Wave packet calculation using finite element method based on unstructured mesh

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Acknowledge: J. Chen [5], F. Zonca [3,4], T. Hayward-Schneider [1], A. Könies [2], R. Kleiber [2], A. Ratnani [1], E. Fable [1], L. Villard[6], B.D. Scott [1], E. Poli [1], O. Maj [1] , O. Pan [1], G. Vlad[3], M. Falessi[3] , H. Wang [7], A. Bierwage [7], A. Biancalani [1], C. Angioni [1]

NLED project (F. Zonca), NAT project (Ph. Lauber)

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Ringberg Theory Seminar

19th -23rd, Nov., 2018, Ringberg

Max-Planck-Institut für Plasmaphysik

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Outline

- Motivation
- Finite element method on unstructured mesh
  - Basic concept
  - Examples of unstructured mesh
- Eigenvalue approach: TAE and ITG
  - Toroidicity induced Alfén eigenmode
  - Ion temperature gradient mode
- Initial value approach: PIC simulation
  - Model and numeric method
  - Applications to zonal flow residual and symmetry breaking studies
- Fluid electron model for EP driven Alfvén modes and application to AUG
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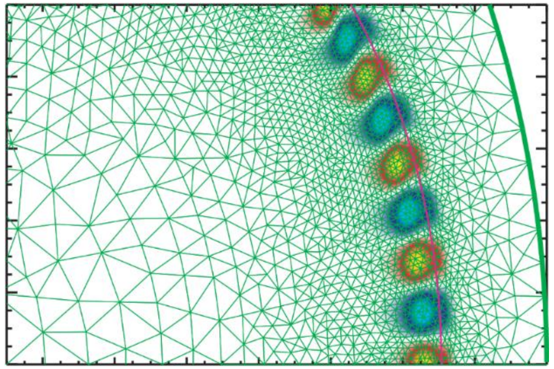
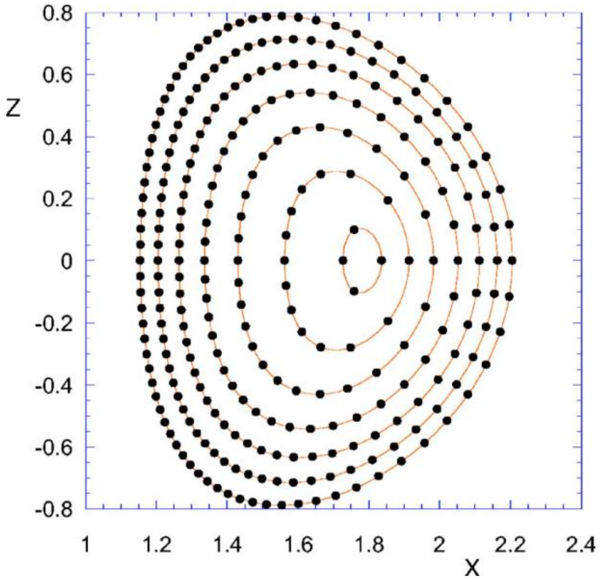
Motivation

- Finite element method (FEM) for Unstructured Mesh : a useful numerical tool
  - Magnetic axis: no singularity although grids aligned on flux surface
  - Complicated boundary: plasma wall, with separatrix
  - Good description of localized wave packet (broad Fourier spectrum needed for narrow beam)
  - For studies of Nonlinear interaction of Alfvénic and turbulent fluctuations (NAT) and meso-scale physics (MET) in burning plasmas: for resolving non-Fourier mode structures
- Useful for Wave Packet Calculation and mode structure symmetry breaking in addition to Mode Structure Decomposition (MSD) method and kinetic PIC simulation
  - It can be useful for studies of micro-instability, energetic particle driven modes and radio frequency wave propagation & absorption [Lu POP'12, 13; Bao, Lin, Lu PPCF'14, Lu POP'17, Lu NF'18]
- Complement to available codes and methods
  - Codes using FEM and Unstructured Mesh: M3D, M3D_C^1, XGC, GTS (PPPL); GTC (UCI)
  - European codes ORB5, LIGKA, HMGC, EUTERPE etc: based on structured grids



A peeling-ballooning eigenmode calculated using M3D-C ^{1} [Ferraro POP'10]



GTS grids for unstructured mesh [W. Wang POP'06]

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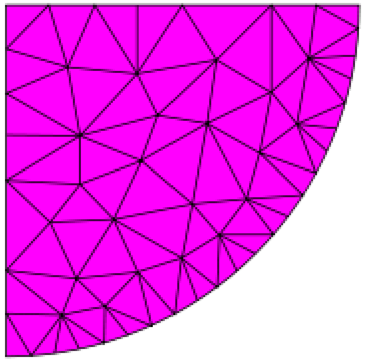
Finite element method on unstructured mesh

- Unstructured mesh
  - Unstructured mesh: A tessellation of a part of the Euclidean plane or Euclidean space by simple shapes, such as triangles or tetrahedra, in an irregular pattern



[Example of unstructured grid]

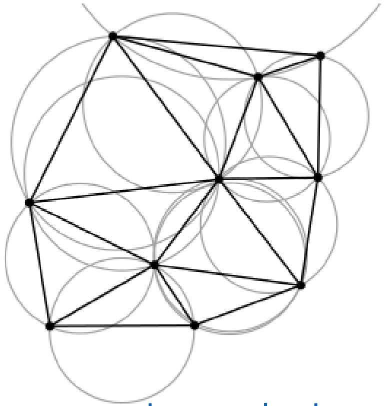
- Finite element method for Unstructured mesh
  - Equation to be solved: $L(\boldsymbol{R})y(\boldsymbol{R}) = S(\boldsymbol{R})$, where $L(\boldsymbol{R})$: operator, $S(\boldsymbol{R})$: known, $y(\boldsymbol{R})$: to be solved
  - Basis functions N_i are defined in each local shape, e.g., triangle
  - Solution y is represented as the superposition of basis functions: $y(\boldsymbol{R}) = \sum_i y_i N_i(\boldsymbol{R})$
  - Coefficients y_i obtained from weak form: $\int dS N_j \{L(\boldsymbol{R}) \sum_i y_i N_i(\boldsymbol{R}) = S(\boldsymbol{R})\}$

TRIMEG: TRiangular MEsh based Gyrokinetics

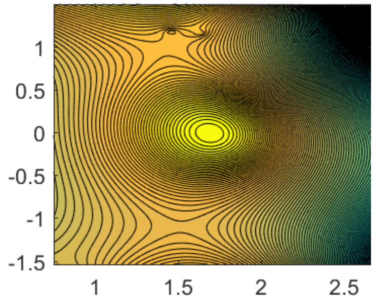
- Purpose: test the finite element method for unstructured mesh
- Object oriented programing: capsulated equilibrium, field, particle classes
- Field class: eigenvalue solver, initial value solver⋯
- Particle class: particle pusher ⋯

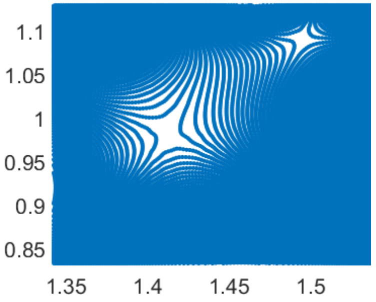
Delaunay triangulation

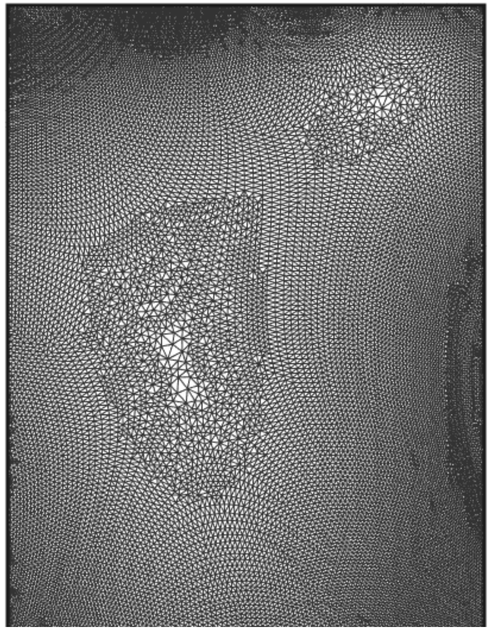
- Delaunay triangulation
  - Delaunay triangulation for a given set P of discrete points in a plane is a triangulation DT(P) such that no point in P is inside the circumcircle of any triangle in DT(P)
- Several examples (TRIMEG: vertex initialization, field solver, particle pusher, with external library for mesh generation)

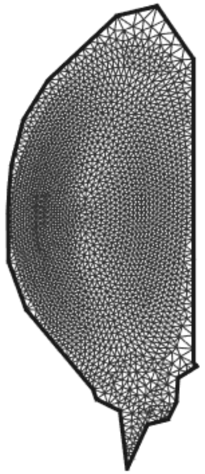


[A Delaunay triangulation in the plane with circumcircles shown](#)

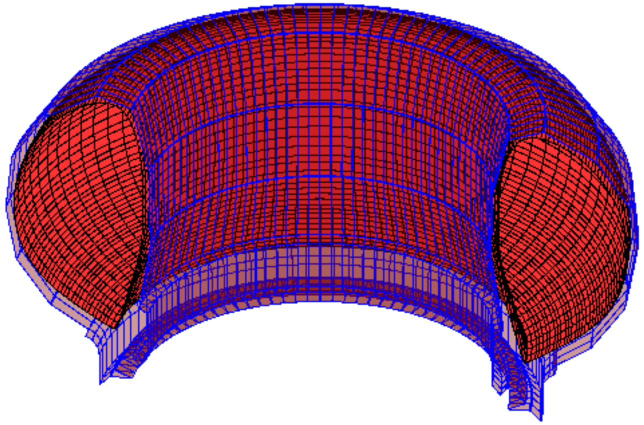




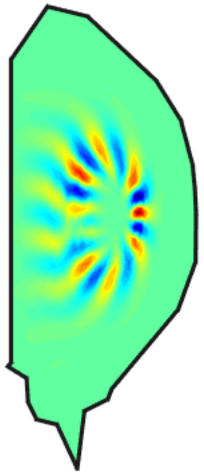


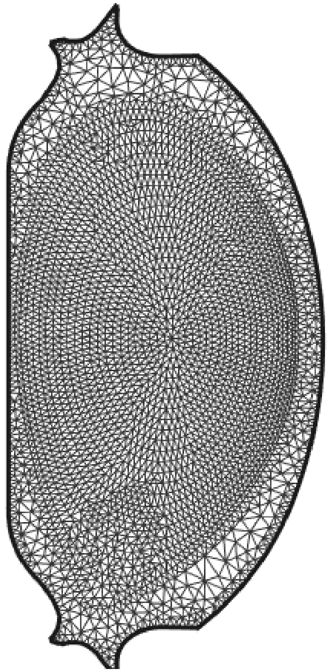


TRIMEG results: for ASDEX Upgrade upper snow flake divertor (data from O. Pan, IPP; Lunt et al, Nuclear Materials and Energy 12 (2017): 1037)



Eigenmode calculated using TRIMEG for CFETR (data from Z. Li, PKU)





TRIMEG results: DTT (data from G. Vlad , M. Falessi, ENEA)

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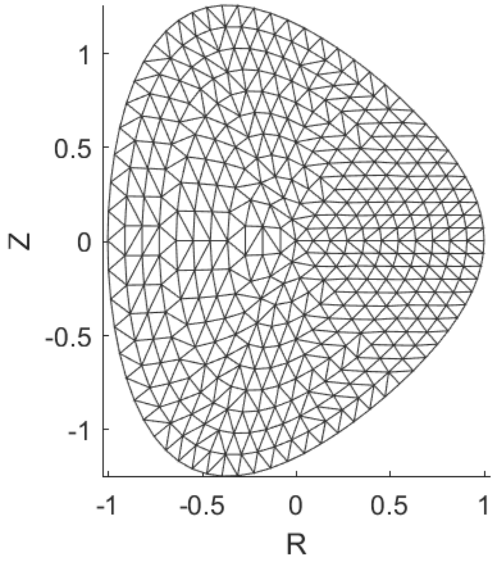
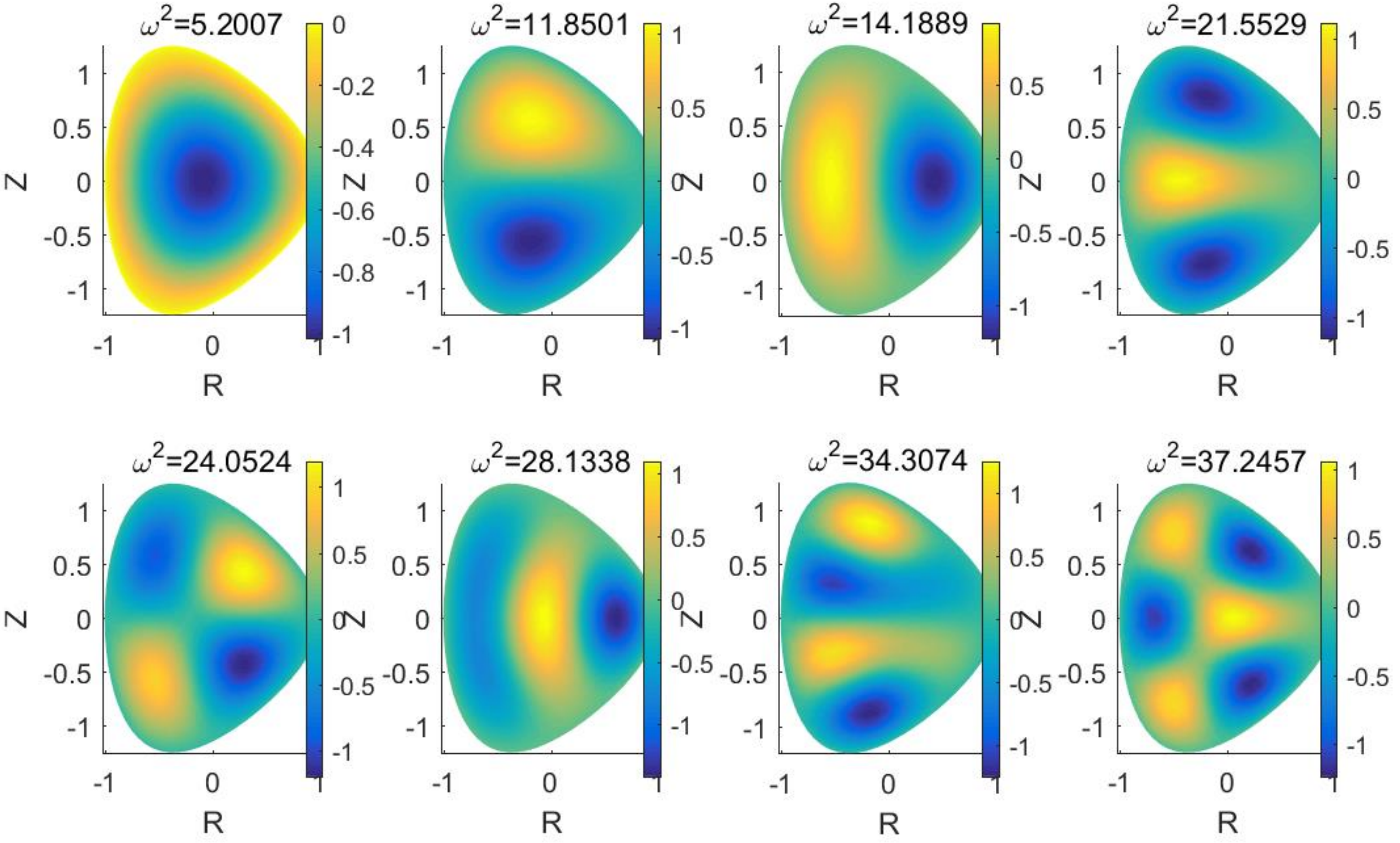
Solution of eigenvalue problem: different eigenstate

- Helmholtz equation:
  $\nabla^2\delta\phi_{\omega_p} - \omega^2\delta\phi_{\omega_p} = 0$
- 2D eigenmodes with Dirichlet BC

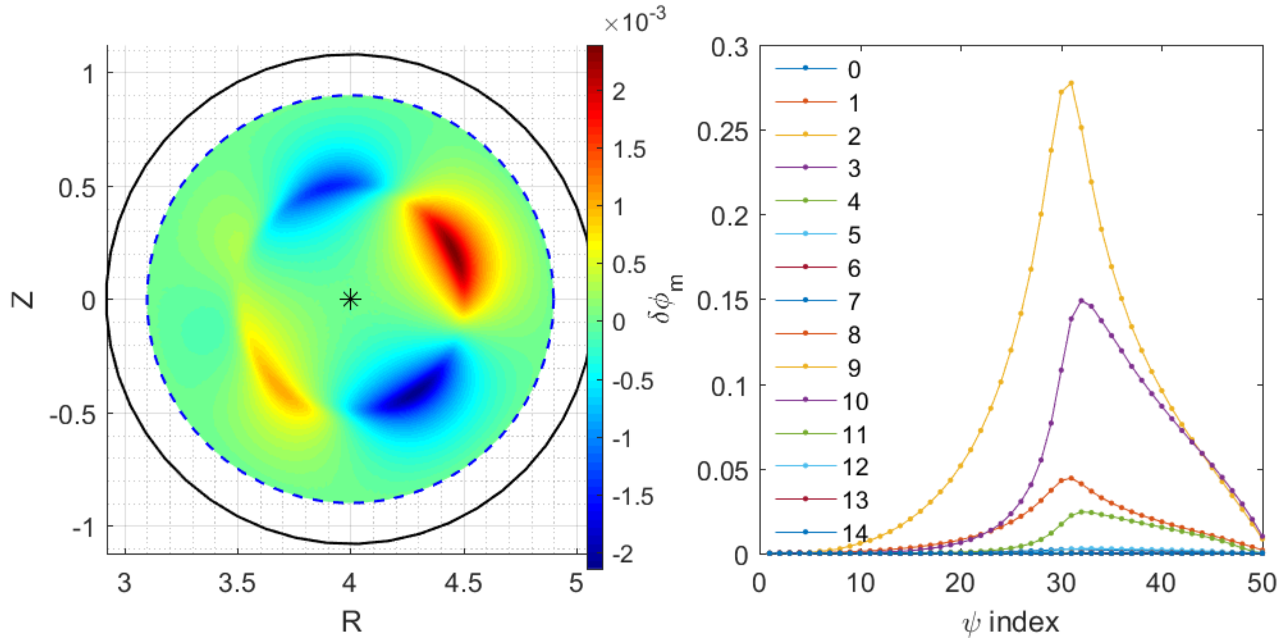




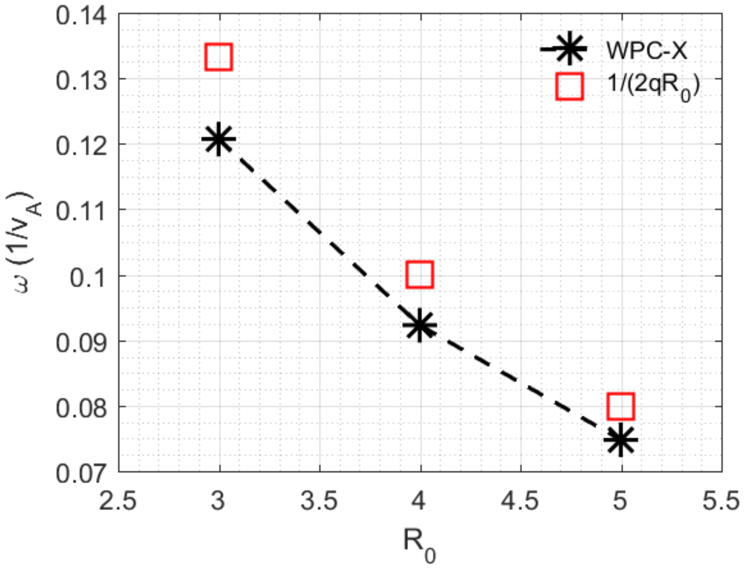
Mode structure symmetry property of different eigenstates for KBM studied in [Xie, Lu, Li POP 25(7) 072106 (2018)]

Eigenvalue approach: TAE

- Toroidal Alfvén eigenmodes (TAE): $\nabla_\perp \cdot \frac{\omega^2}{v_A^2} \nabla \delta\psi + B\partial_\parallel \frac{\nabla_\perp^2}{B} \partial_\parallel \delta\psi = 0$



Comparison with HYMAGYC (X. Wang&ENEA), LIGKA (Ph. Lauber) in plasma core: in progress



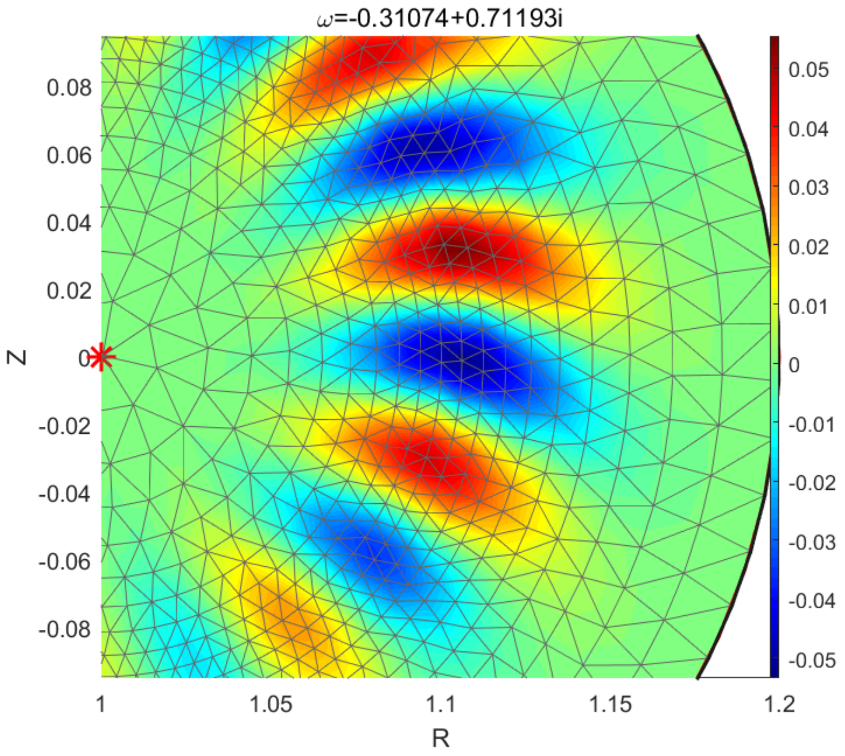
WPC-X: Wave Packet Calculation code (under TRIMEG framework)

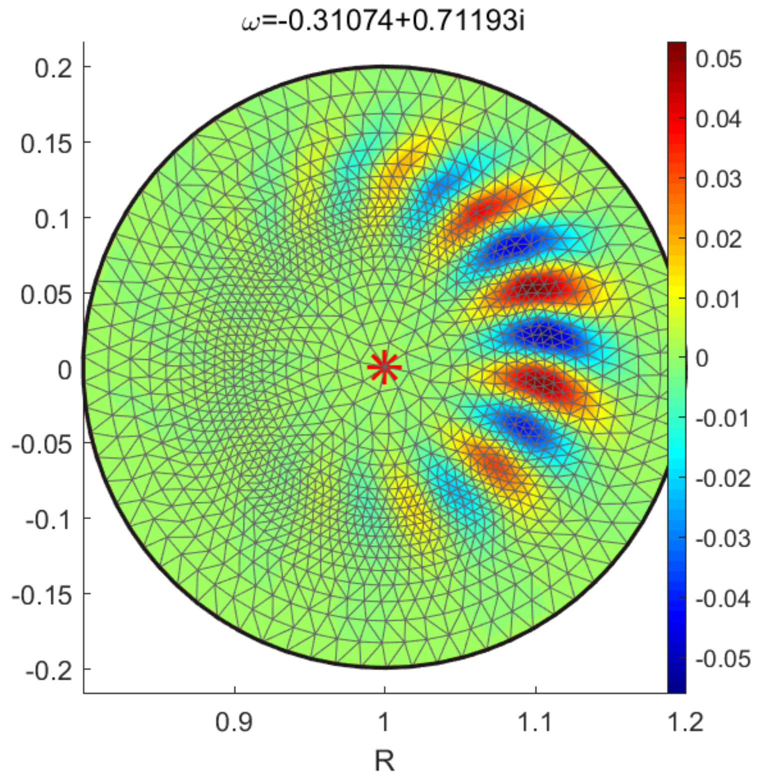
Eigenvalue approach: ITG (fluid-like ions)

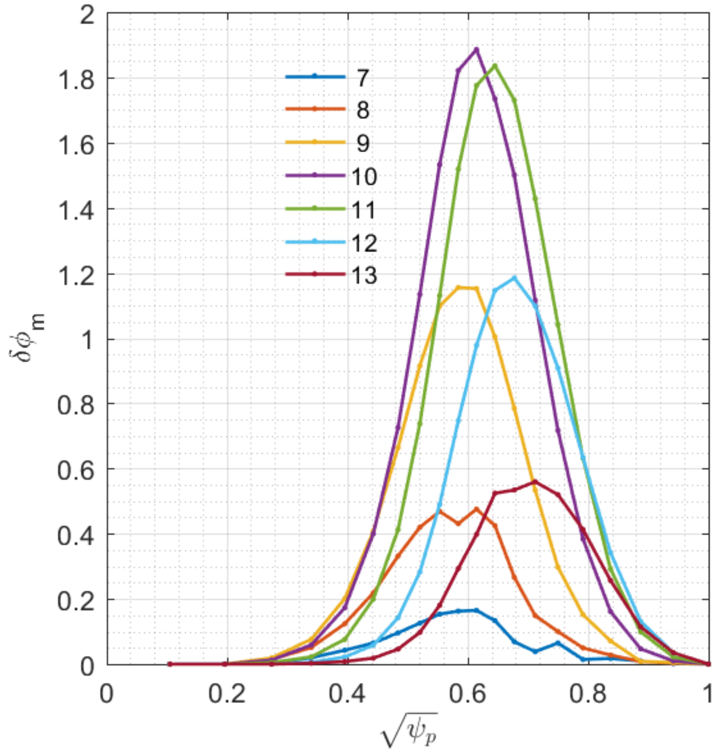
- Ion temperature gradient (ITG) mode

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

Denser grids adopted in maximum mode amplitude region







Comparison with LIGKA (Ph. Lauber) in plasma core: in progress

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Initial value approach: PIC simulation

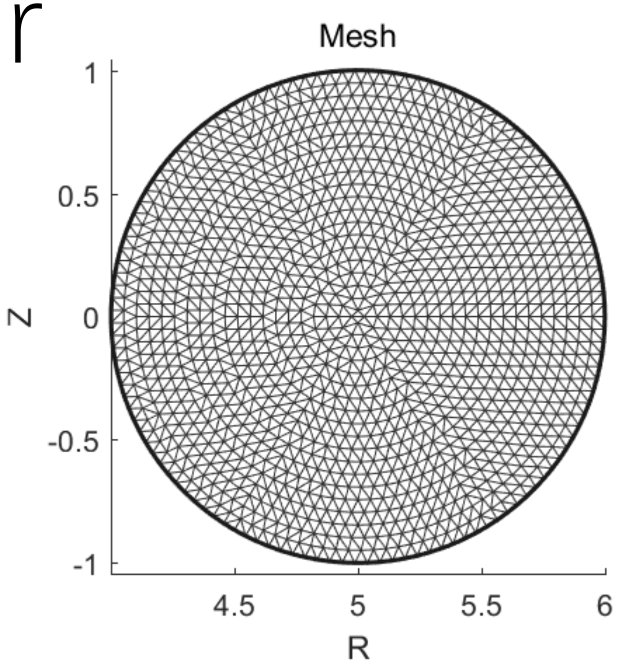
- Models
  - Delta f method $\frac{\mathrm{d}\delta f}{\mathrm{dt}} = -\dot{\boldsymbol{r}} \cdot \nabla f_0 - \dot{v}_\parallel \frac{\partial}{\partial v_\parallel} f_0$
  - Long wavelength approximation for ion polarization density

    $-\nabla_\perp \cdot \frac{q_i n_0}{B\Omega_i} \nabla_\perp \delta\phi = \delta\, \bar{n}_i$-$\delta n_e$; adiabatic $\delta n_e = \frac{e}{T_e}(\delta\phi - \langle\delta\phi\rangle_\psi)$
  - Particle-in-cell in (R, Z) plane (unstructured mesh), Particle-in-Fourier (PIF) in ϕ direction

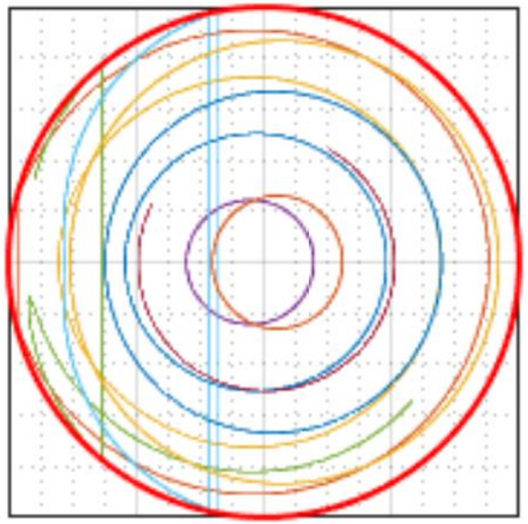
- Simplification for axisymmetric (n=0) problem (GAM/EGAM)
  - Ad-hoc equilibrium (A. Bottino, ORB5)
  - Linearized gyrokinetic equation; only lowest order for GAM problem [Z. X. Lu et al, PPCF submitted]
  - Long wave length approximation for ion polarization
  - No gyro average in particle equation of motion, i.e., $\langle\delta\phi\rangle_{Gyro} \approx \delta\phi$ (small $k_r \rho_i$ limit)

Coordinates, mesh and RK4 integrator

- Hybrid coordinates: equation of motion in (R, Z, ϕ) [Chang, POP'04]; grids along flux surface
- Intermediate structured grid (r, θ) for charge deposition [W.X. Wang POP'06]
- Reflected particles (up-down symmetric) for touching-wall particles
- Particle motion: Runge-Kutta 4th order, coupled to Poisson solver



Particle trajectory



Particle coordinates increment k

Field value $\delta\phi$

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

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

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

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

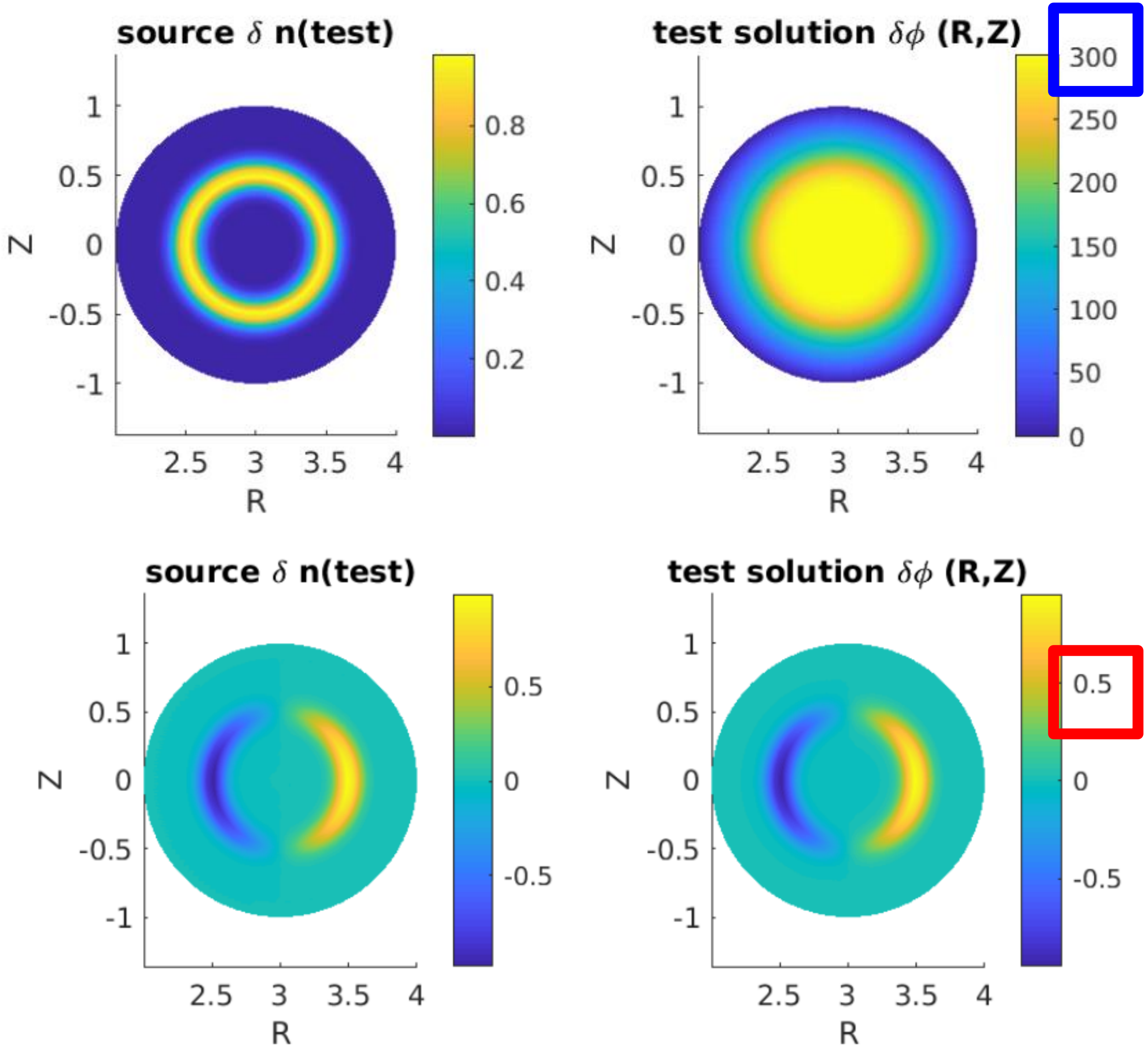
$$k_3 = h\, f\left(t_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right),$$

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

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

Field solver with flux surface average: important for Zonal component calculation

- m=0
- m=1



- $\delta\phi$ response to $\delta n(m=0)$ is much larger than that to $\delta n(m\neq 0)$

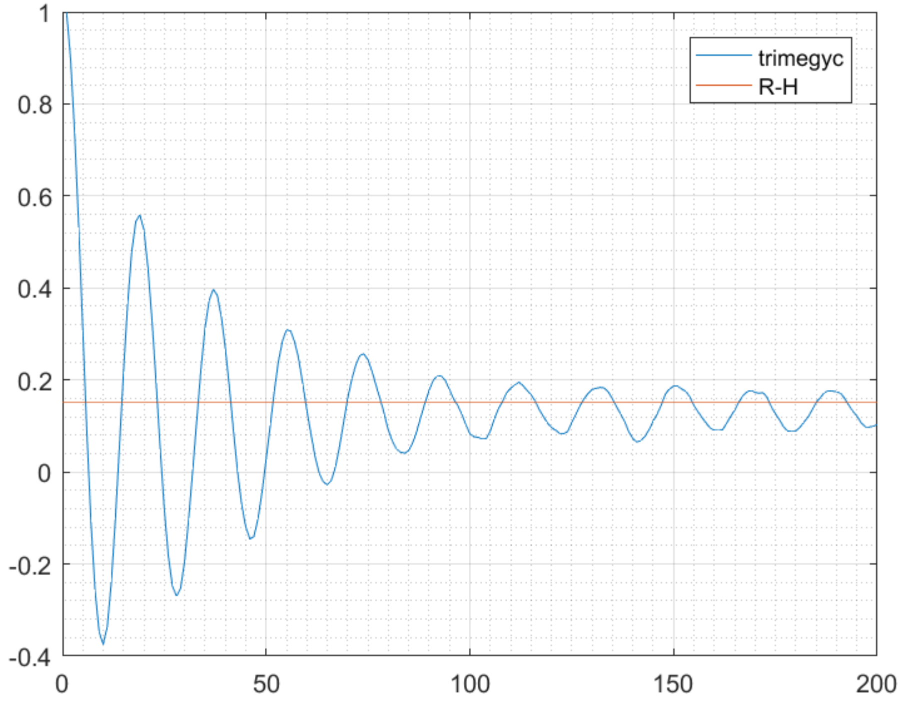
$$-\nabla_\perp \cdot \frac{q_i n_0}{B\Omega_i}\nabla_\perp \delta\phi = \delta\,\bar{n}_i\text{-}\delta n_e$$

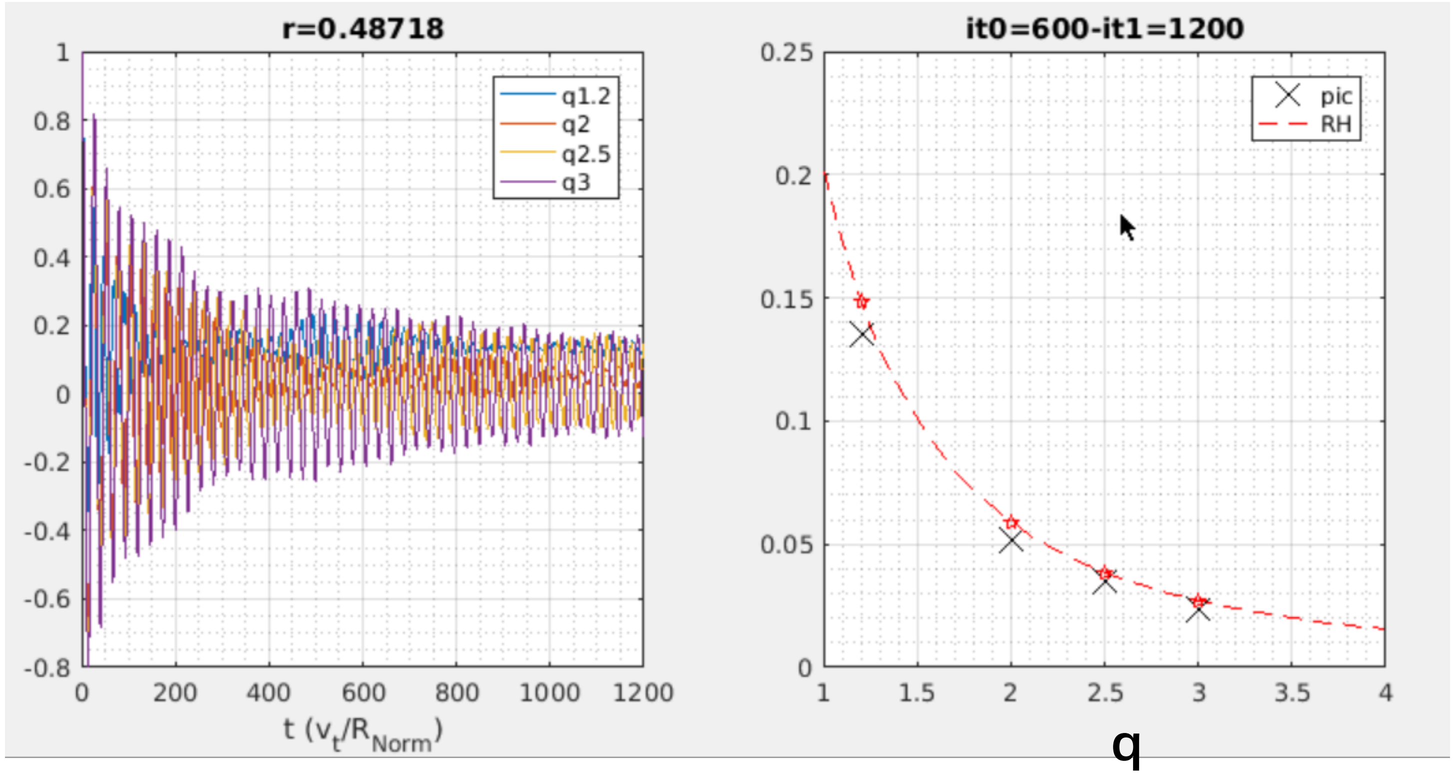
Adiabatic electrons:

$$\delta n_e = \frac{e}{T_e}(\delta\phi - \langle\delta\phi\rangle_\psi$$

Single species test: GAM residual level

- Maxwellian species, low $k_r \rho_{Ti}$ limit
  - Residual level predicted by Rosenbluth-Hinton (R-H) results

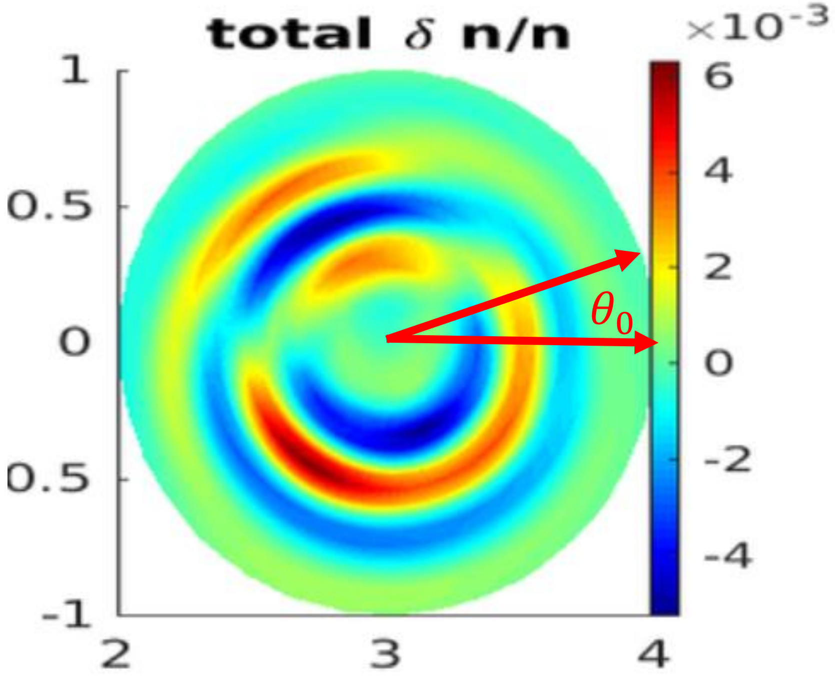


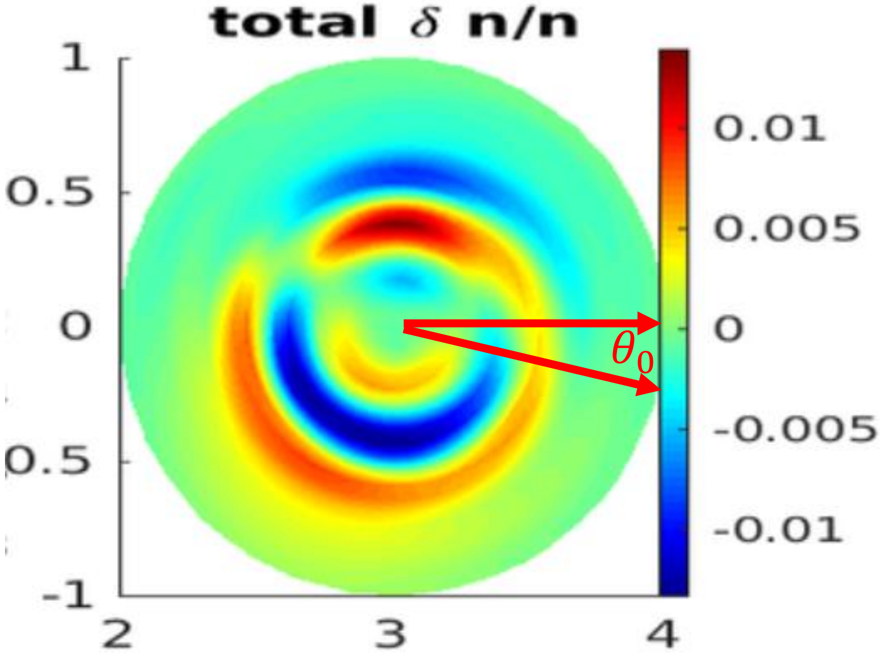


Implementation directed by theoretical derivation: dominant terms kept [Z.X. Lu et al, NF' 18]
Gyro average needs to be added for Finite Larmor radius and orbit width effects [Zonca EPL'08]

EGAM mode structure symmetry breaking

- Tilting angle changes directions when injected EP direction changes
- Single bump-on-tail EP source: $f_{EP} = \frac{1}{\pi^{1.5} v_t^3} \exp\{-\frac{(v-u_\parallel)^2}{v_t^2}\}$





- 2D mode structure tilting angle θ_0 changes its sign for $u_\parallel = 3v_{th}$ (left) and for $u_\parallel = -3v_{th}$ (right)
- EGAM mode structure symmetry breaking effects on particle/momentum/heat transport discussed theoretically [Z.X.Lu et al PPCF submitted]

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Fluid electron model: fluid electron, gyrokinetic energetic particle

- Field equation with EP contribution

$$\partial_t \delta A_\parallel = -\hat{b} \cdot \nabla_\parallel \delta\phi \ (1)$$

$$\partial_t \left\{ \nabla \frac{m_i n_0}{B^2} \cdot \nabla_\perp \delta\phi \right\} + B \partial_\parallel \frac{1}{B\mu_0} \nabla_\perp^2 \delta A_\parallel = \nabla_\perp \cdot \delta J_{\perp,EP} \ (2)$$

- $\delta J_{\perp,EP}$: calculated from the evolving EP information

$$\partial_t \delta f = -f_0 \kappa(\Upsilon)\dot{\Upsilon} + \frac{\partial f_0}{\partial \epsilon} \dot{\epsilon} \quad (3)$$

- Similar to the ``minimum'' e-fluid model in ORB5 [Mishchenko, Bottino et al]

Field integrator: verification using Helmholtz equation

- Model equation for testing implicit scheme:

$$\partial_t^2 \delta\phi + \nabla^2 \delta\phi = 0 \ (1)$$

- Explicit V.S. implicit scheme
  - Discretization for $\partial_t \delta\phi = L(\boldsymbol{R})\delta\phi$
    L: a linear operator, represented as mass and stiffness matrices in unstructured mesh
  - Explicit (Euler method): $\frac{\delta\phi_i^{t+\Delta t} - \delta\phi_i^t}{\Delta t} = L\delta\phi_i^t$
  - Implicit: $\frac{\delta\phi_i^{t+\Delta t} - \delta\phi_i^t}{\Delta \mathrm{t}} = \frac{L\delta\phi_i^{t+\Delta t} + L\delta\phi_i^t}{2}$
- Accuracy test: comparing with eigenvalue solution

$$\nabla^2 \delta\phi_{\omega_p} - \omega^2 \delta\phi_{\omega_p} = 0$$

  - Solution of Eq. (1): $\delta\phi = \sum_p \delta\phi_{\omega_p} e^{-i\omega_p t}$
  - Eigenvalue and initial value problem connected with each other closely

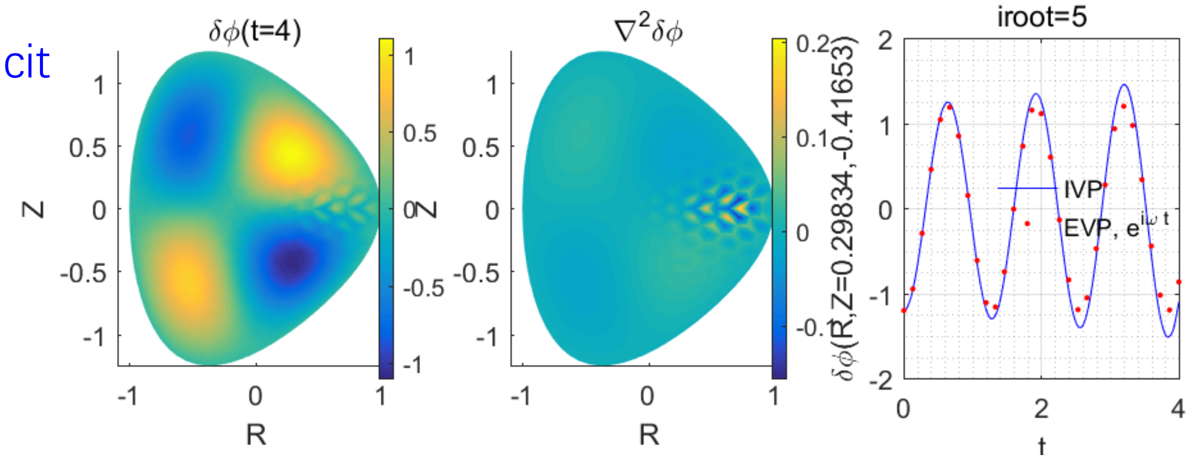
[Vlad, G., F. Zonca, and S. Briguglio. *La Rivista del Nuovo Cimento (1978-1999)* 22.7 (1999): 1]

Explicit v.s. implicit schemes

- Comparison

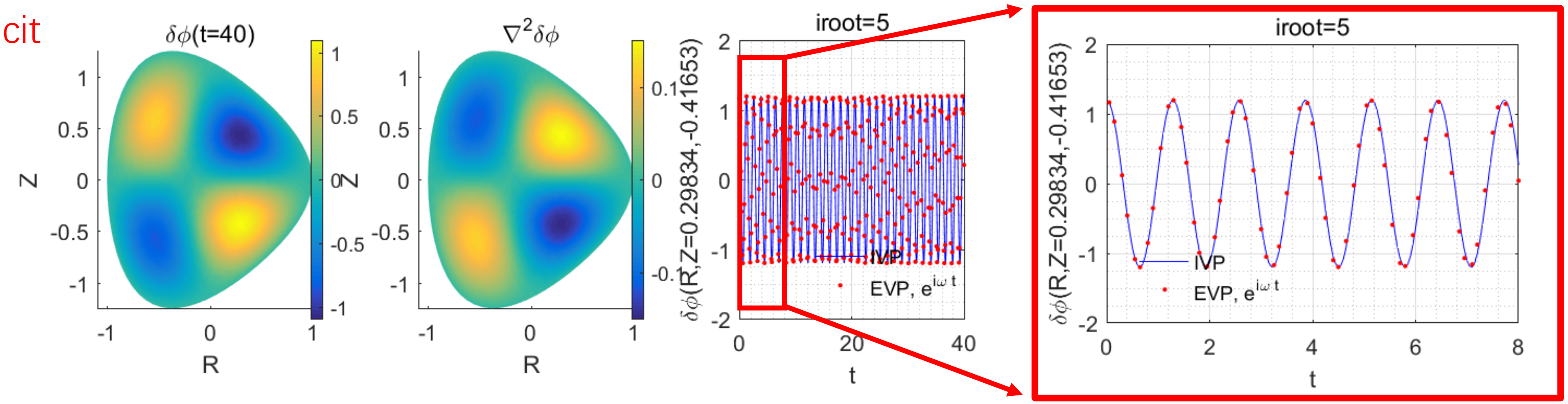
	dt	t end
Explicit	0.005	4
Implicit	0.05	40

Explicit



Numerical instability after t=5 (explicit)
Red dots: theoretical results;
blue line: initial value approach

Implicit

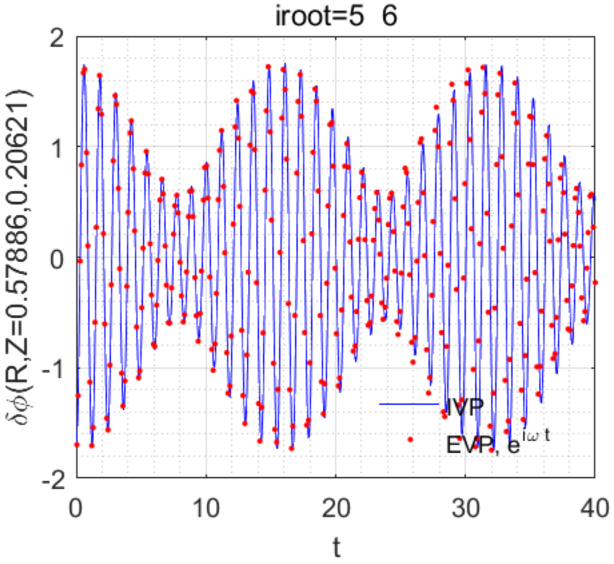


Time evolution of multiple eigenmodes

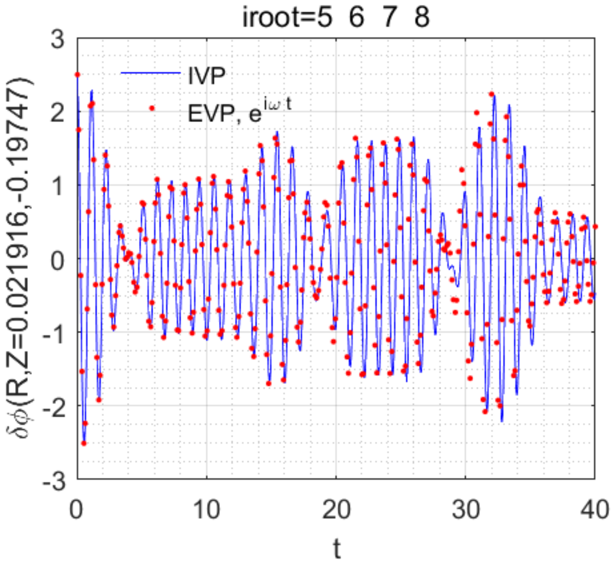
- Superposition of a band of eigenmode

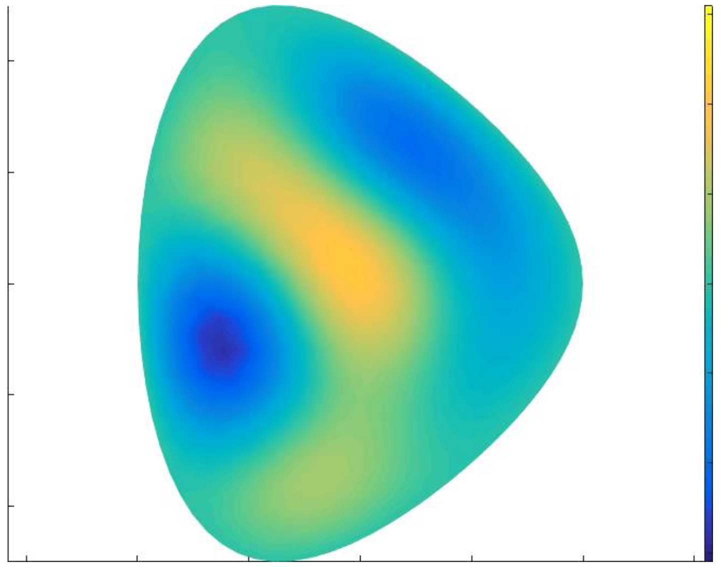
iroot=5,6,7,8

Two eigenmodes as initial value



Four eigenmodes as initial value





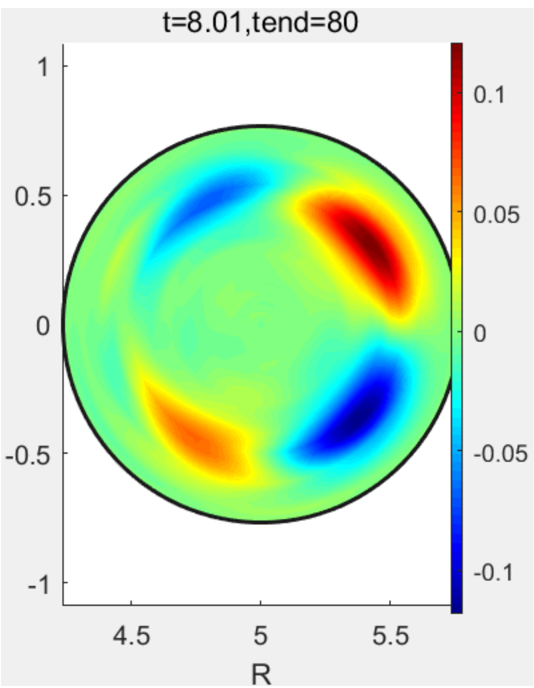
- The implicit time scheme produces accurate time evolution

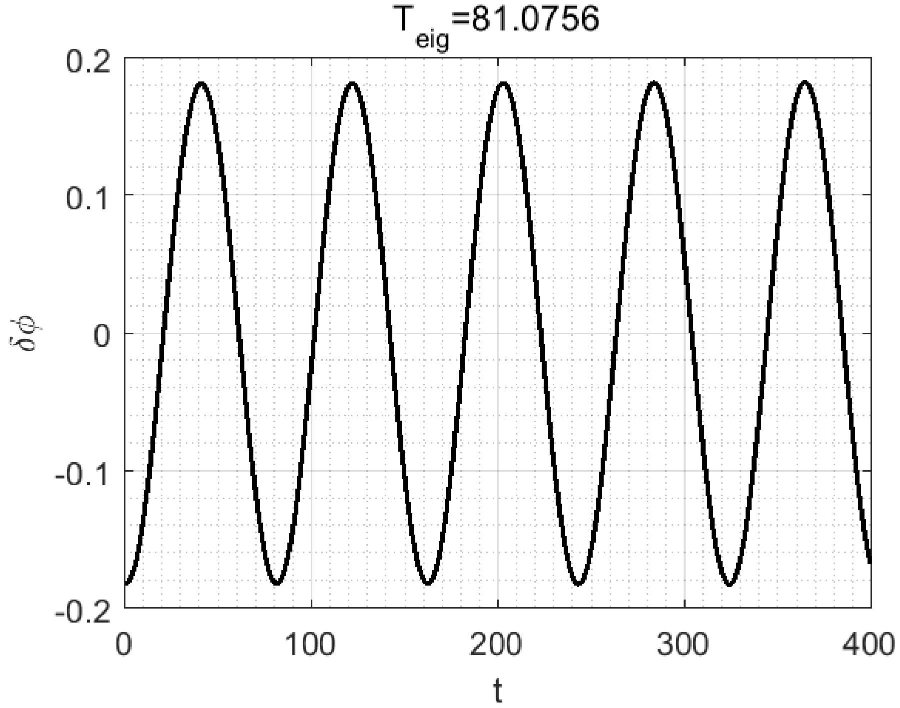
Results of TAE evolution w/o EPs

- For zero EP density: $\partial_t^2 \nabla_\perp \cdot \frac{1}{v_A^2} \nabla \delta\psi = B \partial_\parallel \frac{\nabla_\perp^2}{B} \partial_\parallel \delta\psi$, i.e., $\nabla \cdot \delta j = 0$

- It corresponds to the eigenvalue problem $\nabla_\perp \cdot \frac{\omega^2}{v_A^2} \nabla \delta\psi + B \partial_\parallel \frac{\nabla_\perp^2}{B} \partial_\parallel \delta\psi = 0$

- 2D mode structure and time evolution (explicit scheme)



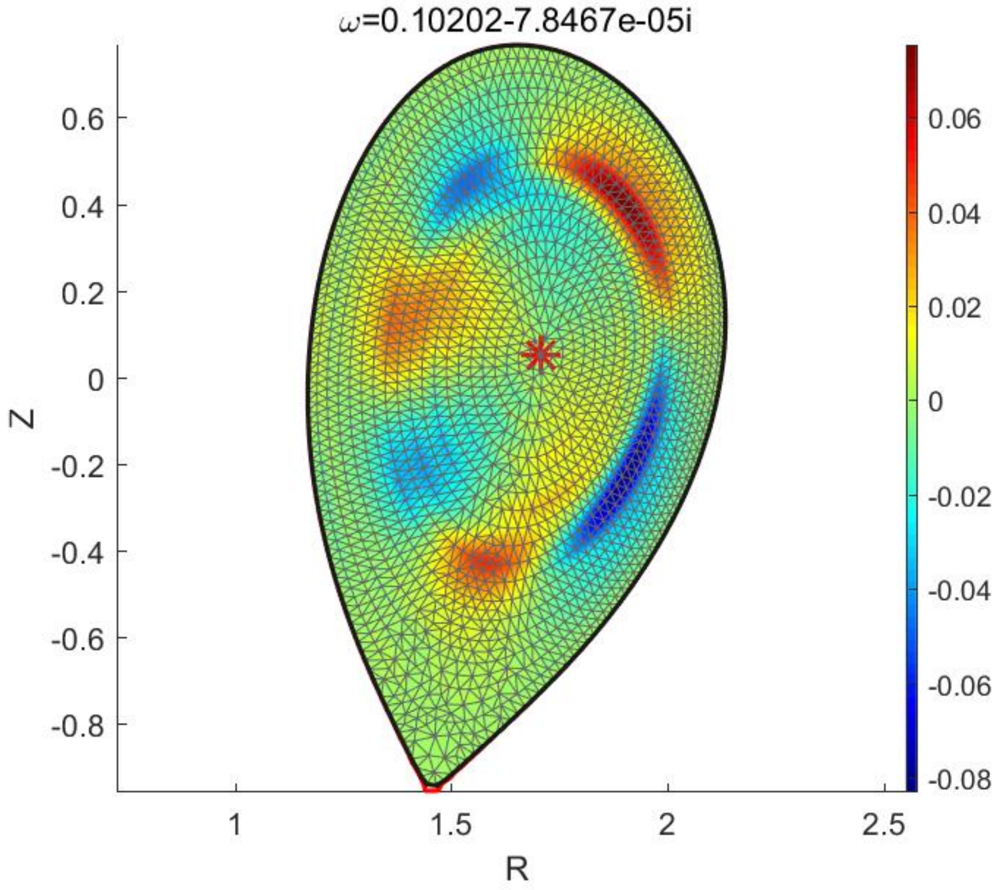


Preliminary results of TAE calculation for AUG plasma

- Strongly non-linear energetic particle dynamics in ASDEX Upgrade with core impurity accumulation has been studied [Lauber et al, 27th IAEA FEC, 2018]

- Simulation using ORB5 is important for identifying the nonlinear physics
  - Simulation using AUG discharge 034924.036 is in progress, following the DIII-D benchmark case [Taimourzadeh et al, submitted to NF]

- TAE studies using finite element method for unstructured mesh is in progress
  - TAE eigenvalue and 2D mode structure obtained using AUG discharge 034924.03600
  - Simulation using initial value approach with EP effect in progress



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- Aim: a numerical tool for wave packet calculation, mode structure symmetry breaking studies and energetic particle physics

- Finite element method for unstructured mesh implemented
- Field class and particle class tested in Eigenvalue and initial value problems
- Physics problems tested
  - ITG/TAE eigenvalue problem
  - Particle-in-cell simulation: GAM residual level and symmetry breaking
  - Toroidicity induced Alfven eigenmode for ad-hoc equilibrium and for AUG

Outlook

- Numerical improvement
  - For better efficiency, sparse matrix solver in Fortran (WSMP/PETSC/PARDISO) is needed (PETSC serial solver implemented)
  - C^0 high order basis or C^1 basis needed for higher differential operators
  - Realistic tokamak geometry and plasma profiles

- Physics targets
  - Wave packet calculation (propagation & absorption)
  - Mode structure symmetry breaking and momentum transport with EP effects
  - Analyses of experimental data for EGAM, AEs (NAT project)
  - Edge physics (contribution to ORB5&EUTERPE…)?

- Your suggestions are appreciated

Backup

- A brief introduction to TRIMEG
- Delaunay triangulation examples
- Multiple species simulation: preliminary results
- Petsc solver (for 2D structured mesh test, finite difference)
- Boundary condition

A brief introduction to TRIMEG

- TRIMEG: TRIangular MEsh based Gyrokinetics
  - Object Oriented Programming: capsulation considered for equilibrium, field and particle classes; inheritance and polymorphism: less demanding in the present stage
  - Aim: a computational tool with physics targets

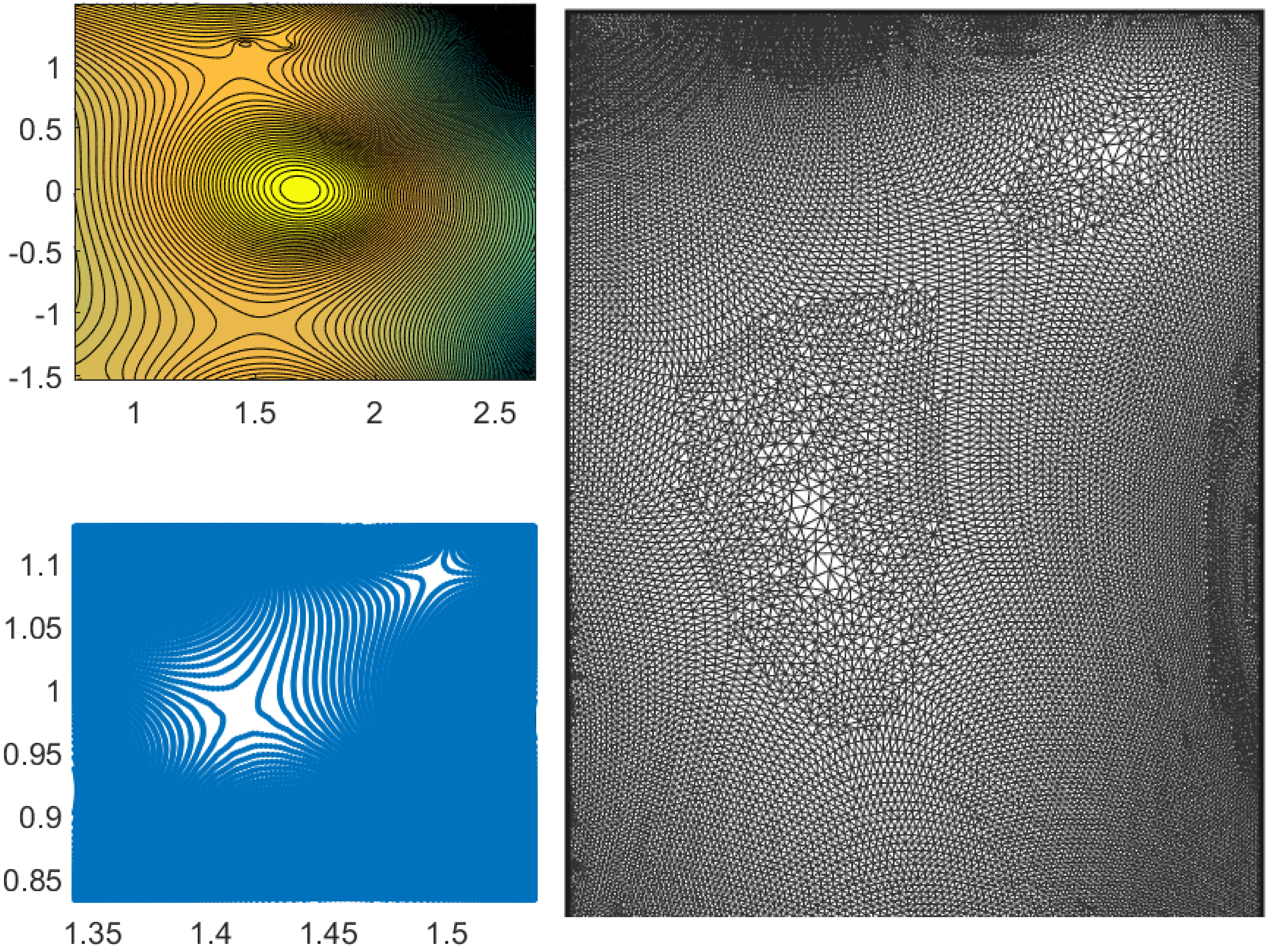
Numerical features	**Present status**
1 Unstructured mesh	Mesh generated using Fortran/Matlab libraries
2 Finite element method	C0 linear/quadratic basis implemented, linear one routinely used
3 Initial value problem: RK4 or/and implicit treatment	RK4: circular PIC code; implicit: 2D FEM Poisson solver
4 Multi languages: Fortran&Matlab (Lu), Python (Wang)	Most in Matlab, Fortran version works for GAM, python in progress
5 Scalability using ScaLapack/PETSC/WSMP	MKL Lapack full matrix solver tested in Fortran; PETSC interface tested for Helmholtz equation (preliminary)

A brief introduction to TRIMEG

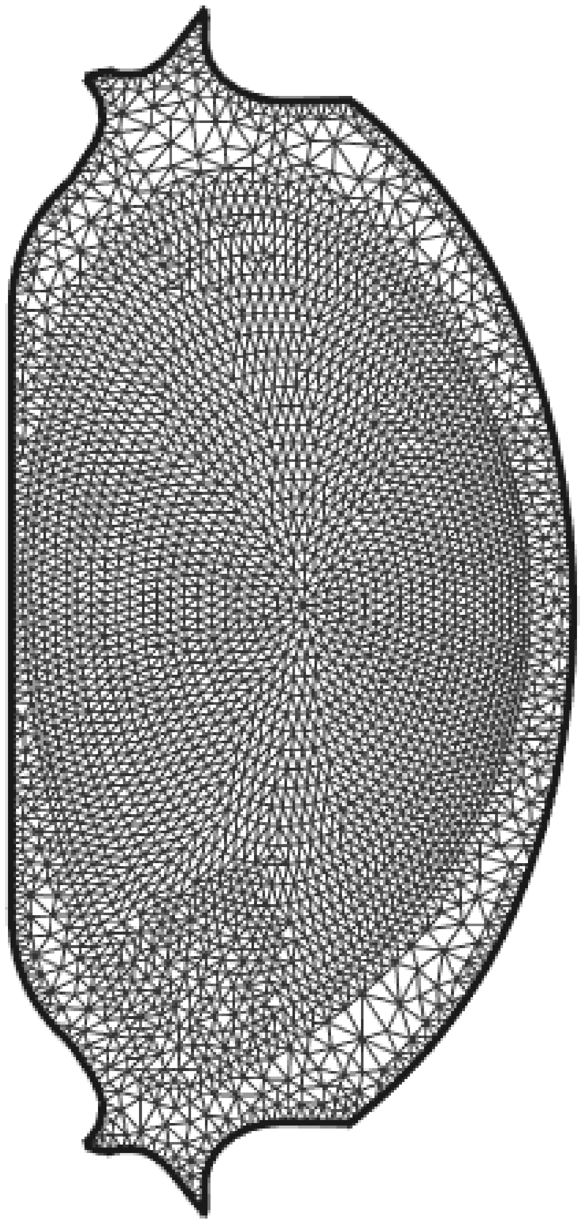
- TRIMEG: TRIangular MEsh based Gyrokinetics

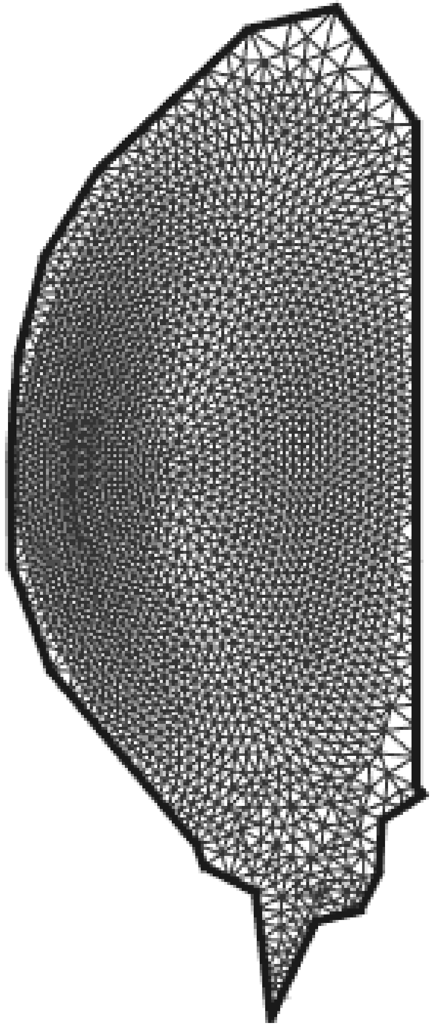
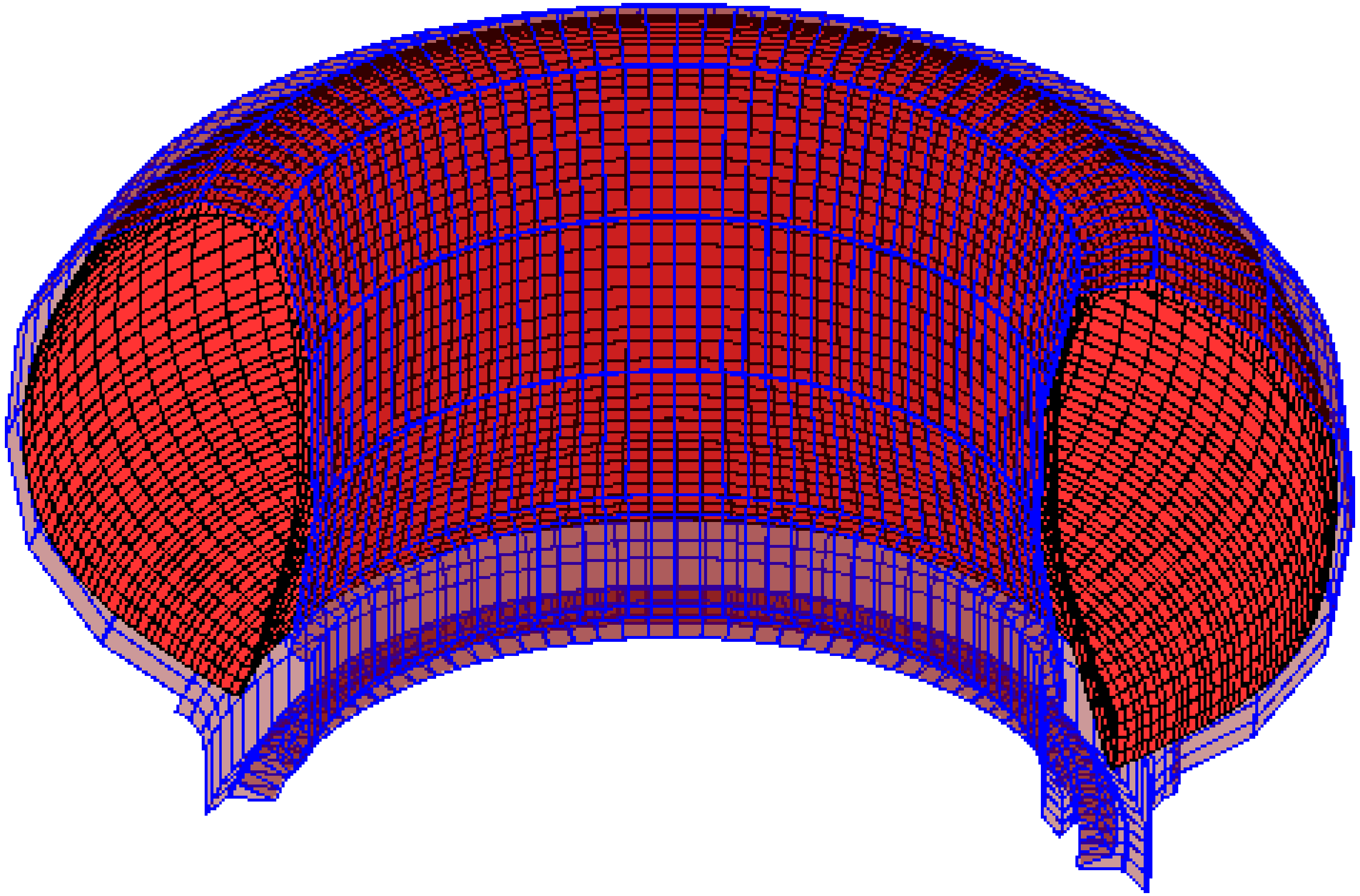
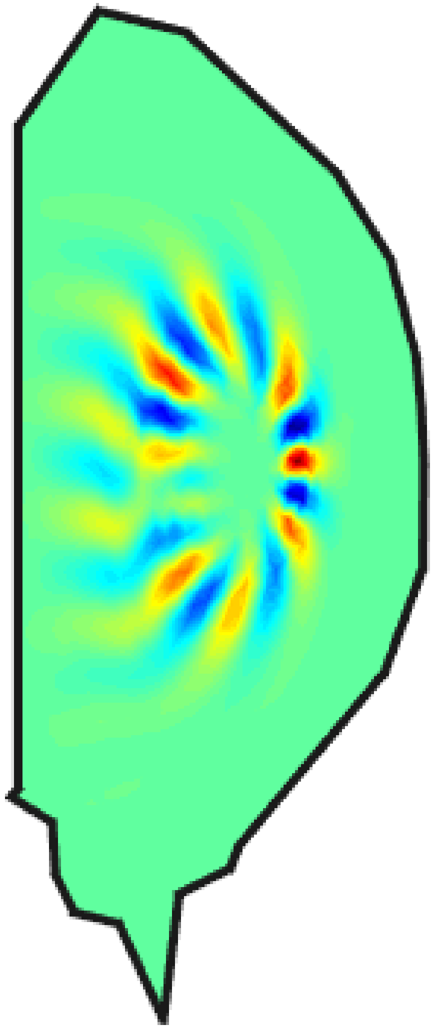
Physics targets	Present status
1 Realistic tokamak geometry	Ad-hoc/EQDSK equilibrium in Matlab; ad-hoc in Fortran
2 Wave Packet Calculation (forced oscillation & instability)	TAE 4^{th} order eigenvalue equation solved (to do: comparison with LIGKA); ITG fluid equation solved
3 Mode structure symmetry breaking & momentum transport	ITG mode structure tilting observed (to do: flux calculation along EGAM momentum transport derivation)
4 Multiple species (energetic particle physics)	EP effects in ZF residual (trends observed in Matlab PIC)
5 More challenging (but important): nonlinear physics, GeFi	To do: collaboration with Philipp on AUG cases; collaboration of Gefi (Yu Lin, F. Zonca); ORB5 simulation

Acknowledge: J. Chen (FEM, mesh); T. Hayward-Schneider (particle positioning), Ph. Lauber, X. Wang, A. Bottino, W.X. Wang, G. Meng (RBQ), R. Kleiber, B.D.Scott, G. Vlad, F. Zonca for instructive feedback



ASDEX Upgrade upper snow flake divertor (data from O. Pan, IPP; Lunt et al, Nuclear Materials and Energy 12 (2017): 1037)


DTT (data from G. Vlad , M. Falessi, ENEA)

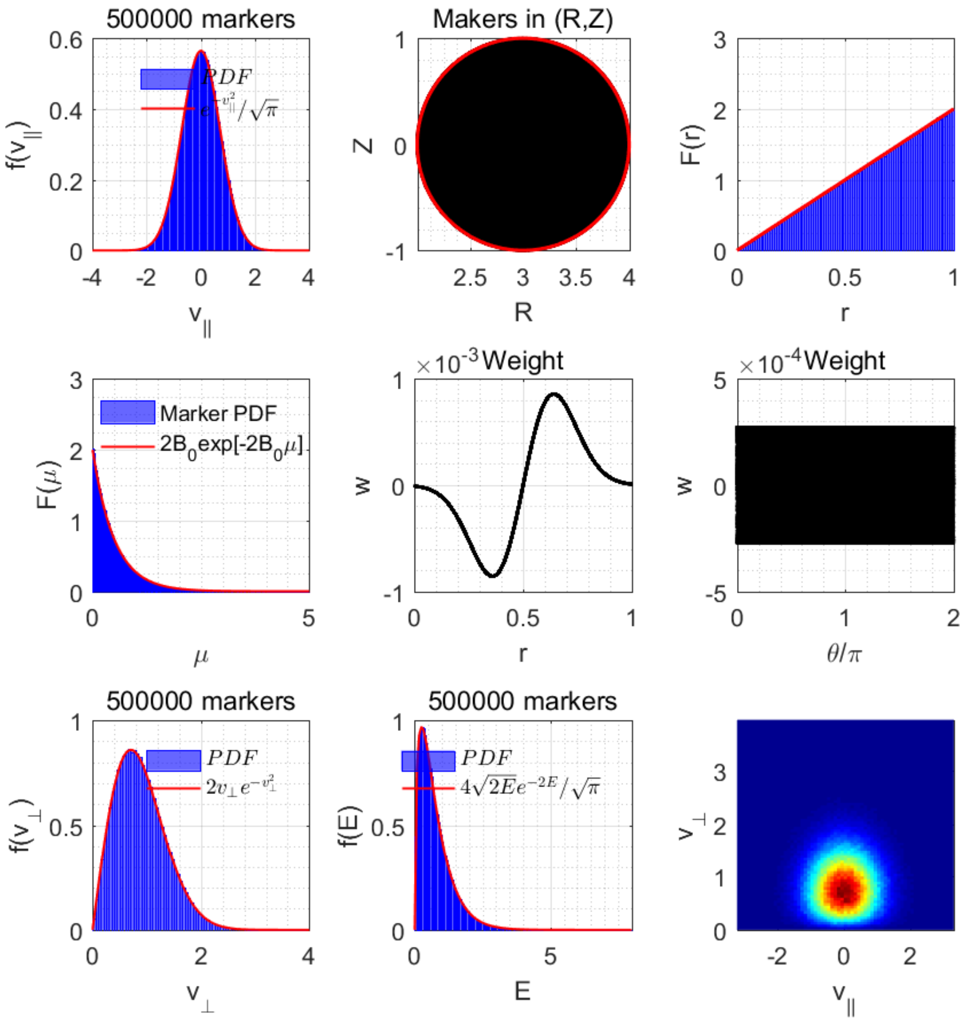




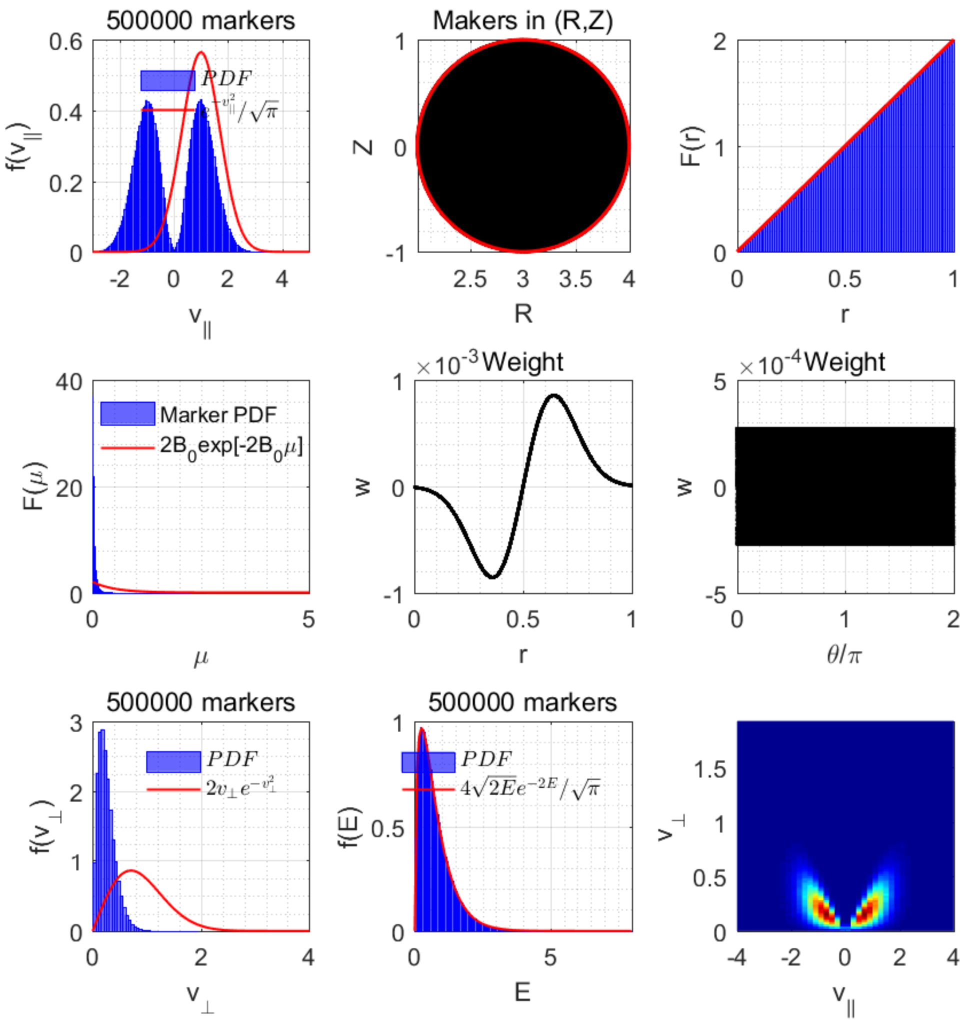
CFETR (data from Z. Li, Peking University)

Particle loading for Maxwellian and anisotropic species

- Maxwellian species
- Anisotropic species

0.5 million markers



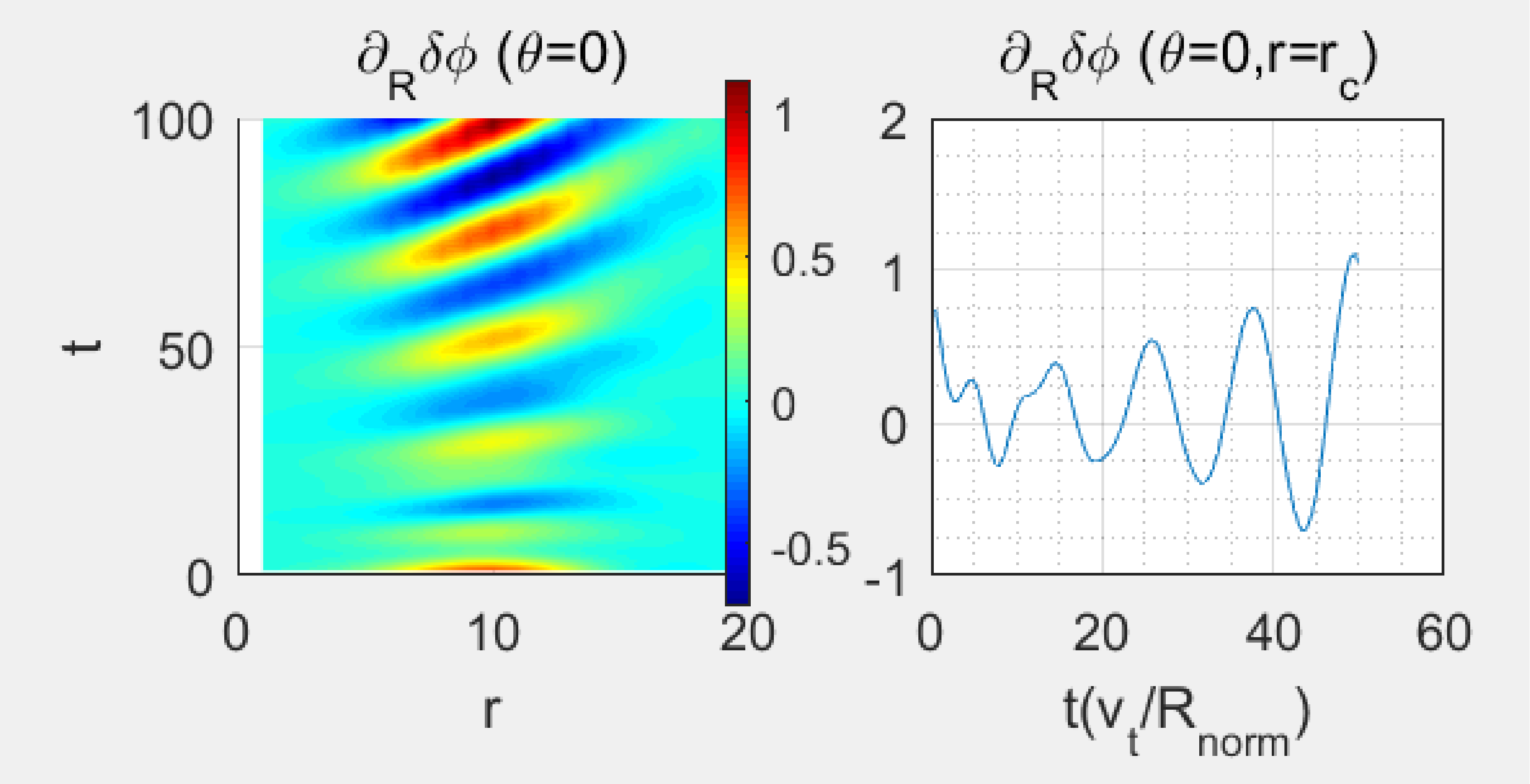


Different loading scheme worthwhile trying (inspired by Alberto)

Multiple species simulation: preliminary results

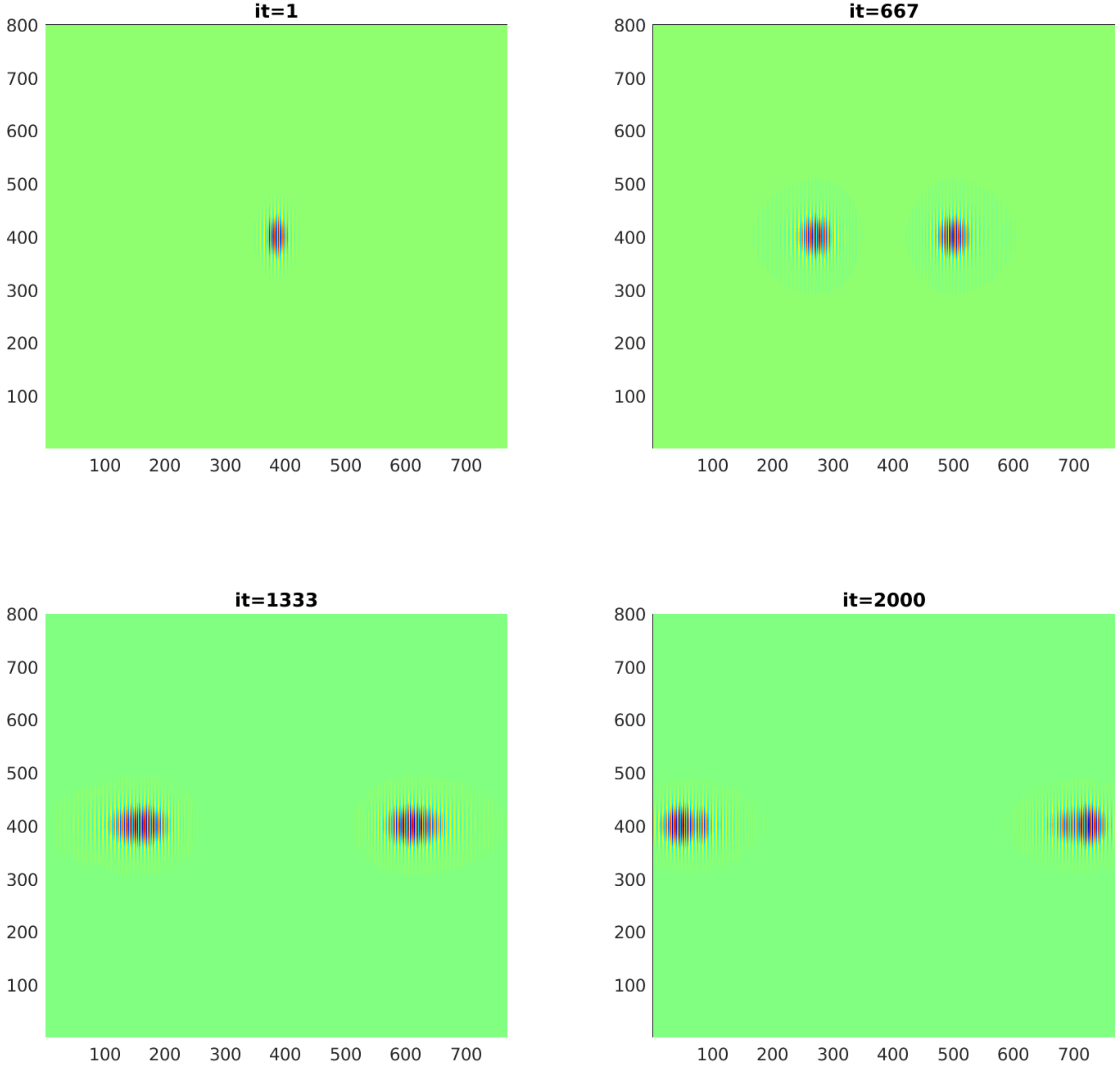
- Expected picture: EGAM excitation with thermal ions & EPs
- EP: shifted Maxwellian
- Instability observed (preliminary)

To be compared with [Zarzaso NF'14, Biancalina NF'14]



Petsc solver: test for 2D wave propagation

- Solver tested for 2D wave packet propagation; finite difference
- Sparse matrix used, KSP solver
- Total DOF: 800*768; 2000 steps finished in <30 mins (serial version)
- Coupling to TRIMEG: in progress
- Scalability: as reference, an available physics study case is Alctor C-Mod ITG/TEM simulation using GTS [Lu NF 55, 093012 (2015)]
    - Radial domain: [0.2,0.8], radial grid #: 70-110; 40 markers/cell; 400~600 L_T/v_{ti}; typical core hours: ~0.1 million



Dirichlet, Neumann or mixed boundary condition

- Linear equation: $L(x)y(x) = b(x)$
- $y(x) = \sum_i y_i N_i(x)$, $y_i = \binom{Y^I}{Y^E}$, Y^I & Y^E : values on Internal & External vertices
- For $M_{ij} y_i = b_i$, (1) where $M_{ij} = \begin{pmatrix} M^{I,I}, M^{I,E} \\ M^{E,I}, M^{E,E} \end{pmatrix}$
- Boundary condition described by $(M^{E,I}, M^{E,E}) \binom{Y^I}{Y^E} = b_i^E$, (2a)

  i.e., $Y^E = (M^{E,E})^{-1} M^{E,I} Y^I$ (2b)
- Then (1) → $M^{I,I}\, Y^I + M^{I,E}\, (M^{E,E})^{-1} M^{E,I} Y^I = b_i^I$ (3)