ITPA-EP TAE benchmarking using a new gyrokinetic code TEK

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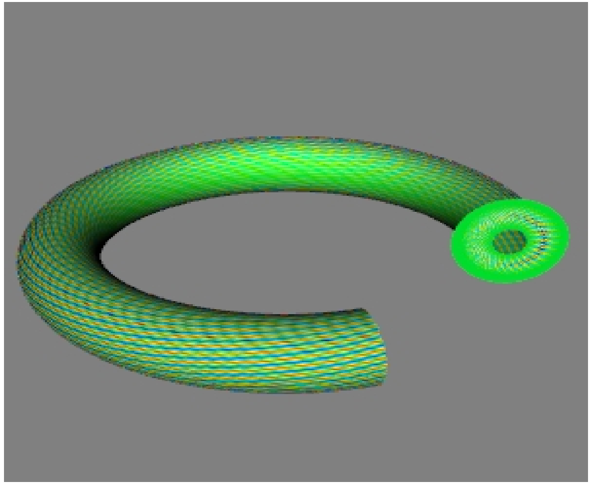
δf gyrokinetic PIC code: TEK

- **Electromagnetic perturbations** (using the **mixed-variable pullback** mitigation)
- **Both ions and electrons are treated with gyrokinetic model (FLR neglected for electrons)**
- **Multiple ion species (EPs, impurities)**
- **Arbitrary numerical configurations and profiles**
- **Verified with other codes in simulating：**
  - **Kinetic Ballooning Modes (KBMs)**
  - **EP-driven modes (e.g.,TAEs)**
- **Open source: https://github.com/Youjunhu/TEK**



TEK uses field-aligned coordinates (similar to GENE, GYRO, GEM)

$x = \psi$ → **Arbitrary magnetic surface label**

$z = \theta$ → **Arbitrary poloidal angle**

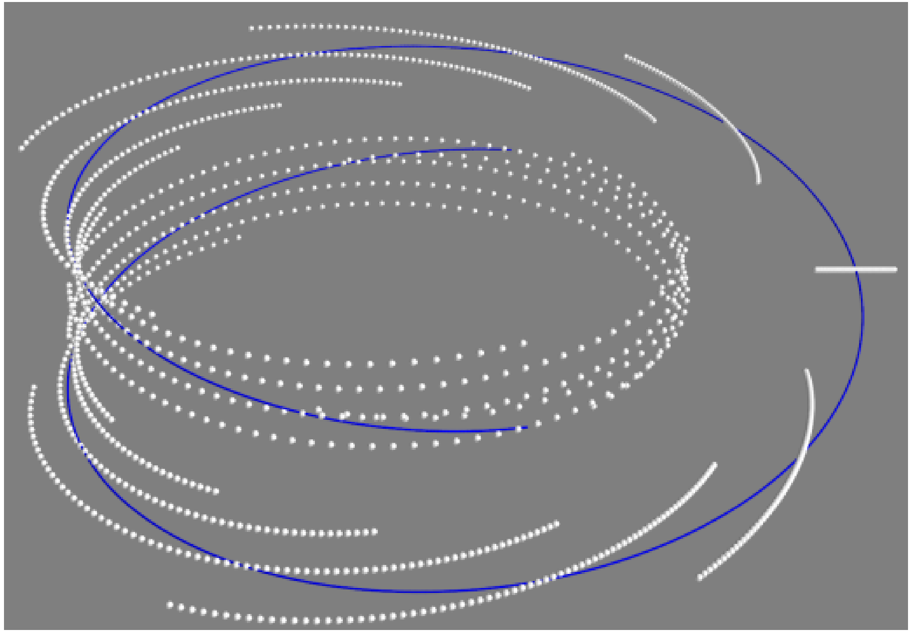
$y = \phi - \int_0^\theta \frac{\mathbf{B}\cdot\nabla\phi}{\mathbf{B}\cdot\nabla\theta} d\theta$ → **Generalized toroidal angle**

$\frac{\partial \mathbf{r}}{\partial x}|_{y,z} \longrightarrow$ combination of the usual radial and toroidal direction → **Sine expansion**

$\frac{\partial \mathbf{r}}{\partial y}|_{x,z} \longrightarrow$ usual toroidal direction, $\hat{\phi}$ → **Fourier expansion**

$\frac{\partial \mathbf{r}}{\partial z}|_{x,y} \longrightarrow$ field line direction → **Finite difference**

Spatial grid example (x, y, z) = (64 x 1 x 16)



- Gridpoints (white dots) for a fixed value of y.
- The blue line is a field line: $\partial \mathbf{r} / \partial z$

Neglecting the displacement current, Maxwell' equations in Coulomb gauge $(\nabla \cdot \mathbf{A} = 0)$ are written as

$$-\nabla^2 \delta\Phi = \frac{\delta\rho_c}{\varepsilon_0},$$ → **from gyrokinetic**

$$-\nabla^2 \delta\mathbf{A} = \mu_0 \delta\mathbf{J},$$

with $\delta\mathbf{E}$ and $\delta\mathbf{B}$ given by

$$\delta\mathbf{B} = \nabla \times \delta\mathbf{A},$$

$$\delta\mathbf{E} = -\nabla\delta\varphi - \frac{\partial\delta\mathbf{A}}{\partial t},$$

Conventional gyrokinetic simulations keep only the parallel component of $\delta\mathbf{A}$, and Ampere's law is approximated as

$$-\nabla_\perp^2 \delta A_\parallel = \mu_0 \delta J_\parallel$$ → **from gyrokinetic**

Frieman-Chen gyrokinetic equation (for the special case $\partial F_0/\partial\mu|_\varepsilon = 0$)

$$\frac{\partial \delta G}{\partial t} + \Bigg(v_\parallel \mathbf{e}_\parallel + \mathbf{V}_D - \underbrace{\frac{q}{m}\nabla\langle\delta L\rangle \times \frac{\mathbf{e}_\parallel}{\Omega}}_{\text{nonlinear}} \Bigg) \cdot \nabla \delta G$$

$$= \underbrace{\left(\frac{q}{m}\nabla\langle\delta L\rangle \times \frac{\mathbf{e}_\parallel}{\Omega}\right) \cdot \nabla F_0}_{\text{spatial-drive}} - \frac{q}{m}\frac{\partial\langle\delta L\rangle}{\partial t}\frac{\partial F_0}{\partial \varepsilon}.$$

where $\delta G(\mathbf{X}, \varepsilon, \mu, t)$ is related to the distribution function perturbation δF by

$$\delta F = \frac{q}{m}\delta\Phi\frac{\partial F_0}{\partial \varepsilon} + \delta G,$$

where the first term is called "adiabatic part".

Time derivative of unknowns. Problematic for simulation

$$\langle\delta L\rangle = \langle\delta\Phi\rangle - v_\parallel\langle\delta A_\parallel\rangle$$

$$\varepsilon = \frac{v^2}{2}, \mu = \frac{v_\perp^2}{2B_0}$$

$\langle\ldots\rangle$ **is gyro-average operator**

Eliminate $\partial\langle\delta\Phi\rangle/\partial t$ ———> Polarization term

It turns out that $\partial\langle\delta\Phi\rangle/\partial t$ can be eliminated by defining another gyro-phase independent function δf by

$$\delta f = \frac{q}{m}\langle\delta\Phi\rangle\frac{\partial F_0}{\partial\varepsilon} + \delta G$$

Then

$$\begin{aligned}
&\left[\frac{\partial}{\partial t} + (v_\parallel \mathbf{e}_\parallel + \mathbf{V}_D + \delta\mathbf{V}_D)\cdot\nabla\right]\delta f \\
= \ & -\delta\mathbf{V}_D\cdot\nabla F_0 \\
+ \ & \frac{q}{m}\frac{\partial F_0}{\partial\varepsilon}\left[\frac{\partial\langle v_\parallel\delta A_\parallel\rangle}{\partial t} + \left(v_\parallel\mathbf{e}_\parallel + \mathbf{V}_D + \frac{q}{m}\nabla\langle v_\parallel\delta A_\parallel\rangle\times\frac{\mathbf{e}_\parallel}{\Omega}\right)\cdot\nabla\langle\delta\Phi\rangle\right].
\end{aligned}$$

Eliminate $\partial \langle v_\| \delta A_\| \rangle / \partial t$ —–> skin current (bad)

Define

$$\delta f^{(p_\|)} = \delta f - \frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}\langle v_\| \delta A_\| \rangle.$$

Then

$$\left[\frac{\partial}{\partial t} + (v_\| \mathbf{e}_\| + \mathbf{V}_D + \delta \mathbf{V}_D)\cdot\nabla\right]\delta f^{(p_\|)}$$

$$= \quad -\delta\mathbf{V}_D\cdot\nabla F_0 + \frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}(v_\| \mathbf{e}_\| + \mathbf{V}_D)\cdot\nabla\langle\delta\Phi\rangle$$

$$- \quad \frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}[v_\|(v_\| \mathbf{e}_\| + \mathbf{V}_D)\cdot\nabla\langle\delta A_\|\rangle - \langle\delta A_\|\rangle\mu\mathbf{e}_\|\cdot\nabla B_0],$$

which is called "$p_\|$ formulism" —–> cancellation problem in Ampere's law

Summary of distribution function split

$$F = F_0 + \delta F$$

$$\delta F = \delta f^{(p_\parallel)} + \frac{q}{m}\left(\delta\Phi - \langle\delta\Phi\rangle\right)\frac{\partial F_0}{\partial \varepsilon} + \frac{q}{m}\langle v_\parallel \delta A_\parallel\rangle\frac{\partial F_0}{\partial \varepsilon},$$

Polarization density
(good for simulation),
Makes Poisson'equation easy to solve.

$$\mu_0 \delta j_\parallel^{(\mathrm{skin})} = -\frac{\omega_p^2}{c^2}\delta A_\parallel,$$

Skin current (bad for simulation)
Cancellation error
makes Ampere's law hard to solve

Mixed-variable pull-back*: mitigate cancellation error

Mixed-variables:

$$\delta A_\parallel^{(h)} = \delta A_\parallel - \delta A_\parallel^{(s)},$$

$$\frac{\partial \delta A_\parallel^{(s)}}{\partial t} = -\mathbf{e}_\parallel \cdot \nabla \delta \Phi.$$

$$\delta f^{(\mathrm{mv})} = \delta f - \frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}\langle v_\parallel \delta A_\parallel^{(h)} \rangle.$$

$$\left[\frac{\partial}{\partial t} + (v_\parallel \mathbf{e}_\parallel + \mathbf{V}_D + \delta \mathbf{V}_D)\cdot\nabla\right]\delta f^{(\mathrm{mv})}$$
$$= -\delta \mathbf{V}_D \cdot \nabla F_0 + \frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}(\mathbf{V}_D + \delta \mathbf{V}_D)\cdot\nabla\langle\delta\Phi\rangle$$
$$-\frac{q}{m}\frac{\partial F_0}{\partial \varepsilon}\left[v_\parallel (v_\parallel \mathbf{e}_\parallel + \mathbf{V}_D + \delta \mathbf{V}_D)\cdot\nabla\langle\delta A_\parallel^{(h)}\rangle - \langle \delta A_\parallel^{(h)}\rangle \mu \mathbf{e}_\parallel \cdot \nabla B_0\right].$$

Parallel Ampere's law: $$\left(\left(\sum_j \frac{\omega_{pj}^2}{c^2}\right) - \nabla_\perp^2\right)\delta A_\parallel^{(h)} = \nabla_\perp^2 \delta A_\parallel^{(s)} + \mu_0 \sum_j \delta J_{\parallel j}^{(\mathrm{mv})},$$

At each time-step:

$$\delta A_{\parallel \mathrm{new}}^{(s)} = \delta A_{\parallel \mathrm{old}}^{(s)} + \delta A_{\parallel \mathrm{old}}^{(h)}.$$

$$\delta A_{\parallel \mathrm{new}}^{(h)} = 0.$$

Potential reset

$$\delta f_{\mathrm{new}}^{(\mathrm{mv})} = \delta f_{\mathrm{old}}^{(\mathrm{mv})} + \frac{q}{m}\langle v_\parallel \delta A_{\parallel \mathrm{old}}^{(h)} \rangle \frac{\partial F_0}{\partial \varepsilon}.$$

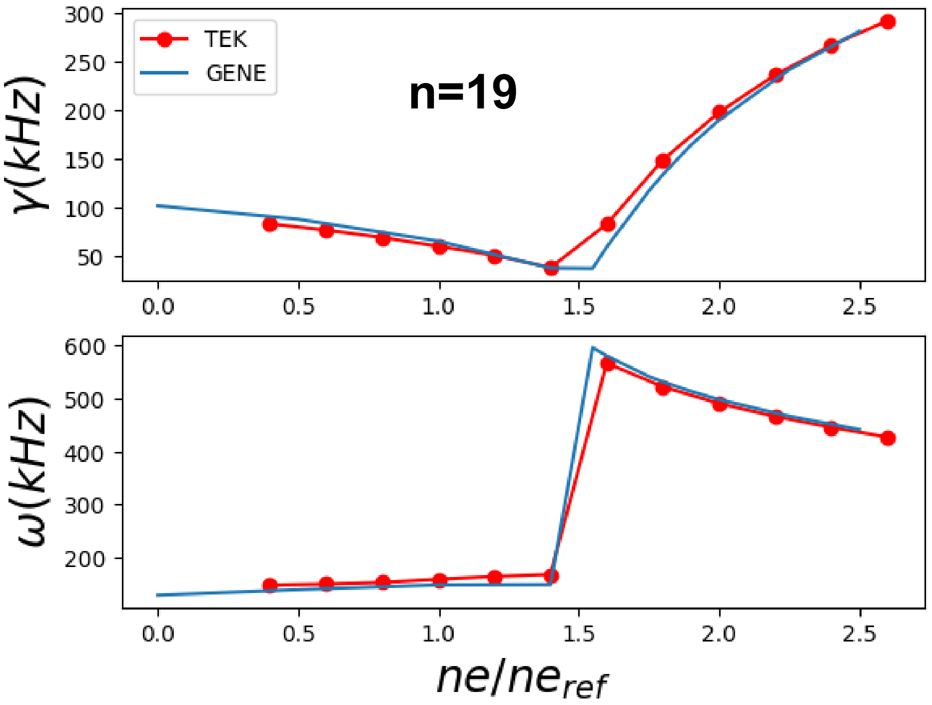
pull-back

* Easy to understand
* Easy to implement in codes

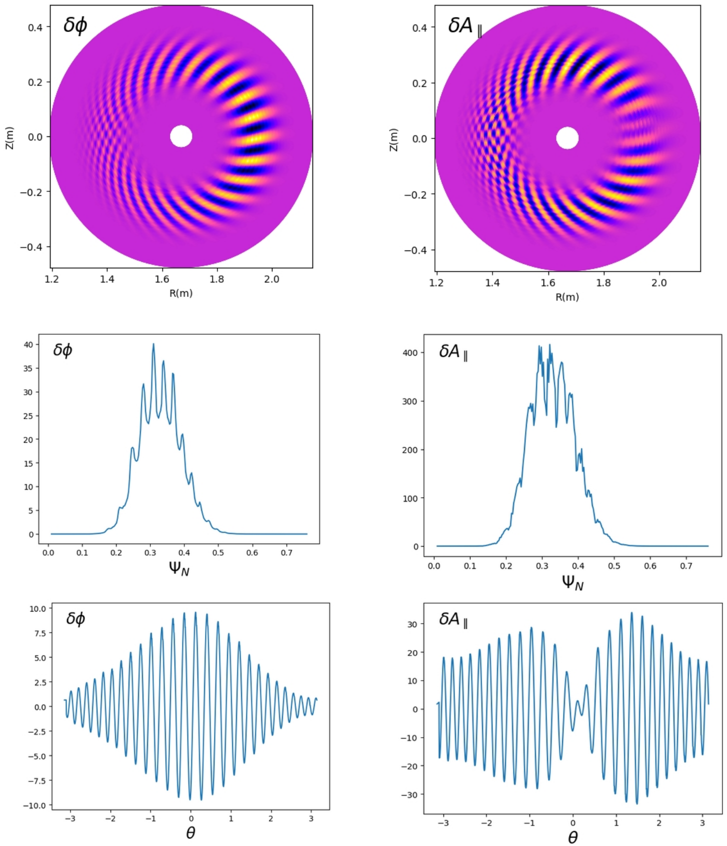
* A. Mishchenko et al., CPC(2019)

KBM benchmark in DIII-D cyclone base case

ITG-KBM transition in density scan



n=19 KBM mode



Circular and concentric tokamak for the ITPA-EP TAE benchmark

R_0	a	$B_{\rm axis}$	$q(r)$	$g(r) \equiv B_\phi R$
$10m$	$1.0m$	$3.0T$	$1.71 + 0.16(r/a)^2$	$30Tm$

$$R(r,\theta) = R_0 + r\cos\theta,$$

$$Z(r,\theta) = r\sin\theta,$$

Poloidal flux:

$$\Psi_p(r) = \Psi_p(0) + \int_0^r \frac{1}{q(r)} \frac{2\pi g r}{\sqrt{R_0^2 - r^2}} dr$$

Toroidal flux:

$$\Psi_t(r) = 2\pi g\left(\sqrt{R_0^2} - \sqrt{R_0^2 - r^2}\right)$$

Magnetic field:

$$\mathbf{B}_0 = \frac{1}{2\pi}\nabla\Psi_p \times \nabla\phi + g\nabla\phi$$

$$= \nabla r \times \nabla\phi \frac{1}{q(r)} \frac{g r}{\sqrt{R_0^2 - r^2}} + g\nabla\phi$$

$$\rho_t = \sqrt{\frac{\Psi_t(r)}{\Psi_t(a)}} = \sqrt{\frac{R_0 - \sqrt{R_0^2 - r^2}}{R_0 - \sqrt{R_0^2 - a^2}}}.$$

In the limit of $r/a \to 0$, then $\rho_t = r/a$.

*** TEK does not use analytic equilibrium.**

*** Polidal flux and g are written as a numerical gfile, then TEK reads it**

Profiles of thermal and energetic species

*** All 3 species are of Maxwellian in velocity space.**

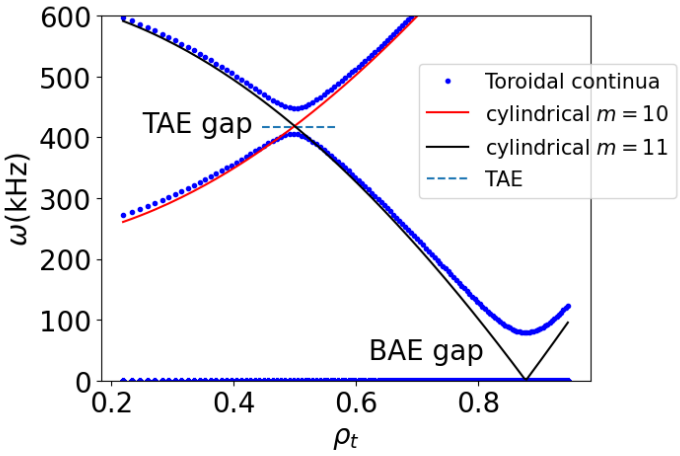
*** Only EP density is radially nonuniform; all others are uniform.**

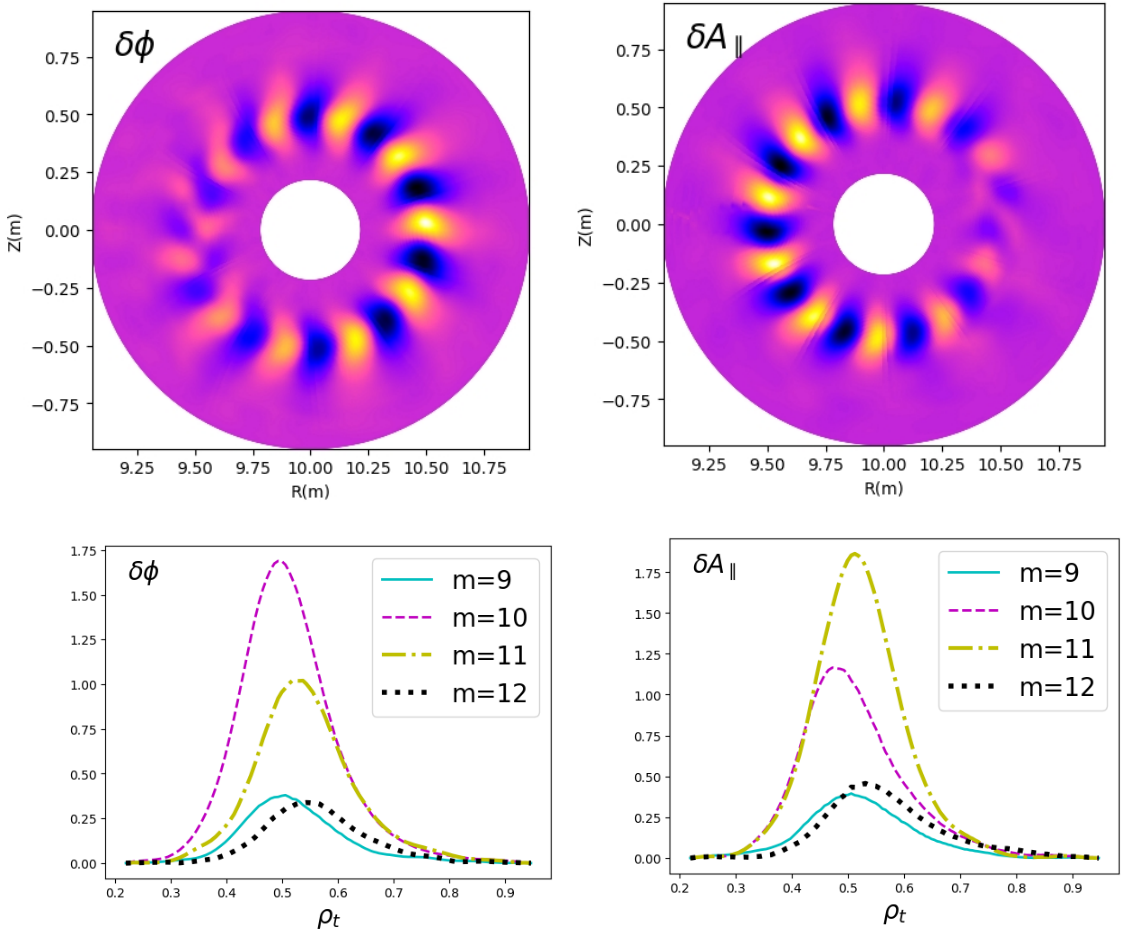
	Electron	Hydrogen	Deuterium
Mass (kg)	$9.10938*10^{-31}$	$1.67355*10^{-27}$	$3.34358*10^{-27}$
Charge (e)	-1	+1	+1
Temperature (keV)	1	1	100, 200,…,**400**,...800
Number density	$2*10^{19}m^{-3}$	$2*10^{19}m^{-3}$	$n_0 c_3 \exp\left[-\frac{c_2}{c_1}\tanh\left(\frac{\rho_t - c_0}{c_2}\right)\right]$

$$n_0 = 1.44131 \times 10^{17} m^{-3},$$
$$c_0 = 0.49123,\ c_1 = 0.298228,\ c_2 = 0.198739,\ c_3 = 0.521298$$

All parameters are the same as in A. Könies et al., NF 2018.

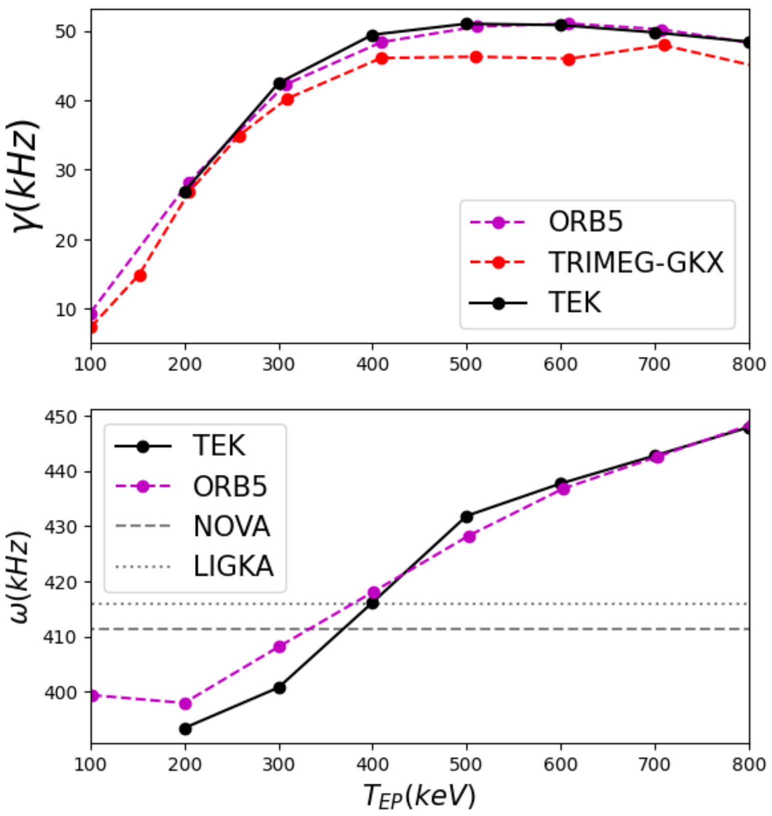
n=6 TAE in the case of T_{EP} = 400keV





Linear benchmark of n=6 TAE with ORB5 and TRIMEG-GKX

Growth rate and frequency vs. EP temperature

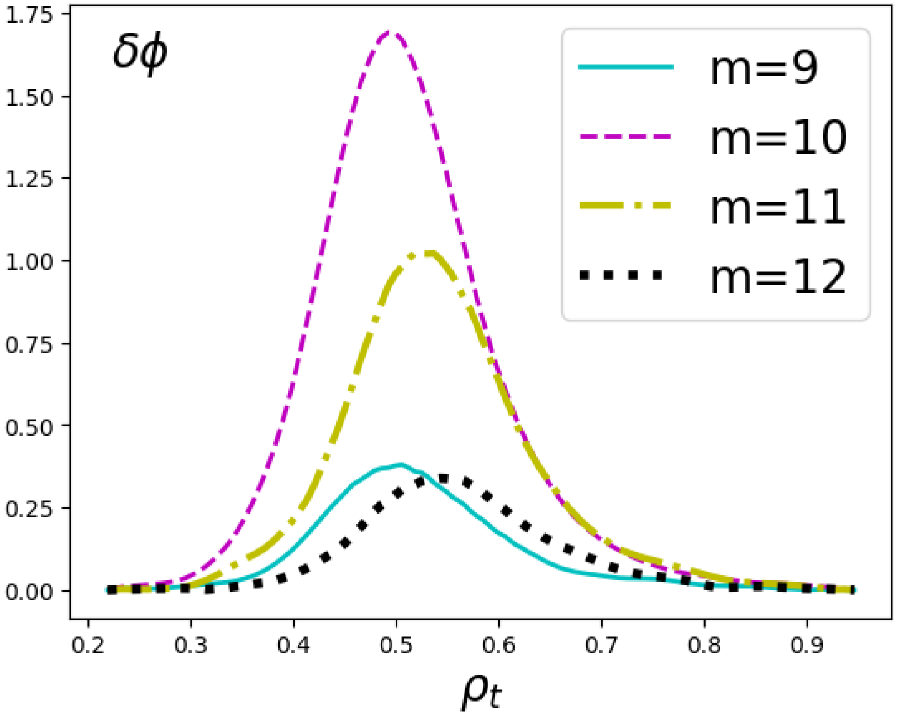


*** Reasonable agreement with other codes in growth rate and frequency for the EP temperature scan.**

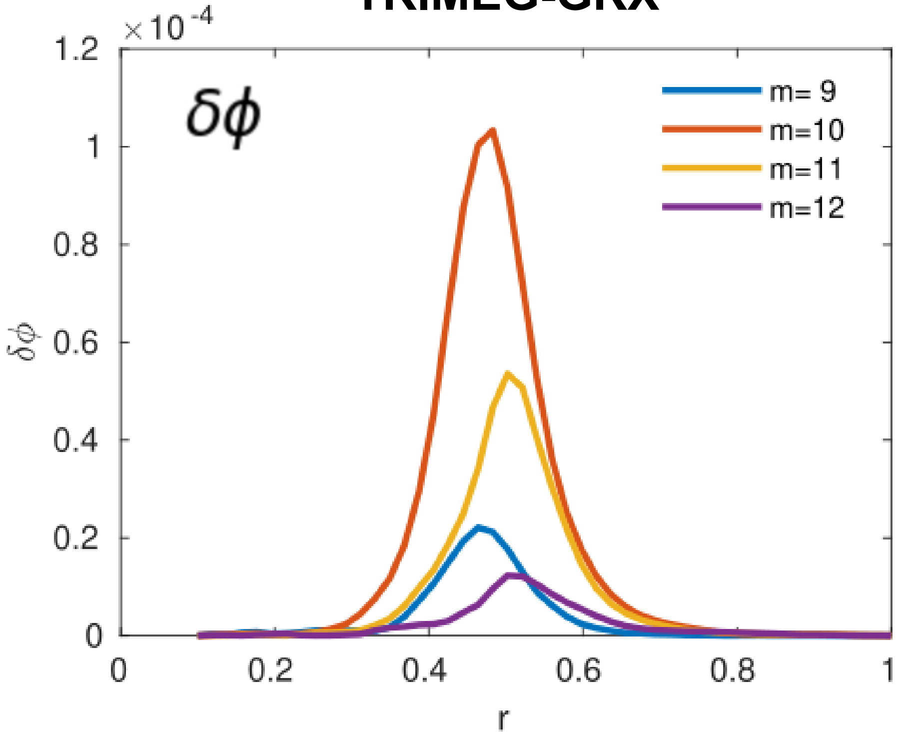
Results other than TEK simulations are from A. Könies' 2018 NF paper, and Z. Lu's 2023 PPCF paper.

Mode structure comparison

TEK

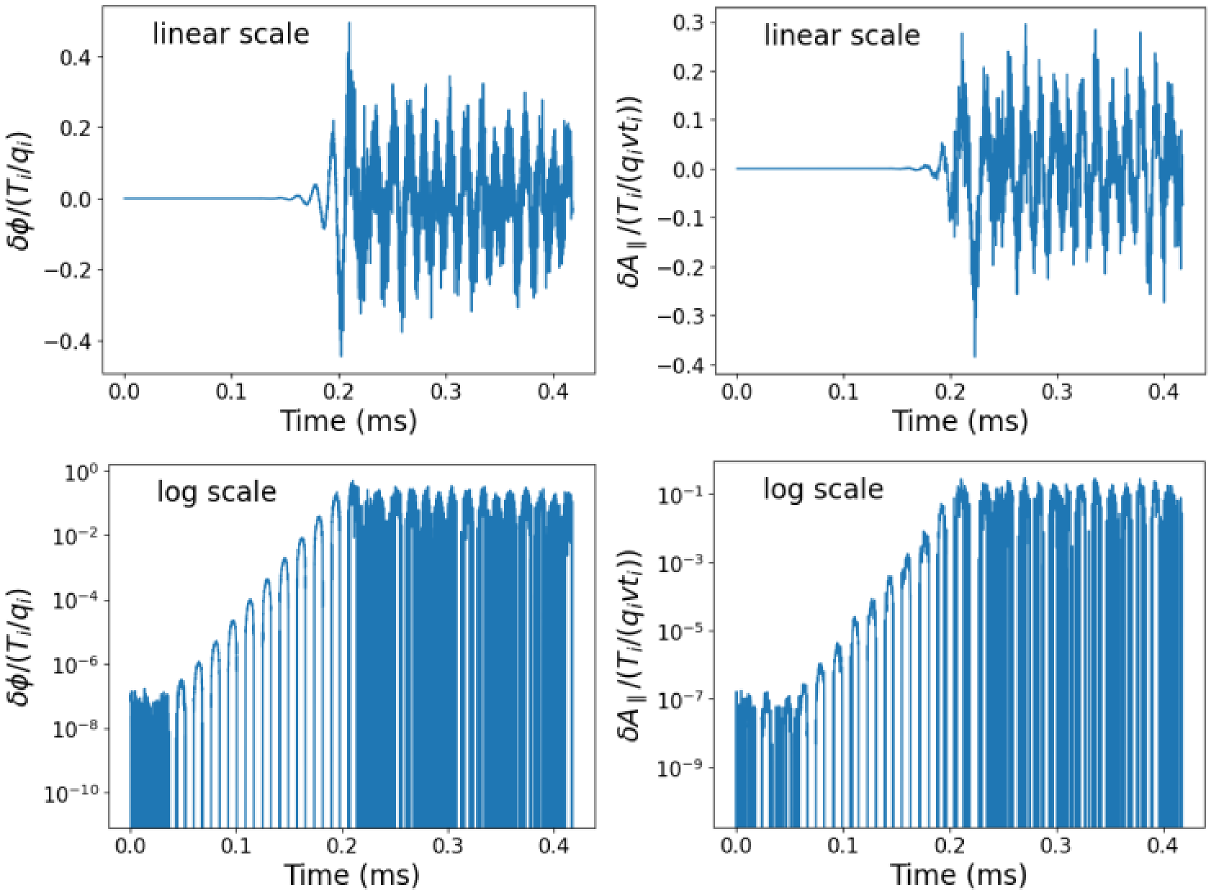


TRIMEG-GKX



Z. Lu et al, PPCF 65 (2023) 034004

Single-n (n=6) TAE nonlinear saturation

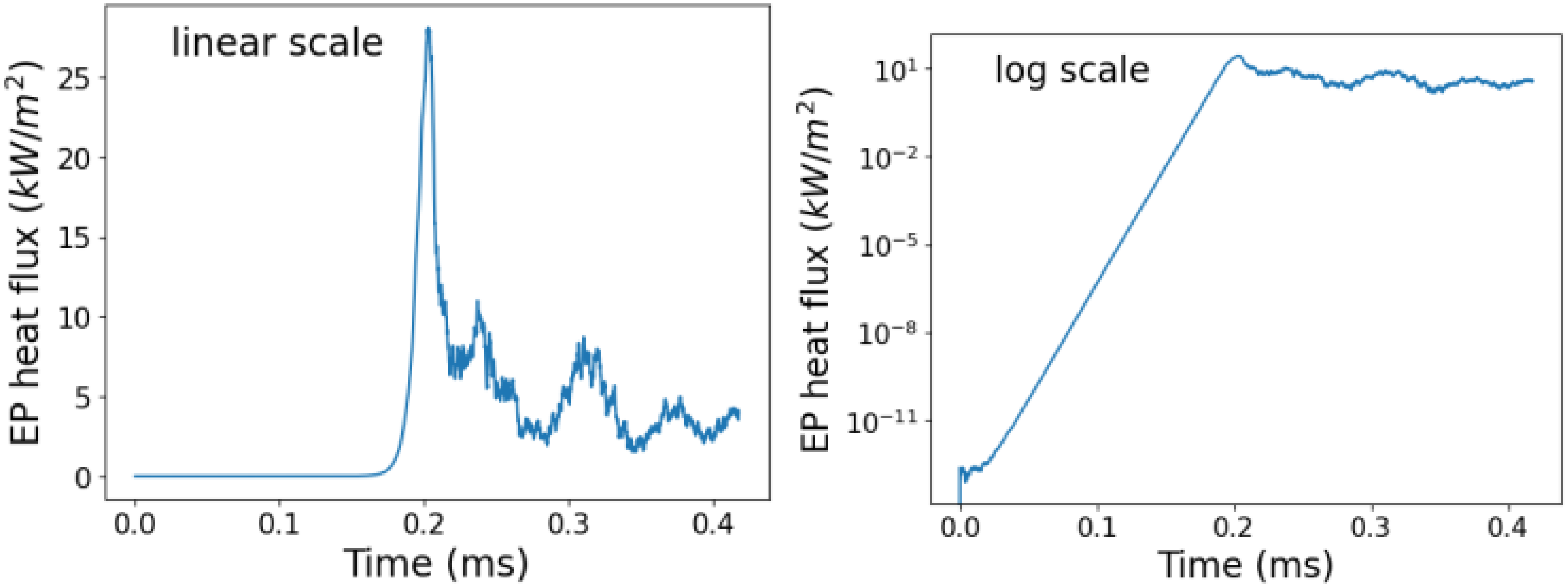


Signal at low-field side midplane

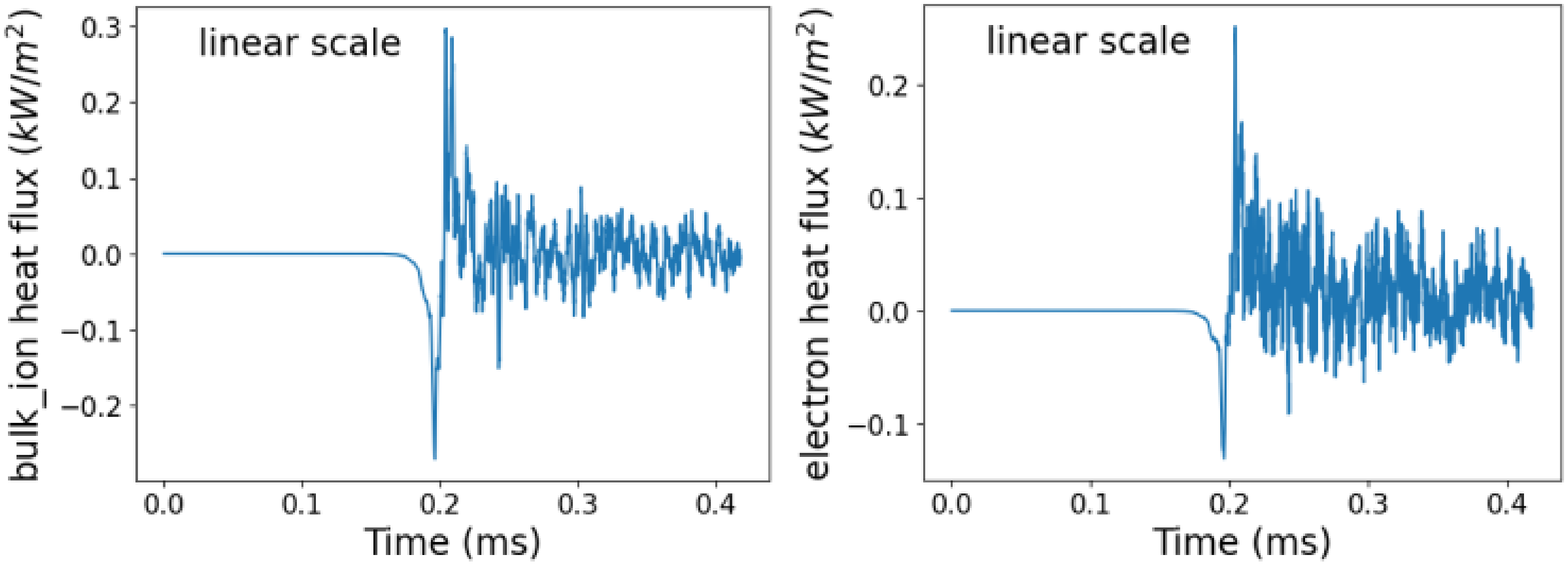
EP heat flux due to single n=6 TAE

Radial heat flux definition: $$Q \equiv \int \delta \mathbf{V}_D \cdot \frac{\nabla \psi}{|\nabla \psi|}\left(\frac{1}{2} m v_\parallel^2 + \mu B_0\right)\delta f d^3\mathbf{v},$$

Volume-averaged radial heat flux



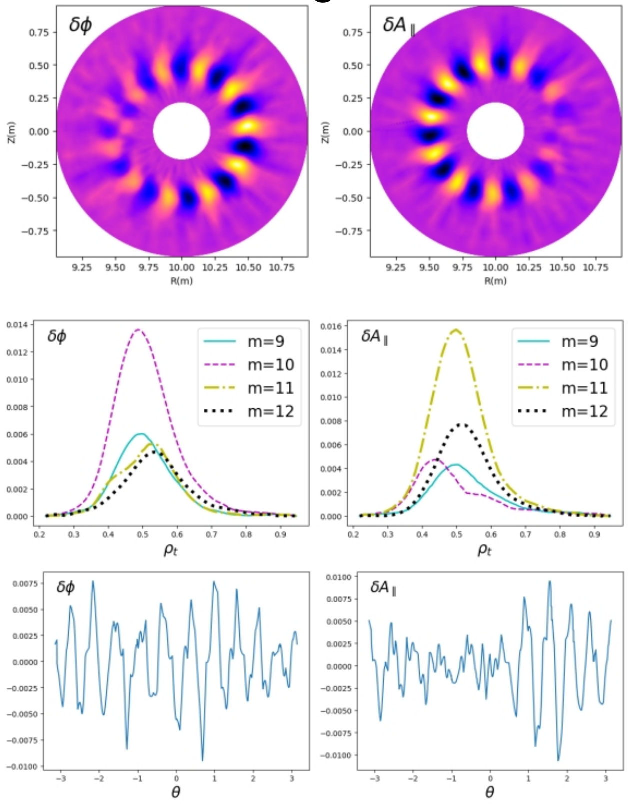
Thermal ions and electrons heat flux generated by TAE are negligible



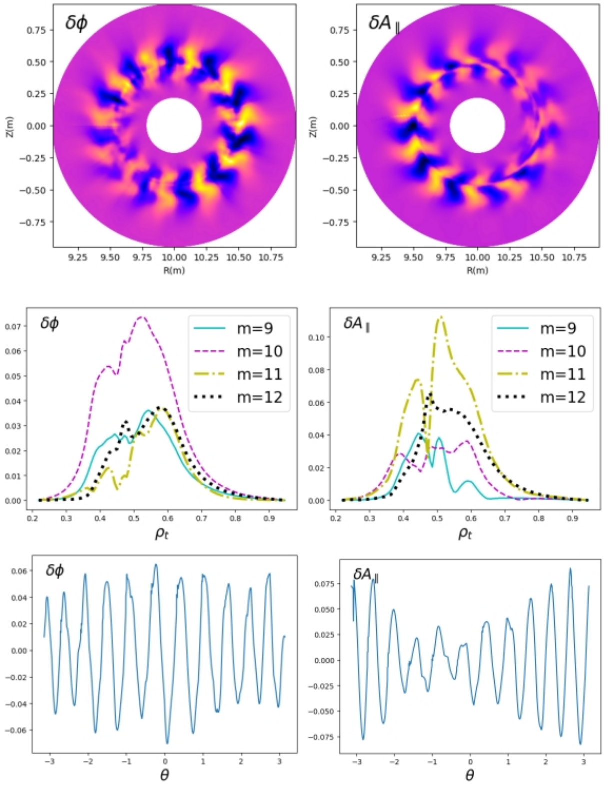
*** The flux is inward in the linear phase**

Nonlinear evolution in real space

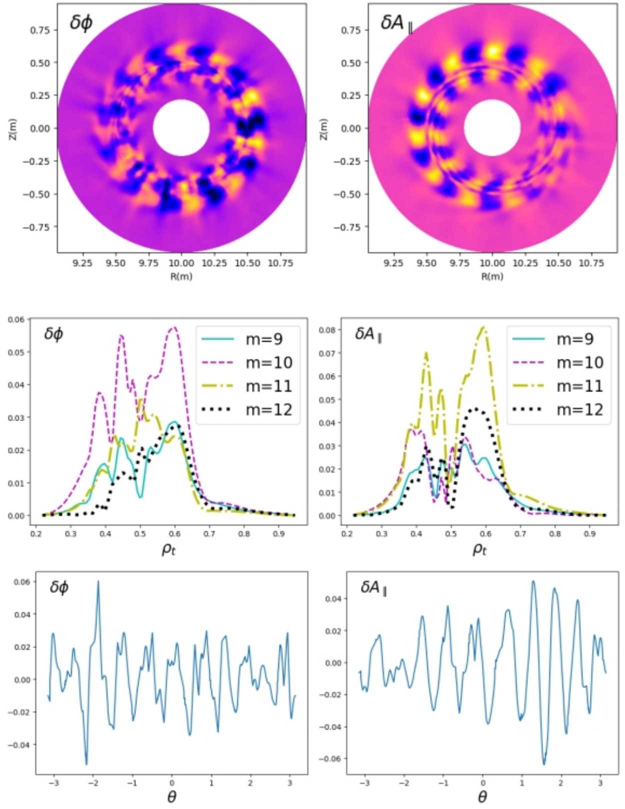
Linear stage



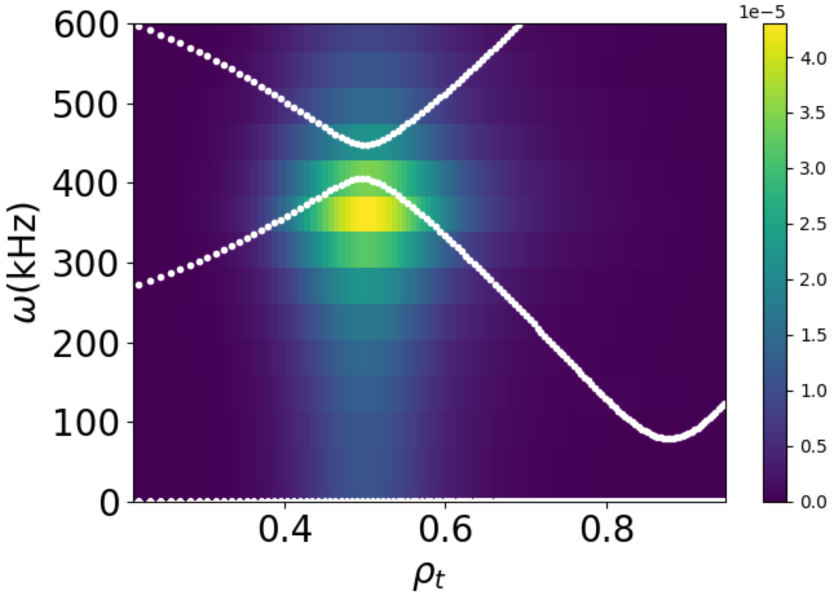
Early nonlinear stage



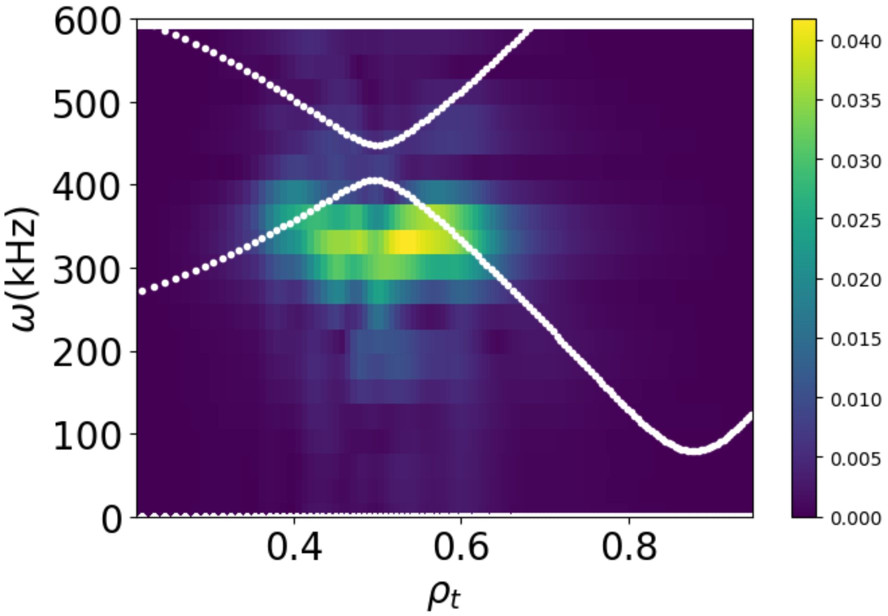
Late nonlineare stage



Frequency goes down in the nonlinear stage

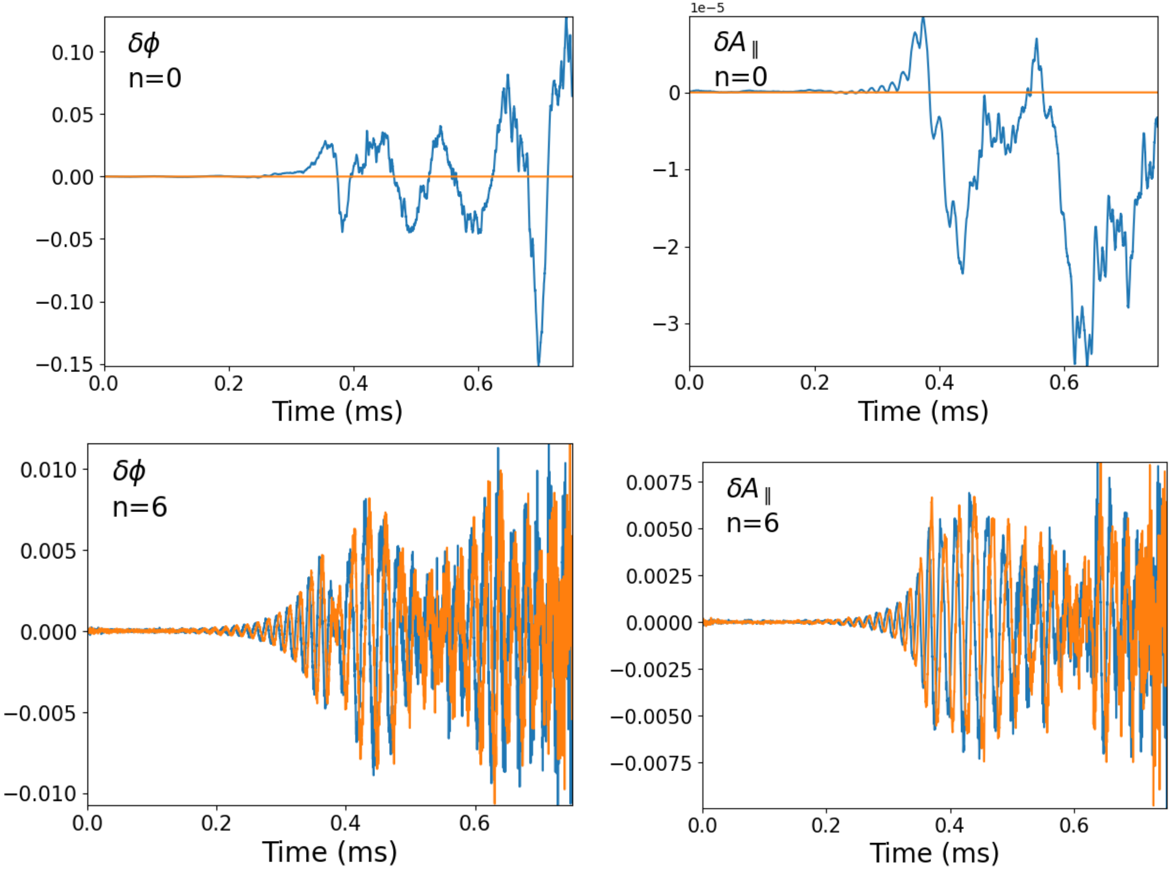


Linear stage



Nonlinear stage

Multiple-n (n = 0, 6, 12, 18) nonlinear saturation



Diagnosed at radial-center in low-field-side midplane

Numerical parameters:

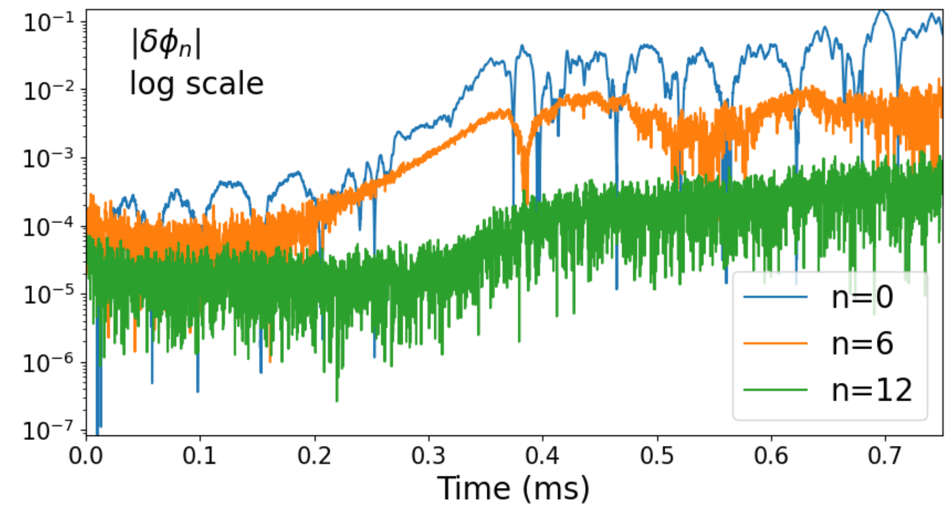
*** Spatial grid: (nx, ny, nz) = (258, 64, 32)**

*** Particle number per-cell for each species:**

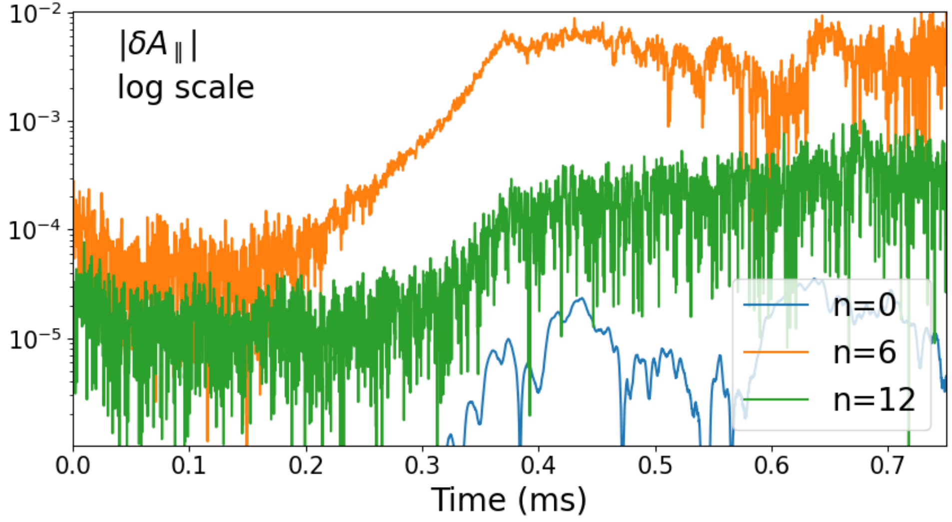
(ions, electrons, EPs) = (40, 80, 40)

*** Time step size:** $dt\Omega_{i,\mathrm{axis}} = 2$

- **The n=0 harmonic is filtered by retaining only its zonal component (i.e., magnetic surface average)**
- **Without the filtering, the simulation exploded**

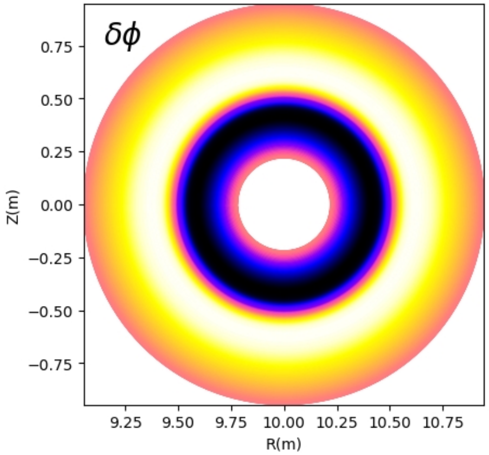


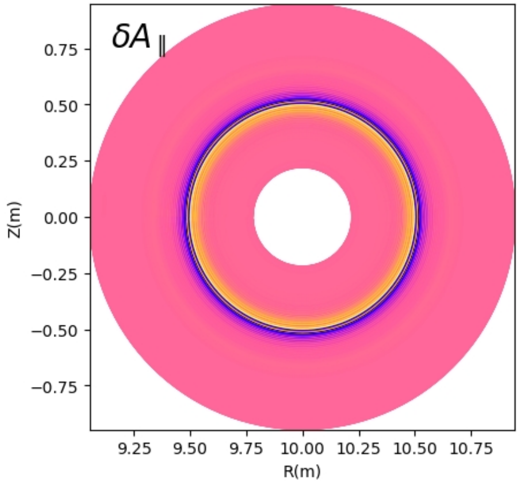
n=0 harmonic is dominant

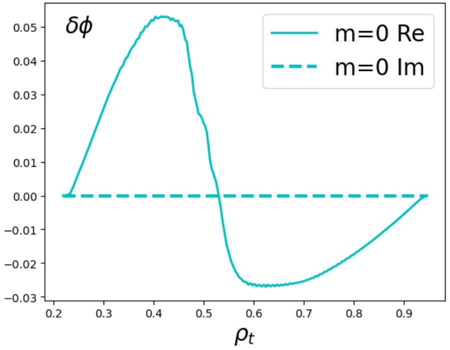


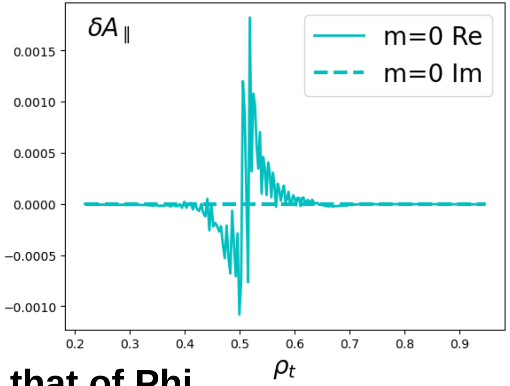
n=6 harmonic is dominant

n=0 mode structure (magnetic surface average of Phi and Apara)



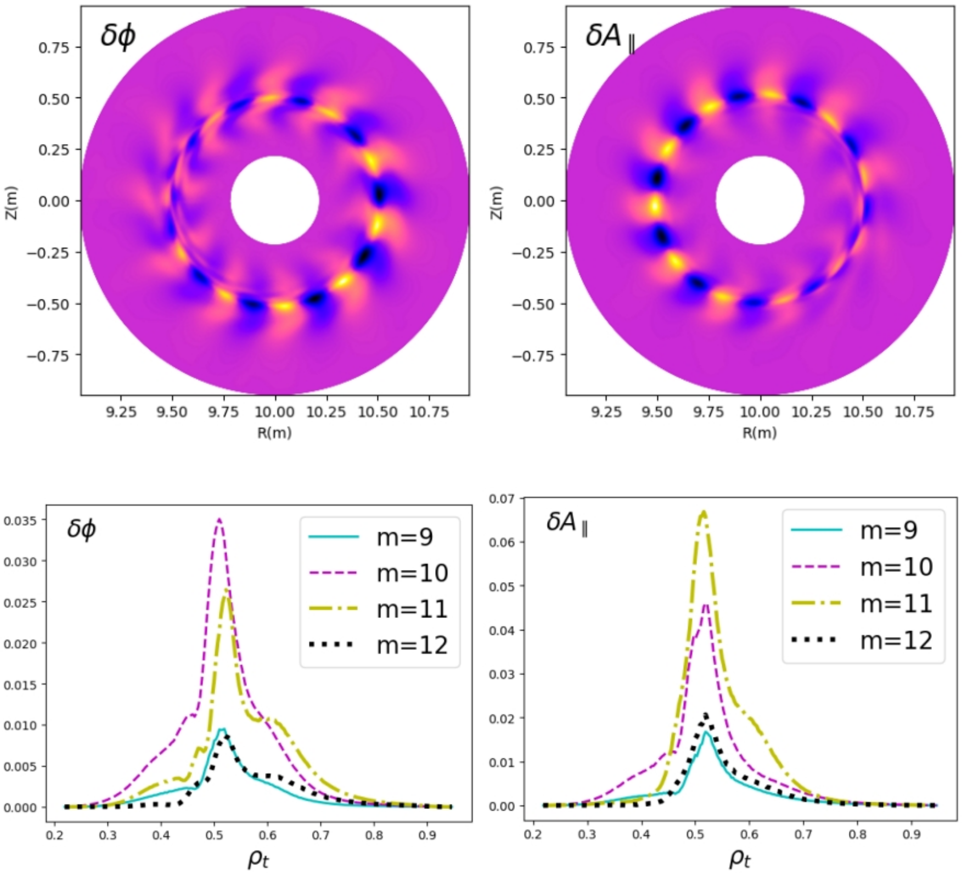




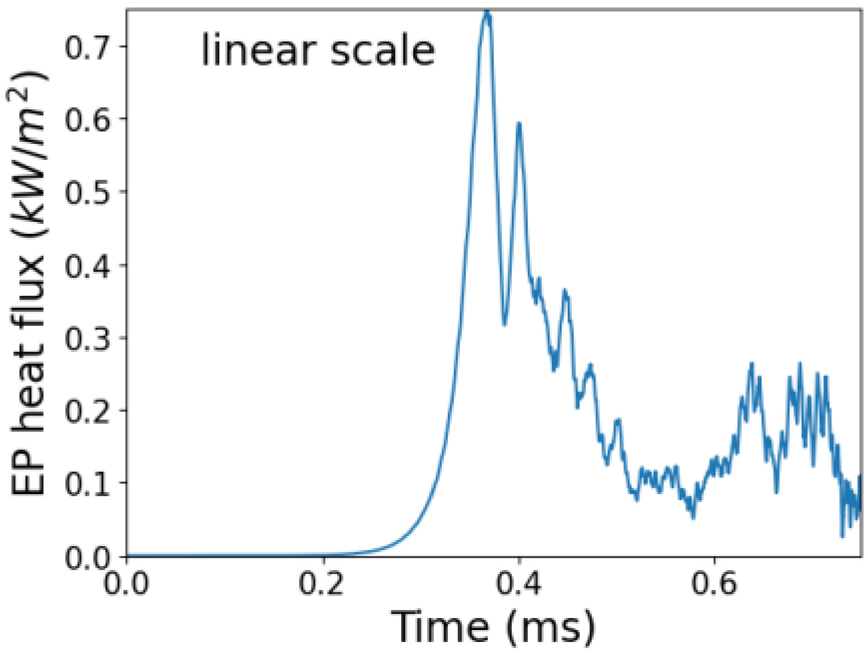


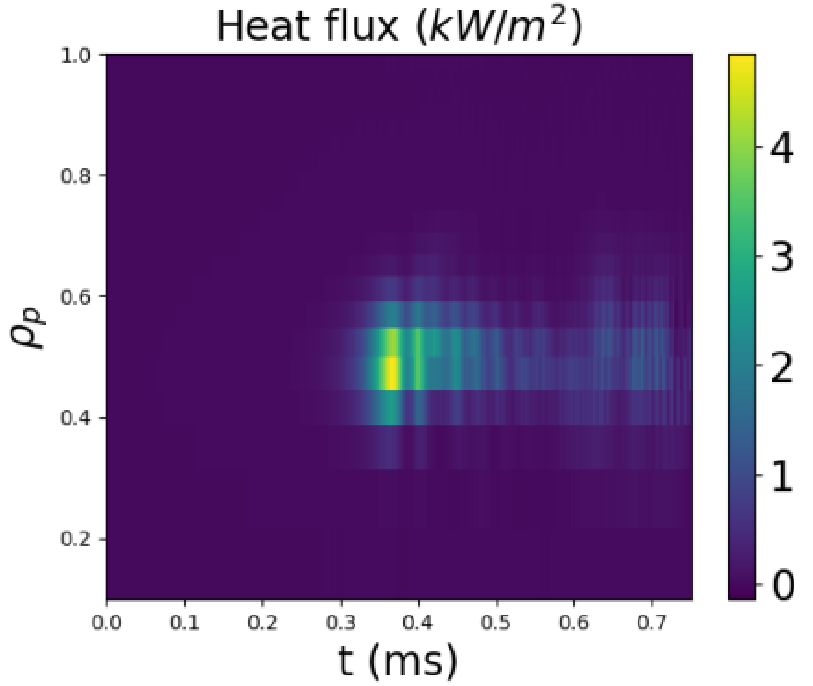
Observation: Apara has larger kr than that of Phi

$n \neq 0$ mode structure



EP heat flux in multiple-n simulations





*** The flux is 1 order smaller than that in single-n simulation**

Numeical parameters: markers per-cell for ions, electrons, Eps: (40,40,80)

Summary

- **Linear benchmark has no uncertainty.**
- **Nonlinear simulations without the n=0 harmonic seem robust.**
- **Nonlinear simulations with the n=0 harmonic are tricky, needing filtering to get reasonable results.**
- **Saturation level convergence over phase-space resolution (especially for electrons) need further verification. Are 80 markers per-cell enough?**

Thank you for your attention.