Pullback approach for gyrokinetic electromagnetic simulations

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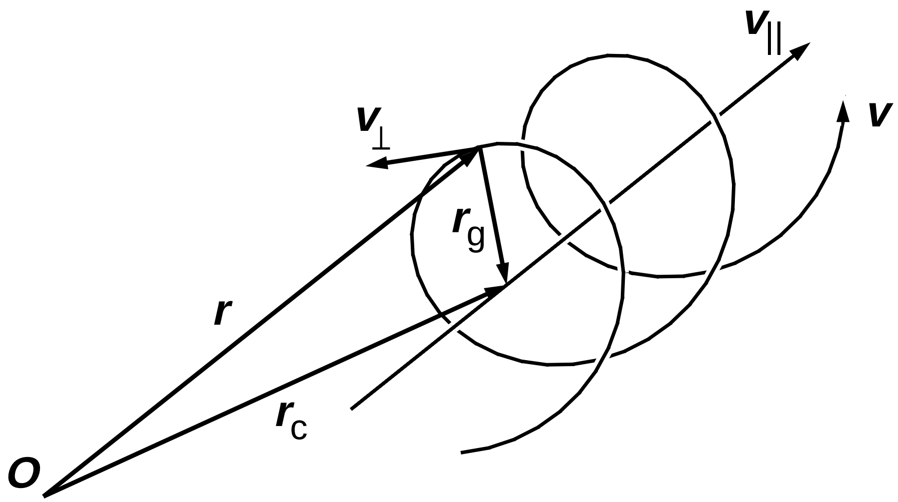
Physical Context

- **Kinetic effects on MHD instabilities**
  - **Finite ion gyroradius (e. g. comparable to boundary layer width – kink)**
  - **Finite electric field (electron inertia, electron pressure, collisionality)**
  - **Non-fluid "compressibility": trapped-particle effect (kink, ballooning)**
- **Kinetic destabilisation of MHD-stable modes**
  - **Fast-ion destabilisation of Alfvén eigenmodes: TAE, HAE, GAE, BAE**
  - **Lower MHD destabilisation thresholds: KBM**
  - **Interaction between (marginal) MHD and fast ions: fishbones**
- **EM microturbulence:** **global profile evolution (drift-Alfvén)**

1. Global approach is needed (intrinsic for MHD; needed for profiles)

2. Kinetic approach is needed (to address relevant physics)

Physical scales



$$\epsilon_B = r_g / L_B \ll 1$$

$$\epsilon = \omega/\omega_c \sim k_\parallel / k_\perp \sim q\delta\phi/T \sim \delta B/B \ll 1$$

Perturbative elimination of fast gyro-scale $\Rightarrow$ **Gyrokinetics**

Gyrokinetic SPC-IPP global PIC code suite

- **1995: GYGLES is developed at SPC(CRPP) with adiabatic electrons**
- **1997: kinetic electrons implemented in GYGLES at IPP**
- **1999: ORB5 is developed at SPC**
- **1999: EUTERPE is developed at SPC**
- **2004: EUTERPE implemented for W7-X at IPP**
- **2004: GYGLES becomes electromagnetic at IPP**
- **2008: ORB5 becomes electromagnetic, joint development IPP/SPC/UW**
- **2009: EUTERPE becomes electromagnetic at IPP**

All the codes share the equations solved, physics addressed and the discretisation principles applied. Deeper core routines are often very similar. Normalisation in EUTERPE and ORB5 is almost identical.

$$\gamma = q\vec{A}^*(\vec{R}) \cdot \mathrm{d}\vec{R} + \frac{m}{q}\mu \mathrm{d}\theta - \left(\frac{mv_\parallel^2}{2} + \mu B\right)\mathrm{d}t + qA_\parallel(\vec{x})\vec{b} \cdot \mathrm{d}\vec{x} - q\phi(\vec{x})\mathrm{d}t$$

$$\vec{A}^* = \vec{A}_0 + \frac{mv_\parallel}{q}\vec{b}\,, \quad \vec{x} = \vec{R} + \vec{\rho}(\theta)$$

- $\vec{x} = \vec{R} + \vec{\rho}(\theta) \Rightarrow$ **gyro-dependent correction is not small, when** $k_\perp \rho \geq 1$
- **Eliminate fast gyro-phase dependence from the Lagrangian**
- **U S E L I E T R A N S F O R M:** $\Gamma = e^{\hat{G}}\gamma + dS$

$$\underline{p_\parallel - GK} : \Gamma = q\vec{A}^*\mathrm{d}\vec{R} + \frac{B}{\Omega}\mu d\theta - \left(\frac{mv_\parallel^2}{2} + \mu B + q\langle\phi\rangle - qv_\parallel\langle A_\parallel\rangle\right)\mathrm{d}t$$

$$\underline{v_\parallel - GK} : \Gamma = q\vec{A}^*\mathrm{d}\vec{R} + \frac{B}{\Omega}\mu d\theta + \langle A_\parallel\vec{b}\rangle\mathrm{d}\vec{R} - \left(\frac{mv_\parallel^2}{2} + \mu B + q\langle\phi\rangle\right)\mathrm{d}t$$

T. S. Hahm (1988), A. J. Brizard (1988, 1994, 2000)

Gyrokinetic equations ($v_\parallel$-formulation)

- **Gyrokinetic Vlasov equation:** **method of characteristics**

$$\frac{\partial f_{1s}}{\partial t} + \dot{\vec{R}} \cdot \frac{\partial f_{1s}}{\partial \vec{R}} + \dot{v}_\parallel \frac{\partial f_{1s}}{\partial v_\parallel} = -\dot{\vec{R}}^{(1)} \cdot \frac{\partial F_{0s}}{\partial \vec{R}} - \dot{v}_\parallel^{(1)} \frac{\partial F_{0s}}{\partial v_\parallel}$$

- **Gyrocenter trajectories:** $\partial\langle A_\parallel\rangle/\partial t$ **appears in** $v_\parallel$**-GK!**

$$\dot{\vec{R}} = v_\parallel \vec{\tilde{b}}^* + \frac{1}{q_s \tilde{B}_\parallel^*} \vec{b} \times \left[\mu \nabla B + q_s \left(\nabla \langle \phi \rangle + \frac{\partial \langle A_\parallel \rangle}{\partial t} \vec{b} \right) \right]$$

$$\dot{v}_\parallel = -\frac{1}{m_s} \vec{\tilde{b}}^* \cdot \mu \nabla B - \frac{q_s}{m_s} \left(\vec{\tilde{b}}^* \cdot \nabla \langle \phi \rangle + \frac{\partial \langle A_\parallel \rangle}{\partial t} \right)$$

$$\vec{\tilde{B}}^* = \vec{B} + \frac{m_s}{q_s} v_{\parallel s} (\nabla \times \vec{b}) + \vec{b} \cdot \nabla \times A_\parallel \vec{b} = B_\parallel^* + \vec{b} \cdot \nabla \times A_\parallel \vec{b}$$

- **Gyrokinetic field equations:** $\delta_{\rm gy} = \delta(\vec{R} + \rho - \vec{x})$

$$\sum_{s=i,f} \int \frac{q_s^2 F_{0s}}{T_s} \left(\phi - \langle \phi \rangle \right) \delta_{\rm gy} \, \mathrm{d}^6 Z = \sum_{s=i,e,f} q_s \bar{n}_s \,, \quad -\nabla_\perp^2 A_\parallel = \mu_0 \sum_{s=i,e,f} \bar{j}_{\parallel s}$$

- **Gyrokinetic Vlasov equation:** **method of characteristics**

$$\frac{\partial f_{1s}}{\partial t} + \dot{\vec{R}} \cdot \frac{\partial f_{1s}}{\partial \vec{R}} + \dot{v}_\| \frac{\partial f_{1s}}{\partial v_\|} = -\dot{\vec{R}}^{(1)} \cdot \frac{\partial F_{0s}}{\partial \vec{R}} - \dot{v}_\|^{(1)} \frac{\partial F_{0s}}{\partial v_\|}.$$

- **Gyrocenter trajectories:** $\partial\langle A_\|\rangle/\partial t$ **does not appear in** $p_\|$**-GK!**

$$\dot{\vec{R}} = \left(v_\| - \frac{q}{m}\langle A_\|\rangle\right)\vec{b}^* + \frac{1}{qB_\|^*}\vec{b} \times \left[\mu\nabla B + q\left(\nabla\langle\phi\rangle - v_\|\nabla\langle A_\|\rangle\right)\right]$$

$$\dot{v}_\| = -\frac{1}{m}\left[\mu\nabla B + q\left(\nabla\langle\phi\rangle - v_\|\nabla\langle A_\|\rangle\right)\right] \cdot \vec{b}^*$$

- **Gyrokinetic field equations:**

$$\int \frac{q_i F_{0i}}{T_i}\left(\phi - \langle\phi\rangle\right)\delta(\vec{R} + \rho - \vec{x})\,\mathrm{d}^6 Z = \bar{n}_i - \bar{n}_e$$

$$\frac{\beta_i}{\rho_i^2}\langle\overline{A_\|}\rangle_i + \frac{\beta_e}{\rho_e^2}A_\| - \nabla_\perp^2 A_\| = \mu_0\left(\bar{j}_{\|i} + \bar{j}_{\|e}\right)$$

Discretization

- **“Klimontovich” representation for perturbed distribution function:**

$$\delta f_s(\vec{R}, v_\parallel, \mu, t) = \sum_{\nu=1}^{N_p} w_{s\nu}(t)\delta(\vec{R} - \vec{R}_\nu)\delta(v_\parallel - v_{\nu\parallel})\delta(\mu - \mu_\nu) \ ,$$

- **Maxwellian distribution for all species:**

$$F_{0s} = n_0 \left(\frac{m}{2\pi T_s}\right)^{3/2} \exp\left[-\frac{m_s v_\parallel^2}{2T_s}\right] \exp\left[-\frac{m_s v_\perp^2}{2T_s}\right]$$

- **Finite-element discretization for fields:**

$$\phi(\vec{x}) = \sum_{l=1}^{N_s} \phi_l(t)\Lambda_l(\vec{x}) \ , \quad A_\parallel(\vec{x}) = \sum_{l=1}^{N_s} a_l(t)\Lambda_l(\vec{x}) \ ,$$

Cancellation problem: particles vs. grid

$$\underbrace{\frac{\beta_i}{\rho_i^2} A_\parallel + \frac{\beta_e}{\rho_e^2} A_\parallel - \nabla_\perp^2 A_\parallel}_{\text{finite-element grid}} = \underbrace{\mu_0 \left(\bar{j}_{\parallel i} + \bar{j}_{\parallel e} \right)}_{\text{particles}}$$

- **Very large skin terms are "generated" by $p_\parallel$-formulation:** **Not physics!**

$$\frac{\beta_e}{\rho_e^2} A_\parallel = \frac{\mu_0 n_0 e^2}{m_e} A_\parallel$$

- **Adiabatic currents are "generated" by $p_\parallel$-formulation:** **Not physics!**

$$\bar{H}_1 = q_s \left(\langle \phi \rangle_s - v_\parallel \langle A_\parallel \rangle_s \right) \;, \quad F_e^{(\mathrm{ad})} = F_{0e}\, e^{-\bar{H}_1/T_e} \approx - \frac{q_e F_{0e}}{T_e} \left(\phi - v_\parallel A_\parallel \right)$$

- **Adiabatic current coincides with the skin terms** **Must cancel each other!**

$$\mu_0 \bar{j}_{\parallel s}^{(\mathrm{ad})} = \mu_0 q_s \int v_\parallel F_s^{(\mathrm{ad})} \mathrm{d}^3 v = \frac{\mu_0 n_0 e^2}{m_e} A_\parallel = \frac{\beta_e}{\rho_e^2} A_\parallel$$

Solution of the cancellation problem

- True-particle distribution function f_s can be expressed through gyrokinetic $\bar{f}_s$ by $p_\|$-transform: Also in quasineutrality!

$$f_{1s} = \underbrace{\bar{f}_{1s} + \frac{q_s \langle A_\| \rangle}{m_s} \frac{\partial F_{0s}}{\partial v_\|}}_{\text{discretize with particles}} + \{S_1, F_{0s}\} \ , \quad \omega_{cs} \frac{\partial S_1}{\partial \theta} = q_s \left(\widetilde{\phi} - v_\| \widetilde{A}_\| \right)$$

- Ampere's law in terms of the true-particle distribution function

$$\underbrace{-\nabla_\perp^2 A_\|}_{\text{grid}} = \underbrace{\mu_0 \int v_\| \left[\bar{f}_{1s} + \frac{q_s \langle A_\| \rangle}{m_s} \frac{\partial F_{0s}}{\partial v_\|} \right] \delta(\vec{R} + \vec{\rho} - \vec{x}) \mathrm{d}^6 Z}_{\text{particles}}$$

- Discretize skin terms with particles in Ampere's law and quasineutrality

$$\bar{f}_{1s}(Z) = \sum_{\nu=1}^{N_p} w_\nu \delta(Z - Z_\nu(t)) \ , \quad F_{0s}(Z) = \sum_{\nu=1}^{N_p} F_{0s}(Z_\nu) \zeta_\nu \delta(Z - Z_\nu(t))$$

Mixed-variable gyrokinetics: derivation

- **Split the magnetic potential into the 'symplectic' and 'Hamiltonian' parts:**

$$A_\| = A_\|^{(\mathrm{s})} + A_\|^{(\mathrm{h})}$$

- **The perturbed guiding-center phase-space Lagrangian**

$$\gamma = q\vec{A}^* \cdot \mathrm{d}\vec{R} + \frac{m}{q}\mu\,\mathrm{d}\theta + q\,A_\|^{(\mathrm{s})}\vec{b}\cdot\mathrm{d}\vec{x} + q\,A_\|^{(\mathrm{h})}\vec{b}\cdot\mathrm{d}\vec{x} - \left[\frac{mv_\|^2}{2} + \mu B + q\phi\right]\mathrm{d}t$$

- **"Mixed" Lie transform: $A_\|^{(\mathrm{h})} \rightarrow$ Hamiltonian, $A_\|^{(\mathrm{s})} \rightarrow$ symplectic structure**

$$\Gamma = q\vec{A}^* \cdot \mathrm{d}\vec{R} + \frac{m}{q}\mu\,\mathrm{d}\theta + q\left\langle A_\|^{(\mathrm{s})}\right\rangle \cdot \mathrm{d}\vec{R} - \left[\frac{mv_\|^2}{2} + \mu B + q\left\langle \phi - v_\| A_\|^{(\mathrm{h})}\right\rangle\right]\mathrm{d}t$$

Mixed-variable formulation: equations

- **The corresponding perturbed equations of motion are**

$$\dot{\vec{R}}^{(1)} = \frac{\vec{b}}{B_\|^*} \times \nabla \left\langle \phi - v_\| A_\|^{(\mathrm{s})} - v_\| A_\|^{(\mathrm{h})} \right\rangle - \frac{q}{m} \langle A_\|^{(\mathrm{h})} \rangle \, \vec{b}^*$$

$$\dot{v}_\|^{(1)} = -\frac{q}{m} \left[\vec{b}^* \cdot \nabla \left\langle \phi - v_\| A_\|^{(\mathrm{h})} \right\rangle + \frac{\partial}{\partial t} \left\langle A_\|^{(\mathrm{s})} \right\rangle \right] - \frac{\mu}{m} \frac{\vec{b} \times \nabla B}{B_\|^*} \cdot \nabla \left\langle A_\|^{(\mathrm{s})} \right\rangle$$

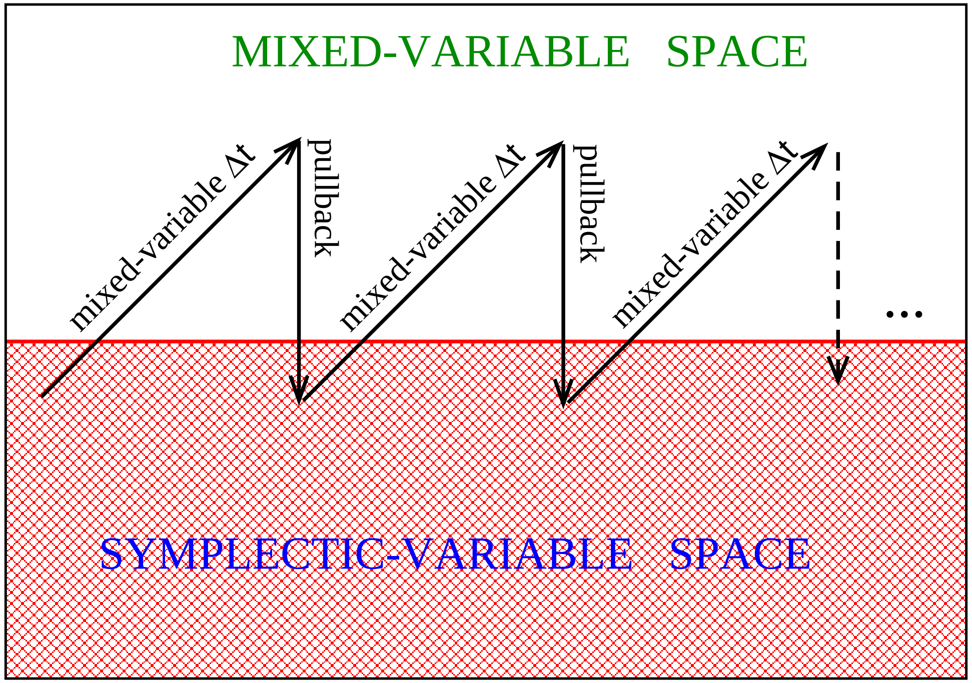
- **An equation for $\partial A_\|^{(\mathrm{s})} / \partial t$ is needed**

$$\frac{\partial}{\partial t} A_\|^{(\mathrm{s})} + \vec{b} \cdot \nabla \phi = 0$$

- **Ampere's law takes the form**

$$\sum_{s=i,e,f} \frac{\beta_s}{\rho_s^2} \left\langle \overline{A}_\|^{(\mathrm{h})} \right\rangle_s - \nabla_\perp^2 A_\|^{(\mathrm{h})} = \mu_0 \sum_{s=i,e,f} j_{\|1s} + \nabla_\perp^2 A_\|^{(\mathrm{s})}$$

Mixed-variable formulation: nonlinear algorithm



$$f_{1s}(Z_s, A_\|^{(s)}) = f_{1m}(Z_m, A_\|^{(s)}, A_\|^{(h)})$$

$$v_\|^{(\mathrm{s})} = v_\|^{(\mathrm{m})} - \frac{e}{m}\left\langle A_\|^{(\mathrm{h})}\right\rangle$$

Additional nonlinear terms appear in equations of motion [R. Kleiber et al, PoP 2016] (symplectic-hamiltonian equivalence at the 2nd order)

1. Push coordinates and weights in mixed-variable space (nonlinear)

2. Transform coordinates into symplectic space keeping weights constant

3. Set $A_{\|(\mathrm{new})}^{(\mathrm{s})}(t_i) = A_\|(t_i) = A_{\|(\mathrm{old})}^{(\mathrm{s})}(t_i) + A_{\|(\mathrm{old})}^{(\mathrm{h})}(t_i)$ **and** $A_{\|(\mathrm{new})}^{(\mathrm{h})}(t_i) = 0$**.**

Conservation laws in mixed-variable gyrokinetics

A gyrokinetic field theory is obtained from action principle

$$\delta\mathcal{A} = \delta\int_{t_1}^{t_2}\mathcal{L}\,\mathrm{d}t = 0$$

where $\mathcal{A}$ is called the action and $\mathcal{L}$ the Lagrangian

$$\mathcal{L}[\vec{R}, U_\|, \mu, \alpha, \phi, A_\|^s, A_\|^h] = \sum_\sigma \int \mathrm{d}W_0\mathrm{d}V_0 f_{\sigma,0}(\mathrm{Z}_0) L_\sigma(\mathrm{Z}, \dot{\mathrm{Z}})$$

$$+\int \mathrm{d}V \frac{q_i\rho_i^2}{k_\mathrm{B}T_i}|\nabla_\perp\phi|^2 - \frac{1}{2\mu_0}\int \mathrm{d}V|\nabla_\perp A_\||^2 + \int \mathrm{d}V\lambda\left(\frac{\partial A_\|^s}{\partial t} + \vec{b}\cdot\nabla\phi\right)$$

GK single-particle Hamiltonian and Lagrangian are

$$H_\sigma = \frac{mU_\|^2}{2} + \mu B(\vec{R}) + q_\sigma(\langle\phi\rangle - U_\|\langle A_\|^h\rangle) + \frac{q_\sigma^2}{2m_\sigma}\langle A_\|^h\rangle^2 - \frac{q_i\rho_i^2}{2T_i(\vec{R})}\nabla_\perp|\phi|^2$$

$$L_\sigma(\vec{R}, U_\|, \mu, \dot{\vec{R}}, \dot{\alpha}) = q_\sigma\vec{A}_\sigma^\star\cdot\dot{\vec{R}} + \frac{m_\sigma^2}{q_\sigma}\mu\dot{\alpha} - H_\sigma$$

Derivation of the equations from the Lagrangian

Liouville theorem follows from variational principle:

$$\frac{\partial B^\star_{\|,\sigma}}{\partial t} + \nabla\cdot\left(B^\star_{\|,\sigma}\frac{\mathrm{d}\vec{R}}{\mathrm{d}t}\right) + \frac{\partial}{\partial U_\|}\left(B^\star_{\|,\sigma}\frac{\mathrm{d}U_\|}{\mathrm{d}t}\right) = 0$$

Thanks to the Liouville theorem the gyro-center distribution function of each particle species $f_\sigma(t,\vec{r},u_\|,\tilde{\mu})$ satisfies the gyrokinetic Vlasov equation

$$\frac{\mathrm{d}f_\sigma}{\mathrm{d}t} = \frac{\partial f_\sigma}{\partial t} + \frac{\mathrm{d}\vec{R}}{\mathrm{d}t}\cdot\nabla f_\sigma + \frac{\mathrm{d}U_\|}{\mathrm{d}t}\frac{\partial f_\sigma}{\partial u_\|} = 0$$

Lagrange multiplier for Ohm's law constrain satisfies:

$$\int \mathrm{d}V\frac{\partial\lambda}{\partial t}\tilde{A}_\| = 0 \quad \forall\tilde{A}_\| \quad \Rightarrow \quad \frac{\partial\lambda}{\partial t} = 0$$

Taking zero as an initial condition for λ, which can be defined arbitrarily, Lagrange multiplier λ vanishes: $\lambda = 0$.

Energy conservation

GK Lagrangian does not explicitly depend on time.
There is a conserved energy related to Noether theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_\sigma \int \mathrm{d}W_0 \mathrm{d}V_0 f_{\sigma,0}(\mathrm{Z}_0)\left[\frac{\partial L_\sigma}{\partial \dot{\vec{R}}}\cdot \dot{\vec{R}}\right] - \mathcal{L}\right) = 0$$

This implies that the following energy is conserved

$$\mathcal{E}(t) = \sum_\sigma \int \mathrm{d}W_0 \mathrm{d}V_0 f_{\sigma,0}(\mathrm{Z}_0) H_\sigma - \int \mathrm{d}V \frac{q_i \rho_i^2}{k_\mathrm{B} T_i} |\nabla \phi|^2 + \frac{1}{2\mu_0}\int \mathrm{d}V |\nabla_\perp A_\parallel|^2$$

This energy is split into kinetic energy and potential energies.

Energy conservation

$$\mathcal{E}_{\text{pot}}(t) = \frac{1}{2}\int \mathrm{d}V \left(qn\langle\phi\rangle + j_\parallel \langle A_\parallel^s\rangle - j_\parallel \langle A_\parallel^h\rangle - \sum_\sigma \frac{q_\sigma^2 n_\sigma}{m_\sigma}\langle A_\parallel^h\rangle\langle A_\parallel^s\rangle \right)$$

$$\mathcal{E}_{\text{kin}} = \sum_\sigma \int \mathrm{d}W_0 \mathrm{d}V_0 f_{\sigma,0}(\mathrm{Z}_0) H_{\sigma,0} = \sum_\sigma \int \mathrm{d}u_\parallel \, \mathrm{d}\mu \, \mathrm{d}V \, f_\sigma(\mathrm{Z}, t) \left[\frac{m u_\parallel^2}{2} + \mu B(\vec{R}) \right]$$

Energy conservation implies

$$\frac{\mathrm{d}\mathcal{E}_{\text{kin}}}{\mathrm{d}t} = -\frac{\mathrm{d}\mathcal{E}_{\text{pot}}}{\mathrm{d}t} = -\sum_\sigma \int \mathrm{d}u_\parallel \mathrm{d}\mu \mathrm{d}V \, f_\sigma(\mathrm{z}, t)$$
$$\left[\frac{q_\sigma}{m_\sigma}\langle A_\parallel^h\rangle \vec{B}_\sigma^\star \cdot \nabla\left(\mu B + q_\sigma\langle\phi\rangle - q_\sigma u_\parallel \langle A_\parallel^h\rangle\right) \right.$$
$$\left. + B_{\parallel,\sigma}^\star \left(\frac{q_\sigma}{m_\sigma} u_\parallel \frac{\langle \partial A_\parallel^s\rangle}{\partial t} + \dot{\vec{R}} \cdot \nabla\left(q_\sigma\langle\phi\rangle - q_\sigma u_\parallel \langle A_\parallel^h\rangle\right)\right)\right]$$

Conservation of total angular momentum

As the background fields do not depend on the toroidal angle in a tokamak, the total canonical angular momentum is conserved.

$$\delta \mathcal{L} = \frac{\delta L}{\delta \vec{R}} \cdot \vec{R}_\varphi = 0, \qquad \text{for } \vec{R}_\varphi = (0, 0, R_\varphi), \quad \text{with } R_\varphi \text{ any constant.}$$

Knowing that the Euler-Lagrange equations are satisfied, yields

$$\frac{\delta L}{\delta \vec{R}} \cdot \vec{R}_\varphi = \frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}W_0 \mathrm{d}V_0 f_{\sigma,0}(\mathrm{Z}_0) \left[\frac{\partial L_\sigma}{\partial \dot{\vec{R}}} \cdot \vec{R}_\varphi \right]$$

The conserved angular momentum in mixed-variable formulation is

$$\mathcal{P}_\varphi = \sum_\sigma q_\sigma \int \mathrm{d}W \mathrm{d}V f_\sigma(\mathrm{z}, t) \left[A_\varphi + \left(\frac{m_\sigma}{q_\sigma} u_\| + \langle A_\|^s \rangle \right) b_\varphi \right]$$

Numerical properties of pullback scheme

f_0 is Maxwellian; $\vec{B}_0 = B_0 \vec{e}_z$, electrons are the only dynamical species,

$$\Phi, A_\|, \delta f \sim \exp\left[\mathrm{i}(k_\perp x + k_\| z) - \mathrm{i}\omega t\right]$$

Linearized GK equations in $v_\|$-formulation:

$$\dot{z} = v_\| \ , \quad \dot{v}_\|^{(1)} = \frac{q_\mathrm{e}}{m_\mathrm{e}} \left(\frac{\partial \Phi}{\partial z} + \frac{\partial A_\|}{\partial t} \right) \ , \quad \frac{\partial \delta f_\mathrm{e}}{\partial t} + v_\| \frac{\partial \delta f_\mathrm{e}}{\partial z} = -\dot{v}_\|^{(1)} \frac{\partial f_{e,0}}{\partial v_\|}$$

$$\frac{m_\mathrm{i} n_0}{B^2} k_\perp^2 \Phi = q_\mathrm{e} \int \delta f_\mathrm{e} \, \mathrm{d}v_\| \ , \quad k_\perp^2 A_\| = \mu_0 q_\mathrm{e} \int v_\| \delta f_\mathrm{e} \, \mathrm{d}v_\|$$

Well-known exact dispersion relation ($v_{\mathrm{th,e}} = \sqrt{2T_\mathrm{e}/m_\mathrm{e}}$, $\tilde{\mu} = m_e/m_i$):

$$D_\mathrm{exact} = 1 - \frac{2\beta}{\bar{k}_\perp^2} \left(\bar{\omega}^2 - \frac{\tilde{\mu}}{\beta} \right) (1 + \bar{\omega} Z(\bar{\omega})) = 0$$

Consider kinetic shear Alfvén wave in slab geometry

Numerical properties of pullback scheme

Implicit Euler scheme with step-size Δt and $t = t_n = n\Delta t$

$$\left.\frac{\partial A_\parallel}{\partial t}\right|_n \approx \frac{A_{\parallel,n} - A_{\parallel,n-1}}{\Delta t} = -\mathrm{i}\Omega_+ A_n \;, \quad \Omega_\pm = \pm\mathrm{i}\frac{1-\mathrm{e}^{\pm\mathrm{i}\omega\Delta t}}{\Delta t}.$$

Equations of motions $z_n = z_{n-1} + v_{\parallel,n-1}\Delta t$ and $v_{\parallel,n} = \mathrm{const}$,

$$\left.\frac{\mathrm{d}\delta f_\mathrm{e}}{\mathrm{d}t}\right|_n \approx \frac{\delta f_{\mathrm{e},n} - \delta f_{\mathrm{e},n-1}}{\Delta t} = -\mathrm{i}K_+ f_{\mathrm{e},n} \;, \quad K_\pm = \pm\mathrm{i}\frac{1-\mathrm{e}^{\pm\mathrm{i}(\omega - k_\parallel v_\parallel)\Delta t}}{\Delta t}$$

The numerical dispersion relation (converges to D_exact for $\Delta\bar{t} \to 0$)

$$D_{v_\parallel} = 1 - \frac{2\beta}{\bar{k}_\perp^2}\sum_{l=-\infty}^{\infty}\left(\bar{\Omega}_+ F_{1,l} - \frac{\tilde{\mu}}{\beta}F_{0,l}\right) = 0$$

$$F_{0,l} = \mathrm{e}^{-y^2+2\mathrm{i}xy}\left[1 + xZ(x+\mathrm{i}y)\right]$$

$$F_{1,l} = \mathrm{e}^{-y^2+2\mathrm{i}xy}\left[x^2 Z(x+\mathrm{i}y) + x - \mathrm{i}y\right]$$

$$x = \bar{\omega} - 2\pi l/\Delta\bar{t} \;, \quad y = -\Delta\bar{t}/4 \;, \quad \bar{t} = t k_\parallel v_{\mathrm{th},e}$$

Numerical properties of pullback scheme

The equations to be solved in this scheme are

$$\dot{z} = u_\parallel \,, \quad \dot{u}_\parallel^{(0)} = 0 \,, \quad \dot{u}_\parallel^{(1)} = \frac{q_\mathrm{e}}{m_\mathrm{e}} u_\parallel \frac{\partial A_\parallel^\mathrm{h}}{\partial z} \,, \quad \frac{\mathrm{d}\delta f_\mathrm{e}}{\mathrm{d}t} = -\dot{u}_\parallel^{(1)} \frac{\partial f_{\mathrm{e},0}}{\partial u_\parallel}$$

with the field equations

$$\left(k_\perp^2 + \frac{\mu_0 n_0 q_\mathrm{e}^2}{m_\mathrm{e}} \right) A_\parallel^\mathrm{h} = \mu_0 q_\mathrm{e} \int u_\parallel \delta f_\mathrm{e} \, \mathrm{d}u_\parallel - k_\perp^2 A_\parallel^\mathrm{s} \,, \quad \frac{m_\mathrm{i} n_0}{B^2} k_\perp^2 \Phi = q_\mathrm{e} \int \delta f \, \mathrm{d}u_\parallel$$

Ohm's law

$$\frac{\partial A_\parallel^\mathrm{s}}{\partial t} = -\frac{\partial \Phi}{\partial z}$$

and pullback transformation has to be applied at end of each time step

$$\delta f_\mathrm{e}^* = \delta f_\mathrm{e} + \frac{q_\mathrm{e}}{m_\mathrm{e}} \frac{\partial f_{\mathrm{e},0}}{\partial u_\parallel} A_\parallel^\mathrm{h} \,, \quad A_\parallel^{\mathrm{s}*} = A_\parallel^\mathrm{s} + A_\parallel^\mathrm{h} \,, \quad A_\parallel^\mathrm{h} = 0$$

Numerical properties of pullback scheme

The transformed quantities have to be used for time derivatives:

$$\left.\frac{\partial A_\|^{\rm s}}{\partial t}\right|_n \approx \frac{A_{\|,n+1}^{\rm s} - A_{\|,n}^{\rm s*}}{\Delta t}$$

Explicit Euler scheme with step-size Δt and $t = t_n = n\Delta t$.

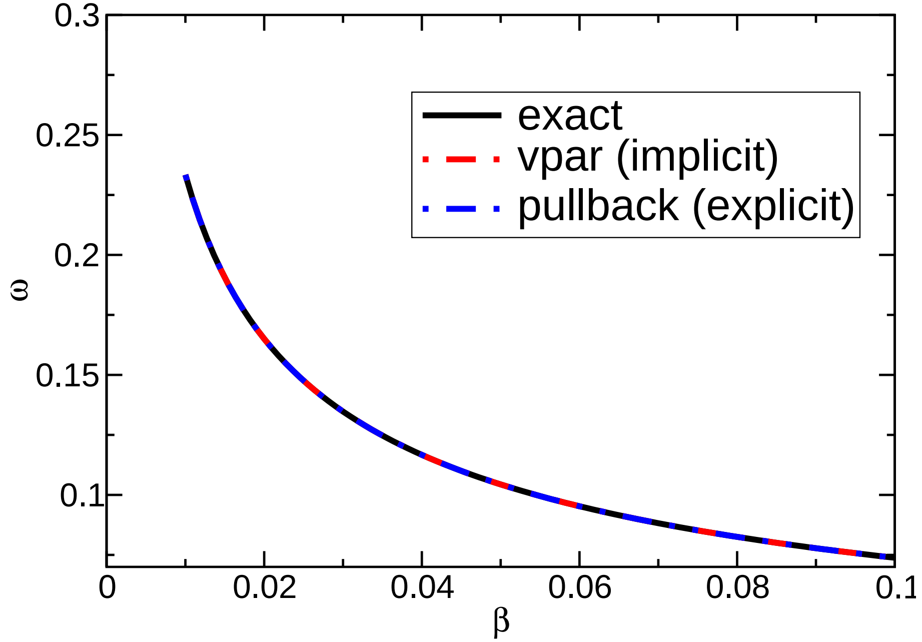
$$\delta f_{{\rm e},n} = \frac{\rm i}{\Delta t K_-} \frac{q_{\rm e}}{m_{\rm e}} A_{\|,n}^{\rm h} \frac{\partial f_{{\rm e},0}}{\partial u_\|}\,, \quad A_{\|,n}^{\rm s} = \frac{\rm i}{\Delta t \Omega_-}\left(A_{\|,n}^{\rm h} - {\rm i} k_\| \Phi_n \Delta t\right)$$

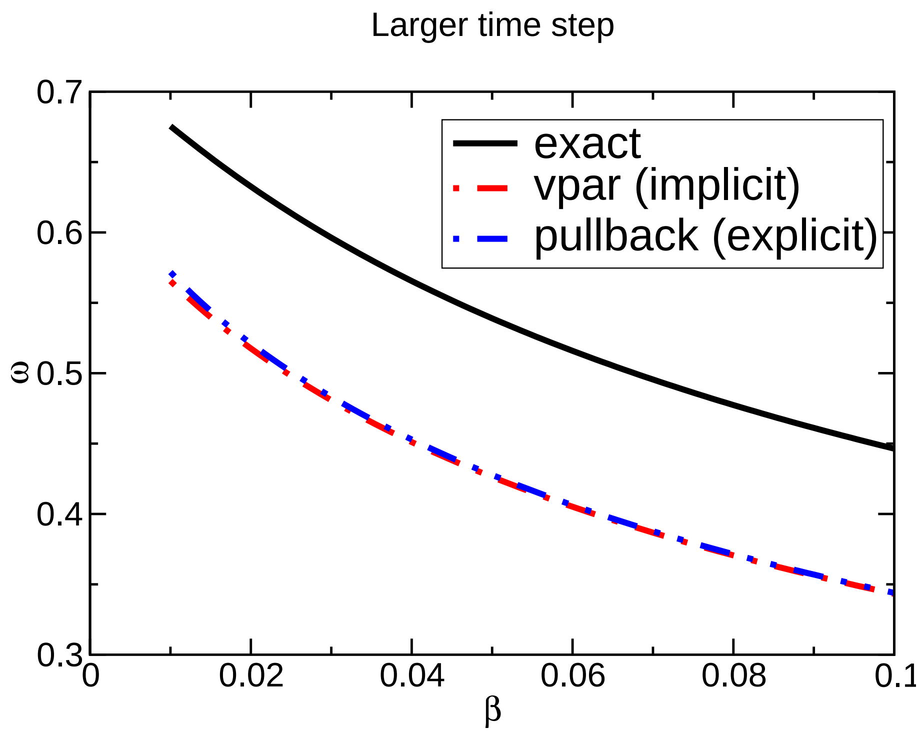
Important result $A_\|^{\rm h} \sim \Delta t$! Putting everything together leads finally to the numerical dispersion relation for the PT-scheme

$$D_{\rm PT} = 1 - {\rm i}\bar{\Omega}_- \Delta t \left(1 + \frac{\beta}{\bar{k}_\perp}\right) - \frac{2\beta}{\bar{k}_\perp^2} \sum_{l=-\infty}^{\infty} \left(\bar{\Omega}_- F_{1,l} - \frac{\tilde{\mu}}{\beta} F_{0,l}\right) = 0.$$

where $F_{0,l}$, $F_{1,l}$ now must be evaluated using $y = \Delta\bar{t}/4$.

Numerical properties of pullback scheme





- **Explicit discretisation for the $v_{\|}$-scheme possible but leads to strong numerical instabilities.**
- **$v_{\|}$- and PT-scheme give same results.
Hence, both schemes are equivalent but PT-scheme is explicit.**

Collisions in electromagnetic PIC (EUTERPE)

- **collisions important for realistic description of fusion plasmas**
- **electromagnetic simulations with EUTERPE including collisions had been unsuccessful in the past**
- **benchmark of EUTERPE against grid code based on decomposition of $f_e^{(1)}$ into Legendre polynomials (EF of pitch-angle collision operator)**

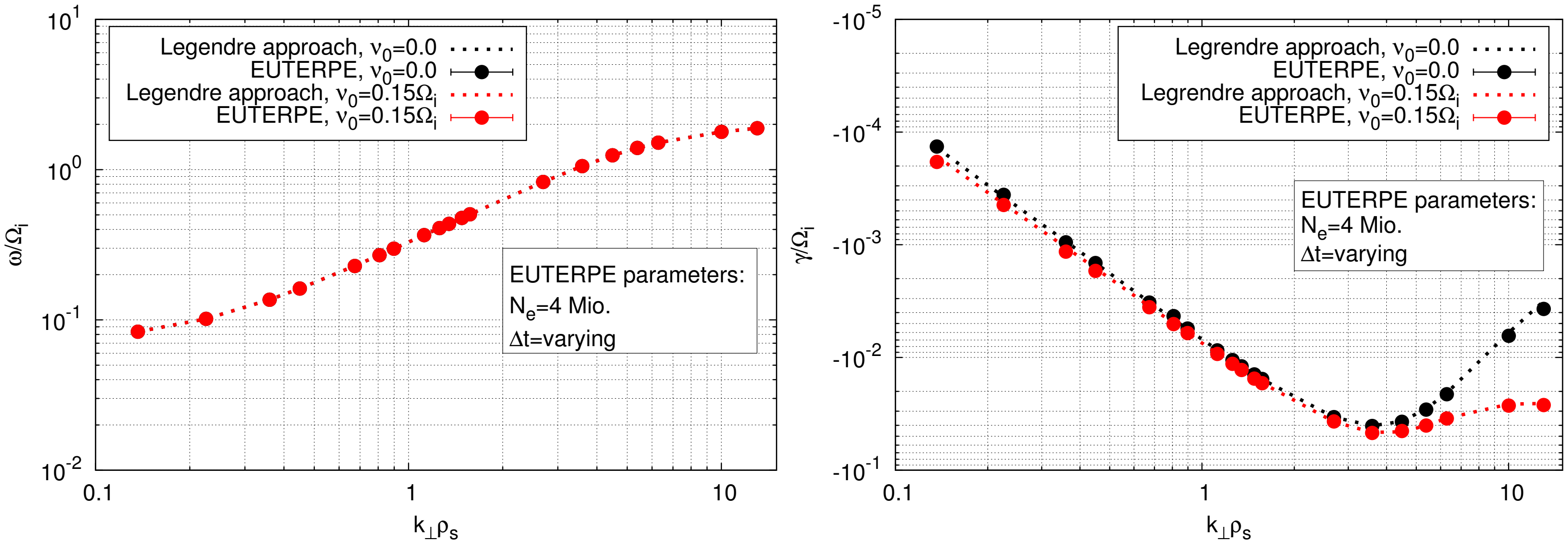
$$\frac{\partial f_e}{\partial t} + \dot{\vec{R}} \cdot \nabla f_e + \dot{u}_\parallel \frac{\partial f_e}{\partial u_\parallel} = \mathcal{L}(f_e), \quad \mathcal{L}(f_e) = \frac{\nu}{2} \frac{\partial}{\partial \xi} \left(1 - \xi^2\right) \frac{\partial f_e}{\partial \xi}, \quad \xi = \frac{v_\parallel}{v}$$

$$f_e^{(1)} = \sum_{l=0}^{N_l} f_l\,(u, t)\, P_l\,(\xi')\, F, \quad P_l \ldots l^{\text{th}} \text{ Legendre polynomial}$$

- **kinetic Alfvén wave subject to electron pitch-angle collisions**

J. W. Banks et al., Phys. Plasmas 23, 032108 (2016)

Results – with and without pitch-angle collisions



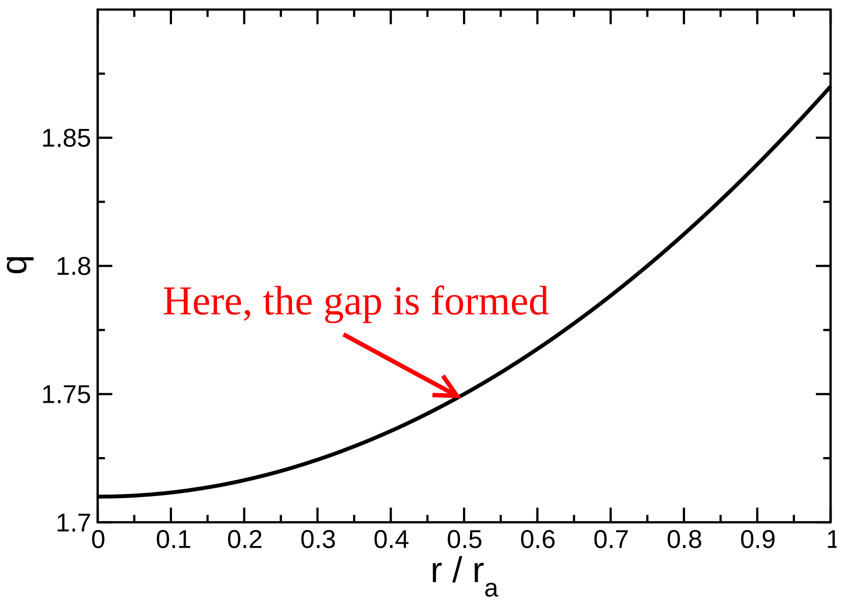
- **real frequency not affected by collisions**
- **collisions lead to collisional damping for all $k_\perp \rho_s$**
- **large $k_\perp \rho_s$ (small scales) effectively damped by pitch-angle collisions**
- **EUTERPE and the Legendre approach agree very well**
- **stochastic scheme replaces Runge-Kutta: weaker convergence in Δt**

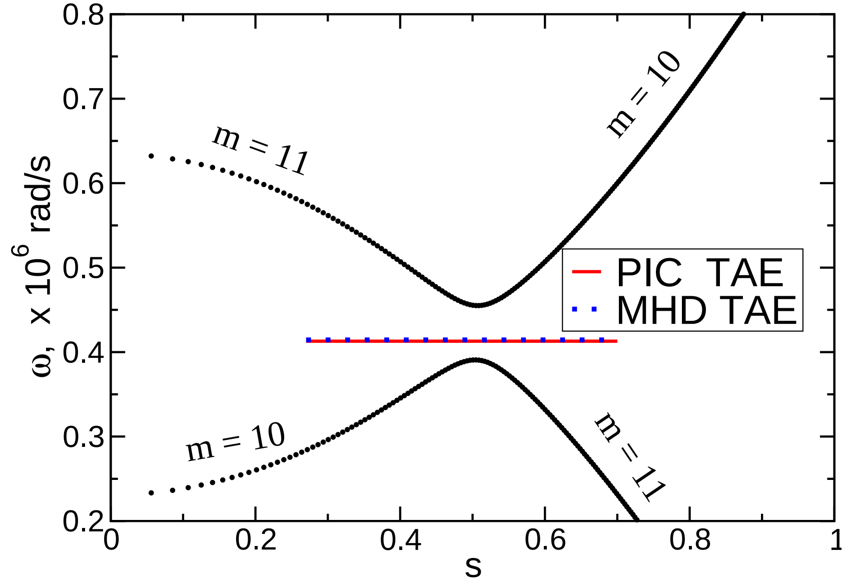
C. Slaby et al., Comp. Phys. Comm. 218, 1-9 (2017)

S I M U L A T I O N S

Toroidal Alfvén Eigenmode
Energetic Particle Mode
Internal Kink Mode
Collisionless Tearing Mode
Stellarators (EM drift modes)

Tokamak configuration





Large-aspect-ratio, circular cross-sections

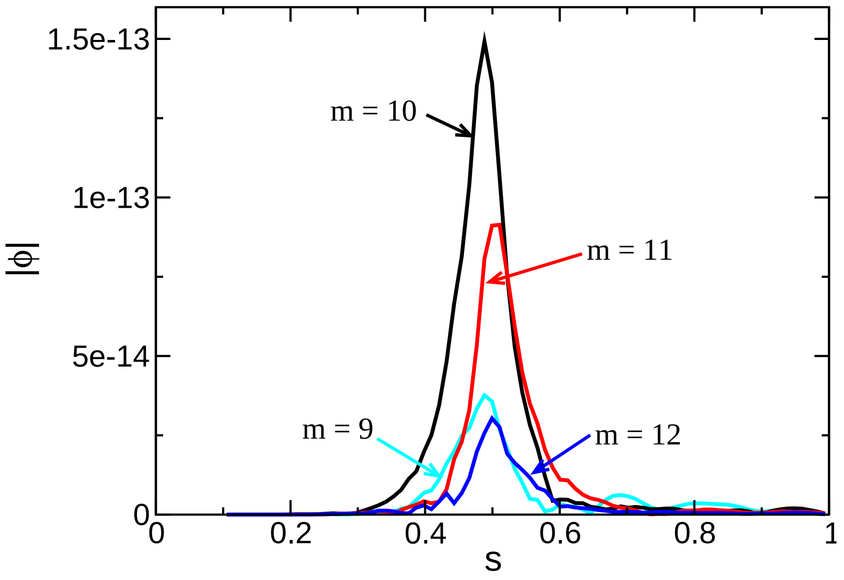
Major radius $R_0 = 10$ m, minor radius $r_a = 1$ m

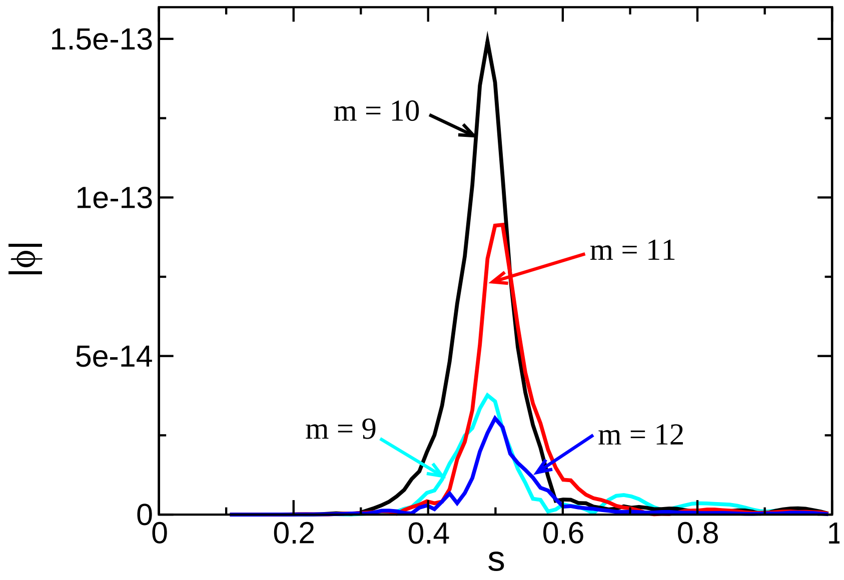
Magnetic field on the axis $B_0 = 3.0$ T, flat density $n_0 = 2 \times 10^{19}\ \mathrm{m}^{-3}$

Flat bulk-plasma temperature and density ($\beta_{\mathrm{bulk}} \approx 0.18\%$) , Hydrogen

Toroidal mode number $n = 6$

Radial structure (GYGLES, EUTERPE, ORB5)

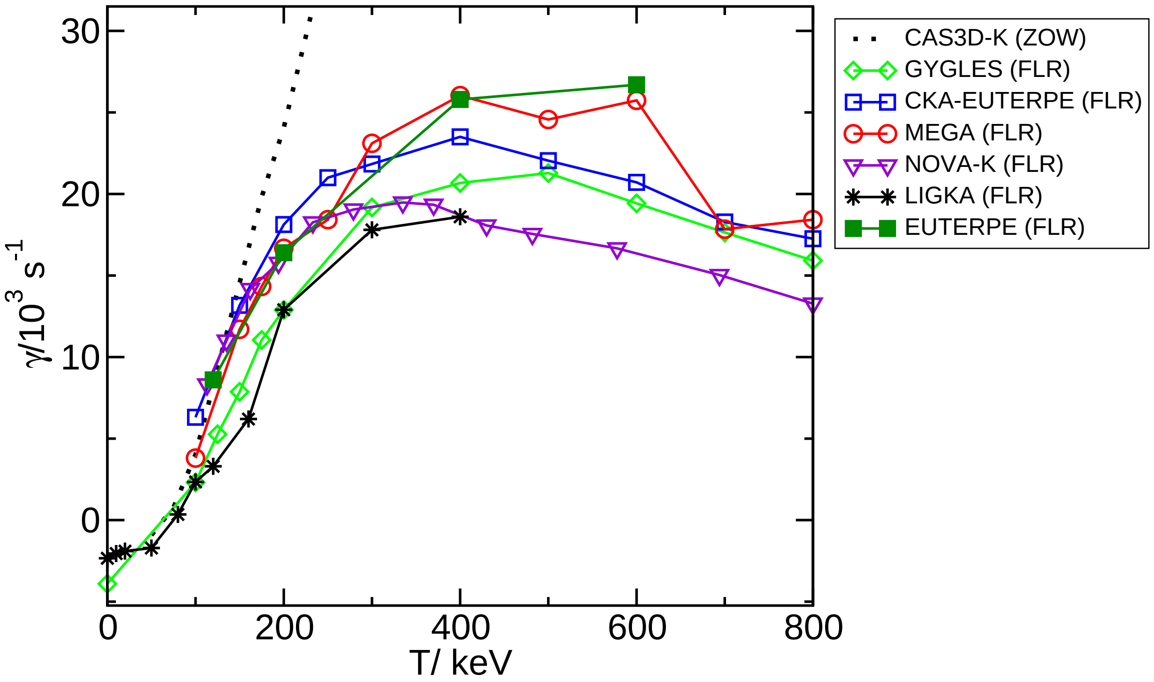


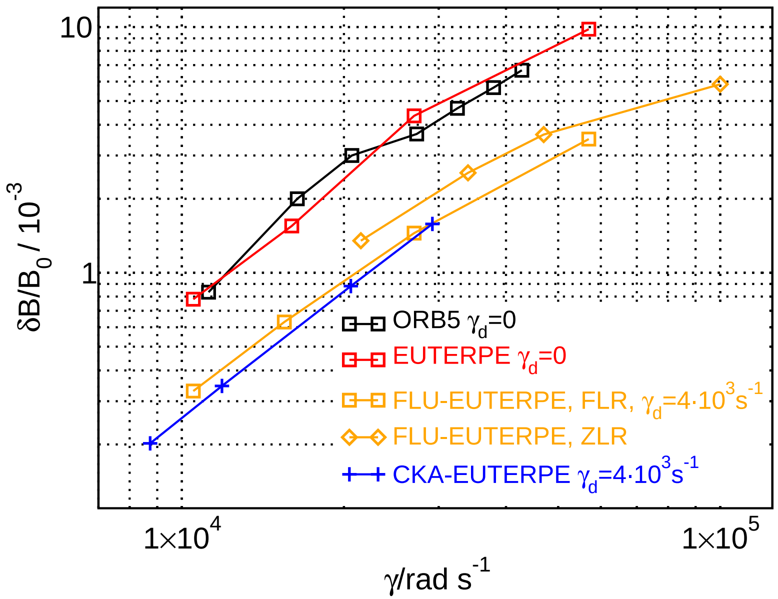


Radial pattern resulting from the PIC simulations (in some particular point of time)

It resembles a typical TAE structure.

ITPA benchmark (GYGLES, EUTERPE, ORB5)



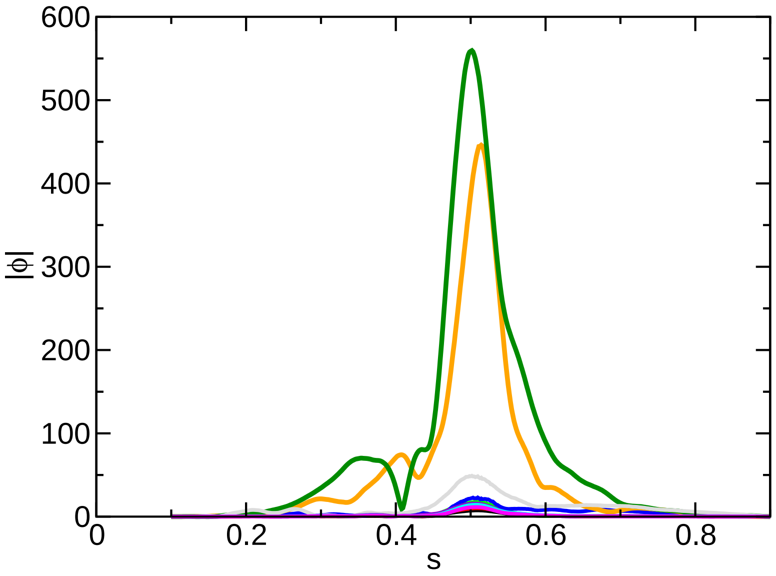


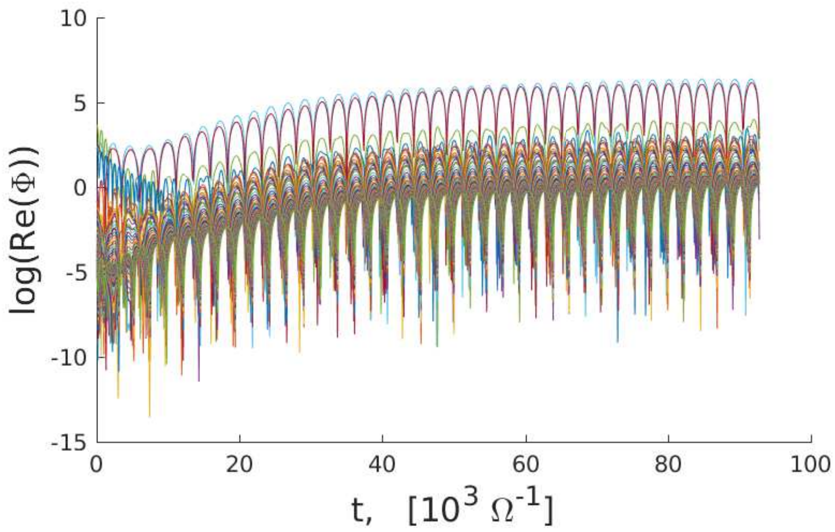
Successful worldwide benchmark (ITPA framework)

Linear with and without FLR

Nonlinear (EUTERPE vs. ORB5; GK vs. reduced models)

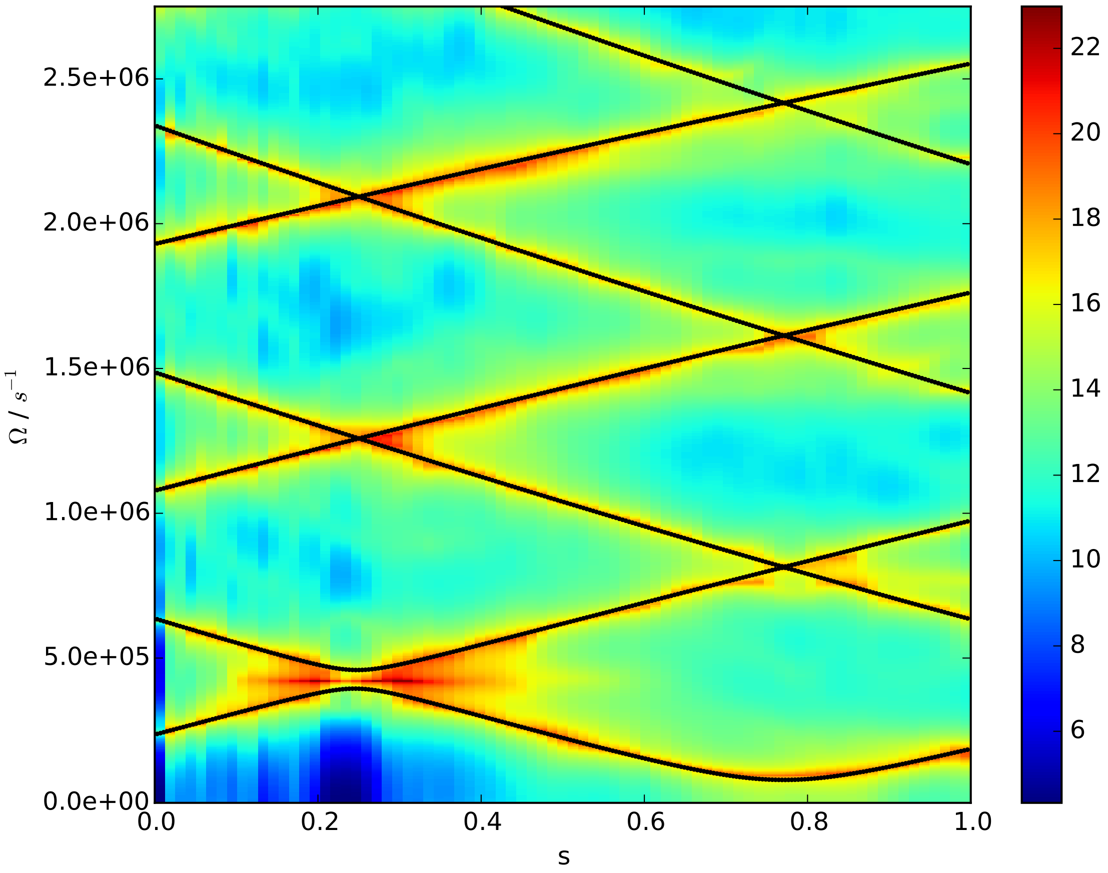
Nonlinear simulations (ORB5, EUTERPE)





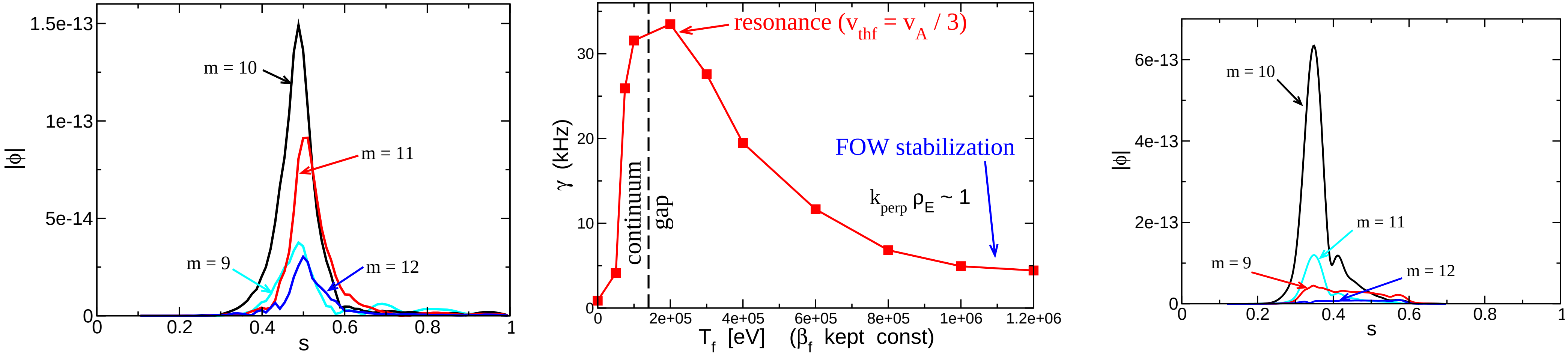
Nonlinear mode structure (fast-particle nonlinearity)
Mode saturation through resonance detuning and radial decoupling
(Fulvio Zonca talk; this conference)

Long-time simulations (EUTERPE)



ITPA benchmark case (tokamak, n=-6 TAE)
Fully GK simulations using EUTERPE
DMUSIC algorithm (parametric method superior to FFT)
GK DMUSIC spectrum compared with MHD continuum

TAE-EPM transition (GYGLES, ORB5)



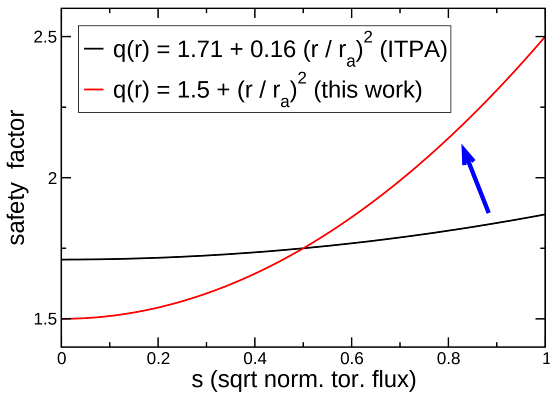
Dependency on the fast-particle temperature ($\beta_f = 0.134\%$ kept constant)

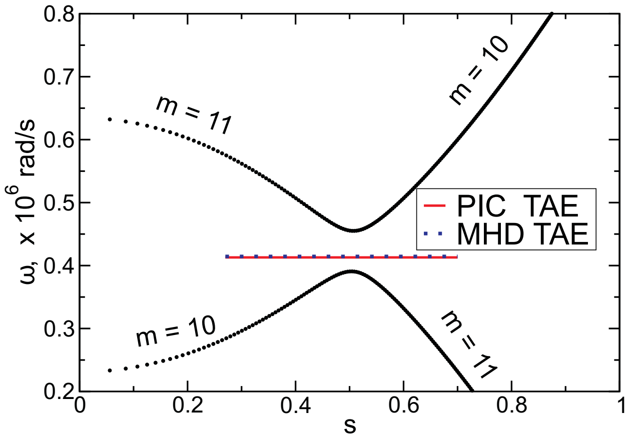
Destabilization is most effective near the resonance $v_{thf} \approx v_A/3$

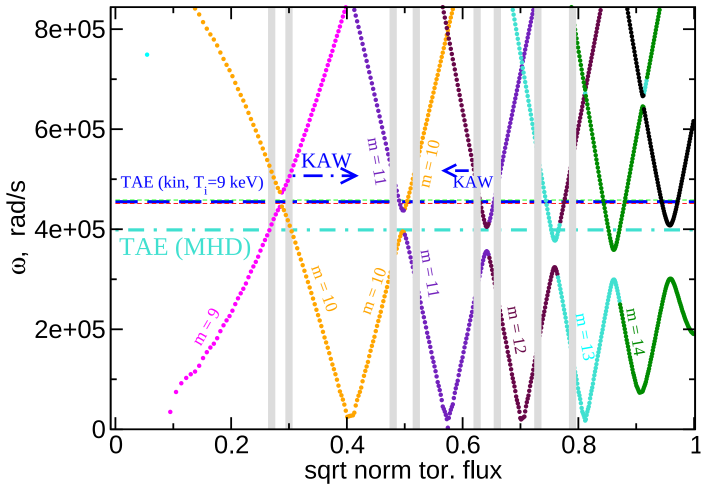
At large T_f, finite-orbit-width (FOW) stabilization is seen

At smaller T_f (larger n_f to keep β_f constant), an EPM appears

Safety factor and SAW continuum

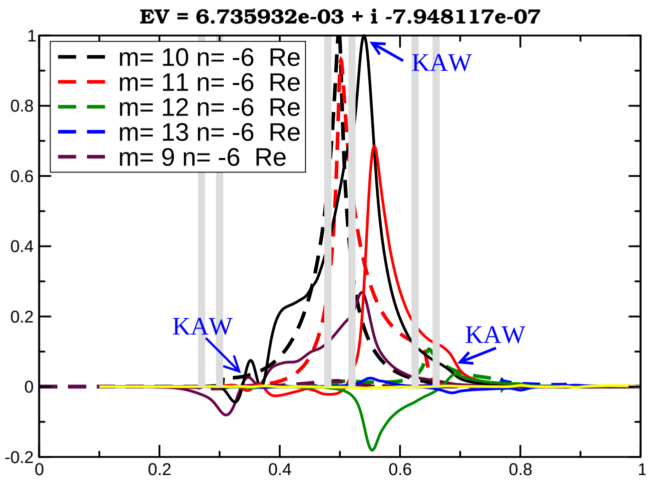


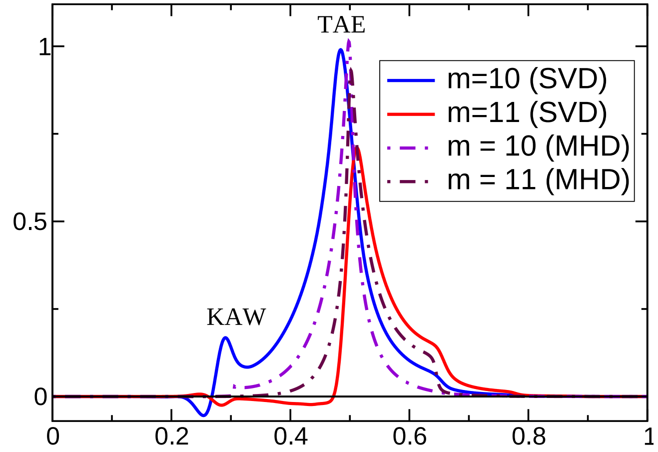


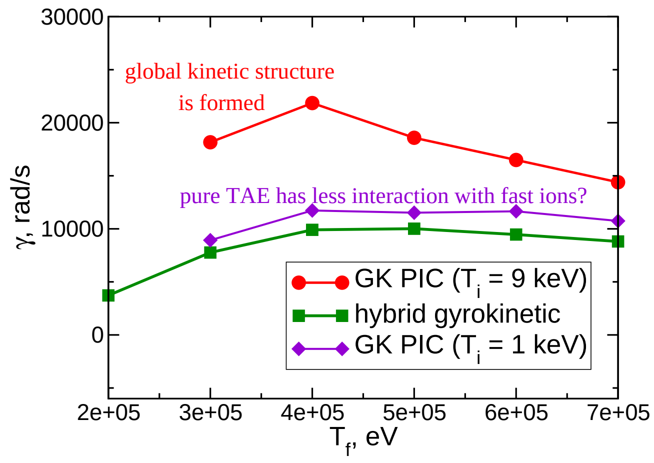


- **Simulation Concept**
  - **Modify the ITPA benchmark parameter safety factor (magnetic shear)**
  - **But: use flat bulk plasma density and temperature (same v_A as ITPA)**
- **New physics (compared to ITPA)**
  - **The resulting continuum is much more complicated than ITPA**
  - **The gap is deformed and involves many modes; <u>continuum resonances</u>**

Gyrokinetic Eigenmode (GYGLES, EUTERPE, ORB5)

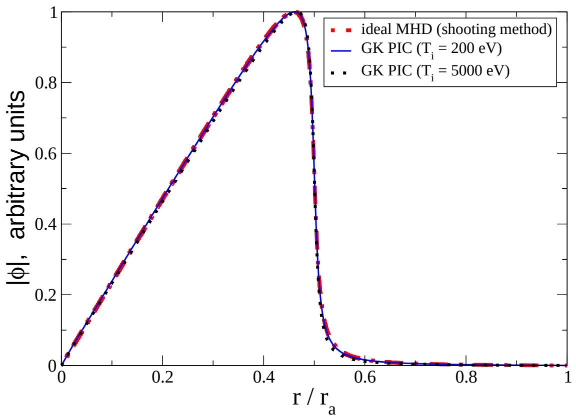


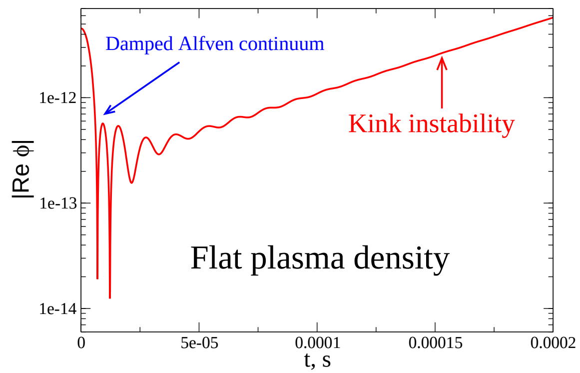


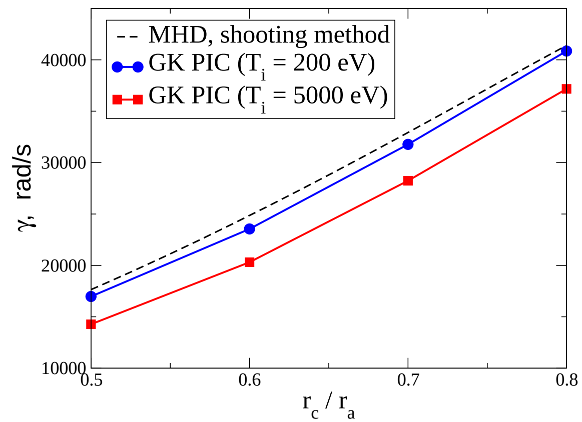


- **Electrostatic radial pattern at different times**
- **KAWs are excited at continuum resonances**
- **Resonantly excited KAWs mix with the global eigenmode (interference)**
- **Kinetic mode is wider comparing to ideal mode (KAW admixtures)**

Internal kink mode (GYGLES)





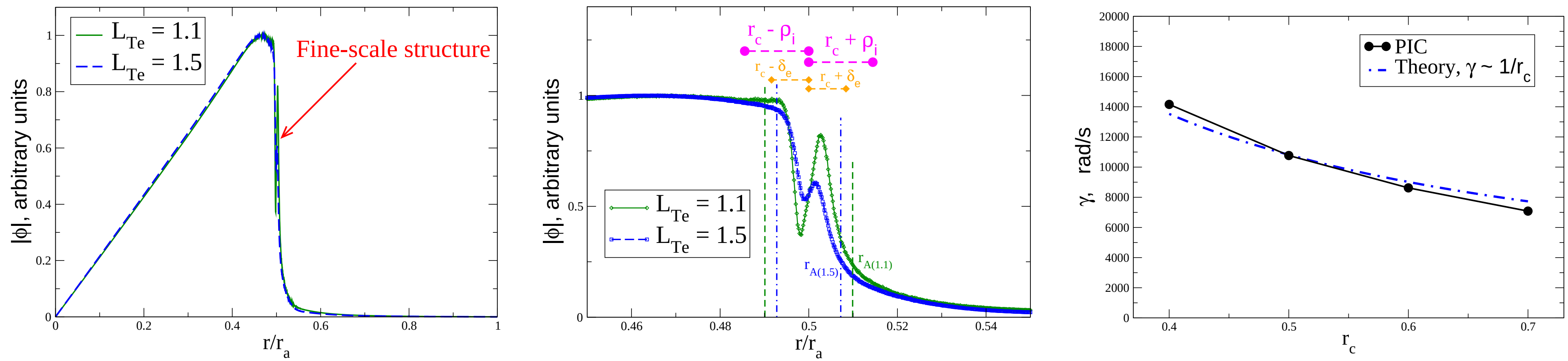


Ideal-MHD internal kink mode equation:

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\left[\underbrace{\mu_0 m_i n_0 \gamma^2}_{\text{small}} + (\vec{k}\cdot\vec{B})^2\right] r^3 \frac{\mathrm{d}\xi}{\mathrm{d}r}\right) - g(r)\xi = 0\,, \quad \xi \propto \phi/r$$

- **Intertial layer: plasma inertia can compete with magnetic tension**
- **Poloidal plasma rotation with $v_\theta \propto \partial\phi/\partial r$ resolves the MHD singularity**
- **The width of the intertial layer $\underline{\lambda_H \propto \delta W_{\mathrm{MHD}}}$**
- **"MHD regime": λ_H exceeds all microscopic kinetic scales (ρ_i, δ_e etc)**

Collisionless $m = 1$, $n = 1$ tearing mode (GYGLES)

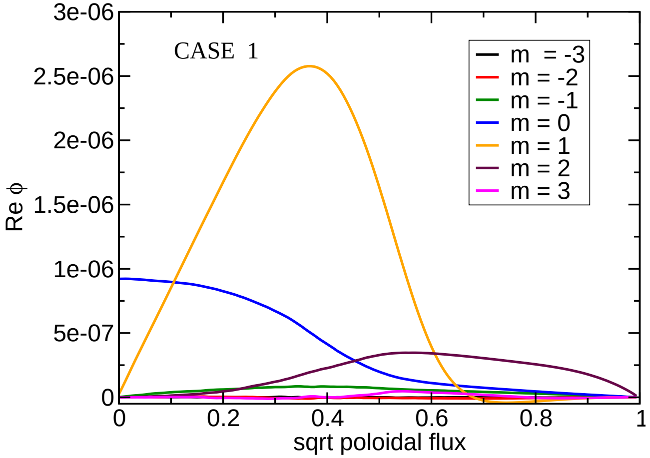


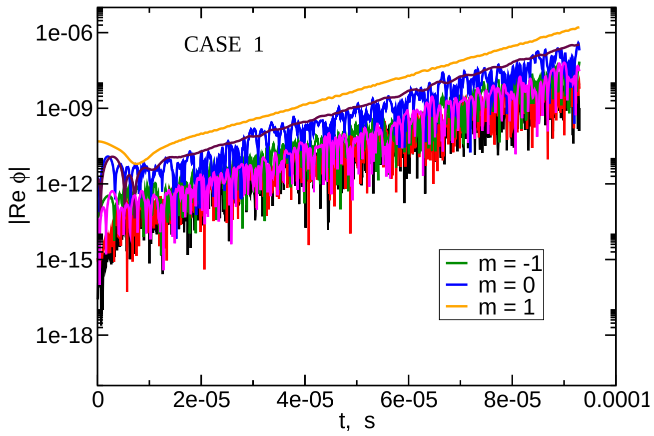
"Collisionless $m = 1$ tearing mode" [Porcelli 91]

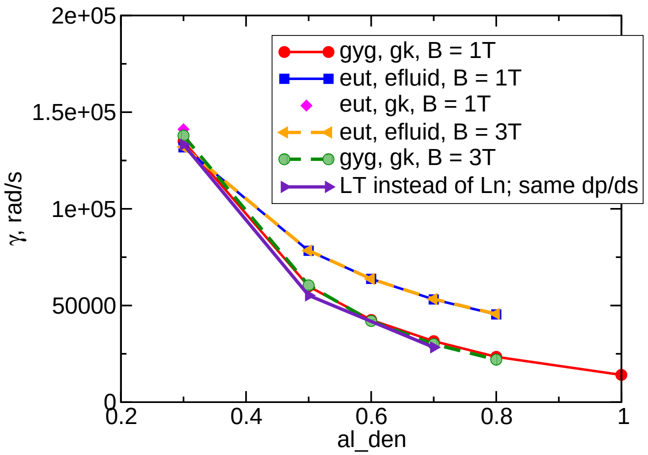
$$\gamma = \frac{\hat{s}_q(r_c) v_A(r_c)}{R_0} \frac{(\delta_e \rho_i^2)^{1/3}}{r_c}, \quad v_A = \frac{B_0^2}{\sqrt{\mu_0 m_i n_0}}, \quad \hat{s}_q = \frac{r}{q}\frac{\mathrm{d}q}{\mathrm{d}r}$$

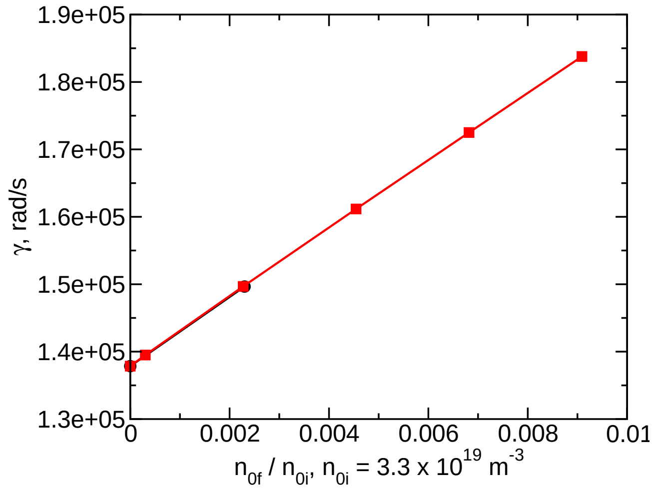
- **Drift-kink mode: fine scale feature at resonant flux surface**
- **Sub-gyro scales are involved – Kinetic Alfvén Waves (KAW) resonantly excited by the drift-kink mode**
- **Mode dynamics as a combination of MHD dynamics, reconnection and the KAW excitation ("continuum damping")**

Internal kink mode in tokamak (GYGLES)



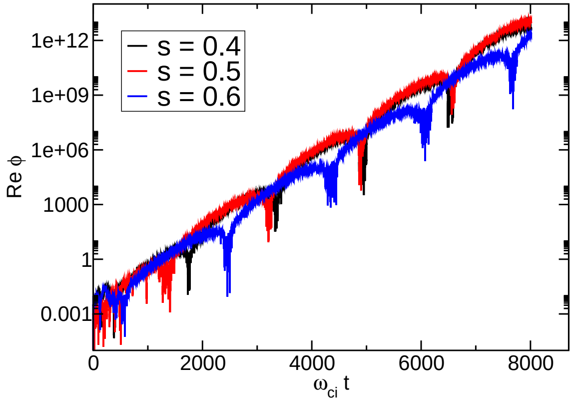


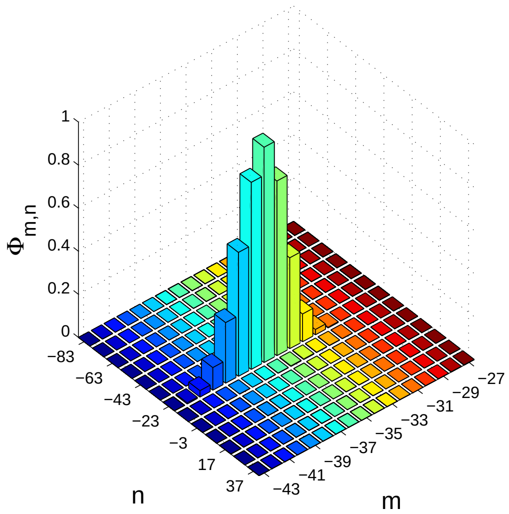




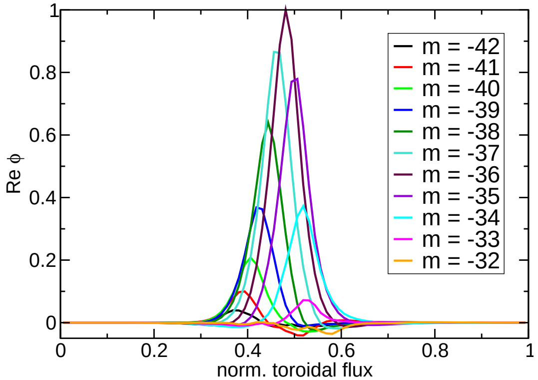
Internal kink mode in tokamak geometry ($R_0/r_a = 10$); strong MHD drive (pressure+current); GK-efluid comparison; fast-ion effect: MHD drive p'_{fast}

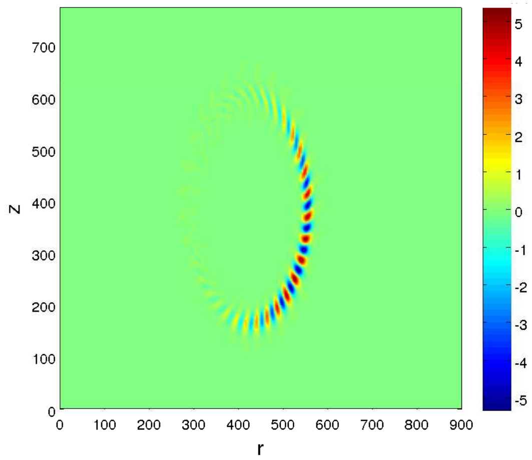
KBM/ITG in LHD-like geometry (EUTERPE)





Clean instability; ballooning in Fourier

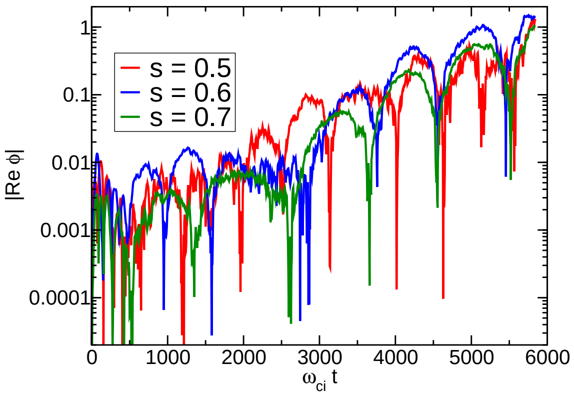


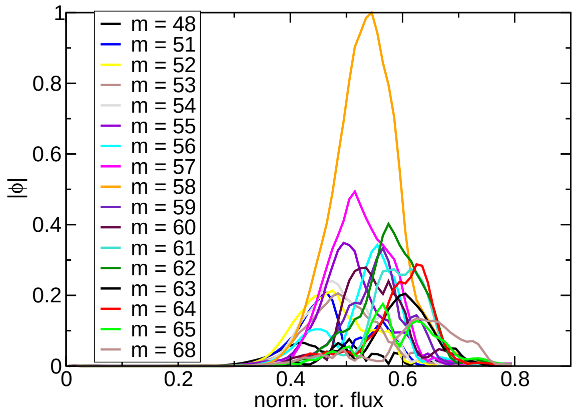


Ballooning mode (radial pattern)

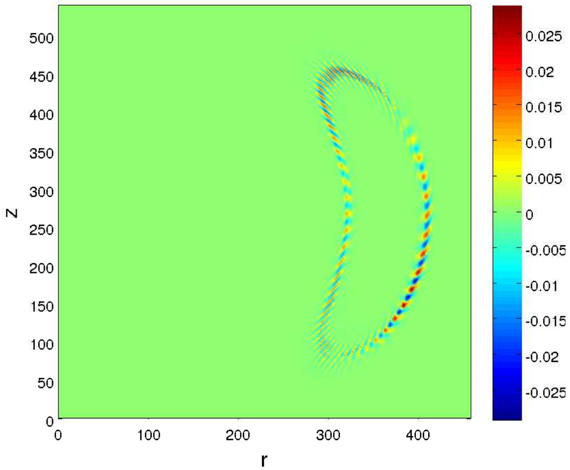
A. Mishchenko et al, Phys. Plasmas 21, 092110 (2014)

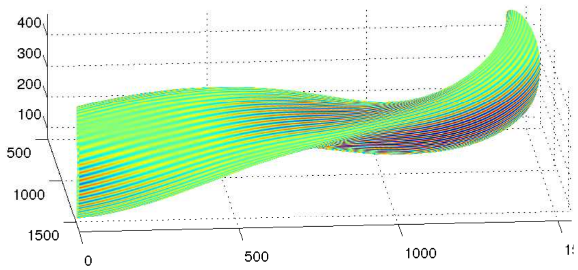
KBM/ITG in W7-X stellarator (EUTERPE)





Electromagnetic ITG;
left: evolution;
right: mode structure





left: cross-section
right: flute-like mode

Outlook: going mainstream

- Cancellation problem has prohibited large-scale effort on GK EM global PIC simulations (Reynders 1992, Cummings 1995)
- Reduced models have been widely used to circumvent the problem: hybrid kinetic-MHD, fluid-electron models
- Limitations of reduced models: closure issues, no micro-tearing physics

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- A lot of work has been done to mitigate the cancellation problem: control variate, mixed-variable pullback scheme; US schemes
- The mitigation schemes can be used both in linear and nonlinear regimes
- The mitigation schemes have been validated on many examples, including the international ITPA benchmark

Global gyrokinetic EM PIC simulation schemes approach mainstream

Mixed-variable formulation: the algorithm

1. At the end of each time step, redefine the magnetic potential splitting:

$$A^{(s)}_{\|(\mathrm{new})}(t_i) = A_{\|}(t_i) = A^{(s)}_{\|(\mathrm{old})}(t_i) + A^{(h)}_{\|(\mathrm{old})}(t_i)$$

2. As a consequence, redefine $A^{(h)}_{\|(\mathrm{new})}(t_i) = 0$

3. New mixed-variable distribution function coincides with symplectic one (pullback 0-form): $f_1^{(s)}(Z^{(s)}, A_{\|}^{(s)}) = f_1^{(m)}(Z^{(m)}, A_{\|}^{(s)}, A_{\|}^{(h)})$

$$f^{(m)}_{1(\mathrm{new})}(t_i) = f_1^{(s)}(t_i) = f^{(m)}_{1(\mathrm{old})}(t_i) + \frac{q\,\langle A^{(h)}_{\|(\mathrm{old})}(t_i)\rangle}{m}\frac{\partial F_0}{\partial v_{\|}}$$

4. Proceed, explicitly solving the mixed-variable system of equations at the next time step $t_i + \Delta t$ in a usual way, but using the symplectic coordinates as the initial conditions.

Solution of the cancellation problem (iterative scheme)

- **Ampere's law computes $A_\parallel$. But $p_\parallel$-transform depends on $A_\parallel$!**

$$-\nabla_\perp^2 A_\parallel = \mu_0 \int v_\parallel \left[\bar{f}_{1s} + \{S_1, F_{0s}\} + \frac{q_s \langle A_\parallel \rangle}{m_s} \frac{\partial F_{0s}}{\partial v_\parallel} \right] \delta(\vec{R} + \vec{\rho} - \vec{x}) \mathrm{d}^6 Z$$

- **Solution: introduce an easy-to-compute estimator for transform (β_e/ρ_e^2)**

$$(s + L)a = j \Rightarrow (s + L)a = j + (\hat{s} - \hat{s})a \Rightarrow (\hat{s} + L)a = j + (\hat{s} - s)a$$

- **Employ $\|\hat{s} - s\| = \mathcal{O}(\epsilon)$ and solve Ampere's law iteratively**

$$a = a_0 + \epsilon a_1 + \epsilon^2 a_2 + \ldots\ , \quad (\hat{s} + L)a_0 = j\ , \quad (\hat{s} + L)a_1 = j + (\hat{s} - s)a_0\ , \ldots$$

$$\hat{s}_{kl} = \int \frac{\beta_e}{\rho_e^2} \Lambda_k(\vec{x}) \Lambda_l(\vec{x})\, \mathrm{d}^3 x\ , \quad j_k = \sum_{\nu=1}^{N_\mathrm{p}} v_{\parallel\nu}\, w_\nu \langle \Lambda_k \rangle_\nu$$

$$j_k - s_{kl} a_l^{n-1} = \sum_{\nu=1}^{N_\mathrm{p}} v_{\parallel\nu} \left(w_\nu + \frac{q_s \langle A_\parallel^{(n-1)} \rangle}{m_s} \frac{\partial}{\partial v_\parallel} F_{0s}(Z_\nu) \zeta_\nu \right) \langle \Lambda_k \rangle_\nu$$