Gyrokinetic simulation using unstructured mesh (Fortran version)

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MET meeting

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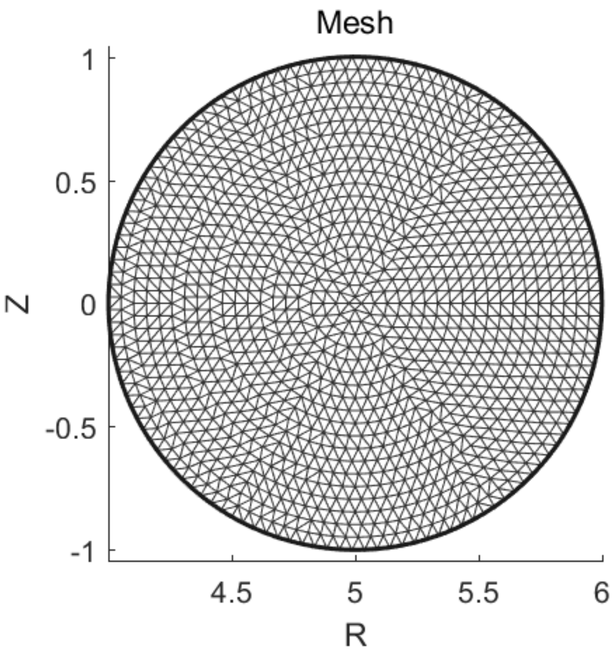
Outline

- Motivation
- Gyrokinetic simulation using unstructured meshes
- Simulation using realistic equilibrium & simplified n, T profiles
- Kinetic electron model
- Outlook

TRIMEG: TRIangular Mesh based Gyrokinetics as a testbed

- TRIMEG: a particle code, written from scratch as a testbed, inspired by other codes
- Hybrid coordinates: equation of motion in (R, Z, ϕ) [Chang, POP'04]; grids along flux surface except refinement grids
- Intermediate structured grid (r_i, θ_j) or (R_i, Z_j) for projection of marker weight to field quantities δn, $\delta \boldsymbol{j}$
- Particle motion: Runge-Kutta 4th order, coupled to Poisson solver



Particle coordinates increment k

$$k_1 = h\, f(t_n, y_n),$$

$$k_2 = h\, f\left(t_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right),$$

$$k_3 = h\, f\left(t_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right),$$

$$k_4 = h\, f\left(t_n + h, y_n + k_3\right).$$

Field value $\delta\phi$

$$\nabla_\perp \cdot C \nabla_\perp \delta\phi_{n,1} = \delta n(y_n + k_1/2)$$

$$\nabla_\perp \cdot C \nabla_\perp \delta\phi_{n,2} = \delta n(y_n + k_2/2)$$

$$\nabla_\perp \cdot C \nabla_\perp \delta\phi_{n,3} = \delta n(k_3)$$

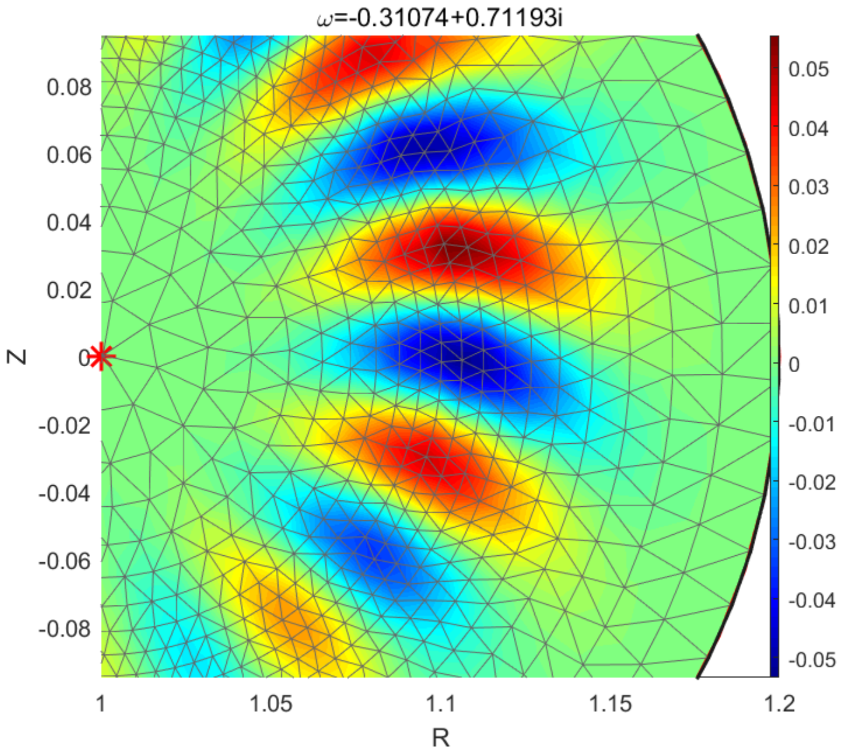
Non uniform mesh for eigenvalue problem

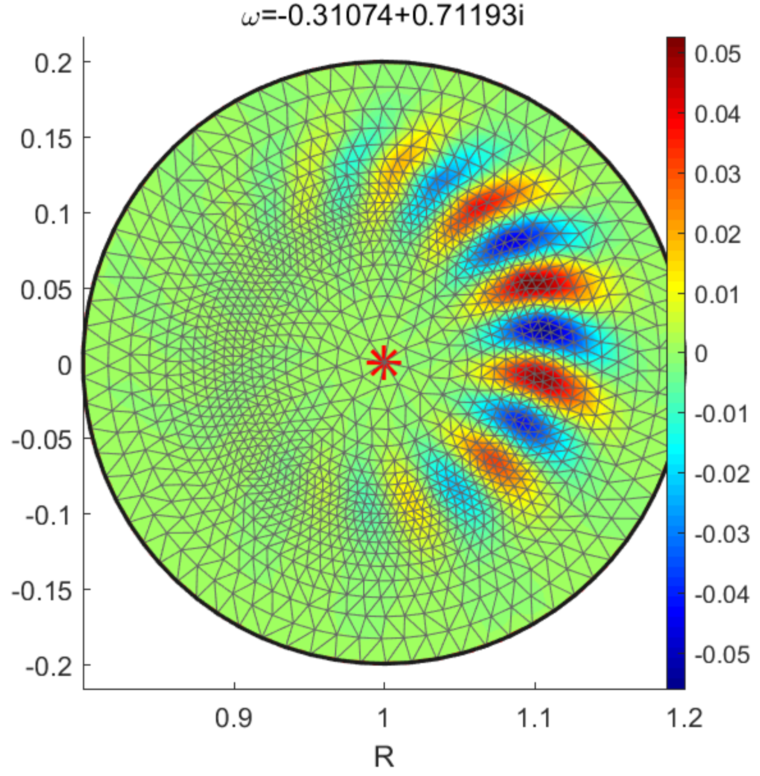
- Ion temperature gradient (ITG) mode

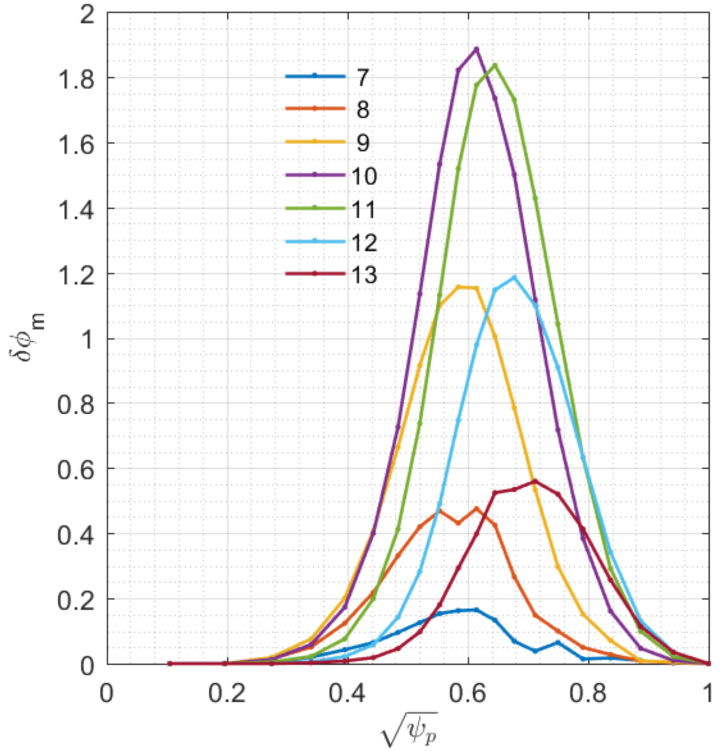
- $$\left\{\frac{R^2}{\Omega^2}\partial_\parallel^2 + \frac{\tau^{-1}\Omega+\Omega_{*i}}{\Omega-\Omega_{*pi}} - \rho_{Ti}^2\nabla_\perp^2 + \frac{i\rho_{Ti}\boldsymbol{e_Z}\cdot\nabla}{\Omega}\right\}\delta\phi = 0$$

Denser grids adopted in maximum mode amplitude region

[Equation used in Lu Phys. Plasmas 22 (5), 052118 (2015) and other early Refs. therein]



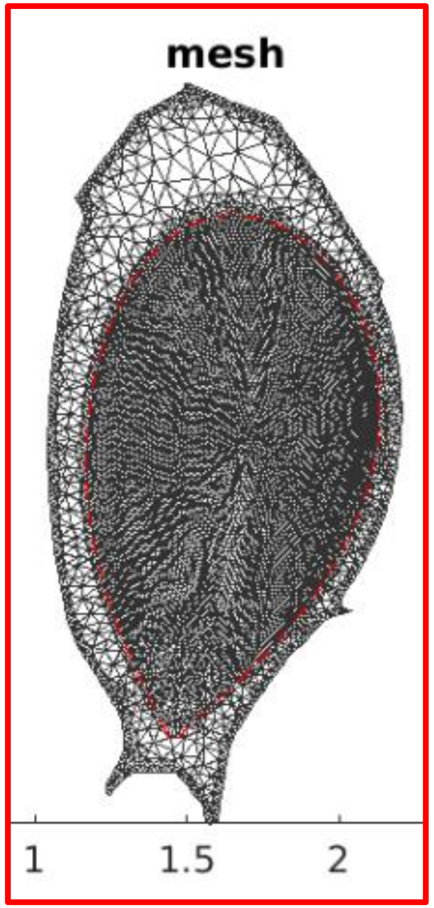




Extension to Fortran version

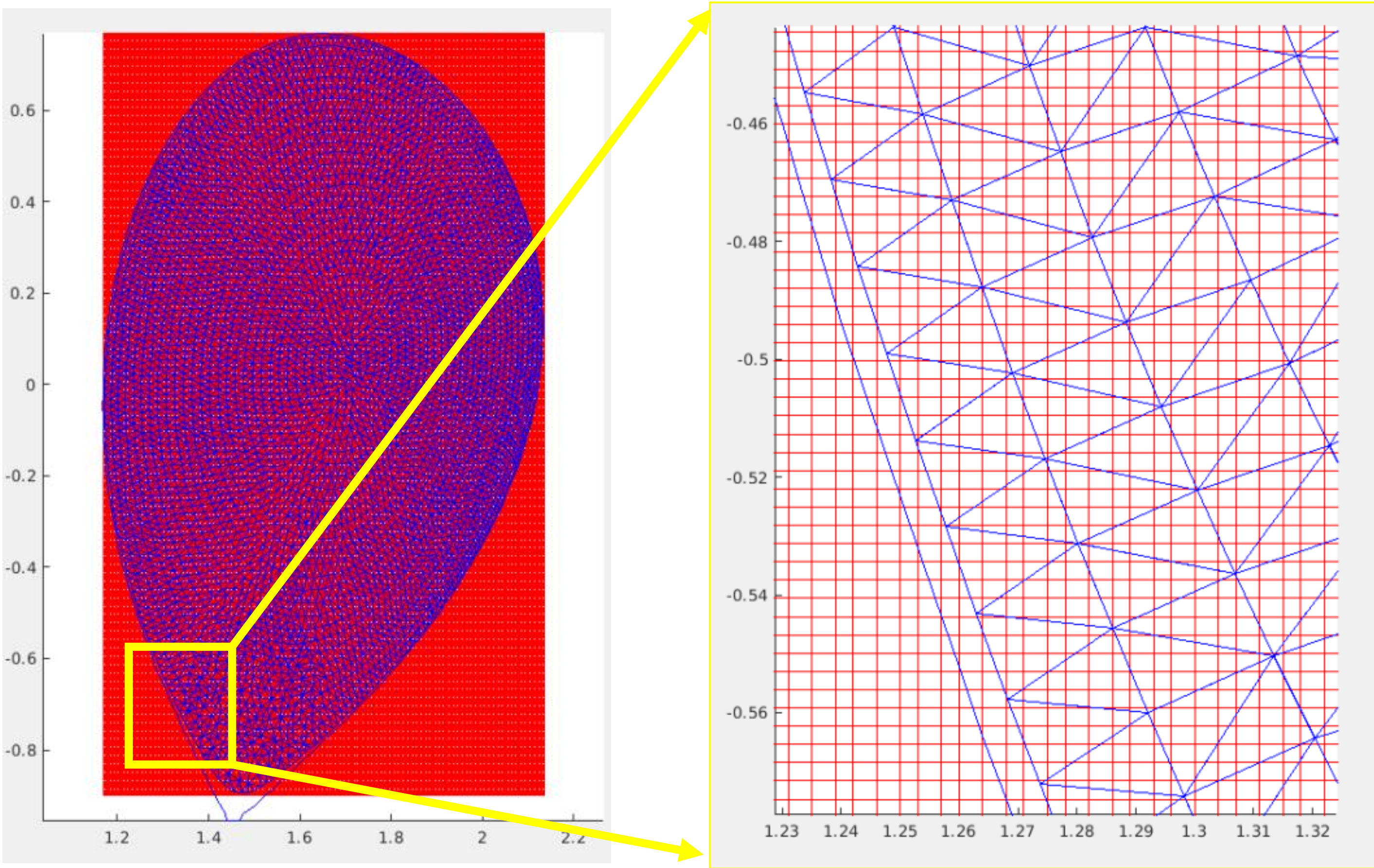
- Matlab version is for small scale cases
  - Field degree of freedom ~1e4, i.e., radial grid # <50; particle # < 5 millions; serial
- Fortran version for large scale cases; aiming for whole device simulation
  - Field degree of freedom > 1e5, i.e., radial grid # > 100; particle # ~ 16 millions; MPI

Comparable to DIII-D benchmark case [S. Taimourzadeh et al, *Nuclear Fusion*, 59 (6), 066006 (2019)]



Particle positioning (deposition) in unstructured meshes

- Goal: computation cost $\propto \alpha N_p$ for N_g particles, instead of $N_g N_p$ or $N_p\sqrt{N_g}$, α: constant
  - N_g: grid #, N_p: particle #
- Global positioning scheme (GPS, brute force scheme), cost $\propto N_g N_p$
  - For a given particle, check every triangle whether this particle is in this triangle
- Local positioning scheme (LPS), cost $\propto \alpha N_p$
  - Construct boxes and build the box-triangle mapping
  - For a given particle, first find the box, then find the triangle, where the particle is inside of.



Physics model (Particle code)

- Gyrokinetic equation (delta f method $\delta f = f - f_0$)

  $$\partial_t \delta f + \dot{\boldsymbol{x}} \cdot \nabla \delta f + \dot{v}_\parallel \partial_{v_\parallel} \delta f = \delta \dot{\boldsymbol{x}} \cdot \nabla f_0 + \delta \dot{v}_\parallel \partial_{v_\parallel} f_0$$

- Particle equations of motions
  - Gyrokinetic equation with phase space conservation with $D \equiv 1 + v_\parallel \boldsymbol{b} \cdot \nabla \times \boldsymbol{b}/B$ (XGC)

    $$\dot{\boldsymbol{x}} = \frac{1}{D}\left[v_\parallel \boldsymbol{b} + \frac{v_\parallel^2}{\omega_c} \nabla B \times \boldsymbol{b} + \boldsymbol{B} \times \frac{\mu \nabla B - E}{\omega_c B^2} \right]$$

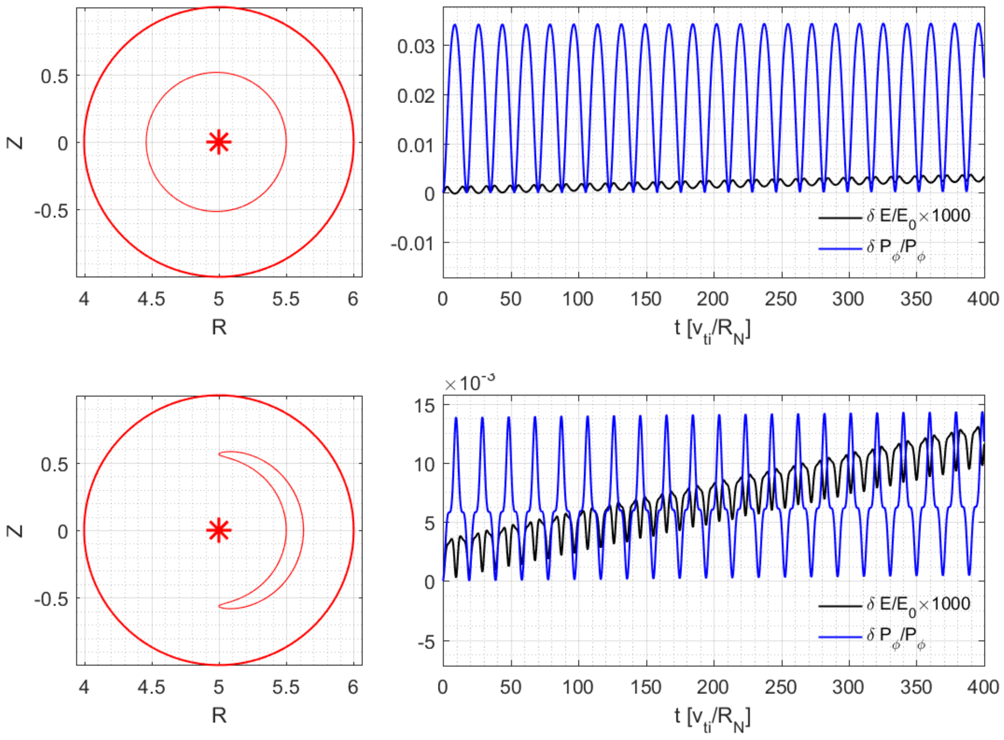
    $$\dot{v}_\parallel = -(\boldsymbol{B} + v_\parallel \nabla B \times \boldsymbol{b}) \cdot (\mu \nabla B - E)$$

  - Lowest order solution (in present TRIMEG version)

    $$\dot{\boldsymbol{x}} = v_\parallel \boldsymbol{b} - \frac{\hat{\boldsymbol{z}}(v_\perp^2 + 2v_\parallel^2)}{2\omega_c} \frac{\partial B}{\partial R} - \frac{\boldsymbol{B} \times E}{\omega_c B^2}$$

    $$\dot{v}_\parallel = -\boldsymbol{B} \cdot (\mu \nabla B - E)$$

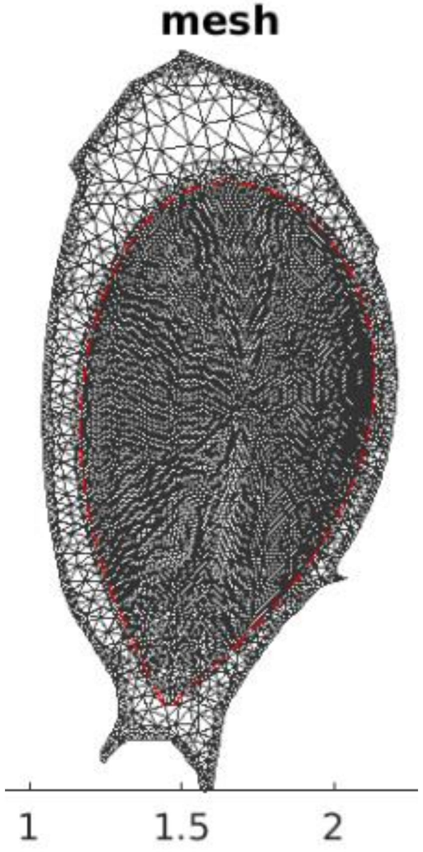
- Poisson equations in the long wavelength limit
  - $-\nabla_\perp \frac{n_0}{\omega_c B} \cdot \nabla_\perp \delta\phi = \delta n_i - \delta n_e$
  - Adiabatic electron: $-\nabla_\perp \frac{n_0}{\omega_c B} \cdot \nabla_\perp \delta\phi + \frac{e\delta\phi}{T_e} = \delta n_i$



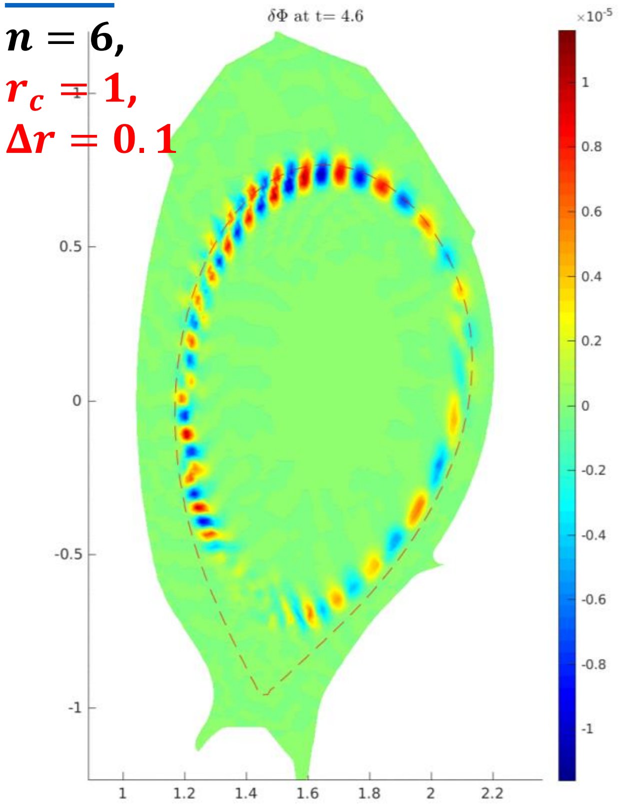
Error of particle integrator (passing & trapped particles)

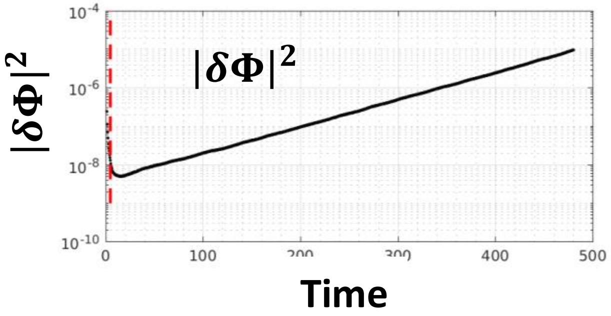
ASDEX Upgrade simulation in the whole plasma volume

- TRIMEG development for large scale simulation
  - Equilibrium: constructed in the whole device using EQDSK
  - Particle equation (dominant terms) implemented
  - Field solver implemented using PETSc library
  - Mixed PIC-PIF scheme: Particle-in-cell in (R,Z); Particle-in-Fourier in toroidal direction
  - Typical nonlinear runs (single n): 640 cores, 25.6 millions markers, 4 hours
- Application to AUG plasma
  - Equilibrium of ENR projects (NLED/NAT) case, Ph. Lauber (AUG Shot 034924)
  - Gradient profile: $\frac{d\ln\{n_i,T_i\}}{dr} = \frac{\kappa_{n_i,T_i}}{R_0}\exp\{-\left(\frac{r-r_c}{\Delta r}\right)^{\alpha}\}$
  - Benchmark with ORB5 in core, fully consistent profiles, comprehensive models (kinetic electrons, phase space conservation): in progress



Linear simulation

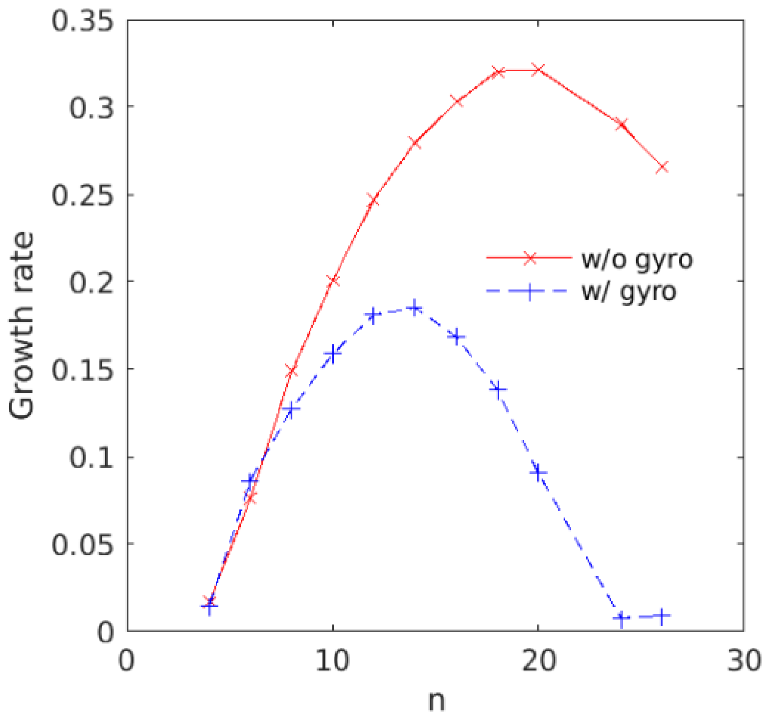




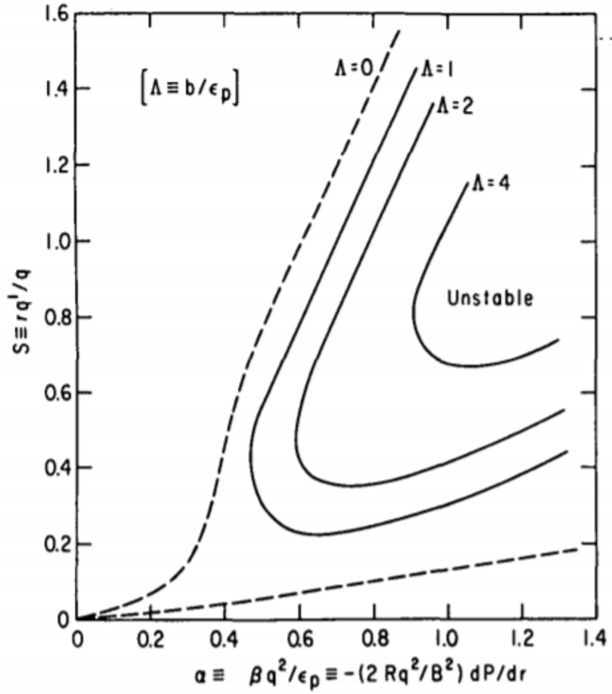
- Ion Temperature Gradient (ITG) mode simulation

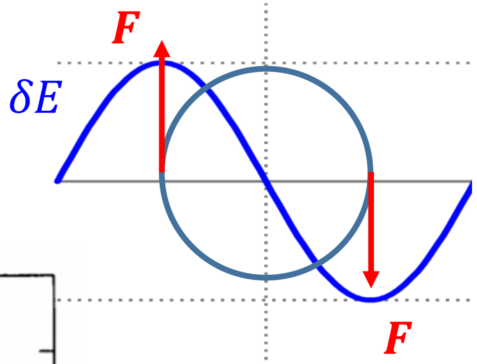
Linear results: stabilization due to FLR

- Essence: gyroaverage weakens the effective field perturbation felt by particles δE → $\langle \delta E \rangle_{gyro} \sim J_0(k_\perp \rho_i)\delta E$
- $k_\perp \rho_i \sim nq\rho_i/r$ indicates strength of FLR



Results from TRIMEG using 4 point gyro average





As $k_\perp \rho_i \to 1$, gyro averaged δE is weakened

FLR stabilization, where $\Lambda = k_\perp^2 \rho_i^2/(2\varepsilon_p)$, $1/\varepsilon_p = -Rd(lnP)/dr$
[Tang, Connor & White NF 81]

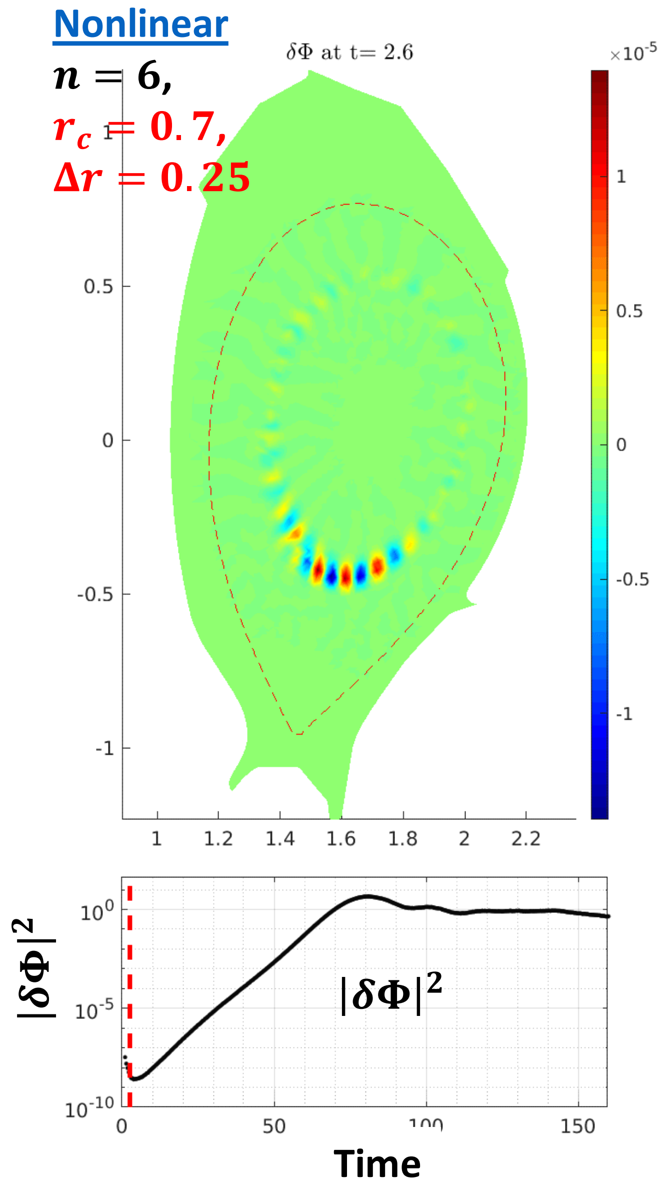
Nonlinear results

- Saturation due to perturbed trajectory related nonlinear term

$$\partial_t \delta f + \boldsymbol{v} \cdot \nabla \delta f + \dot{v}_\parallel \partial_{v_\parallel} \delta f = \delta \boldsymbol{v} \cdot \nabla f_0 + \delta \dot{v}_\parallel \partial_{v_\parallel} f_0$$

$$\boldsymbol{v} \cdot \nabla \delta f = \boldsymbol{v_0} \cdot \nabla \delta f + \delta \boldsymbol{v}_{\boldsymbol{E \times B}} \cdot \nabla \delta f$$

- Zonal flow and equilibrium E_r suppresses turbulence and needs to be added for interpreting experiments



Kinetic electron (electrostatic) model (preliminary)

- Main issue: fast electron motion along $\boldsymbol{B}$
  - $\partial_t \delta f + \boldsymbol{v_0} \cdot \nabla \delta f + \dot{v}_{\parallel,0} \partial_{v_\parallel} \delta f = \delta \boldsymbol{v} \cdot \nabla f_0 + \delta \dot{v}_\parallel \partial_{v_\parallel} f_0$
  - $\boldsymbol{v_0} \cdot \nabla \delta f \sim \boldsymbol{v}_{\parallel,0} \boldsymbol{\partial}_\parallel \delta f$ balances $\delta \dot{v}_\parallel \partial_{v_\parallel} f_0 = \frac{e}{T} v_\parallel f_0 \partial_\parallel \delta \phi$ in $m_e = 0$, uniform plasma limit; thus fast electron motion along $\boldsymbol{B}$ should be simulated accurately
  - Solution I: decrease time step to resolve the $\omega - H$ mode [Lee 1987]
  - Solution II: fluid electron model [Chen, Lin, GTC; Mishchenko et al]
  - Solution III: separation of adiabatic electrons [Lewandovski, Lee et al GTC]
  - Solution IV: separation of passing/trapped electrons [Bottino et al, ORB5]
  - …

  - Another question: any lessen from pull-back scheme?
    - For electrostatic modes, $\delta A_\parallel^s + \delta A_\parallel^h = \delta A_\parallel = 0.$

→ Should $\partial_t \delta A_\parallel^s + \partial_\parallel \delta \phi = 0$ be chosen (but then $\delta A_\parallel^s$=-$\delta A_\parallel^h$)?

Kinetic electron (electrostatic) model (preliminary)

- Iterative scheme in this work
  - Field equation: $-\nabla_\perp \frac{n_0}{\omega_c B} \cdot \nabla_\perp \delta\phi + \frac{e\delta\phi}{T_e} = \delta\, n_i - \delta n_e^{NA}$, $\delta n_e^{NA} = \delta n_e \; - \frac{e\delta\phi}{T_e}$
  - For $\delta n_e^{NA} \ll \frac{e}{T_e}\delta\phi$, solve $\delta\phi = \delta\phi^{(0)} + \delta\phi^{(1)} + \delta\phi^{(2)} + \cdots$ order by order

$$-\nabla_\perp \frac{n_0}{\omega_c B} \cdot \nabla_\perp \delta\phi^{(0)} + \frac{e}{T_e}\delta\phi^{(0)} = \delta n_i \quad ,$$

$$-\nabla_\perp \frac{n_0}{\omega_c B} \cdot \nabla_\perp \delta\phi^{(1)} + \frac{e}{T_e}\delta\phi^{(1)} = \delta n_e^{NA,(1)} \quad ,$$

$$\cdots$$

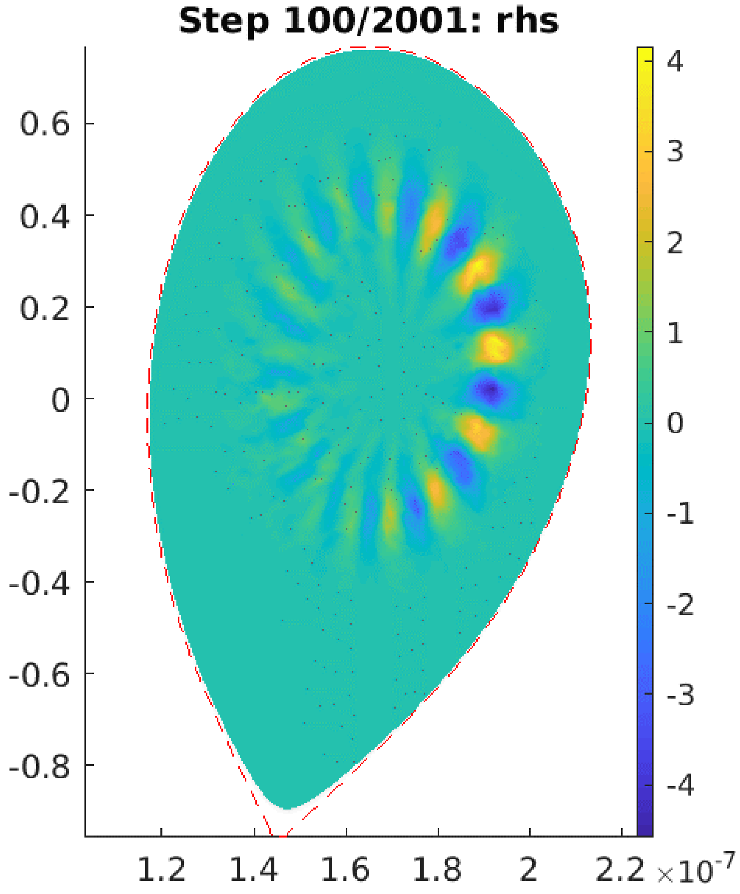
where $\delta n_e^{NA,(1)} = \delta n_e - e\delta\phi^{(0)}/T_e$, δn_e is calculated using δf_e.

- Main concern: applicability of this scheme? $n_e^{NA} \ll \frac{e}{T_e}\delta\phi$ can break down!
- Better scheme?

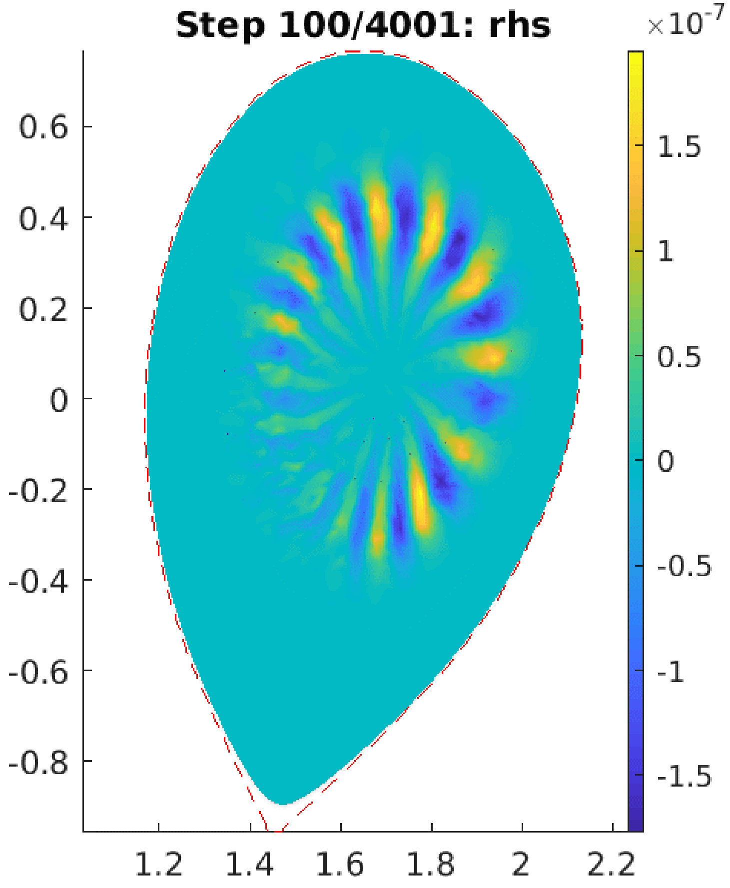
Simulation results (w/ kinetic e^-)

- AUG equilibrium, analytical T, n gradient profiles

ITG



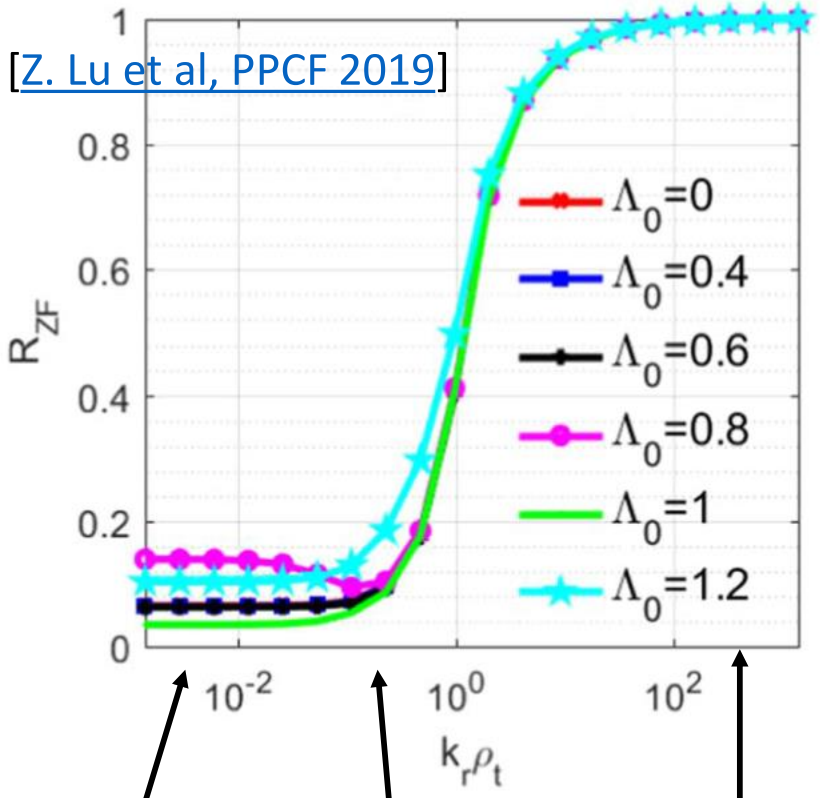
TEM



- More tests are needed

Outlook

[Z. Lu et al, PPCF 2019]



- Code capabilities
  - Electrostatic, kinetic electrons: schemes and tests, more realistic experiments profiles (E_r, consistent profiles)
- Possible physics studies related to EP physics
  - ITG/TEM induced EP transport and particle/heat flux on the wall
  - Anisotropic EP effects on zonal flow residual
    - Is it possible / how to use ICRF to enhance ZF and reduce turbulence?
  - And more?

More analyses needed

	Macroscale	Mesoscale	Microscale
Ansotropic EP effects on ZF	large	Moderate	Small
Flow shear effects on turbulence suppression	small	moderate	large

Thank you

- Comments are welcome