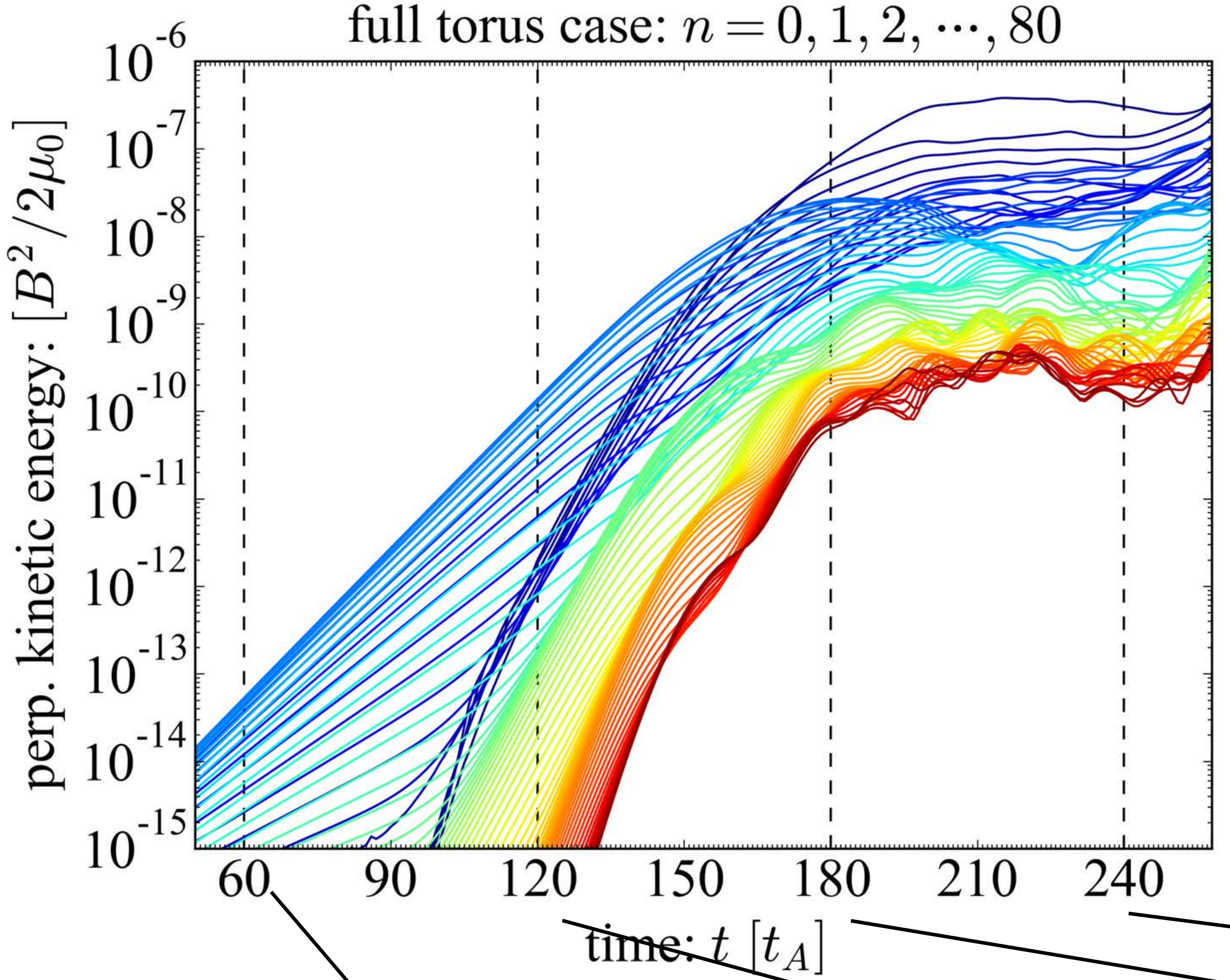


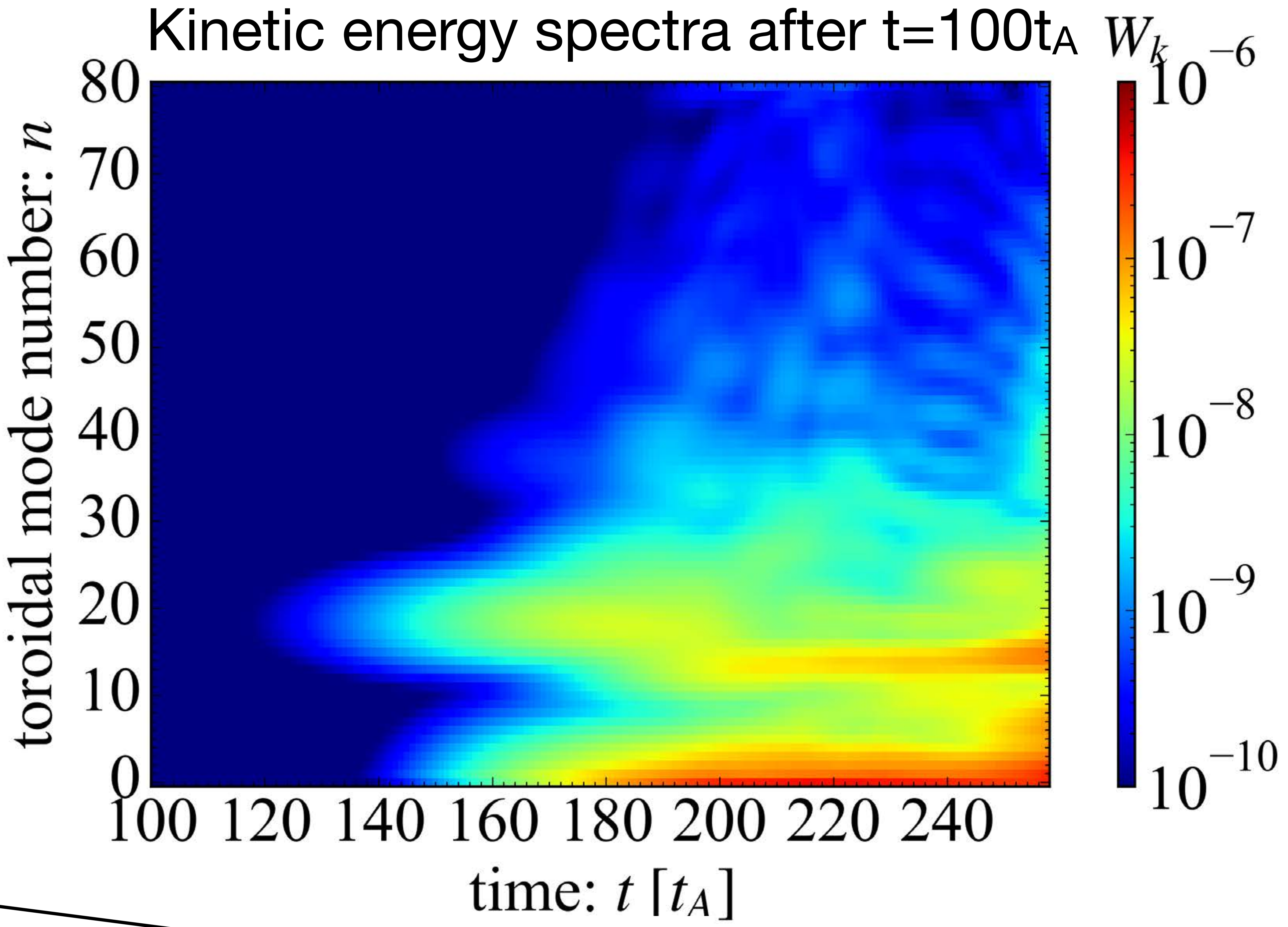
Electromagnetic oscillations (ZF -> turb.) rather than electrostatic oscillations (turb. -> ZF)

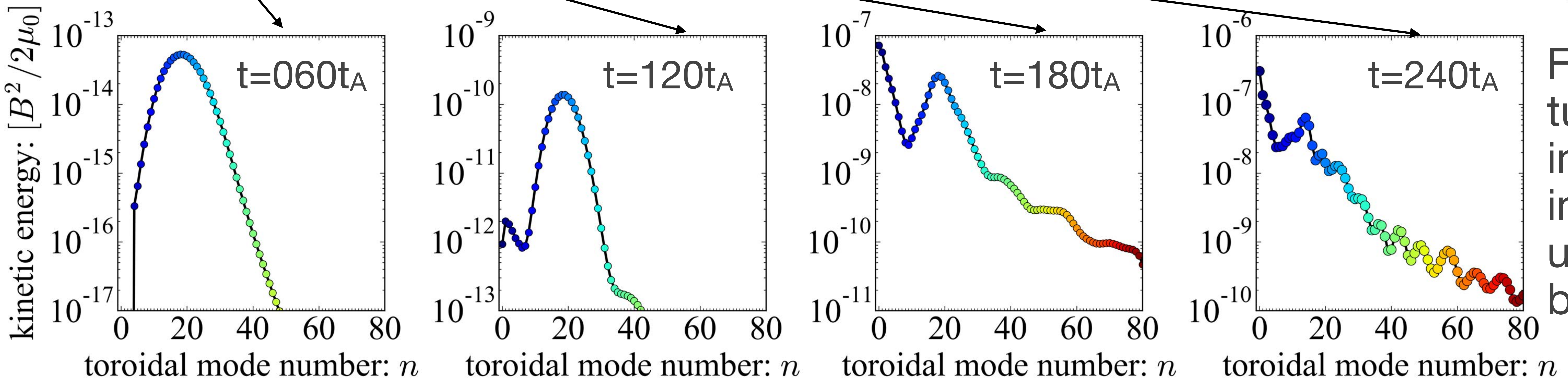
Fluctuation intensity: $\mathcal{S}(\psi) = \sqrt{\sum_{n\neq 0}\sum_{m} \phi(\psi,m,n)\phi(\psi,-m,-n)}$

- Turbulence bursts with cyclic oscillation between ZF and turbulence are observed in all cases
- n=1 fluctuation has global structure whose peak is located at turbulence bursts in full torus case

Kinetic energy grows in reasonable manner and low-n modes get excited







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