Verification of long wavelength electromagnetic modes with a gyrokinetic-fluid hybrid model in the XGC code

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As an alternative option to kinetic electrons, the gyrokinetic total-f particle-in-cell (PIC) code XGC1 has been extended to the MHD/fluid type electromagnetic regime by combining gyrokinetic PIC ions with massless drift-fluid electrons analogous to Chen and Parker [Phys. Plasmas 8, 441 (2001)]. Two representative long wavelength modes, shear Alfvén waves and resistive tearing modes, are verified in cylindrical and toroidal magnetic field geometries. Published by AIP Publishing.

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This article describes the verification of two important MHD/fluid type, long-wavelength, electromagnetic modes after the addition of an optional kinetic-fluid hybrid model to the gyrokinetic particle-in-cell (PIC) code XGC1. This work complements—as a more economical alternative—the fully implicit, fully kinetic electromagnetic formulation, that is also being developed for XGC1.

The importance of MHD/fluid type electromagnetic modes in magnetically confined fusion devices, which operate regularly at moderate to high \( \beta = 2 \mu_0 P / B^2 \) (the ratio of thermodynamic to magnetic pressure), is widely recognized. Examples are neoclassical tearing modes, sawtooth oscillations, and edge localized modes (ELMs). Gyrokinetic electromagnetic codes such as GYRO, GS2, GENE, and GEM have been available with increasing physics capability for more than a decade and have also been used to study those modes. However, their application in long wavelength MHD/fluid type instabilities has been difficult, especially for PIC codes, due to the so called “cancellation problem.” Recently, several methods were developed to overcome the cancellation problem with kinetic electrons for PIC codes, due to the so called “cancellation problem.” The cheapest way to study these modes is to use fluid electrons instead of electron particles. The electron density continuity equation is given by

\[
\frac{\partial n_e}{\partial t} = -n_0 (B + \delta B) \cdot \nabla \left( \frac{\nabla^2 A \parallel}{e \mu_0 n_0 B} + \frac{u_{\parallel} B}{B} \right) + \frac{2n_0}{B^2} (B \times \nabla B) \cdot \nabla \delta \phi + \frac{2}{e B^3} (B \times \nabla B) \cdot \nabla \delta P_e,
\]

where \( B \) is the axisymmetric background magnetic field, \( \delta B = B_0 \times \hat{\mathbf{b}} \) is the perturbed magnetic field, \( \hat{\mathbf{b}} = B / B_0 \), and \( A_\parallel \) is the component of the perturbed vector potential along the background magnetic field, \( \mu_0 \) is the vacuum permeability, \( u_{\parallel} \) is the parallel ion fluid flow, \( \delta \phi \) is the perturbed ion guiding center distribution function, \( n_e = n_0 + \delta n_e \) is the electron density, \( j_0 = \hat{\mathbf{b}} \cdot \nabla \times (B / \mu_0) \) is the equilibrium current density, \( \delta P_e = e \delta n_e T_0, e \) is the
perturbed iso-thermal electron pressure, and \( v_E = \frac{1}{2} \mathbf{b} \times \nabla \phi \) is the \( \mathbf{E} \times \mathbf{B} \) drift. We also used the relation \( u_{i,j} = (\nabla^2 \mathbf{A}_j) / (e\mu_0 n_0) + u_{i,j} \). The time evolution of the perturbed vector potential is given by the definition of the electric field and Ohm’s law

\[
\frac{\partial \mathbf{A}_j}{\partial t} = -\mathbf{b} \cdot \nabla \phi - E_j, \tag{2}
\]

\[
E_j = -\frac{\mathbf{b} \cdot \nabla}{\varepsilon_0 n_0} e \mathbf{P}_e - \frac{\mathbf{b} \cdot \nabla}{\varepsilon_0 n_0} (P_{0,e} - \varepsilon_0 \phi) + \eta_j \mathbf{J}_j. \tag{3}
\]

Here, \( \mathbf{b} = \mathbf{b} + \Delta \mathbf{b} / B, P_{0,e} = \varepsilon_0 T_{0,e} \) is the background electron pressure, and \( \mathbf{b} \) is the background electron kinetic Poisson equation in the long wave length limit is

\[
-\nabla \left( \frac{\varepsilon_0 k_0}{e} \nabla \phi \right) = \delta n_i - \delta n_e, \tag{4}
\]

where \( \delta = (\rho_0 / \lambda_0) \) is the ion electric susceptibility, \( \rho_0 \) is the ion gyro radius, \( \lambda_0 \) is the Debye length, and \( \varepsilon_0 = B / (\mu_0 n_0) \) is the Alfvén speed. The ion density is \( \delta n_i = \int dt_0 \mathbf{v}(\delta f) \rho \), where \( \langle \ldots \rangle \rho \) indicates gyro-averaging. The massless electron approximation is valid in the limit \( v_{ei} / v_{e} \rightarrow 0 \) or \( \beta_i m_i / m_e \gg 1 \), where \( \beta_i = 2 \mu_0 e / B^2 \).

The fluid equations are implemented by using a mixed finite-difference (FD) finite-element (FE) method. Terms of the form \( \mathbf{a} \cdot \nabla \) and \( \mathbf{b} \cdot \nabla \) use a second order FD derivative. Parallel derivatives are set up by field-line tracing and exploiting the field-following property of the XGC meshes.33,34 The Poisson equation and the Laplacian \( \nabla^2 \phi \) retain only derivatives with respect to \( R \) and \( Z \) and are evaluated with linear finite elements on a planar triangular mesh.

In the \( \delta f \) formalism, the nonlinear terms in the electron fluid equations, e.g., \( v_{e} \cdot \nabla \delta n_e \), are a potential complication compared to the particle weight evolution equation,1 which is formally linear with the non-linearity entering through the perturbed particle orbits. Based on preliminary nonlinear studies of KBM turbulence, we expect this will not cause numerical problems. However, in some cases, numerical problems might arise and require adjustments to the implementation of the nonlinear terms, e.g., by casting the nonlinear terms in the electron continuity equation in a conservative form as in the GEM code.

Both explicit and implicit time integrators have been implemented. A second order Runge–Kutta (RK2) method has been utilized for the time integration of the combined particle–fluid system for many of the results discussed in this work. In the first step, \( \delta n_i(t + \Delta t/2) \) and \( A_j(t + \Delta t/2) \) are evaluated using, \( \phi(t) \), \( \delta n_i(t) \) and \( u_{i,j}(t) \). Then the particles are pushed for a half time step to evaluate \( \delta n_i(t + \Delta t/2) \) and \( u_{i,j}(t + \Delta t/2) \). In the second step, we evaluate \( \phi(t + \Delta t/2) \) and then push the particles for a full time step to obtain \( \phi(t + \Delta t), \delta n_i(t + \Delta t) \) and \( u_{i,j}(t + \Delta t) \).

Implicit time stepping methods have been implemented using the PETSc TS framework to overcome the restrictions in the time step of explicit methods. The particle terms \( \delta n_i \) and \( u_{i,j} \) are treated as non-linear contributions to the system of electron fluid equations and are fully integrated into PETSc’s nonlinear solver residual, but only the electron fluid terms are included in the Jacobian. The Newton method is used to solve the non-linear equations, which requires one particle push per evaluation of the residual.

For the verification of shear Alfvén wave physics, we use a minimal system that supports this mode: linearized versions of equations (1)–(3) with the closure \( E_j = \eta_j \mathbf{J}_j \). In addition, we neglect the terms related to the curvature and \( \nabla \mathbf{B} \) drift in Eq. (1). It is straightforward to prove in cylindrical geometry that the dispersion relation of the resulting reduced system yields \( \omega = (v_A k_0^2 - \mathbf{k} \cdot \mathbf{b} / \sqrt{2 / \mu_0}) \mathbf{k}_0^2 + \eta_e / (2 \mu_0) \mathbf{k}_0^2 \). The first verification test of the shear Alfvén dispersion relation was conducted in cylindrical geometry with concentric, circular flux-surfaces with minor radius \( a = 1 \), constant safety factor \( q = 3 \), \( \beta_e = 1.5 \times 10^{-2} \), and \( \eta_e = 10^{-6} \Omega \) m. The simulation was initialized with a global perturbation of \( A_j \) centered around \( \varphi / a = 0.67 \) containing toroidal mode numbers \( n = 1 \ldots 4 \) and poloidal mode numbers \( m = 0 \ldots 4 \). With this large scale variation in the radial and poloidal direction, the low resistivity does not influence the real frequency much but still serves as a check for the resistive dissipation of the reduced shear Alfvén wave system (with \( k_\perp \sim 1/a \)). The time step for this simulation was \( \Delta t = 1.36 \times 10^{-3} \) s \( \approx 10^{-2} \tau_A \), where \( \tau_A = R_0 / \Omega_A \). The total duration of the simulation is \( 1.36 \times 10^{-3} \) s \( \approx 1000 \tau_A \).

Figure 1 shows the shear Alfvén spectrum obtained from this simulation. The parallel wave number was determined as \( k_\parallel = \mathbf{b} \cdot \mathbf{k} = (B_y / B) k_0 + (B_z / B) k_0 \). The mode frequency is the median of the intensity for each value of \( k_\parallel \) and the error bars indicate the decay length of the mode intensity around its median. The increasing width of the error bars at \( k_\parallel > 0.5 \) indicates decreasing overall intensity due to the low toroidal and poloidal mode numbers used to initialize the simulation. The steps in the frequency spectrum are an artifact of the interpolation of the intensity from \( (k_\parallel, k_\perp) \) space to a common \( k_\parallel \) scale.

Similar tests in toroidal geometry have been performed in a slightly modified version of the standard cyclone geometry, with \( R_0 = 1.7, a/R_0 = 0.358, B_0 = 1.9 \), constant \( q = 2, \)

![FIG. 1. The shear Alfvén wave spectrum in cylindrical geometry with concentric circular flux-surfaces. The density plot indicates the mode intensity, the diamonds indicate the median of the intensity at each \( k_\parallel \), and the error bars indicate the decay length of the intensity around the median. The steps in the median frequency are an artifact of the interpolation of the intensity from \( (k_\parallel, k_\perp) \) space to a common \( k_\parallel \) scale.](image-url)
and $T_0 = 2$ keV. The density is varied between $1.875 \times 10^{19} \text{m}^{-3}$ and $6 \times 10^{20} \text{m}^{-3}$ to achieve values of $\beta_e$ between 0.4% and 13.4%. The time step is $\Delta t \approx 5 \times 10^{-2} \tau_A$ and the total simulation time is $\approx 40\tau_A$. The simulation is initialized with an $n = 4, m = 4 \ldots 12$ perturbation of $A_i$. Figure 2 shows the frequency spectrum of the $n = 4$ Alfvén wave for the poloidal wave numbers $m = 6 \ldots 10$. The numerical frequencies agree very well with the (approximate) analytical result $\omega \propto (2n/L_0)(n - m/q)\gamma_A$, where $L_0$ is the parallel connection length for one poloidal circuit. The deviations are caused by the variation of the field line pitch along magnetic field lines. We find that $\delta T_A$ is independent of $\beta_e$ as expected because only the density $n_0$ was varied in this test.

Since the kinetic-fluid hybrid approach is especially useful for the simulation of low-$n$ tearing modes, we benchmarked the $(m, n) = (2, 1)$ tearing mode in cylindrical and toroidal geometry against the GEM code and M3D-K, respectively. We did not consider the effect of kinetic ions in this benchmark. The only term added to the electron fluid equations compared to the terms kept in the shear Alfvén case is the kink drive $\delta B_L \cdot \nabla \left[ j_0 / (eB) \right]$ in Eq. (1) to be consistent with GEM's eigenvalue solver.

For the benchmark against the GEM code, we use the case described in Ref. 32: concentric, circular flux-surfaces in cylindrical geometry, $R_0 = 1.7 \text{m}$, $a = 0.425 \text{m} \quad (R_0/a = 4)$, $B_0 = 1.906 \text{T}$, $q = 1.5 \left[ 1 + (r/a)^2 \right]$, $Z = 1$, $m_i/m_p = 2.5$, and constant density $n_0 = 3.886 \times 10^{20} \text{m}^{-3}$. Since the electron fluid equations used for this benchmark have no temperature dependence, we can use a constant temperature profile $T_0 = 45.63 \text{eV}$, which yields the same on-axis $\beta_e$ of $4 \times 10^{-3}$ and relative domain size $a/r_1 \approx 740$ as in Ref. 32. The resonant surface for the $(2, 1)$ tearing mode is at $(r/a)_c \approx 0.577$ corresponding to the normalized poloidal magnetic flux $\psi_{N,c} = 0.411$. In order to be able to resolve the resonance layer of the $(2, 1)$ tearing mode also at low resistivity, the radial resolution of our computational mesh varies between 0.5 mm around the resonant surface to a maximum of 8 mm far from the resonant surface. The relationship between the normalized resistivity $\eta_N$ and growth rate $\gamma_N$ used in Ref. 32 and the corresponding values $\eta_N$ and $\gamma$ in SI-units are $\eta_N = (e\nu_0/B_0)\eta$ and $\gamma = m_p/(eB_0)\gamma$, where $m_p$ is the proton mass. The results of a resistivity scan of the growth rate of the $(2, 1)$ tearing mode in this geometry are shown in Fig. 3. The growth rates evaluated with XGC1 show excellent agreement with the growth rates computed with GEM's eigenvalue solver that uses the MHD approximation for the ion polarization density (Fig. 3 in Ref. 32).

We did not include an XGC1 data point for $\eta_N = 10^{-7}$ because of the very strict resolution requirements of about $2.5 \times 10^{-4} \text{m}$ or less for this low resistivity. Using the Crank–Nicolson method, the implicit time integrator could speed up these simulations by a factor of more than 10. For $\eta_N = 10^{-6}$ a time step of $\Delta t = 2.7\tau_A$ could be used.

For the benchmark against M3D-K in toroidal geometry, we use a Grad–Shafranov equilibrium generated with the FLOW code with a fixed circular boundary, $R_0 = 5.76 \text{m}$, $a = 1 \text{m}$, $B_0 = 1 \text{T}$, $q = 1.5 + 2\psi_{N,c}$, $m_i/m_p = 2.5$, and constant $n_0 = 10^{20} \text{m}^{-3}$ and $T_0 = 100 \text{eV}$, so that $\beta_e = 4 \times 10^{-3}$ and $\beta_i/m_i = 18.4$. The resonant surface of the $(2, 1)$ tearing mode is located at $\psi_N = 0.5$. The radial resolution of the computational mesh is 1.5 mm between approximately $\psi_N = 0.4$ and $\psi_N = 0.6$ and up to 1.2 cm away from the tearing layer. For the normalized resistivity of $\eta_{NM3D} = 10^{-4}$ used in Ref. 38 and the corresponding normalization relations, we obtain a resistivity in SI units of $\eta_N = \mu_0 (a^2 / \tau_A)\eta_{NM3D} = 3.01 \times 10^{-4}$. The XGC1 growth rate calculation used a time

![FIG. 2. Poloidal mode number scan ($m = 6 \ldots 10$) of the $n = 4$ shear Alfvén wave in a toroidal cyclone-like geometry for $\beta_e = 3.3 \times 10^{-3}$. The dotted line is the analytical mode frequency in cylindrical geometry.](image-url)
step of $\Delta t = 7 \times 10^{-3} \tau_A$, and ran for a total time of approximately 350 $\tau_A$. Figures 4(a)–4(d) show the mode structure of the growing (2, 1) mode, which exhibits the usual tearing structure. For comparison with Ref. 38, we use reduced MHD quantities, the perturbed current $R_{\theta, e}$, and the velocity stream function $\phi/\beta$. The growth rate we obtain from the XGC1 calculation is $\gamma = 1.12 \times 10^{-2} \tau_A^4$ and compares well to Ref. 38.

The relative difference between the XGC1 and the M3D-K result is 6%.

Verification of linear and nonlinear intermediate wavelength drift-Alfvén modes such as ion temperature gradient-driven modes and kinetic ballooning modes (KBMs) will be presented in a future paper. In order to demonstrate the coupling of the gyrokinetic ion particles to the electron fluid equations, we give one example of linear growth of KBM modes in cyclone geometry with hydrogen ions, $R_0 = 1.7$ m, $a/R_0 = 0.358$, $B_0 = 1.9$ T, $q = 0.854 + 2.184(r/a)^2$, $T_i/T_e = 1$ keV, $\beta_e = 4.4\%$, $R_0/L_n = 2.22$, and $R_0/L_T = R_0/L_{Ti} = 10$. Figure 5 shows the final mode structure of the $n = 10$ mode, which exhibits the usual tearing structure. The frequency and growth rate obtained in this case are $\omega = 2.0 c_s / R_0$ and $\gamma = 0.69 c_s / L_n$.

In order to add gyrokinetic ion effects to electromagnetic fluid/MHD instabilities, the gyrokinetic edge turbulence code XGC1 has been modified by replacing the kinetic electrons by massless drift-fluid electrons. Explicit and implicit time integration methods have been implemented and tested. We verified shear Alfvén wave physics against the analytical solution and benchmarked the massless fluid model for resistive tearing modes against the codes GEM and M3D-K. The hybrid model in XGC will be further developed into a total-f code with the aim of studying the onset of edge localized modes across the magnetic separatrix surface. Verification of the kinetic version of peeling-ballooning

FIG. 4. Mode structure of the (2, 1) tearing mode in toroidal geometry, which compares well to Fig. 1 in Ref. 38. (a) $R_{\theta, e}$ (equivalent to the perturbed current) at $\varphi = 0$, and (b) $\phi/\beta$ (velocity stream function) at $\varphi = 3\pi/2$ plotted along the midplane. The dashed lines indicate the location of the $\psi_{\parallel} = 0.5$ surface. (c) $R_{\theta, e}$ at $\varphi = 0$, and (d) $\phi/\beta$ at $\varphi = 3\pi/2$ in the $(R,Z)$ plane. The dotted circle is the $\psi_{\parallel} = 0.5$ surface.

FIG. 5. Vector potential $A_\parallel$ obtained for the $n = 10$ mode after 65.7 $\tau_A$ in a linear XGC simulation in cyclone geometry with hydrogen ions, $R_0 = 1.7$ m, $a/R_0 = 0.358$, $B_0 = 1.9$ T, $q = 0.854 + 2.184(r/a)^2$, $T_i/T_e = 1$ keV, $\beta_e = 4.4\%$, $R_0/L_n = 2.22$, and $R_0/L_T = R_0/L_{Ti} = 10$.
modes, and kinetic ballooning modes will be reported in a subsequent paper.

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