Particle simulation of radio frequency waves with fully-kinetic ions and gyrokinetic electrons

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Abstract
A toroidal particle-in-cell (PIC) code, suitable for investigating nonlinear phenomena in radio frequency (RF) heating and current drive, is developed and verified thereafter through a series of fidelity tests for field solvers and single particle motions in toroidal geometry, where simulation results show good coincidence with analytical prediction. The RF capability is then demonstrated through the integrated benchmarks with linear lower hybrid wave and ion Bernstein wave theory in cylindrical geometry, where the analytic result is easily available. The frequency and mode structure in the simulations agree well with the theoretical prediction.

Keywords: fully-kinetic, gyrokinetic, radio frequency, particle simulation, lower hybrid, ion Bernstein wave

(Some figures may appear in colour only in the online journal)

1. Introduction

The application of radio frequency (RF) waves to magnetically-confined fusion can be traced back to the very early days of nuclear fusion research \cite{1}. It is critical for achieving steady state operations of a magnetically-confined fusion device, such as international thermonuclear experimental reactor (ITER) \cite{2}, where RF waves, including lower hybrid waves (LHW), ion cyclotron waves (ICW), fast waves and ion Bernstein waves (IBW), play an irreplaceable role in auxiliary heating, current drive, profile control and mitigating MHD instabilities \cite{3}. However, as the power of the RF wave increases, various nonlinear effects emerge, which will dramatically lower the injection efficiency and hinder the application of RF waves to fusion devices.

To investigate these RF waves, simulation works have been conducted employing various simulation schemes including ray-tracing \cite{4}, beam-tracing \cite{5,6}, full-wave \cite{7} and mixed WKB-full-wave \cite{8} methods. For ray tracing and beam tracing, a certain form of oscillation is assumed, and the Eikonal is traced through multiple ‘rays’ or ‘beams’. Coupled with the Fokker–Plank solver, ray-tracing could predict wave’s trajectory and absorption with very low computation power demand. However, the WKB assumption \cite{9} and the concomitant ray-tracing method is violated when the propagating wavelength is larger than or comparable to any of the the curvature radius of the wave front or the characteristic scale length of the system susceptibilities. Furthermore, the diffraction and caustic effect are not included in the ray-tracing code. To address the deficiency of
the ray-tracing code, the full wave approach is proposed by directly solving the Maxwell equations with plasma response \footnote{\[ \nabla \times \nabla \times \mathbf{E} = \omega^2 \varepsilon_0 \mathbf{E} + \left( 4\pi i / \omega \right) \left( \mathbf{J}^p + \mathbf{J}^s \right) \] where \( \mathbf{J}^s \) is the plasma current and \( \mathbf{J}^p \) is the current imposed by the external antenna. The plasma response could be coupled with the Fokker–Plank equation solver to include the non-Maxwellian distribution effect. This method successfully unveils various physical optics features of RF waves including interference and diffraction, but the plasma response is quasi-linear so that the non-linear effects are not included. To address this limitation and take advantage of the ever-growing supercomputing power, the kinetic method is considered to directly solve the Vlasov–Maxwell equation systems, which captures nonlinear physical phenomena with less assumptions.

For high frequency simulation, the pure gyrokinetic simulation model \footnote{\cite{22}} based on G-gauge theory \footnote{\cite{11}}, which could loosen the requirement of frequency \( \omega < \Omega_c \), has been successfully developed and implemented to inspect high frequency RF waves in magnetized plasmas. Based on the Frieman–Chen nonlinear gyrokinetic theory \footnote{\cite{12}}, Yu Lin \textit{et al} proposed a gyrokinetic electron and fully-kinetic ion combination \footnote{\cite{13}} to bridge the different temporal and spatial scales of electrons and ions. Together with Poisson’s equation, the parallel Ampère’s law, the force balance equation and the perpendicular Ampère’s law, a simulation model GeFi \footnote{\cite{13, 14}} was constructed and coded in slab geometry to investigate the dynamics of the collisionless processes with frequency ranges from the Alfvén frequency to the lower hybrid frequency. Afterwards, Yang Chen \footnote{\cite{15–17}} adopted the gyrokinetic electron and fully kinetic ion combination, Faraday’s equation and Ampère’s law to construct a model for studying turbulent transport. The gyrokinetic toroidal code (GTC) \footnote{\cite{18}} extends its capability with fluid ions and drift-kinetic electrons to investigate the lower hybrid wave physics in cylindrical and toroidal geometries. Then Bao \textit{et al} \footnote{\cite{19, 20}} benchmark linear mode conversion of lower hybrid wave by introducing compressional component \footnote{\cite{20}}. GTC also develops the capability with fully-kinetic particles using the Boris scheme, and the linear dispersion relation and nonlinear effects of the ion Bernstein wave \footnote{\cite{21}} are verified.

Recently, based on Lie-transform gyrokinetic theory, a gyrokinetic electron and fully-kinetic ion simulation model, which is directly closed by using Poisson’s equation and Ampère’s law, is developed in toroidal geometry \footnote{\cite{22}}. This article will report the code development based on this compact toroidal model for investigating nonlinear effects in toroidally-confined fusion plasma devices, such as tokamaks and stellarators.

On the code implementation aspect, this code utilizes the mature parallelization structure and toroidal geometry part of GTC, while the particle pushing, field solver and high order spline interpolation are re-implemented to meet the needs of this work. GTC has been successfully used in studying electrostatic turbulence, energetic particle transport and Alfvén wave physics. These works include the ion temperature gradient \footnote{\cite{23, 24}}, electron temperature gradient \footnote{\cite{25}}, trapped electron mode \footnote{\cite{26}}, turbulence induced energetic particle (EP) transport \footnote{\cite{27}}, toroidicity-induced Alfvén eigenmode (TAE) \footnote{\cite{28, 29}} and beta-induced Alfvén eigenmode (BAE) \footnote{\cite{30, 31}}.

This paper will be organized as follows: the set of Vlasov–Maxwell equations for gyrokinetic electron species and fully-kinetic ion species is introduced in section 2. Section 3 includes the dimensionless formulation for code implementation. In section 4, the preliminary fidelity tests, including unit tests for particle trajectory integrator and field solver, are provided. In section 5, the integrated benchmark will be reported using, for example, the lower-hybrid wave and the ion Bernstein wave. The summary and discussion are then presented in section 6.

2. Simulation model

This section briefly presents a closed Vlasov–Maxwell simulation model using fully-kinetic ions and gyrokinetic electrons. This physical model \footnote{\cite{22}} is derived using the modern Lie perturbative Hamiltonian approach. The electromagnetic fields are purely described with scalar potential \( \delta \phi \) and vector potentials \( \delta \mathbf{A} \) without introducing the intermediate magnetic perturbation \( \delta \mathbf{B} \), in the parallel direction. Both gyrokinetic particles and fully-kinetic particles are described with the canonical description. Temporal and spacial ordering are thoroughly treated with the following ordering parameters: \( \epsilon_B \sim \rho_i / L_i \), \( \epsilon_F \sim \rho_i / L_F \), \( \epsilon_e \sim \omega_p / \Omega_p \), \( \epsilon_L \equiv k_L \rho_e \sim 1 \), \( \delta_b \sim \epsilon_b < 1 \) and \( \epsilon_\delta \sim \Delta_b / B \sim \delta f / f \). These parameters will be used as labels for ordering rather than an actual physical value.

2.1. Vlasov equation for ions and electrons

Provided that the vector potential and scalar potential is decomposed to unperturbed and perturbed components in terms of \( \mathbf{A} = \mathbf{A}_0 + \delta \mathbf{A} \) and \( \phi = 0 + \delta \phi \), respectively, the electron’s gyrocenter distribution function \( F_e \) satisfies the gyrokinetic Vlasov equation:

\[
\frac{\partial F_e}{\partial t} + \mathbf{X} \cdot \frac{\partial F_e}{\partial \mathbf{X}} + \frac{e_e}{m_e} \frac{\partial F_e}{\partial \mathbf{p}_e} = 0,
\]

where \( \mathbf{X} \) is the electron’s gyrocenter position and \( \mathbf{p}_e = m_e v_e \) is the momentum of electrons in the direction parallel to the background magnetic field \( \mathbf{B}_0 \). The electron’s gyrocenter motion equations are

\[
\dot{\mathbf{p}}_e = -\frac{\mathbf{b}^*}{B_0^*} \left[ \frac{\epsilon_e c q_e \left\langle \delta \phi^*_{ge} \right\rangle}{\epsilon_B} \hat{\mathbf{n}} \sim \nabla \mathbf{B}_0 \right],
\]

\[
\dot{\mathbf{X}} = \frac{\mathbf{p}_e}{m_e} + \epsilon_e \frac{d}{dt} \left\langle \delta \phi^*_{ge} \right\rangle \frac{\mathbf{b}^*}{B_0^*} \hat{\mathbf{n}} + \epsilon_e \frac{c}{q_e B_0^*} \mathbf{b}_0 \times \left[ \frac{\epsilon_e c q_e \left\langle \delta \phi^*_{ge} \right\rangle}{\epsilon_B} \hat{\mathbf{n}} \sim \nabla \mathbf{B}_0 \right].
\]

In the equations above, the modified field vector is defined as \( \mathbf{b}^* = \mathbf{b} + \epsilon_B \mathbf{p}_e / (m_e \Omega_e) \nabla \times \mathbf{b} \), \( \mathbf{b}_0^* = \mathbf{b} \cdot \mathbf{b}^* \). Operator \( \langle \cdots \rangle \) means gyroaveraging. Additionally, the effective potential reads
\[ \delta \phi^*_{gc} = \delta \phi_{gc} - \frac{\delta A_{gc}}{c} \left( \frac{\rho_e}{m_e} \hat{b} + \Omega_e \frac{\partial \rho_e}{\partial \Theta} \right), \]

where \( \delta \phi_{gc} \) and \( \delta A_{gc} \) are the perturbed scalar and vector potential evaluated in the guiding-center phase space, \( \rho_{gc} = (2 \mu B_0/m_e)^{1/2}/\Omega_e \) is the gyroradius of the guiding center, \( \mu = m v^2 / (2 B) \) is the particle’s magnetic moment and \( \Theta \) is the guiding-center gyroangle.

Through two steps of transformation [32, 33], guiding-center transformation and gyrocenter transformation, the removing of the gyroangle \( \Theta \) dependence of the Hamiltonian in an equations come from a charged particle and canonical momentum are \( C = \frac{q}{m_e} \). This feature is desired by computation [35] since the directly advancing \( \partial / \partial t \) term is either inaccurate or cumbersome. The additional reason for describing the ion in canonical form is that the \( P_e \) is conserved, since the unperturbed Hamiltonian does not depend on \( \zeta \). The conservation of \( P_e \) will increase the numerical accuracy of the ion in the \( \zeta \) direction.

2.2. Field equation

In particle-in-cell (PIC) simulation, the field is solved based on the marker particle’s information. Since \( k_i \ll k_L \), the Poisson equation reads [22]:

\[ (1 + \sum_e \frac{\omega_{pe}^2}{\Omega_e^2}) \nabla^2 \delta \phi + \sum_e \frac{4 \pi q_e N_0}{B_0} \nabla \cdot (\delta A \times \hat{b}) = -4 \pi \left( \sum_i q_i \delta n_i + \sum_e q_e \delta N_e \right). \]  

(7)

where \( \rho_0 = v_\perp / \Omega_0 \) is the gyroradius vector, which is quantitatively equal to the local gyroradius and points from the gyrocenter to the particle, and \( \mathbf{a}_i \) is a gyroangle-dependent dyadic tensor [34]. In the absence of fluctuations, the magnetic moment in particle \( \mu_0 = \mu(1 + C_D + C_E)^{-1} \approx \mu(1 - C_D - C_E) \) consists of three components: a constant term \( \mu \), a slowly-varying drift term \( C_D \), which is proportional to \( v_\perp \), and a quickly-varying gyromotion term \( C_E \) related to \( \rho_0 \) and \( \mathbf{a}_i \).

For ions, since the frequency of waves, such as lower hybrid waves and ion cyclotron waves, is beyond the ion’s gyrofrequency, the full kinetic model is adopted by directly advancing the ion’s position and its canonical momentum in 6-dimensional phase space. The fully-kinetic ion’s Vlasov equation is

\[ \frac{\partial f_i}{\partial t} + \hat{x}_i \cdot \frac{\partial f_i}{\partial \mathbf{x}_i} + \hat{p}_i \cdot \frac{\partial f_i}{\partial \mathbf{p}_i} = 0, \]  

(5)

Here, \( f_i \) is the ion’s distribution function, and the ion’s position and canonical momentum are \( \mathbf{x}_i \) and \( \mathbf{p}_i \), respectively. Ion motion equations come from a charged particle’s Hamiltonian in an electromagnetic field, \( H = \mathbf{p}_i - (q_i/c) \mathbf{A} / (2m_i) - q_i \delta \phi \).

\[
\begin{align*}
\frac{d \mathbf{p}_i}{d t} &= -q_i \frac{\partial \delta \phi}{\partial \mathbf{x}_i} + \frac{q_i}{c} \frac{\partial \mathbf{A}}{\partial \mathbf{x}_i} \cdot (\mathbf{p}_i - (q_i/c) \mathbf{A}), \\
\frac{d \mathbf{x}_i}{d t} &= \frac{1}{m_i} (\mathbf{p}_i - q_i/c \mathbf{A}).
\end{align*}
\]

(6)

It is notable that here, both the ion and electron are described using canonical momentum instead of velocity. The major advantage of using canonical momentum in the gyrokinetic formulation is that the \( \partial \mathbf{A} / \partial t \) term does not appear in the gyrocenter dynamics [32]. This feature is desired by computation.
by ignoring the finite Larmor radius effect in the drift kinetic limit; the homogeneous Maxwellian background is assumed; and high order nonlinear terms are turned off. This assumption is sufficient for the linear benchmark, while analytically simplifying the calculations. The drift-kinetic equations are derived by taking the long wavelength limit $k_{\perp} \rho_e \rightarrow 0$. For simplicity, a uniform background field and particle distribution are also assumed. The dynamics of the electron guiding center reads:

$$
\dot{p}_c = -e_B \left[ \frac{\epsilon s \beta q_e}{m_e} \nabla \hat{\phi} - \mu \nabla B_0 \right],
$$

(9)

$$
\dot{X} = \left( \frac{p_{\parallel}}{m_e} + c_s \frac{\partial \delta \phi_{\parallel}}{\partial p_{\parallel}} \right) b_{\parallel}^* + e_B b_{\parallel} \times \nabla \phi + \frac{e_B}{q_e B_{\parallel}^*} b_{\parallel} \times \nabla \phi_{\parallel} = \epsilon \left( \frac{\delta \phi_{\parallel}}{\epsilon} \nabla B_0 \right).
$$

Thus, equations (1), (5)–(9) form a closed system for the numerical code.

2.4. Formulations in Toroidal geometry

In the toroidal code, the field equation and particle motion are described using the magnetic flux coordinate [36] and the field-line coordinate [37] for better numerical accuracy and the reduced requirement of toroidal resolution. Since these two coordinate systems are essentially non-orthogonal, the equation must be expanded under the general curvilinear coordinate. A curvilinear coordinate may be represented as $q^2$ with $\beta = 1, 2, 3$, and the relation to the Cartesian coordinate $x^\alpha$ ($\alpha = 1, 2, 3$) is $q^2 = q^2(x^\alpha)$. Specific to toroidal geometry, in the magnetic flux coordinate [36], $(q^1, q^2, q^3)$ refers to $(\psi_p, \theta, \zeta)$, and the magnetic field can be expressed as $\mathbf{B} = g \hat{\nabla} \theta + f \hat{\nabla} \zeta$. $\mathbf{A} = \psi_p \hat{\nabla} \theta - \psi_p \hat{\nabla} \zeta$, where $\psi_p$ represents the toroidal magnetic flux and $\psi_p$ the poloidal flux [36].

While expanding the ion’s motion equation, an appropriate canonical transformation could be found using the second kind generation function by assigning $F_2 = q^2(x^\alpha)P_\beta$ [38]:

$$
p^\alpha = \frac{\partial F_2}{\partial x^\alpha} = \frac{\partial q^2}{\partial x^\alpha} P_\beta,
$$

$$
q^\beta = \frac{\partial F_2}{\partial P_\beta} = q^2(x^\alpha).
$$

The new Hamiltonian is

$$
\mathbf{H}' = \mathbf{H}(x^\alpha(q^\beta), p^\alpha(q^\beta, P_\beta)) + \frac{\partial F_2}{\partial \phi},
$$

(12)

$$
= -\frac{1}{2m} g^{\beta \delta} \left( P_\beta - e c A_\beta \right) \left( P_\delta - e c A_\delta + e \phi \right).
$$

Then the particle motion in this coordinate reads:

$$
\dot{q}^\gamma = \frac{1}{m} g^{\beta \gamma} \delta_{\gamma \delta} \left( P_\beta - e c A_\beta \right)
$$

(13)

Thus, the Vlasov equation in toroidal geometry can be written as follows:

$$
\frac{\partial f_i}{\partial t} + \frac{q^i}{q^2} \frac{\partial f_i}{\partial q^i} + \frac{\partial p_{\alpha}}{\partial p_{\alpha}} \frac{\partial f_i}{\partial p_{\alpha}} = 0.
$$

(14)

The ion’s motion, $\dot{q}^i$ and $P_\alpha$, can be substituted with equation (13). For a better numerical property, the $\delta_f$ method is used by decomposing the total distribution function $f_i$ into the equilibrium part $f_{i0}$ and the perturbed part $\delta_f$, $f_i = f_{i0} + \delta_f$, where $s$ denotes particle species. Instead of directly solving the above distribution function, the particle’s weighting function, $W_i = \delta_f / f_s$, is solved. For a local Maxwellian distribution with temperature $T_i$, the evolution of the ion’s weight $W_i$ is governed by the following equation

$$
\frac{dW_i}{dt} = (W_i - 1) \left[ \dot{q}_i \left( \kappa_i + \frac{P_{\alpha} - P_{\alpha1}}{T_i} \right) - \frac{\partial p_{\alpha1}}{\partial T_i} \frac{\partial q^2}{\partial q^2} \right],
$$

(15)

$$
\kappa_i = \frac{1}{n_0} + \frac{1}{T_i} \frac{\partial T_i}{\partial q^2} \left( E_i - \frac{3}{2} \right),
$$

(16)

$$
\dot{q}_i = -e \frac{q_i}{cm_i} \partial \mathbf{A}^\alpha,
$$

(17)

$$
\dot{p}_{\alpha} = e s \frac{q_i}{cm_i} \left( \frac{p_{\alpha} \partial \mathbf{A}^\beta}{\partial q^2} - \frac{q_i}{c} \frac{\partial \mathbf{A} \partial \mathbf{A}^\beta}{\partial q^2} \right) - \frac{\partial \phi}{\partial q^2}.
$$

(18)

The electron motion equations in the magnetic coordinate read [22]:

$$
\mathbf{B}_0^s = \left( 1 - e_B \frac{B_0 p_{\parallel}}{m_e \Omega_{e0} \partial \psi_p B_0} \frac{g}{\partial \psi_p} \right) \nabla \psi_p \times \nabla \theta,
$$

$$
+ \left( e + e_B \frac{B_0 p_{\parallel}}{m_e \Omega_{e0} \partial \psi_p B_0} \right) \nabla \psi_p \times \nabla \theta,
$$

$$
\psi_p = e_B \frac{c \mu}{q_i B_0} \left( \frac{\partial B_0}{\partial \zeta} - \frac{g \partial B_0}{\partial \theta} \right) + e c \left( \frac{\partial (\delta \phi^\gamma)}{\partial \zeta} - \frac{\partial (\delta \phi^\gamma)}{\partial \theta} \right).
$$
\[ \dot{\theta}_c = \frac{B_0}{D} \left( \frac{p_{\|}}{m_e} + \epsilon_B \frac{\partial (\delta \phi_{\|}^*)}{\partial p_{\|}} \right) \left( 1 - \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) + \epsilon_B \frac{\partial \mu}{q_D} \frac{\partial}{\partial \psi_p} B_0 + \epsilon_B \frac{g_{\parallel}}{D} \frac{\partial}{\partial \psi_p} B_0, \]

\[ \dot{\zeta}_c = \frac{B_0}{D} \left( \frac{p_{\|}}{m_e} + \epsilon_B \frac{\partial (\delta \phi_{\|}^*)}{\partial p_{\|}} \right) \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 - \epsilon_B \frac{q_D}{D} \frac{\partial}{\partial \psi_p} B_0 \right), \]

\[ p_{\|} = \frac{\partial q_B}{q_D} \left[ \left( 1 - \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) + \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) \frac{\partial}{\partial \psi_p} B_0 \right]. \]

The electron’s weighting equation is

\[ \frac{dW_e}{dt} = \left( W_e - 1 \right) \left( \dot{\psi}_{pe1} \kappa_{e\psi} - \dot{p}_{\|} \epsilon_{p_{\|}} \frac{p_{\|}}{m_e T_c} \right), \] (19)

where

\[ \kappa_{e\psi} = \frac{1}{N_{e0}} + \frac{1}{T_e} \frac{\partial T_e}{\partial \psi_p} \left( \frac{E_e}{T_e} - \frac{3}{2} \right) - \frac{\mu}{T_e} \frac{\partial B_0}{\partial \psi_p}, \]

\[ \dot{\psi}_{pe1} = \frac{\epsilon}{D} \left( \frac{1}{T_e} \frac{\partial}{\partial \psi_p} \frac{\partial (\delta \phi_{eB}^*)}{\partial \psi_p} \right), \]

\[ \dot{p}_{\|} = \frac{q_B}{D} \left[ \left( \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) + \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) \frac{\partial}{\partial \psi_p} B_0 \right]. \]

For field equations, the vector Laplacian operator in arbitrary (non-orthogonal) curvature coordinate \( \varphi \) is

\[ \nabla^2 \mathbf{V} = \nabla (\nabla \cdot \mathbf{V}) - \nabla \times \nabla \times \mathbf{V}, \]

\[ (\nabla^2 \mathbf{V})^m = \xi^{m\alpha} \partial_{\alpha} (g_{\alpha\beta} \xi^{\beta} \partial_{\beta} V_k) \]

\[ -g^{\alpha\beta} \partial_{\alpha} (J^{-1} \partial_{\beta} (g^{\gamma\delta} V_k)). \] (20)

Here, the Einstein summation convention is utilized, and \( J \) stands for the Jacobian. \( \xi^{\alpha \beta} = (\nabla \varphi \times \nabla \varphi ') \cdot \nabla \varphi \) is the Levi–Civita symbol with the Jacobian included, and \( g^\alpha \) and \( g_\beta \) are the contravariant and covariant metric tensor, respectively.

### 3. Formulation in dimensionless form

In this section, we provide a dimensionless form of the drift-kinetic formulation, specifically for code implementation. The normalization includes the basic units:

**Time** \( \dot{\tau} = \Omega_0 t = \left[ \frac{m_e}{(eB_0)} \right] t \)

**Length** \( l = \frac{1}{\Omega_0} \)

**Mass** \( m = m/m_p \)

**Charge** \( Z = q/e \)

and two additional units:

**Magnetic field** \( B = B/B_n \)

**Number density** \( \bar{n} = n/N_{eu} \)

where \( B_n, N_{eu}, \omega_{pea} \) and \( \Omega_{pa} \) are the magnetic field, electron density, proton plasma frequency and proton gyro frequency measured on the magnetic axis; other terms with subscript \( a \) also mean that the value is evaluated on the magnetic axis. \( m_p \) is the mass of the proton, and \( e \) represents the elemental charge. For conciseness, the hat symbol \( \hat{\cdot} \) for normalized properties is omitted in the following equations.

**Ion motion equations**:

\[ \dot{q}^i = \frac{1}{M} g^{ij} \left( \partial^i (P_{\beta} - ZA_{\beta}) \right), \]

\[ \dot{P}_{\gamma} = -\left( \frac{1}{2M} g^{ij} \partial^i (P_{\beta} - ZA_{\beta}) \right) + \frac{Z}{M} g^{ij} A_{\beta,\gamma} (P_{\beta} - ZA_{\beta}) + Z \dot{\varphi}_{\beta,\gamma} \right]. \] (22)

**Ion weight evolution**:

\[ \frac{dW_i}{dt} = -\left( 1 - W_i \right) \frac{1}{T} \left[ (\dot{q}^i)(\dot{\varphi}_{\alpha}) - (\dot{\varphi}_{\alpha})(\dot{q}^i) + (\dot{q}^i)H \nabla \ln T \right] \] (23)

**Electron motion equations**:

\[ \dot{\psi}_{pe1} = \frac{\mu}{q_D} \frac{\partial B_0}{\partial \psi_p} - \frac{g}{D} \frac{\partial}{\partial \psi_p} B_0 + \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) \frac{\partial}{\partial \psi_p} B_0 \]

\[ \dot{\psi}_{pe1} = \frac{\epsilon}{D} \left( \frac{1}{T_e} \frac{\partial}{\partial \psi_p} \frac{\partial (\delta \phi_{eB}^*)}{\partial \psi_p} \right), \]

\[ \dot{p}_{\|} = \frac{q_B}{D} \left[ \left( \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) + \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) \frac{\partial}{\partial \psi_p} B_0 \right]. \]

**D = 1 + qg + \frac{B_0 p_{\|}}{m_e \Omega_0} \left[ \left( q + \epsilon_B \frac{B_0 p_{\|}}{m_e \Omega_0} \frac{\partial}{\partial \psi_p} B_0 \right) \frac{\partial}{\partial \psi_p} B_0 \right] . \]
\[
\frac{dW_e}{dt} = (1 - W_e)
\]
\[
\left\{ \left( \frac{\Omega_{\phi} \delta A_{\phi}}{B^*_{\parallel}} + \frac{b_0}{B^*_{\parallel}} \times \nabla \delta \phi_1 \right) \cdot \nabla \ln F \right\} - \frac{1}{b^*_{\parallel}} \left[ \delta b^* \cdot (\mu \nabla B_0) + b^*_0 \cdot (e \nabla \delta \phi_1) \right] \frac{\partial \ln F}{\partial p} \right\}.
\]

Poisson equation:
\[
(1 + \sum_e \frac{\omega_{pe,0} N_e}{\Omega_{\phi,0} B^2}) \nabla^2 \delta \phi = -\frac{\omega_{pe,0} N_e}{\Omega_{\phi,0} B^2} \nabla \cdot (\delta A \times \hat{b}) - \frac{\omega_{pe,0}^2}{\Omega_{\phi,0}^2} \sum_i Z_i \delta n_i - \sum_e \delta N_e.
\]

Ampère’s law:
\[
(1 + \beta_{\omega}) \nabla \times A - \frac{\delta \beta_{\omega} \bar{F}}{c^2} \left( \frac{Z_n}{M_i} \delta A + \frac{N_e}{M_i} \delta A_{\phi} \right) + \frac{\delta \omega_{pe,0}}{c^2} \bar{b}_0 \times \nabla \delta \phi = -\frac{\delta \beta_{\omega} \bar{F}}{c^2} \delta \bar{J}_e.
\]
\[
\delta J_e = \left[ \frac{N_e}{M_i} \int \rho_e \delta F d\rho + \delta M_i \bar{J}_0 + \frac{Z_n}{M_i} \int \rho_e \delta \bar{F} d\rho \right]
\]

4. Fidelity test

The fidelity of this code was first verified through two sets of benchmarks. The first two tests were single fully-kinetic particle dynamics in a given electromagnetic field. Then, the last test was the verification of the field solver.

4.1. Marker energy conservation test

In this work, the standard Runge–Kutta (RK) method was chosen to integrate the marker particle’s trajectory with the single precision in the simulations throughout this article.

The RK algorithm has been applied to integrate the ordinary differential equations (ODE) since the early days of the numerical computation. Due to its simplicity and easy implementation, the Runge–Kutta method has been regarded as a de facto ‘standard’ way of integrating a general ODE system. By directly using the RK algorithm on equation (22), the symmetry in the toroidal direction will automatically be preserved in linear simulations. However, compared with modern symplectic algorithms and the Boris scheme, one major weak point in the RK algorithm might be the error accumulation, where the total error will accumulate and finally invalidate the whole simulation even though the error is bounded at each time step.

In order to assess the error accumulation quantitatively, a time step convergence test was conducted in toroidal geometry using a trapped marker particle, whose detailed trajectory is shown in figure 3. The convergence test (figure 1) shows that particle energy conservation quickly converges to an acceptable level when the time-step changes from 1/50 to 1/75, 1/100 and 1/200. This benchmark indicates that time step \( \Omega_i \Delta t = 1/75 \) is a good balance between accuracy and performance sufficient for simulation within 4000 ion gyro periods or roughly six bounce periods. A zoomed history on the right with time step \( \Omega_i \Delta t = 2\pi /100 \) shows a detailed stochastic-like behavior and indicates that in this case, the numerical truncation error dominates. These test results suggest that RK4 is good enough for investigating short-time single- or multi-pass wave propagation process, which is still inadequately investigated due to the lack of a proper simulation tool.

The Boris scheme has recently been proven to be a promising algorithm, which preserves phase-space volume [39] and has better numerical properties. The benchmark of [40] showed that the 1/32 gyroperiod per step is arguably enough for conserving particle energy. However, Kuley’s benchmark [21] suggested that there is no such clear convergence dependence on time step \( \Delta t \) in the particle energy conservation tests. The relative error of the marker particle’s energy provided in that benchmark is about \( 2.5 \times 10^{-5} \) for 80 gyro periods; whilst in this work, the relative error level using the RK4 method is about \( 4 \times 10^{-5} \) for the same time span. These two simulations indicate that the error level and the energy convergence behavior of RK4 are comparable to the Boris scheme. In addition, the Boris algorithm is complicated and hard to implement in general geometry and consumes more computing power [40]. At the same time, a perturbed magnetic
is set to \( \mu_0 \equiv v^2_r / (2B_0) \) is not constant for fully-kinetic marker particles, which usually perform fast cyclotron motion, intermediate drift and slow bounce motions simultaneously in an equilibrium tokamak magnetic field. The simulation duration is 4000 gyro- or about six bounce-periods; a zoomed magnetic field strength in particle space. In the figure, the magnetic moment is also shown on the uppermost panel with the red dot. The gyroaveraged momentum expression in equation (4) is found to be an exact constant for fully-kinetic particles, as shown in our simulations through figure 2. In the simulation, the magnetic moment was measured using normalized variables as \( \mu_0 \equiv (2E - m\hat{v}\cdot\hat{b}) / (2B_0) \), where \( E \) is the particle’s energy, \( \hat{v} = \hat{m} \cdot (\hat{p} - \hat{A}) \), and \( B_0 \) denotes the background magnetic field strength in particle space. In the figure, the magnetic moment is plotted with relative error \( (\mu_0 - \mu_0^{(0)})/\mu_0^{(0)} \), where \( \mu_0^{(0)} \) is the magnetic moment measured at \( t = 0 \). In our benchmark, a trapped particle was chosen with the banana orbit large enough to fully examine the fidelity of the orbit integrator for fully-kinetic particles, since a larger banana orbit will lead to a relatively larger flutter in \( \mu_0 \) according to \( \mu_0 \) expression (4). At time \( t = 0 \), particles were initialized with pitch \( \nu_p/\nu_L = 0.1 \) at \( \theta = 0 \) on the low field side, marked with LF labels in figures 2 and 3. The particles then drifted counterclockwise to the upper turning point (UT), high field side (HF), lower turning point (LT) and then back to LF in a iterative manner, as shown in figures 2 and 3.

In the equilibrium tokamak magnetic field, the particles are usually found to perform fast cyclotron motions and slow drift motions simultaneously. The slow drift motions are shown in the middle upper panel and the red lines in the top panel of figure 2, as well as the red lines of left panel of figure 3. The fast gyration is shown in the dense black curves superposed on the red drift motions in the top panel, the fast oscillations in the bottom panel of figure 2 and the blue lines of figure 3. Its amplitude, the local gyroradius, is mainly described by the slow varying curve in the middle lower panel of figure 2. In the simulation, the particle drifted to the upper turning point, where the particle obtained its maximum local gyroradius. After it turned back, the particle drifted to the high field side, where the magnetic moment oscillation amplitude was minimized due to the minimum local gyroradius. Considering the magnetic moment expression in equation (4), those three components are easily identified:

1. The magnetic moment \( \mu \) in the gyrocenter phase space is conserved;
2. The gyroaveraged momentum (red dots in figure 2) oscillates both over the banana bounce time scale and the gyration time scale, which corresponds to the term \( C_p = -\nu_p \Omega^{-1} \hat{b} \cdot \nabla \times \hat{b} \). Since the \( \nu_p \) slowly varies along the banana bounce trajectory, the red dot shows an
oscillation at drift time; the \( v_\parallel \) also performs a fast oscillation at the gyration time scale due to the non-uniformity of the background field, which explains the fast oscillation of the gyroaveraged magnetic moment. In addition, the averaged \( \mu_0 \) obtains the maximum at point HF and the minimum at LF. This is caused by the \( v_\parallel \) obtaining its maximum in the opposite direction at points HF and LF, since the magnetic curvature is approximately the same; this term will reach the maximum with the opposite sign at these locations. The analytical plot of \( (C_d^{(0)} - C_d)/(1 + C_e^{(0)} + C_e^{(0)}) \approx (C_d^{(0)} - C_d) \) based on the particle’s position and parallel velocity (figure 2) is in accord with this explanation.

3. The fast oscillation of \( \mu_0 \) is attributed to the fast variation of gyroradius vector \( \mathbf{p}_\parallel \). Since in this case \( v_\parallel \ll v_{\perp} \), the terms \( 2(v_\parallel /v_{\perp})^2 \mathbf{b} \cdot \nabla \mathbf{b} \) and \( v_\parallel \Omega \cdot \mathbf{a}_1 \): \( \mathbf{b} \) is negligible. Therefore, \( \mathbf{p}_\parallel \nabla \ln B_\parallel \) determines the amplitude of this oscillation, and the amplitude of this term is also analytically plotted in the lower middle panel of figure 2, which qualitatively match the fast oscillation behavior in the \( \mu_0 \) plot.

As a summary, the time history of the magnetic moment over several bounce times shows an overall conservation with fast oscillating motions with the amplitude slightly (\( \pm 1\% \)) modulated slowly. Thus, the first adiabatic invariant \( \mu_0 \) is still a good approximation over a time scale of several bounce periods, which is in accord with the classical adiabatic invariant picture. The slow oscillation at the drift time scale and the fast oscillation at the gyro time scale of \( \mu_0 \) is also observed, which is high order behavior and could be explained by modern gyrokinetic theory.

Next, the properties of a banana/trapped particle were checked. The four positions ‘LF’, ‘UT’, ‘HF’ and ‘LT’ shown on the left panel of figure 3 correspond to the same positions as in figure 2. With \( q = 1.0, r = 0.1R_0 \), where \( R_0 \) is the major radius, the particle’s bounce frequency and orbit/banana width were measured using normalized dimensionless values \( \omega_b/\Omega_\parallel \) and \( \Delta r/\rho \). The result is depicted with solid dots in the right panel of figure 3. One coarsely theoretical estimation of the bounce frequency of a trapped particle is \( \omega_b = \sqrt{r/(2R_0)}v_{\perp}/(qR_0) \), and half the banana width is \( \Delta r/\rho = (v_\parallel B_\parallel)/(v_{\perp} B_\parallel) \), which are shown with a solid line on the right panel of figure 3. The trends of the measured simulation data and theoretical prediction are the same; meanwhile, a gradual discrepancy is discovered in both benchmark. The reason is that expressions used for calculating banana bounce frequency and radius are only reliable for deeply-trapped particles. With the increase of the banana width or bounce period, these theoretical estimations are gradually becoming insufficient, and more effects needed to be taken into account, such as curvature drift and the variance of the particle’s radio position.

Multiple particle drift motions were also thoroughly benchmarked for \( \nabla \mathbf{B} \) drift, curvature drift, \( \mathbf{E} \times \mathbf{B} \) drift and polarization drift. Results are shown with blue oscillating lines in figure 4. The theoretical speeds of these four drift motions are \( [42] \), \( v_{\nabla B} = \pm \frac{1}{2} \mathbf{v}_\perp \mathbf{r}_\parallel (\mathbf{B} \times \nabla \mathbf{B})/|\mathbf{B}|^2 \) for \( \nabla \mathbf{B} \) drift, \( v_B = mv_\parallel q^{-2}B^{-2}(|\mathbf{R}_\perp \times \mathbf{B}|/(R_\parallel^2)) \) for curvature drift, where \( \mathbf{R}_\perp \) is the curvature of the magnetic field line, \( v_\parallel = \mathbf{E} \times \mathbf{B}/|\mathbf{B}|^2 \) for \( \mathbf{E} \times \mathbf{B} \) drift and \( v_p = \pm (\Omega B)^{-1}d\mathbf{E}/dr \) for polarization drift. The theoretical guiding-center drift trajectory is drawn with the red line in figure 4. In these four cases, the simulation result (blue line) oscillating along the theoretical guiding-center (red line), which indicates the numerical result, matches well with the theoretical result.

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**Figure 3.** The trajectory (left panel) of a trapped fully-kinetic marker particle is traced with blue dots, whereas the slowly-drifting guiding-center is rendered with red dots. The right panel shows the measured bounce frequency (upper right with dots) and banana width (lower right with dots), where the theoretical bounce frequency \( \omega_b/\Omega_\parallel = \sqrt{2/2R_0}/(qR) \) and the theoretical banana width \( \Delta r/\rho = v_\parallel B_\parallel/(v_{\perp} B_\parallel) \) are shown as solid lines. Four labels LT, UT, HF and LF are the acronyms of lower turning point (LT), upper turning point (UT), high field side (HF) and low field side (LF).
4.3. Field operator check with the analytic source term

For field equations, it is worth noting that the vector Laplacian operator (20) is rather complicated when expressed in the non-orthogonal curvature coordinate. Discretizing it in toroidal geometry with the 11-point scheme [43] makes the final finite difference expression even more complex. To ensure the fidelity, the vector Laplacian solver was thoroughly checked on all three direction. Tests were conducted in cylindrical geometry; the toroidal effect was temporarily omitted for simplicity and theoretical viability. By analytically setting the source term \( B = \nabla \times X \) and solving the vector Laplacian \( \nabla^2 \times X = B \), we could compare the result of the numerically-solved \( X \) with the analytical setup. The test source \( B \) was set to be:

\[
\begin{align*}
\nabla^2 \times (f_{\text{test}}, 0, 0), \\
\nabla^2 \times (0, f_{\text{test}}, 0), \\
\nabla^2 \times (0, 0, f_{\text{test}}),
\end{align*}
\]

in three independent tests, respectively, with \( f_{\text{test}} = \sin \left( \frac{8\pi}{a_1 - a_0} \cos(m\theta) \right) \). The corresponding 2D numerical solution together with the 1D comparison of the simulation results and the analytical curve are shown in figure 5. The 2D solution pattern matches well with the analytical source term. A detailed comparison in the 1D radio cut shows that, at \( \theta = \pi \), where the mode amplitude obtains the maximum, the numerical result (black dots) matches well with the analytical expression.
The dispersion relation of the LH wave is

\[ \omega^2 = \omega_{LH} \left( 1 + \frac{m_i k_\perp^2}{m_e k_\perp^2} \right), \]

where \( \omega_{LH} = \sqrt{\omega_{pi}^2/(1 + \omega_{ce}^2/\Omega_L^2)} \) is the lower hybrid resonance frequency.

In this benchmark, we use an artificial antenna to impose the external scalar potential in the form

\[ \phi = \Phi(r) \cos(m\theta - n\zeta) \cos(\omega t), \]

where \( \omega \) is the frequency of the antenna. If this frequency is equal to the system’s eigenfrequency, the driven mode will gain a maximal growth rate without beating between the eigenfrequency and the driving frequency. The parameter used for the benchmark is \( \omega_{pi}/\omega_{ci} = 14.5, \omega_{ce}/\omega_{ci} = 0.337, \) with the antenna set to \( k_\perp = 5.58 \text{ cm}^{-1}, k_\parallel = 0.14 \text{ cm}^{-1} \) (\( m = 4, n = 7 \)). The theoretical frequency is \( \omega = 1.46\omega_{LH} = 20.19\Omega_i \). Simulation results are shown in figure 6, the mode structure in the right panel indicates a good agreement to the theoretical structure of the antenna. The time history of \( \phi \) is shown in the left panel. Maximal growth is obtained when \( \omega = 2\Omega_i \). The discrepancy of the simulation result is due to the finite oscillation cycles in the limited simulation duration; in this case, one ion gyro period (left panel of figure 6); the maximum resolution in the frequency space is \( \Omega_i \).
As a further benchmark, electron linear Landau damping was benchmarked in the lower hybrid frequency range. The theoretical damping rate could be expressed as 
\[ \gamma = -\frac{D_i}{\partial D_R / \partial \omega}, \]
where \( D_i, D_R \) denote the imaginary and real part of the dispersion relation, respectively. Considering only the electron’s thermal effect in the parallel direction, they could be expressed as [44]
\[
D_i = 2\sqrt{\pi} \frac{\omega_p e}{k_i v_i} \exp \left\{ -\frac{\omega^2}{k_i^2 v_i^2} \right\},
\]
\[
D_R = \left\{ \frac{\omega_p^2}{\omega^2} \left[ 1 + \frac{3}{2} \frac{k_i v_i}{\omega} + \frac{15}{4} \left( \frac{k_i v_i}{\omega} \right)^4 + \frac{105}{8} \left( \frac{k_i v_i}{\omega} \right)^6 \right] \right\} \frac{k_i^2}{\omega^2} + \left[ 1 + \left( \frac{\omega_p}{\Omega_i} \right)^2 - \left( \frac{\omega_p}{\Omega_i} \right)^2 \right] \frac{k_i^2}{\omega^2}.
\]

The simulation was taken in a cylindrical geometry using an artificial antenna stimulating a lower hybrid wave. The simulation parameter was chosen as \( \omega_p v_i / \Omega_i = 0.25 \), and the LH wave number was \( k_i = 1 \) cm\(^{-1} \), \( k_\perp = 14.96 \) cm\(^{-1} \). The temperature of the electron varied from 7 keV to 15 keV, corresponding \( \chi_i = \omega_i / (k_i v_i) \) varying from 2.57 to 1.95; meanwhile, \( \chi_i = \omega_i / (k_i v_i) \) was approximately \( 10^2 \), which meant that the ion’s contribution to the dispersion relation was negligible. As shown in figure 7, the simulation result matches well with the theoretical curve. The small discrepancy of the two furthest right dots in the high temperature region (11 keV and 13 keV) was due to the difficulty of measuring the exact damping rate from a strongly-damped mode, since the signal was quickly attenuated to the numerical noise level in several oscillations.

5.2. Ion Bernstein wave

The dispersion relation of the ion Bernstein wave can be written as [44]
\[
1 - \frac{4\pi n_i m_i c^2}{B_0^2} \frac{\alpha(q_i, \lambda_i)}{\lambda_i} + \frac{4\pi n_n m_e c^2}{B_0^2} = 0,
\]
\[
\alpha(q, \lambda) = 2 \sum_{n=1}^{\infty} e^{-\lambda} I_n(\lambda) \frac{n^2}{q'^2 - n^2},
\]

6. Summary and discussion

In this article, a fully-kinetic-ion/gyrokinetic-electron simulation code, with electromagnetic capability, has been developed to study radio frequency waves inside toroidal fusion devices. This code could be an efficient tool for the investigation of nonlinear phenomena with \( \omega_i < \Omega_i \) and \( k_\parallel \ll k_\perp \). The code implements the general curvilinear description of the field and particle model, makes it more suitable for, but not limited to, simulating toroidally-confined plasma. With the artificial antenna approach, the code is verified with eigenmode simulations of LHW and IBW predicted by linear cold plasma theory.

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