Alfvén wave simulation using implicit particle scheme: from 1D to torus geometry

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MET Project Mid-Term Workshop
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Ongoing work for MET project

1. Development of full f, implicit, mixed Particle-in-Cell-Particle-in-Fourier (PIC-PIF) method for simulation of Alfven wave and EP physics (2019,2020)	WP2-WP3
2. Anisotropic EP effects on zonal flow residual (mainly in 2019; paper to be written in 2020)	WP1

This talk is for Part. 1

Background and motivation

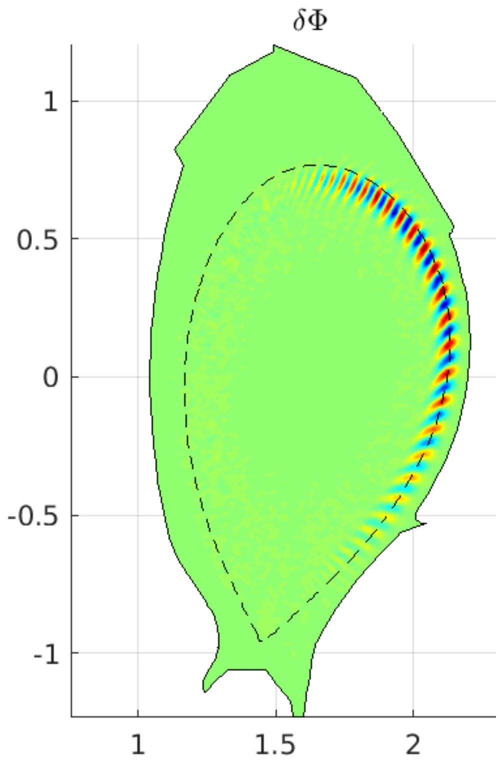
- Related work on implicit scheme

  [Günter JCP09, Kleiber POP16, Perse, Numkin19, ELMFIRE, XGC]

- Implicit scheme can be complementary to CT, pullback…
  - For a system with N_G field grids and N_p particles, the total Degree of Freedom (DOF) is $(N_G + N_p)$
  - The direct implicit solver requires solving a linear system with DOF=$N_G + N_p$. Matrix size is $\left(N_G + N_p\right)^2$!!!
  - Solution: "particle enslavement" [Chen, et al, J. Comput. Phys. 230 (2011) 7018]
  - Particles (x, v) represented as functions of field $F(x)$

    ➔ DOF reduced to N_G !!!

- This work: study the minimum cost of implicit scheme
  - Focus on Darwin model, instead of Vlasov-Maxwell [Perse, et al, Numkin 2019]
  - Focus on Alfven modes, kinetic electron, realistic β/m_e
  - Derive general equations for FEM-particle-implicit scheme, useful for TRIMEG and also other codes (Finite difference in [Chen 2011])



Present TRIMEG version: electrostatic, δf, mixed PIC-PIF, unstructured mesh, FEM, as a testbed. [Z.X. Lu, Ph. Lauber, T. Hayward-Schneider, A. Bottino, M. Hoelzl, *Phys. Plasmas* , 26, 122503 (2019)]

Models and equations

- Normalized equations
  - Parallel electron motion:

$$\frac{dl}{dt} = v_{||};\ l\text{: parallel coordinate}$$

$$\frac{dv_{\parallel}}{dt} = \partial_{\parallel}\delta\phi + \partial_t \delta A_{\parallel}$$

  - Ampere's law & quasi-neutrality

$$\nabla_{\perp}^2 \delta A_{\parallel} = \mathrm{C_A} \delta J_{||}$$

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

  - Normalization units
    - $R_N = 1m, v_N = \sqrt{2T_e/m_e}$
    - $\delta\phi$ normalized to $m_e v_N^2/e$

- Crank-Nicolson scheme (implicit)

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

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

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

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

- Total Degree of Freedom: $(N_G + N_p)!$

Analytic treatment in iteration: “moment enslavement”

- Iteration steps

i: iteration #

$$\xrightarrow{1} \begin{Bmatrix} \delta\Phi^{start}(t+\Delta t) \\ \delta A_{\parallel}^{start}(t+\Delta t) \end{Bmatrix}^{i} \xrightarrow{2} \begin{Bmatrix} l(t+\Delta t) \\ v_{\parallel}(t+\Delta t) \end{Bmatrix}^{i} \xrightarrow{3} \begin{Bmatrix} \delta N^{end}(t+\Delta t) \\ \delta J^{end}(t+\Delta t) \end{Bmatrix}^{i} \xrightarrow{3} \begin{Bmatrix} \delta\Phi^{end}(t+\Delta t) \\ \delta A_{\parallel}{}^{end}(t+\Delta t) \end{Bmatrix}^{i} \xrightarrow{4} \begin{Bmatrix} \delta\Phi^{start}(t+\Delta t) \\ \delta A_{\parallel}^{start}(t+\Delta t) \end{Bmatrix}^{i+1}$$

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. Fields $\{F^{start}(t+\Delta t)\}^{i+1}$ are set so that $|\{F^{start}(t+\Delta t)\}^{i+1} - \{F^{end}(t+\Delta t)\}^{i+1}| \rightarrow 0$ in the next iteration.

Analytic form for setting $\{F^{start}(t+\Delta t)\}^{i+1}$: $\{\delta\phi^{start}, \delta A_{\parallel}^{start}\}^{i+1} = \{\delta\phi^{end}, \delta A_{\parallel}^{end}\}^{i} + \{\Delta\delta\phi, \Delta\delta A_{\parallel}\}$, with

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

$(N_G + N_p)^2$ matrix inversion: unacceptable → particle enslavement [G. Chen 2011]

$$\bar{\bar{M}}_c \approx \begin{bmatrix} \frac{k_{\parallel}^2\Delta t^2}{4}, & -i\frac{k_{\parallel}\Delta t}{2} \\ i\frac{k_{\parallel}\Delta t}{2}, & 1 \end{bmatrix}$$

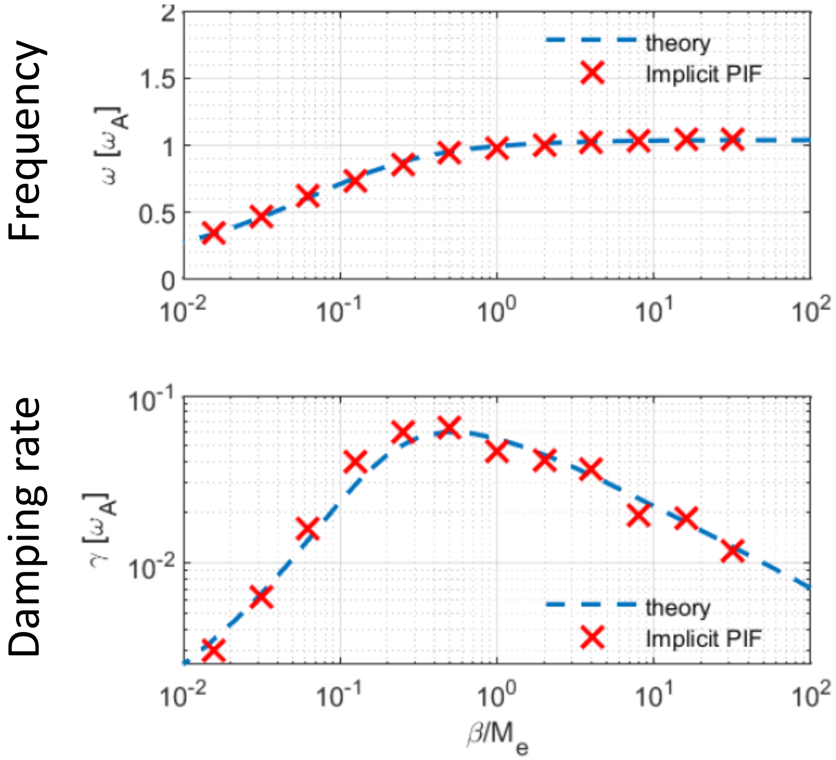
obtained analytically!

$\bar{\bar{M}}_c$ calculation $(N_G \times N_p)$: not cheap → analytic acceleration here, i.e., “moment enslavement”

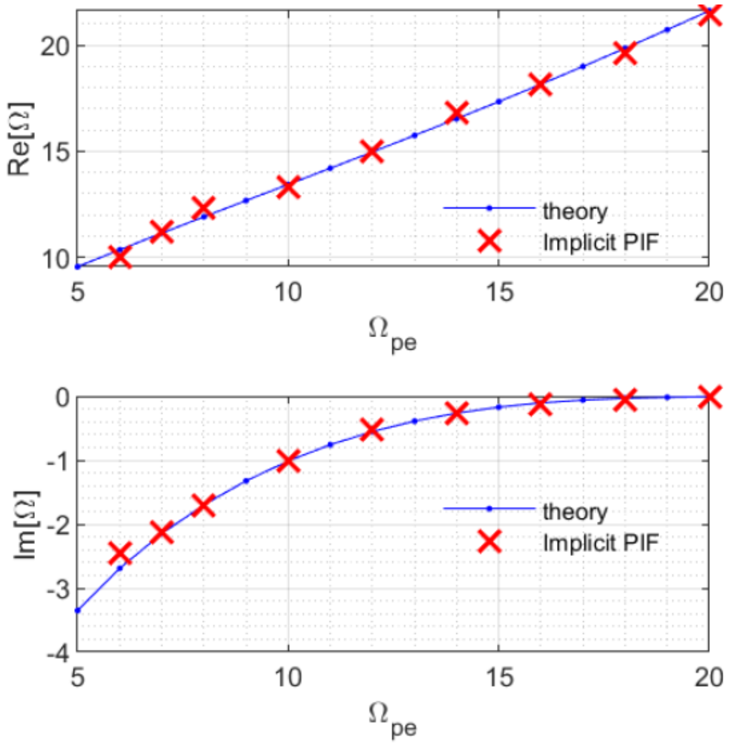
Otherwise more expensive by a factor of N_p/N_G, i.e., particle/grid number ratio, if calculating $\bar{\bar{M}}_c$ using particles.

Shear Alfven wave simulated

- 1D Shear Alfven wave simulated
  - Accessible β/M_e=32, i.e., $\beta = 0.01$, $M_e \equiv \frac{m_e}{m_i} = 1/3200$



Shear Alfven wave



Electron Langmuir wave

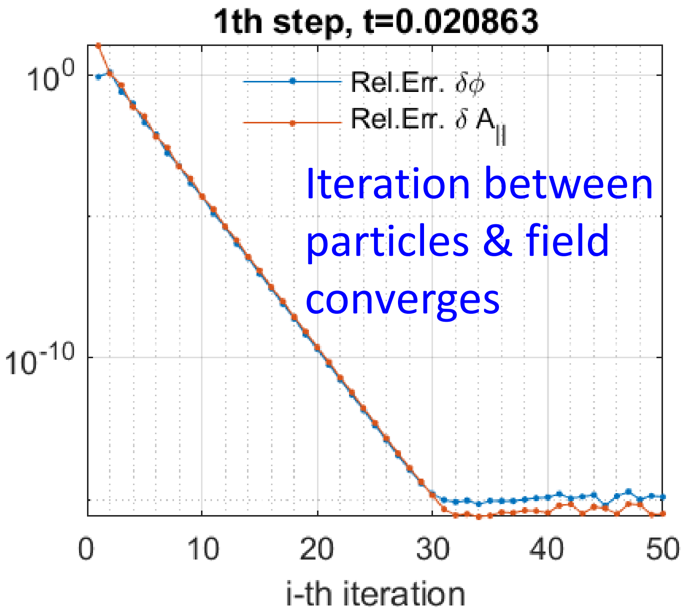
Non uniform loading needed for resolving wave-particle resonance

Shear Alfven wave simulation (prototype version)

- Simplified model for Toroidicity induced Alfven Eigenmode (TAE) simulation
  - Ion response: only polarization density
  - Electron: full f, parallel nonlinear motion kept (zero drift & ExB motion; zero mirror force)

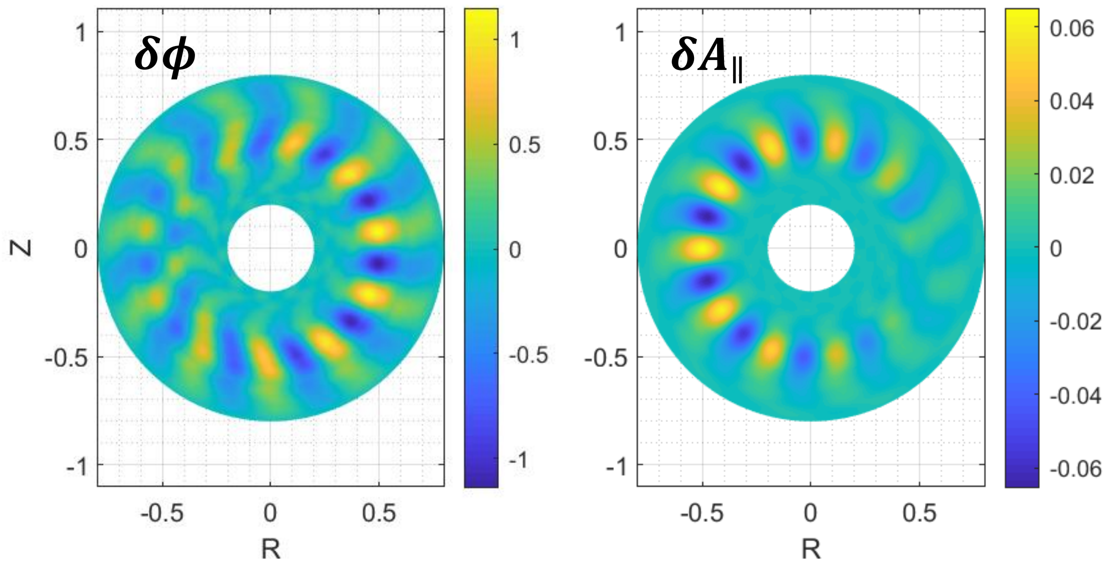
Parameters: aims for ITPA case [Koenies et al 58, 126027(2018)]

- Convergence of the implicit scheme



$$Rel.Err.\{\delta\phi\} = \frac{\sqrt{\int |\Delta\delta\phi|^2 dS}}{\sqrt{\int |\delta\phi|^2 dS}}$$

- TAE 2D mode structure (w/o EPs)



Caveat: reduced β/m_e value with $m_e = 0.002$, $\beta = 0.001$.
Fourier in (θ, ϕ), FEM in r direction. Toroidal mode #: $n = -6$.
Only 2 poloidal harmonics kept.

Mixed explicit (Runge-Kutta)-implicit scheme in torus

- Treat the equilibrium particle motion explicitly but the perturbed one implicitly

$$\frac{d\boldsymbol{R}}{dt} = v_\parallel \boldsymbol{b} + \boldsymbol{v}_d + \frac{\boldsymbol{b}}{B} \times \nabla(\delta\phi - v_\parallel \delta A)$$

$$\frac{d\boldsymbol{v}_\parallel}{dt} = -\mu\partial_\parallel B - \frac{e_s}{m_s}(\partial_\parallel \delta\phi + \partial_t \delta A)$$

It is possible to treat all terms implicitly, but not necessary

- Equilibrium particle motion (explicit)

$$\frac{d\boldsymbol{R}_\mathbf{0}}{dt} = v_\parallel \boldsymbol{b} + \boldsymbol{v}_d$$

$$\frac{d\boldsymbol{v}_{\parallel\mathbf{0}}}{dt} = -\mu\partial_\parallel B$$

- Perturbed particle motion (implicit)

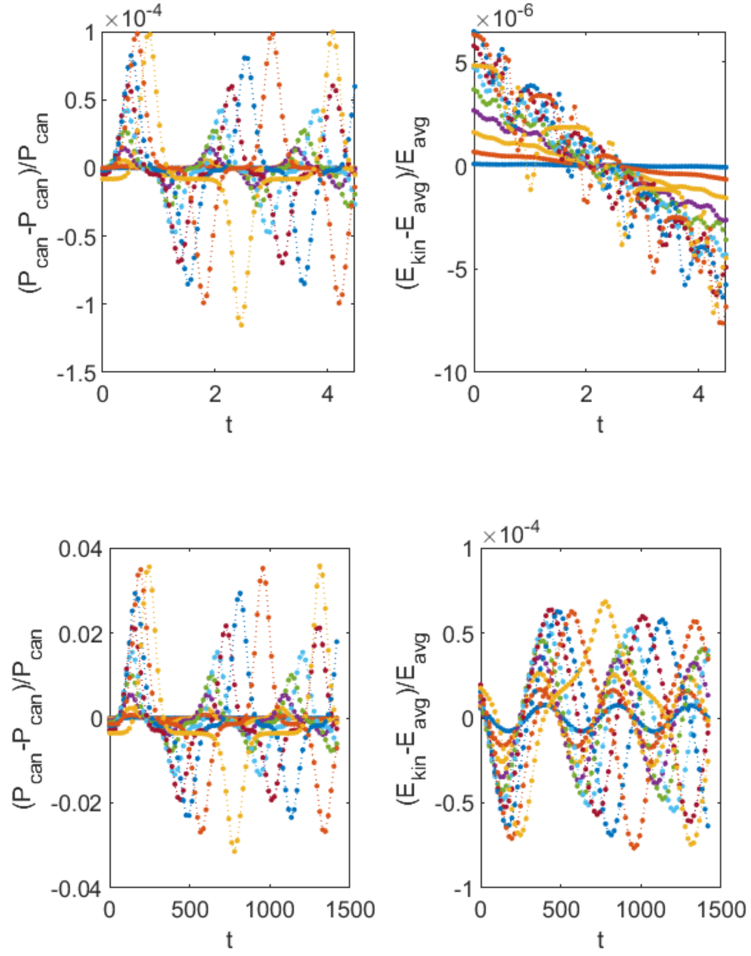
$$\frac{d\boldsymbol{R}_\mathbf{1}}{dt} = \frac{\boldsymbol{b}}{B} \times \nabla(\delta\phi - v_\parallel \delta A)$$

$$\frac{d\boldsymbol{v}_{\parallel 1}}{dt} = -\frac{e_s}{m_s}(\partial_\parallel \delta\phi + \partial_t \delta A)$$

Runge-Kutta 4th order implemented
Geometric scheme of interest

RK4 particle integrator, implicit particle-field iteration

- RK4 integrator gives reasonable conservation of canonical momentum (P_ϕ) & energy (E)

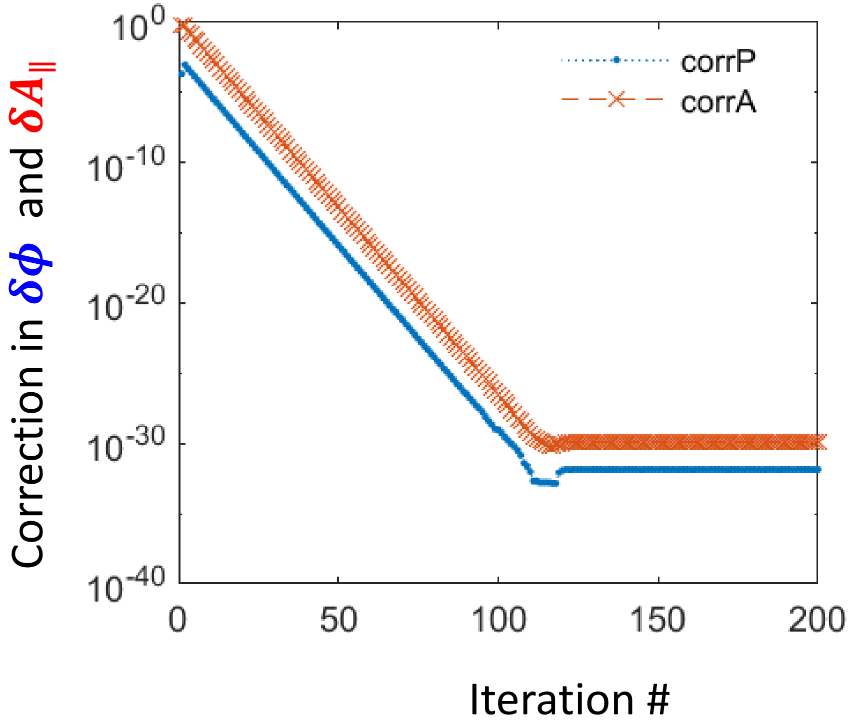


$\rho_t = 6.3e-5$

$\rho_t = 0.02$

ρ/a terms needed for larger ρ_t

- The implicit field-particle solver shows reasonable convergence
  - Radial component of $\delta \boldsymbol{v}$ included
  - More tests for large β/m_e ongoing



Outlook

- Possible contributions to MET in 2020

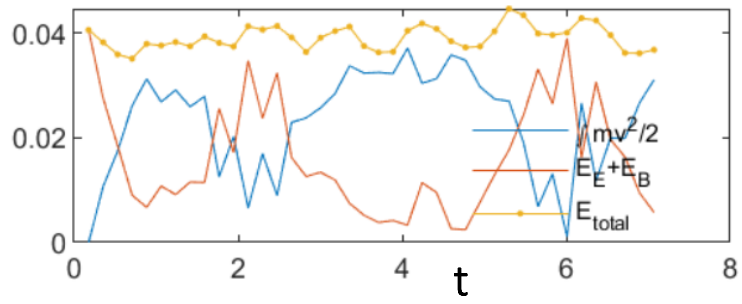
  - Full f, implicit, nonlinear particle simulation of Alfven waves, driven by EPs
    - Caveat: single n (particle-in-Fourier in toroidal direction); ad-hoc equilibrium
    - In parallel with HAGIS full f simulation
  - Anisotropic EP distribution effects on zonal flow residual

    Previous IAEA work to be finalized [Z. Lu et al, Effects of anisotropic energetic particles on residual zonal flow]

- Comments & suggestions are welcome

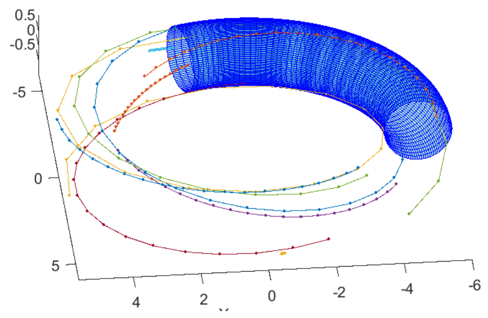
Four tests of implicit scheme (full f)

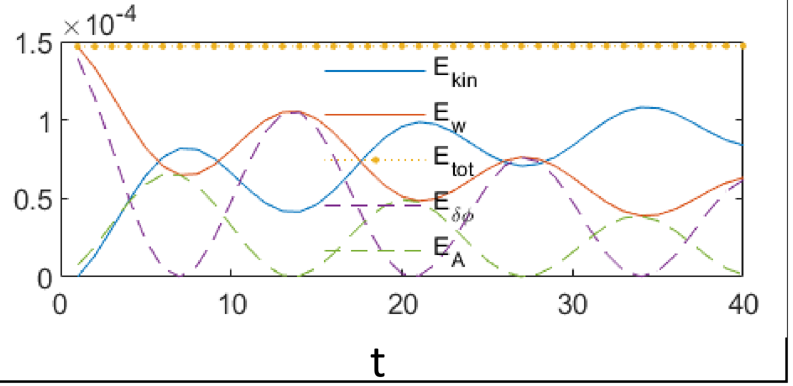
- 1D case, gyrokinetic electrons
  - Shear Alfven wave, SAW (done)
  - Current driven mode (to do)



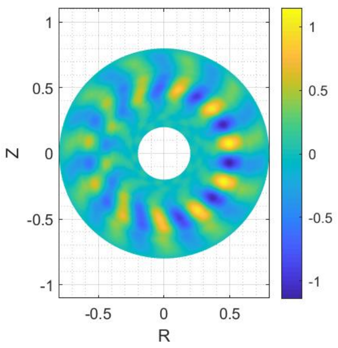
An extreme case: **2 steps per wave period**

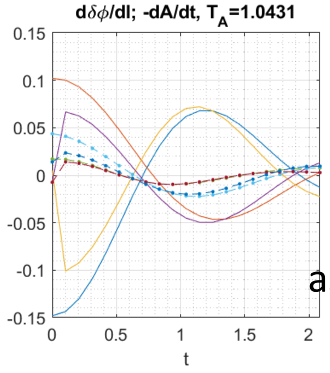
- 2D Single flux surface (cylinder limit)
  - Shear Alfven wave simulated (well passing particle limit)





- 3D circular geometry (tokamak)
  - TAE structure, simplified model
  - Need improvement for large β/m_e





$\beta = 0.001,$
$\frac{m_e}{m_i} = 0.01$
$\partial_t \delta A + \partial_{||}\delta\phi \to 0$
as $\beta/m_e \to \infty$

- 3D realistic tokamak
  - Need more time in 2020
  - Goal: tests of electromagnetic, full f, implicit, kinetic e^- model
  - Complementary to other codes