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Particle and moment enslavement in the implicit full f particle simulations

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Background/Motivation

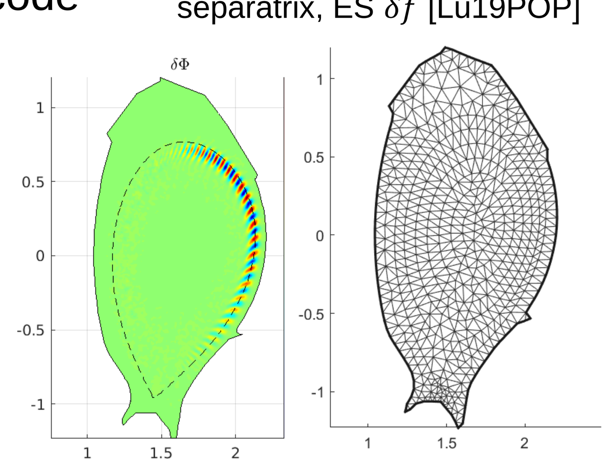
- Early gyrokinetic PIC codes adopted explicit δf as the main scheme
- Full f implicit scheme enables studies of specific physics problems
  - Particle/heat/momentum source and sink; arbitrary distributions
  - Significant profile change during simulation (flux driven simulations)
  - (Semi) implicit scheme or/and full f scheme have attracted numerous efforts [GK5D, GENE; EUTERPE&ORB5, GEMPIC, ELMFIRE, XGC, ECSIM …]
- Implicit scheme: good in conservation properties, large Δt but
  - For a system with N_G field grids and N_p particles, the computational cost is too high: DOF=$N_G + N_p$; matrix size is $(N_G+N_p)^2$.
  - Solution: "particle enslavement" [Chen&Chacon, J. Comput. Phys. 230 (2011) 7018]
    - Particles (x, v) represented as functions of field $F(x)$ → DOF reduced to N_G
  - Open issue: efficient convergence of the implicit particle-field system
    - XGC: preconditioned Picard iteration (numerical); δf [Sturdenvant 2021POP]
    - Our work: analytical treatment of the iteration scheme (rigorous); full f
- The development of the implicit kinetic full f scheme for Alfvén wave/energetic particle physics has not been reported

From ES δf to EM full f TRIMEG

TRIMEG: TRIangular MEsh based Gyrokinetic code

TRIMEG(before 2020)	TRIMEG(since 2020)
• δf, electrostatic, explicit • Unstructured mesh • Adiabatic electrons [Lu et al, POP2019]	• Full f, electromagnetic, implicit • Structured mesh • EM unstructured will be reported elsewhere [Lu et al,JCP2021]

ITG simulation near separatrix, ES δf [Lu19POP]



Conclusions

- The implicit scheme has been implemented for the full f electromagnetic simulations of Alfvén waves and EP physics.
- Using the analytical derivation based implicit scheme "moment enslavement", good convergence of the field-particle solver is achieved
- By applying to the 1D shear Alfvén wave problem, this implicit scheme shows good energy conservation and capabilities of calculating the frequency and damping rate properly in a broad range of β/M_e values, including the small electron mass condition
- The application of this method to the TAE problem shows its applicability for electromagnetic simulations with/without EPs. The TAE mode structure distortion due to the non-perturbative effects of the EPs is observed, consistent with previous simulations and theoretical studies

[1] [Z.X. Lu, Ph. Lauber, T. Hayward-Schneider, A. Bottino, M. Hoelzl, Phys. Plasmas 26, 122503 (2019)]

[2] Lu, Meng, Hoelzl, Lauber, Journal Comput. Phys. 440 (2021) 110384

Physics model & implementation

Shear Alfvén wave in 1D uniform plasma

- Ampere's law: $\nabla_\perp^2 \delta A_\parallel = C_A \delta J_{||}$
- Quasi-neutrality (QN): $\nabla_\perp \cdot \left(\frac{B_0^2}{B^2}\nabla_\perp \delta\phi\right) = C_P \delta N$
  - $C_A = \beta/\rho_{tN}^2$, $C_P = \frac{1}{\rho_{tN}^2}$
  - Ion polarization density balances electron δN in QN Eq (dominant)
- Parallel electron motion:
  - $\frac{dl}{dt} = v_{||}$; l: parallel coordinate
  - $\frac{dv_\parallel}{dt} = \partial_\parallel \delta\phi + \partial_t \delta A_\parallel$
- Analytical dispersion relation:

$$1 - \frac{2\beta[1+\bar\omega Z(\bar\omega)]}{M_e(k_\perp \rho_{ti})^2}\left(\bar\omega^2 - \frac{M_e}{\beta}\right) = 0,$$

$\beta = v_{ti}^2/v_A^2$, v_{ti}, v_A: thermal, Alfven velocities, $\bar\omega = \omega/\omega_{te}$, $\omega_{te} = v_{te}k_\parallel$

- Crank-Nicolson (C-N) scheme (implicit)

$$\frac{l^{t+\Delta t} - l^t}{\Delta t} = \frac{v_{||}^{t+\Delta t} + v_{||}^t}{2}$$

$$\frac{v_{||}^{t+\Delta t} - v_{||}^t}{\Delta t} = \partial_{||}\frac{\delta\phi^{t+\Delta t} + \delta\phi^t}{2} + \frac{\delta A_\parallel^{t+\Delta t} - \delta A_\parallel^t}{\Delta t}$$

$$\nabla_\perp^2 \delta A_\parallel^{t,t+\Delta t} = C_A \delta J_\parallel^{t,t+\Delta t}$$

$$\nabla_\perp \cdot \left(\frac{B_0^2}{B^2}\nabla_\perp \delta\phi^{t,t+\Delta t}\right) = C_P \delta N^{t,t+\Delta t}$$

  - Total Degree of Freedom: $(N_G + N_p)$
- First simplification using "particle enslavement": $(l, v_\parallel)^{t+\Delta t}$ written as functions of $(\delta\phi, \delta A_\parallel)^{t+\Delta t}$; then DOF reduced to N_G [Chen&Chacon JCP 2011]
- Second simplification: "moment enslavement" developed in this work
  - DOF ($>10^5$) in TRIMEG is large; aiming for low cost

Particle & moment enslavement

Workflow of the implicit particle-field solver

- Iterations start with an explicit solution at i=1, aiming for solution to C-N scheme.

$$\xrightarrow{1}\begin{Bmatrix}\delta\Phi^{start}\\ \delta A_\parallel^{start}\end{Bmatrix}^i \xrightarrow{2}\begin{Bmatrix} l\\ v_\parallel\end{Bmatrix}^i \xrightarrow{3}\begin{Bmatrix}\delta N^{start}\\ \delta J_\parallel^{start}\end{Bmatrix}^i \xrightarrow{3}\begin{Bmatrix}\delta\Phi^{end}\\ \delta A_\parallel^{end}\end{Bmatrix}^i \xrightarrow{4}\begin{Bmatrix}\delta\Phi^{start}\\ \delta A_\parallel^{start}\end{Bmatrix}^{i+1};$$ all variables are at $t+\Delta t$ — i: iteration #

1. Each iteration starts with the given field $\{F^{start}(t+\Delta t)\}^i$, where $F \equiv \{\delta\phi, \delta A_\parallel\}$
2. Push particles implicitly from t to $t+\Delta t$
3. In the end of each iteration, fields $\{F^{end}(t+\Delta t)\}^i$ are solved
4. Set $\{F^{start}(t+\Delta t)\}^{i+1}$ so that $|\{F^{start}(t+\Delta t)\}^{i+1} - \{F^{end}(t+\Delta t)\}^{i+1}| \to 0$ in the next iteration

Step 4: good estimate of the field for next iteration $\{F^{start}(t+\Delta t)\}^{i+1}$: key of good convergence

Analytic treatment in iteration: "moment enslavement":

- Particle enslavement: $l = l(\delta\phi, \delta A_\parallel)$, $v_\parallel = v_\parallel(\delta\phi, \delta A_\parallel)$, at $t+\Delta t$
  - $(N_G + N_p)^2$ matrix inversion: unacceptable → "particle enslavement" [Chen&Chacon 2011]
- Moment enslavement: $\delta N^{end} = \delta N^{end}(l, v_\parallel) = \delta N^{end}(\delta\phi, \delta A_\parallel)$, at $t+\Delta t$

Step 4: analytic form for $\{F^{start}\}^{i+1}$: $\{\delta\phi^{start}, \delta A_\parallel^{start}\}^{i+1} = \{\delta\phi^{end}, \delta A_\parallel^{end}\}^i + \{\Delta\delta\phi, \Delta\delta A_\parallel\}$, with

$$\left[\begin{pmatrix}\frac{1}{C_P}\nabla_\perp^2, & 0\\ 0, & \frac{1}{C_A}\nabla_\perp\cdot\frac{B_0^2}{B^2}\nabla_\perp\end{pmatrix} - \bar{\bar{M}}_c\right]\cdot\begin{bmatrix}\Delta\delta\phi\\ \Delta\delta A_\parallel\end{bmatrix} = \begin{bmatrix}\delta N^{end} - \delta N^{start}\\ \delta J^{end} - \delta J^{start}\end{bmatrix}^i, \quad \bar{\bar{M}}_c = \begin{bmatrix}\frac{\partial\delta N^{end}}{\partial\delta\phi}, & \frac{\partial\delta N^{end}}{\partial\delta A_\parallel}\\ \frac{\partial\delta J^{end}}{\partial\delta\phi}, & \frac{\partial\delta J^{end}}{\partial\delta A_\parallel}\end{bmatrix} \approx \begin{bmatrix}\frac{k_\parallel^2\Delta t^2}{4M_e}, & -i\frac{k_\parallel\Delta t}{2M_e}\\ i\frac{k_\parallel\Delta t}{2M_e}, & \frac{1}{M_e}\end{bmatrix}$$

- $\bar{\bar{M}}_c$ obtained analytically; rigorous form can be readily obtained
- Numerical calculation of $\bar{\bar{M}}_c$, cost: $(\alpha N_G \times N_p/\text{cell})$: not cheap; complicated in implementation
- Analytic acceleration here, cost: N_G, i.e., "moment enslavement"

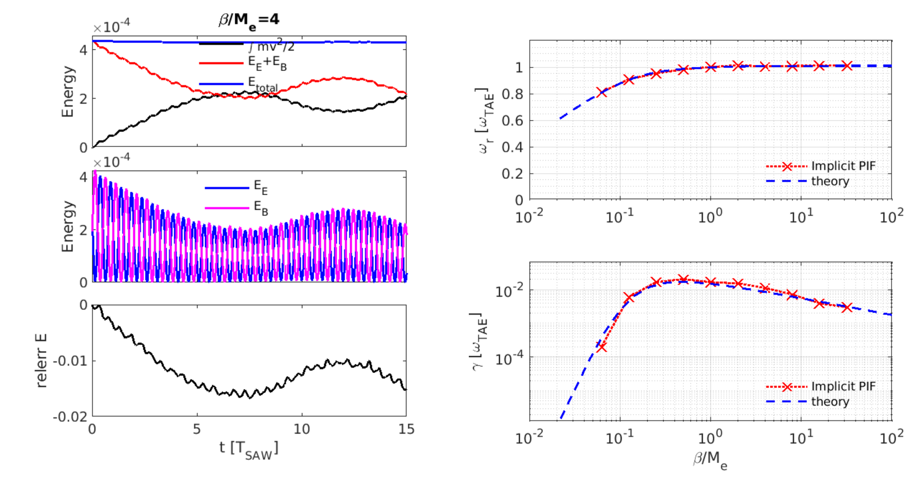
Another way: push particles and calculate $\bar{\bar{M}}_c$; more expensive by a factor of αN_p/cell, $\alpha > 1$.

1D Shear Alfven wave simulations

The implicit scheme is capable of simulating SAW in a broad range of $\frac{\beta}{m_e}$

- The relative error in total energy is bounded (< 0.02)
- Damping rate and real frequency properly simulated

- $k_\perp \rho_N = 0.2$, $\beta/M_e \in \left[\frac{1}{16}, 32\right]$, marker #: 10^5, $dt = 0.01T_{SAW}$
- Parameters relevant to tokamak plasmas, $\beta = 1\%$, $M_e = \frac{1}{1836}$
- Using implicit scheme, SAW is simulated
- For high β/M_e, more iterations needed for convergence
- The challenge in high β/M_e corresponds to "cancelation" problem in $p_\parallel$ formula.

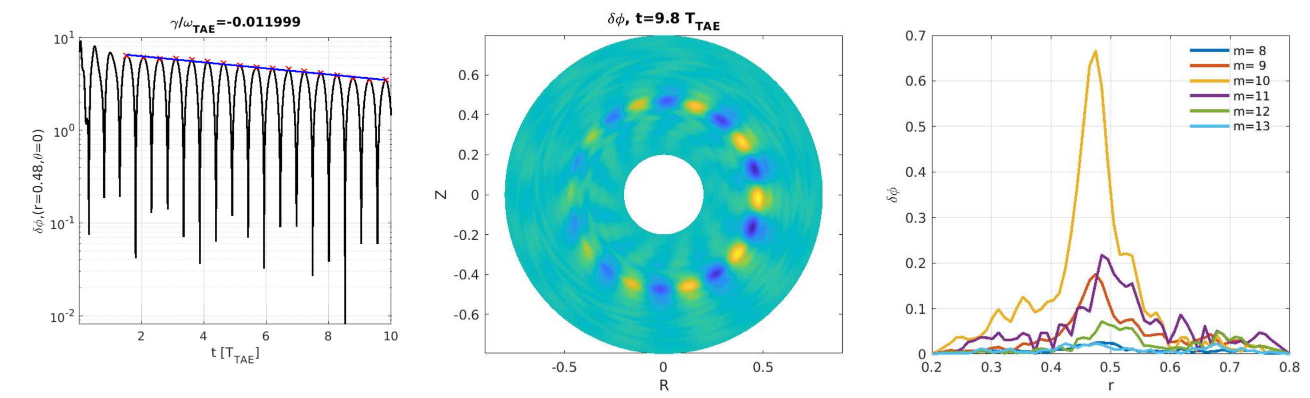


Simulation of TAE damping and excitation in torus

Simulation of TAE/EP using ITPA parameters [Könies et al Nucl. Fusion 58 (2018) 126027]

- $R_0 = 10m$, $a = 1m$, $q = 1.71 + 0.16r^2$, $B_0 = 3T$; $T_{i,e} = 1keV$, $n_e = n_i = 2\cdot 10^{19}/m^3$
- EP density: $n(r) = n_{f0}c_3\exp\{-(c_2/c_1)\tanh[(r-r_0)/c_2]\}$; $\rho_{Ti} = 0.00152m$, $a/\rho_{Ti} = 657.9$; $\beta = 0.0009$; $\beta/M_e k_\perp^2 \rho_{Ti}^2 \gg 1$
- Wave-particle interaction properly simulated by calculating the electron Landau damping
- The Gaussian shape density perturbation is set to be close to the TAE eigenmode

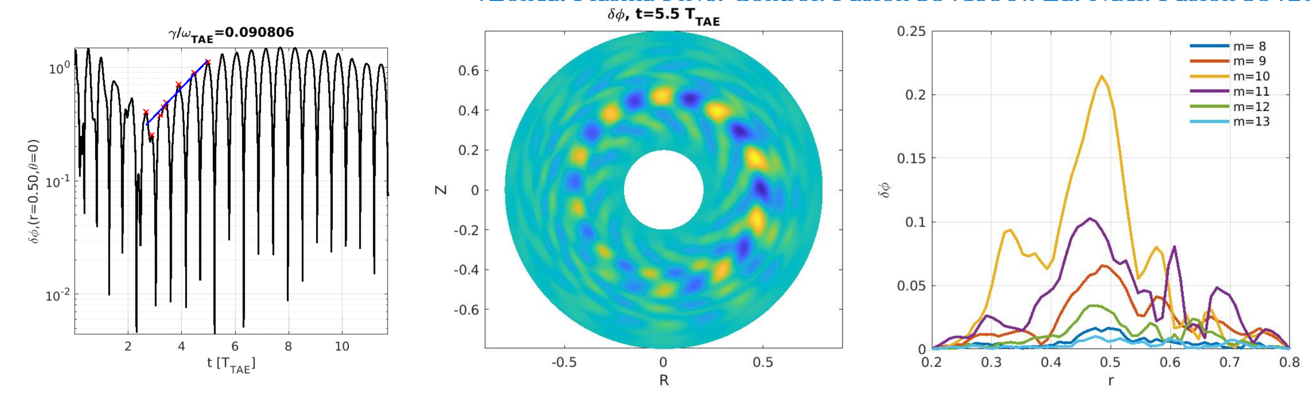
γ/ω_r	$\frac{m_i}{m_e} = 200$	$\frac{m_i}{m_e} = 1836$
LIGKA	−1.293%	−0.5000%
TRIMEG	−1.248%	−0.5008%



Marker #: 16e6e^-, $\frac{m_i}{m_e} = 200, 1836$, on 320 Intel Xeon Gold 6148 processors for 10 or 80 hours

- Clear mode destabilization observed, with reasonable γ/ω_r produced
- Mode radial width (FWHM) $\Delta r \approx 0.12$, larger than that in TAE damping case ($\Delta r \approx 0.06$). It's due to the EP's non-perturbative effects on mode width

[Zonca. Plasma Phys. Control. Fusion 38 (1996); Lu. Nucl. Fusion 58 (2018) 082021 and refs. therein]



Markers #: 128e6 electrons, 32e6 EPs, $\frac{m_i}{m_e} = 200$, on 960 processors for 36 hours

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