Full $f$ and $\delta f$ gyrokinetic particle simulations of Alfvén waves and energetic particle physics

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Abstract

In this work, we focus on the development of the particle-in-cell scheme and its application to the studies of Alfvén waves and energetic particle (EP) physics in tokamak plasmas. The $\delta f$ and full $f$ schemes are formulated on the same footing adopting mixed variables and the pullback scheme for electromagnetic problems. The TRIMEG-GKX code (Lu et al 2021 J. Comput. Phys. 440 110384) has been upgraded using cubic spline finite elements and full $f$ and $\delta f$ schemes. The toroidal Alfvén eigenmode (TAE) driven by EPs has been simulated for the International Tokamak Physics activity (ITPA)-TAE case featured by a small electron skin depth $\sim 1.18 \times 10^{-3}$ m, which is a challenging parameter regime for electromagnetic simulations, especially for the full $f$ model. The simulation results using the $\delta f$ scheme are in good agreement with previous work. Excellent performance of the mixed variable/pullback scheme has been observed for both full $f$ and $\delta f$ schemes. Simulations with mixed full $f$ EPs and $\delta f$ electrons and thermal ions demonstrate the good features of this novel scheme in mitigating the noise level. The full $f$ scheme is a natural choice for EP physics studies, which allows for large variations of EP profiles and distributions in velocity space, providing a powerful tool for kinetic studies using realistic experimental distributions related to intermittent and transient plasma activities.

Keywords: $\delta f$, full $f$, particle-in-cell, Alfvén waves, gyrokinetic simulations, energetic particles, tokamak plasmas

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

1. Introduction

The gyrokinetic particle-in-cell simulation provides a powerful tool for the studies of tokamak plasmas [1]. In order to improve the simulation quality, especially for electromagnetic simulations, various schemes have been implemented, such as the $p_{\parallel}$ formula and the iterative scheme for solving Ampère’s law [2, 3], the noisy matrix [4] and the implicit scheme [5, 6]. Recently, the noise reduction scheme has been summarized comprehensively [3], where various numerical applications have been studied using models with single ion species for linear physics in the fully global linear gyrokinetic simulation code GYGLES, which demonstrates the excellent performance of the control variate method in noise reduction and the enhancement of simulation quality. The pullback scheme using mixed variables is implemented in the global gyrokinetic Lagrangian Particle-In-Cell code ORB5 using the $\delta f$ scheme for the study of energetic particle (EP)-driven toroidal Alfvén eigenmodes (TAEs) [7], demonstrating its capability in the
magnetohydrodynamics (MHD) limit. In table 1, we briefly summarize the discretization schemes (full $f$, control variate or $\delta f$) and the physics models (‘symplectic ($v^i_f$)’ formula, ‘Hamiltonian ($p^i_f$)’ formula or mixed variables with pullback scheme) of some previous works.

| Full $f$ | Control variate | Traditional $\delta f$ |
|----------|-----------------|------------------------|
| $v^i_f$  | [5]             | [6]                    |
| $p^i_f$  | [3]             | [2, 13]                |
| MV w/ PB | [14], this work | [3]                    |
|          | [7], this work  |                        |

While previous work has adopted the $\delta f$ scheme [8], more effort has recently been spent on the full $f$ approach [5, 9, 10]. The full $f$ method does not rely on the separation of the equilibrium and the perturbation, and thus provides a natural way to handle substantial changes in the profiles in the course of a simulation [9]. However, the full $f$ simulations are more expensive and require stricter noise reduction to make simulation studies of tokamak plasma feasible. In particular, the full $f$ model in the MHD limit is still a challenge. In this work, we focus on applications of the noise reduction schemes to the full $f$ and $\delta f$ simulations of Alfvén waves and EP physics. By following the formulation from previous work [3], we implement the pullback scheme using mixed variables in the TRIangular MEsh-based Gyrokinetic (TRIMEG)-Generalized Kinetics eXtended (GKX) code [5, 11]. The TRIMEG code was originally developed using unstructured triangular meshes for the whole plasma volume simulations of the electrostatic ion temperature gradient mode [11] and later was extended to study Alfvén waves and EP physics using the full $f$ electromagnetic model in the testbed TRIMEG-GKX [5]. In the following, the full $f$ and $\delta f$ models are formulated and implemented on the same footing. Although the full $f$ scheme can be applied to all species in the TRIMEG-GKX code, a mixed scheme of full $f$ EPs and $\delta f$ thermal ions and electrons are proposed and applied in the present work. A common phenomenon in experiments is that the EP distribution in velocity space changes substantially, while the background is well described by the Maxwell distribution. With this novel mixed full $f$ and $\delta f$ scheme, the large EP profile variation and the arbitrary distribution in velocity space can be treated in a natural way, and the computational performance is improved when compared with using a full $f$ scheme for all species. The mixed scheme for different species has been implemented in the TRIMEG-GKX code benefiting from its object-oriented programming and modular design of different species.

The paper is organized as follows. In section 2, the equations for the discretization of full $f$ are derived with mixed variables and the pullback scheme adopted. In section 3, the normalized equations are given and the numerical methods are introduced with a rigorous filter derived. In section 4, the $\delta f$ and full $f$ simulations of EP driven toroidicity induced Alfvén eigenmode are performed, demonstrating the features of the schemes and key issues for the accurate description of the EPs in tokamak plasmas.

### 2. Physics models

#### 2.1. Discretization of distribution function

Following the formulation in the previous $\delta f$ work [3, 12], $N$ markers are used with a given distribution,

$$g(z, t) \approx \frac{1}{J_z} \sum_{p=1}^{N} \delta[z_p - z(t)],$$

where $z$ is the phase space coordinate, $\delta$ is the Dirac delta function, $J_z$ is the corresponding Jacobian and $z = (R,v_{\parallel},\mu \equiv v_{\perp}^2/(2B))$ is adopted in this work, $R$ is the real space coordinate. For the full $f$ model, the total distribution of particles is represented by the markers,

$$f(z, t) = C_{gR} P_{tot}(z, t) g(z, t) \approx C_{gR} \sum_{p=1}^{N} p_{p,tot}(t) \frac{\delta[z_p - z(t)]}{J_z},$$

where the constant $C_{gR} \equiv N_f/N_g$, $N_f/N_g$ is the number of particles/markers, and $g$ and $f$ indicate the markers and physical particles respectively. For each marker,

$$P_{p,tot}(t) = \frac{1}{C_{gR}} \frac{f(z_p, t)}{g(z_p, t)} = \text{const},$$

for collisionless plasmas since

$$\frac{d g(z, t)}{dt} = 0, \quad \frac{d f(z, t)}{dt} = 0.$$  

The expression of $P_{tot}(z, t)$ (and consequently, $p_{p,tot}$) can be readily obtained

$$P_{tot}(z, t) = \frac{1}{C_{gR}} \frac{f(z, t)}{g(z, t)} = \frac{n_f}{n_g} \frac{\langle f \rangle_v f_v}{g_v},$$

where $n_f$ is the density profile and $f_v$ is the distribution in velocity space, namely, the particle distribution function $f = n_f(R) f_v(v_{\parallel},\mu) \langle ... \rangle_v$ indicates the volume average. There are different choices of the marker distribution functions as discussed previously [3, 12]. In this work, the markers are randomly distributed in the toroidal direction and in the $(R,Z)$ plane, but the distribution in velocity space is identical to that of the physical particles, which leads to

$$P_{tot}(z, t) = \frac{n_f}{\langle n_f \rangle_v} \frac{R}{R_0}.$$  

The density and parallel current are readily obtained from the markers,

$$\{ n_j \}^{d, j, t, l, o} \equiv \int dV \{ n_j \} (R) N_{io}(r) N_{io}(\theta) N_{io}(\phi) \quad \text{(7)}$$

$$= C_{gR} \sum p_{p,tot} \{ 1, v_{\parallel} \} N_v (r_p) N_{io} (\theta_p) N_{io} (\phi_p),$$

### Table 1. Various works using full $f$ and $\delta f$ schemes. MV and PB indicate mixed variable and pullback schemes, respectively.

| Full $f$ | Control variate | Traditional $\delta f$ |
|----------|-----------------|------------------------|
| $v^i_f$  | [5]             | [6]                    |
| $p^i_f$  | [3]             | [2, 13]                |
| MV w/ PB | [14], this work | [3]                    |
|          | [7], this work  |                        |
where \( d\vec{V} = r \, d\theta \, d\phi \) for an ad-hoc equilibrium, \( N_i, N_e \) and \( N_{\text{ion}} \) are basis functions and \( i_r, i_\theta \) and \( i_\phi \) indicate the indices in \( r, \theta \) and \( \phi \) directions.

For the \( \delta f \) model, the total distribution function is decomposed into the background and perturbed parts, \( f(z,t) = f_0(z,t) + \delta f(z,t) \). The background part can be chosen as the time-independent one, i.e. \( f_0(z,t) = \bar{f}_0(z) \), and one typical choice is the Maxwellian distribution. The background and perturbed distribution functions are represented by the markers as follows,

\[
f_0(z,t) = P(z,t)g(z,t) \approx \sum_{p=1}^{N} p_p(t) \frac{\delta[z_p - \bar{z}_p(t)]}{J_z},
\]

and thus

\[
d \frac{df_0}{dt} = \delta \vec{R} \cdot \left[ \bar{\kappa}_n + \left( \frac{mv^2}{2T} + \frac{m_B B}{T} - \frac{3}{2} \right) \bar{\kappa}_T - \frac{m_B B}{T} \bar{\kappa}_B \right] - \delta \dot{\vec{v}} || \frac{mv^2}{T}, \tag{19}\]

where \( \bar{\kappa}_{n,T,B} \equiv \nabla \ln \{n,T,B\} \). Note that for the Maxwell distribution, without considering the neoclassical physics, the following approximation has been made in the traditional \( \delta f \) scheme,

\[
\frac{df_0}{dt} f_M \approx 0. \tag{20}\]

### 2.2. Physics equations using mixed variables

The mixed variable is defined as follows. The parallel component of the scalar potential is decomposed into the symplectic part and the Hamiltonian part,

\[
\delta A_{||} = \delta A_{||}^b + \delta A_{||}^h, \tag{21}\]

where the symplectic part is chosen to satisfy

\[
\partial_t \delta A_{||}^b + \dot{\theta} \delta \phi = 0. \tag{22}\]

The parallel velocity coordinate of the guiding center is defined as

\[
u = v_{||} + \langle \frac{q_s}{m_s} (\delta A_{||}^h) \rangle, \tag{23}\]

where \( q_s \) and \( m_s \) are the charge and mass of species \( s \), respectively, the subscript \( s \) represents the different particle species, and \( \langle \ldots \rangle \) indicates the gyro average.

The guiding center’s equations of motion are consistent with previous work [3, 7, 12],

\[
\frac{d\vec{R}_0}{dt} = v_{||} \vec{b}^* + \frac{m_B}{q_B} \vec{b} \times \nabla B,
\]

\[
\frac{d\vec{R}}{dt} = \vec{v}_{||} + \frac{m_B}{q_B} \nabla \times \left( \frac{\vec{b}^* \times \vec{B}}{B_{||}} \right), \tag{24}\]

where \( \vec{b} = B / B_{||}, \quad \vec{b}^* = B + (m_s / q_s) v_{||} \vec{B} \times \vec{b} \), \( \vec{b}^* = B^* / B_{||}, \quad v_{||} \) is adopted on the right-hand side, and thus, the term \(- (q_s / m_s) \langle \delta A_{||}^h \rangle \vec{b}^* \) in \( d\vec{R} / dt \) is taken into account in \( d\vec{R}_0 / dt \).

The quasi-neutrality equation is

\[
- \nabla \cdot \left( \sum_s \frac{q_s n_{s,\phi}}{B_0 \omega_{s,\phi}} \right) \approx \sum_s q_s \delta n_{s,\phi}, \tag{24}\]
where $\delta n_s$ is calculated using $\delta f_s(R, v_{\parallel}, \mu)$ (indicated as $\delta f_{s,u}$), namely, $\delta n_s(x) = \int d^2 \delta f_s, \delta(R + \rho - x)$, $\omega_{cs}$ is the cyclotron frequency of species ‘s’ and in this work, we ignore the perturbed electron polarization density on the left-hand side. When the $\delta f$ scheme is adopted, $\delta f_{s,u}$ is obtained from $\delta f_{s,v}$ as follows with the linear approximation of the pullback scheme,

$$\delta f_{s,v} = \delta f_{s,u} + \frac{q_s}{m_s} \frac{\langle \partial A^b \rangle}{\partial v_{\parallel}} f_{0,u} \frac{\partial f_{0,v}}{\partial v_{\parallel}} \frac{\delta(A^b)}{\delta f_{0,u}} \delta f_{s,u}$$

$$- \frac{m_s v_{\parallel}}{T_s} \frac{q_s}{m_s} \langle \delta A^b \rangle f_{0,u}$$

(25)

which is obtained from the more general form,

$$f_{s,v}(v_{\parallel}) = f_{s,u}(v_{\parallel}) + \frac{q_s}{m_s} \langle \delta A^b \rangle$$

(26)

Ampère’s law in $v_{\parallel}$ space is given by

$$- \nabla^2 \delta A^b_{||} = \mu_0 \delta j_{||,v}$$

(27)

where $\delta j_{||,v}(x) = \sum_s \int d^2 \delta f_s, \delta(R + \rho - x)v_{\parallel}$.

For the $\delta f$ model, using the mixed variables and assuming Maxwell distribution, we have

$$\delta j_{||,v} \equiv \sum_s q_s \int d^2 \delta f_{s,v}(v_{\parallel}) \delta(R + \rho - x)v_{\parallel}$$

$$= \sum_s q_s \int d^2 \left[ \delta f_{s,u}(v_{\parallel}) - \frac{v_{\parallel} q_s \langle \delta A^b \rangle}{T_s} f_{0,u} \right] \delta(R + \rho - x)v_{\parallel}.$$  

(28)

Then we can write Ampère’s law as

$$- \nabla^2 \delta A^b_{||} + \sum_s \mu_0 q_s^2 \frac{1}{T_s} \int d^2 v_{\parallel} f_{0,u} \langle \delta A^b \rangle \delta(R + \rho - x)$$

$$= \nabla^2 \delta A^b_{||} + \mu_0 \sum_s q_s \int d^2 v_{\parallel} \delta f_{s,u}(v_{\parallel}) \delta(R + \rho - x).$$

(29)

The integral on the left-hand side can be obtained analytically, yielding

$$- \nabla^2 \delta A^b_{||} + \sum_s \mu_0 \sum_s \frac{1}{d_s^2} \langle \delta A^b \rangle$$

$$= \nabla^2 \delta A^b_{||} + \mu_0 \sum_s q_s \int d^2 v_{\parallel} \delta f_{s,u}(v_{\parallel}) \delta(R + \rho - x),$$

(30)

$$\langle \delta A^b \rangle \equiv \frac{2}{n_{0}v_{\parallel}} \int d^2 v_{\parallel} f_{0,u} \langle \delta A^b \rangle \delta(R + \rho - x),$$

(31)

where $v_{\parallel} = \sqrt{2T_{\parallel}/m_s}$, $d_s$ is the skin depth of species ‘s’ defined as $d_s^2 = c^2 / \omega_{cs}^2 = m_s / (\mu_0 q_s^2 n_{0s})$.

For the full $f$ model, the perturbed current is represented by full $f$,

$$\delta j_{||,v} = \sum_s q_s \int d^3 v_{||} f_{s,v}$$

$$= \sum_s q_s \int d^3 v_{||} \left[ u_{||} - \frac{q_s}{m_s} \langle \delta A^b \rangle \right] f_{s,u} \delta(R + \rho - x).$$

(32)

Ampère’s law yields

$$- \nabla^2 \delta A^b_{||} + \sum_s \mu_0 q_s^2 \frac{1}{T_s} \int d^2 v_{\parallel} f_{0,u} \langle \delta A^b \rangle \delta(R + \rho - x)$$

$$= \nabla^2 \delta A^b_{||} + \mu_0 \sum_s q_s \int d^2 v_{\parallel} \delta f_{s,u}(v_{\parallel}) \delta(R + \rho - x).$$

(33)

The corresponding analytical limit gives the similar form of the equation (30) except for the replacement of $\delta f_{s,u}(u_{||})$ with $f_{s,v}(v_{||})$ and the definition of $\langle \delta A^b \rangle$,

$$- \nabla^2 \delta A^b_{||} + \sum_s \mu_0 \sum_s \frac{1}{d_s^2} \langle \delta A^b \rangle$$

$$= \nabla^2 \delta A^b_{||} + \mu_0 \sum_s q_s \int d^2 v_{\parallel} \delta f_{s,u}(v_{\parallel}) \delta(R + \rho - x).$$

(34)

Using the iterative scheme, the asymptotic solution is expressed as follows,

$$\delta A^b_{||} = \sum_{p=0}^{\infty} \delta A^b_{||,p},$$

(36)

where $\epsilon = |\delta A^b_{||,p+1}/\delta A^b_{||,p}| \ll 1$. Ampère’s law is solved order by order,

$$\left( \nabla^2 - \sum_s \frac{1}{d_s^2} \right) \delta A^b_{||,0} = - \nabla^2 \delta A^b_{||} - \mu_0 \delta j_{||,v},$$

(37)

$$\left( \nabla^2 - \sum_s \frac{1}{d_s^2} \right) \delta A^b_{||,p} = - \sum_s \frac{1}{d_s^2} \delta A^b_{||,p-1} + \sum_s \frac{1}{d_s^2} \langle \delta A^b \rangle_{||,p-1},$$

(38)

$$\langle \delta A^b \rangle_{||,p-1} \equiv \frac{2}{n_{0}v_{\parallel}} \int d^2 v_{\parallel} f_{0,u} \langle \delta A^b \rangle \delta(R + \rho - x),$$

(39)

$$\langle \delta A^b \rangle_{||,p-1} \equiv \frac{1}{n_{0}} \int d^2 v_{\parallel} \delta f_{s,u}(v_{\parallel}) \delta(R + \rho - x),$$

(40)

where $p = 1, 2, 3, \ldots$ and since $2/(n_{0}v_{\parallel}) \int d^3 v_{||} f_{0} = 1$ and $(1/n_{0}) \int d^3 v_{||} f_{0} = 1$ for the Maxwell distribution in the analytical limit, good convergence of the iterative solver is expected.
2.3. Pullback scheme for mitigating the cancellation problem

A more detailed description of the pullback scheme can be found in the previous work [7]. As a brief review, the equations for the \( \delta f \) are listed as follows:

\[
\delta A^s_{\|,\text{new}} = \delta A^s_{\|,\text{old}} + \delta A^h_{\|,\text{old}}, \tag{41}
\]

\[
u_{\text{new}} = \nu_{\text{old}} - \frac{q_s}{m_s} \left( \delta A^h_{\|,\text{old}} \right), \tag{42}
\]

\[
\delta f_{\text{new}} = \delta f_{\text{old}} + \frac{q_s}{m_s} \left( \frac{\delta A^h_{\|,\text{old}}}{v_0} \text{Maxwellian} \right) \rightarrow \delta f_{\text{old}} - \frac{2v_0^2}{v^2} \frac{q_s}{m_s} \left( \delta A^h_{\|,\text{old}} \right), \tag{43}
\]

where equation (43) is the linearized equation for \( \delta f \) pullback, which is from the general equation of the transformation for the distribution function

\[
f_{\text{old}}(u_{\|,\text{old}}) = f_{\text{new}}(u_{\|,\text{new}} = u_{\|,\text{old}} - \frac{q_s}{m_s} \left( \delta A^h_{\|,\text{old}} \right)). \tag{44}
\]

For the full \( f \) scheme, only equations (41) and (42) are needed.

2.4. Kinetic equilibrium in constant of motion coordinates

While the local Maxwellian distribution is widely used in gyrokinetic simulations, its application in the full \( f \) scheme brings in marker relaxation and a consequent lower growth rate for the EP-driven TAE problem. The shifted toroidal canonical momentum has been adopted in the \( \delta f \) particle code ORB5 for the turbulence studies [15]. In this work, we apply this scheme also to the full \( f \) model. To construct the marker distribution in the constant of motion space, we take the shifted toroidal canonical momentum

\[
\psi_{\text{can}} = \psi - \frac{mF}{q_sB} - \text{sign}(v_{\|}) \sqrt{2(E - mB_0) - \frac{mF}{q_sB} (E - mB_0)}, \tag{45}
\]

where \( F \) is the poloidal current function consistent with the magnetic equilibrium field \( B = F \nabla \phi + \nabla \psi \times \nabla \phi, \psi \) is the poloidal magnetic flux function, the last term gives the size of the finite orbit width, and \( H \) is the Heaviside function. For EPs, among the right-hand side terms in equation (45), the second term can be of the same magnitude as the first term and it is a natural choice to bring in the shift (the last term) so that \( \psi_{\text{can}} \) is close to the orbit center. The distribution is specified as

\[
f_{\text{can}}(\psi_{\text{can}}, E, \mu) = n(\psi_{\text{can}}) \exp \left( - \frac{mE}{T(\psi_{\text{can}})} \right), \tag{46}
\]

where the variation along \( \mu \) direction is eliminated for the sake of simplicity. Correspondingly, when loading markers, \( n(r_{\text{can}}) \) replaces \( m(r) \) in equation (5), where \( r_{\text{can}} \equiv (\psi_{\text{can}} - \psi_{\text{axis}})/(\psi_{\text{edge}} - \psi_{\text{axis}}) \), \( r_{\text{can}} \geq 0 \) for \( (\psi_{\text{can}} - \psi_{\text{axis}})/(\psi_{\text{edge}} - \psi_{\text{axis}}) \geq 0 \) and \( r_{\text{can}} < 0 \) for \( (\psi_{\text{can}} - \psi_{\text{axis}})/(\psi_{\text{edge}} - \psi_{\text{axis}}) < 0 \).

3. Numerical schemes

3.1. Normalized equations

The normalization of the variables in the TRIMEG-GKX code is introduced in this section. The length unit is \( R_N = 1 \) m. The particle mass is normalized to \( m_N \) and \( m_N = m_e \). The velocity unit is

\[
\nu_N \equiv \sqrt{2T_N/m_N},
\]

where \( T_N \) and \( m_N \) are the temperature and mass units for normalization. The charge unit is the elementary charge \( e \). Temperature is normalized to \( T_N = m_N \nu_N^2/2 \), namely,

\[
T_s = T_N \frac{\nu_N^2}{2}.
\]

Note another way (not adopted in this work) is to normalize \( T \) to \( 2T_N \), namely, \( T_s = T_N \nu_N^2 = 2T_sT_N \). In addition, \( \mu \) is normalized to \( \nu_N^2/B_{\text{ref}} \),

\[
\mu \equiv \frac{\nu_s^2}{2B} = \frac{\nu_N^2}{B_{\text{ref}}},
\]

where \( B_{\text{ref}} = 1 \) T.

The Maxwell distribution is

\[
f_M = \frac{1}{v^3\pi^{3/2}} \frac{e^{-\frac{v^2 + \nu^2}{T}}}{v^2} = \frac{1}{v^3\pi^{3/2}} \exp \left( - \frac{\nu^2}{T} - 2 \frac{\nu}{T} \frac{m\nu_B}{B_{\text{ref}}} \right), \tag{48}
\]

and correspondingly,

\[
\frac{d}{dt} \ln f_M = \frac{d\bar{R}}{dt} \cdot \left[ \bar{\kappa}_N + \frac{(m\nu_B)^2}{T} + 2\frac{m\nu_B}{T} - \frac{3}{2} \right] \frac{\nu^2}{T} - 2 \frac{\nu}{T} \frac{m\nu_B}{B_{\text{ref}}} \bar{\kappa}_N \tag{49}
\]

The markers are loaded with the same distribution of physical particles in velocity space but uniformly in the poloidal plane and in the toroidal direction. In \( v_{\|} \) direction, a random number generator is used to produce numbers with normal distribution \( f(x) = 1/(\sigma\sqrt{2\pi}) \exp\left( -\frac{(x - x_0)^2}{2\sigma^2} \right) \), where \( x_0 \) and \( \sigma \) are chosen as \( x_0 = 0 \) and \( \sqrt{\sigma^2/2m} \) respectively (note that the 1/2 factor in \( \sqrt{\sigma^2/2m} \) and the 1/2 in the exponent of the normal distribution eventually cancel). In \( \mu \) direction, the uniformly distributed random numbers \( x \) are generated and shifted according to \( \mu = -\ln(x)TB_{\text{ref}}/(2mB) \).

The normalized guiding center’s equations of motion are

\[
\frac{d\bar{R}}{dt} = \bar{v}_N \bar{b}^* + \frac{m_N}{q_s} \frac{B_{\text{ref}}}{B^2} B^2 \cdot \bar{\mu} \times \nabla B, \tag{50}
\]

\[
\frac{d\bar{\mu}}{dt} = -\frac{\bar{\mu}}{B_{\text{ref}}} \frac{B_{\text{ref}}}{B} \times \nabla \left( \bar{\sigma} - \bar{v}_N \bar{A}_{\|} \right), \tag{51}
\]

\[
\frac{d\bar{\sigma}}{dt} = \rho_{\text{ref}} B_{\text{ref}}^2 \times \nabla \left( \delta \phi - \bar{v}_N \bar{A}_{\|} \right), \tag{52}
\]
\[
\begin{align*}
\frac{d\delta \tilde{u}_i}{dr} &= -\frac{\tilde{q}_i}{m_s} \left( \mathbf{b} \cdot \nabla (\delta \tilde{\phi} - \tilde{v}_i \delta A^h_i) + \partial_i \delta A^h_i \right) \\
- \frac{\rho N_c}{B} \nabla \times \nabla \tilde{B} \cdot \nabla (\delta A^h_i),
\end{align*}
\]  
(53)

where \( \nabla = R_N \nabla_r, \delta \phi \) and \( \delta A_i \) are normalized to \( m_N v_N^2 / e \) and \( m_N v_N / e \) respectively.

The normalized quasi-neutrality equation is,
\[
\nabla \cdot \sum n_0 m_s \left( B_{ref} / B \right)^2 \nabla \delta \phi = C_p \sum (-q_i) \delta n_i,
\]  
(54)

where \( C_p = 1 / \rho_c^2 \).

For Ampère’s law, the original normalized equation \( \nabla \vec{E} = C_A \delta J_i, \) is solved using mixed variables, and the iterative scheme (corresponding to equations (37)–(39)),
\[
\left( \nabla^2 - \sum_i \frac{\tilde{q}_i^2}{m_s} C_A \right) \delta A_{i,0}^h = -\nabla^2 \delta A_{i,0}^h - C_A \delta J_i,
\]  
(55)

\[
\left( \nabla^2 - \sum_i \frac{\tilde{q}_i^2}{m_s} C_A \right) \delta A_{i,p}^h = -\sum_i \frac{\tilde{q}_i^2}{m_s} C_A \delta A_{i,p-1}^h + \tilde{G} \delta A_{i,p-1}^h,
\]  
(56)

\[
\tilde{G} \delta A_{i,p-1}^h = C_A \frac{N_0 q_i^2}{T_i} \sum_{p=1}^N \int d\phi w_p (\tilde{R}_p) (\delta A_{i,p-1}^h) \text{ for } \delta f,
\]  
(57)

\[
\tilde{G} \delta A_{i,p-1}^h = C_A \frac{N_0 q_i^2}{m_s} \sum_{p=1}^N \int d\phi \rho_{p,tot} (\tilde{R}_p) (\delta A_{i,p-1}^h) \text{ for full } f,
\]  
(58)

where \( \tilde{R}_p = R_p + \rho_p - x, \rho_p = m_N v_{L-p} / (q_i B) \).

The normalized equations for the pullback treatment are as follows,
\[
\delta A_{i,new}^h = \delta A_{i,old}^h + \delta A_{i,old}^h,
\]  
(59)

\[
u_{new} = \nu_{old} - \frac{\tilde{q}_i}{m_s} \left( \delta A_{i,old}^h \right),
\]  
(60)

\[
\delta f_{new} = \delta f_{old} + \frac{\tilde{q}_i}{m_s} \left( \delta A_{i,old}^h \right) \frac{\partial f_{old}}{\partial \tilde{v}},
\]  
(61)

\[
\text{Maxwellian } \frac{f_{old}}{f_{old}} \rightarrow \delta f_{old} = \frac{2}{T_x} \tilde{v} \left( \delta A_{i,old}^h \right) f_{old},
\]  
(62)

where a factor 2 is from the normalization of \( T \) to \( T_N = m_N v_N^2 / 2 \), and equation (61) is the linearized pullback scheme for the \( \delta f \) model implemented in our work. Studies using the nonlinear pullback scheme are out of the scope of this work and will be addressed in the future.

### 3.2. Finite element method

A three-dimensional solver is developed in this work using the finite element method adopted in the radial, poloidal and toroidal directions. Periodic boundary conditions are adopted in the poloidal and toroidal directions. In the radial direction, the Dirichlet boundary condition with zero value of the function is implemented. The grid size is \( (N_r, N_\theta, N_p) \) and \( (N_{r,FEM}, N_{\theta,FEM}, N_{p,FEM}) \) basis functions are adopted to represent functions in the simulation domain, where \( N_{r,FEM} = N_r + \Delta N \), \( N_{\theta,FEM} = N_\theta \), \( N_{p,FEM} = N_p \), which are consistent with the boundary conditions, where \( \Delta N = 2 \) since cubic splines are adopted. In poloidal and toroidal directions, the cubic finite element basis functions \( N(x) \) are as follows
\[
N_{cubic}(x) = \begin{cases} 4/3 + 2x + x^2 + x^3/6, & \text{if } x \in [-2, -1) \\ 2/3 - x^2 + x^3/2, & \text{if } x \in [-1, 0) \\ 2/3 - x^2 + x^3/2, & \text{if } x \in [0, 1) \\ 4/3 - 2x + x^2 - x^3/6, & \text{if } x \in [1, 2) \end{cases}
\]  
(63)

Along \( \theta \) and \( \phi \), the \( i \)th basis function is \( N_i = N_{cubic}(x + 1 - i) \). In the radial direction, \( N_i \) is the same as those in poloidal/toroidal directions as \( i \geq 4 \) or \( i \leq N_{r,FEM} - 3 \). The first basis function is
\[
N_{cubic}(x) = \begin{cases} 0, & \text{if } x \in [-2, 1) \\ -x^3 + 6x^2 - 12x + 8, & \text{if } x \in [1, 2) \end{cases}
\]  
(64)

The second basis function is
\[
N_{cubic}(x) = \begin{cases} 0, & \text{if } x \in [-2, 0) \\ 7x^3/6 - 3x^2 + 2x, & \text{if } x \in [0, 1) \\ 4/3 - 2x + x^2 - x^3/6, & \text{if } x \in [1, 2) \end{cases}
\]  
(65)

The third basis function is
\[
N_{cubic}(x) = \begin{cases} 0, & \text{if } x \in [-2, -1) \\ -x^3/3 - x^2 + 2x, & \text{if } x \in [-1, 1) \\ x^3/2 - x^2 + 2x, & \text{if } x \in [0, 1) \\ -x^3/6 + x^2 - 2x + 4/3, & \text{if } x \in [1, 2) \end{cases}
\]  
(66)

The last three basis functions are symmetric mapping of the first three basis functions with respect to the middle point of the simulation domain. All radial basis functions are constructed according to \( N_i = N_{cubic}(x + 1 - i) \), where \( i \in [1, N_{r,FEM}] \).

### 3.3. Weak form of field equations

For a partial differential equation,
\[
L(r, \theta, \phi) y(r, \theta, \phi) = b(r, \theta, \phi),
\]  
(67)

where \( L \) is a linear differential operator, the weak form can be written as
\[ \int \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi S(r, \theta, \phi) N_i N_j N_k L(r, \theta, \phi) y(r, \theta, \phi) \]
\[ = \int \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi S(r, \theta, \phi) N_i N_j N_k b(r, \theta, \phi), \quad (68) \]

where \( S(r, \theta, \phi) \) is a function and \( S = 1 \) is chosen in this work. The weak form of the quasi-neutrality equation, Ampère’s law, the iterative equation, and Ohm’s law are
\[ \dot{M}_{p,L,i,j,k,k'} \cdot \delta \theta_{i,j,k'} = C_p \delta N^{j,k}, \quad (69) \]
\[ \ddot{M}_{A,L,i,j,k,k'} \cdot \delta A_{i,j,k'} = \ddot{M}_{A,R,i,j,k,k'} \cdot \delta A_{i,j,k'} + C_A \delta f^{i,k}, \quad (70) \]
\[ \ddot{M}_{B,L,i,j,k,k'} \cdot \delta A_{i,j,k'} = \ddot{M}_{B,R,i,j,k,k'} \cdot \delta A_{i,j,k'} + \dot{M}_{Ohm,L,i,j,k,k'} \cdot \delta \phi_{i,j,k'} + \ddot{M}_{Ohm,R,i,j,k,k'} \cdot \delta \phi_{i,j,k'}. \quad (72) \]

Equations (69)–(72) are solved numerically which provide the perturbed fields for the guiding center’s equations of motion. The Runge–Kutta fourth-order integration is adopted. The matrices and the terms on the right-hand side are as follows,
\[ \ddot{M}_{p,L,i',j',k,k'} = -\sum_i \eta_i \delta_{ij} \frac{B_{ix}^2}{B_{ix}^2} \int \mathrm{d}r \mathrm{d}\theta \mathrm{d}\phi \nabla_i N_{ijk} \nabla_{i'} N_{ijk'}, \quad (73) \]
\[ \ddot{M}_{A,L,i,j,k,k'} = -\sum_i \eta_i \delta_{ij} \hat{N}_{ijk} \hat{N}_{ijk'}, \quad (74) \]
\[ \ddot{M}_{B,L,i,j,k,k'} = \frac{1}{\delta S} \nabla_i \cdot \left( \sum_j \frac{\delta^2}{m_s} C_s \hat{N}_{ijk} \hat{N}_{ijk'} \right), \quad (75) \]
\[ \ddot{M}_{Ohm,L,i,j,k,k'} = \ddot{M}_{Ohm,R,i,j,k,k'} \cdot \delta \phi_{i,j,k'} + \ddot{M}_{Ohm,R,i,j,k,k'} \cdot \delta \phi_{i,j,k'}. \quad (76) \]

3.4. Fourier filter

3.4.1. Filter for moments (particle-in-Fourier). For moment variables (\( \delta n \) and \( \delta \|_n \)), the Fourier components are calculated from markers first as follows,
\[ \{ \delta n_{m,n}, \delta \|_{1,n,m} \} = C_p k \{ \{ 1, V \} \} \mathrm{e}^{-i\theta - i\phi}, \quad (73) \]

where \( m \) and \( n \) are the toroidal and poloidal mode numbers of the filter and \( C_{p_k} \) is the conversion factor from marker to grid variables. The corresponding spline coefficients are readily obtained,
\[ \{ \delta n, \delta \| \}_{1,n,m} = \{ \delta n, \delta \| \}_{1,n,m} T_{n,m} T_{n,m}, \quad (74) \]

where
\[ T_{n,m} = \int_{\theta_{mn}}^{\phi_{mn}} \mathrm{d}\phi \mathrm{e}^{i\phi} N_i(\phi) = \Delta \phi \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}x \mathrm{e}^{i\phi x}, \quad (75) \]

\[ T_{m,n} = \int_{\theta_{mn}}^{\phi_{mn}} \mathrm{d}\phi \mathrm{e}^{i\phi} N_i(\phi) = \Delta \phi \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}x \mathrm{e}^{i\phi x}, \quad (76) \]

where \( n_{eff} = n \Delta \phi, m_{eff} = n \Delta \theta, \Delta \phi \) and \( \Delta \theta \) are the grid size in toroidal and poloidal directions. The analytic results are used for the construction,
\[ \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}x N_i(\phi) \mathrm{e}^{-i\phi x} = \frac{2}{\pi} \mathrm{i} (\cos(2\phi) - \cos(\phi)). \quad (77) \]

3.4.2. Filter for fields. For field variables such as \( \delta \phi \) and \( \delta A_{i,j} \), the physical values are expressed using the spline coefficients, and the Fourier filter is applied to the physical values. The spline coefficients of a variable \( \delta \phi \) are filtered in \( \phi \) and \( \theta \) directions as follows,
\[ \delta \phi_{x_{\text{wid}}} = 2 \text{Re} \{ M_{x_{\text{wid}}} \delta \phi_{x_{\text{wid}}}/\theta_{\text{wid}} \}, \quad (78) \]
\[ \delta \phi_{y_{\text{wid}}} = 2 \text{Re} \{ M_{y_{\text{wid}}} \delta \phi_{y_{\text{wid}}}/\theta_{\text{wid}} \}, \quad (79) \]

where \( \theta_{\text{wid}} \) and \( \phi_{\text{wid}} \) are the widths of the simulation domain in the toroidal and poloidal directions, respectively, \( \phi_{\text{wid}} = 2\pi \) for full torus simulations, \( \theta_{\text{wid}} = 2\pi \), \( M_{i,j} \) is the mass matrix, and the filter is applied at each radial location with the sub-script \( i \) omitted.

3.5. Parallelization and the application of shared memory MPI to field implementation

When markers are distributed among all processes and pushed forward in each process (particle decomposition), each process has access to the whole set of field variables (without domain decomposition). The field variables are stored in the shared memory at each computing node supported by the message passing interface (MPI)-3 standard. This is motivated by the full f simulations, for which the marker number is large and the cost of markers is the biggest part. In addition, the time step size \((\Delta t \sim T_{\text{TAE}}/20)\) allowed is significantly larger using
mixed variables and the pullback scheme than the traditional pure $p_{\parallel}$ form, and a large portion of markers might migrate along magnetic field lines, which leads to significant computational cost if domain decomposition is otherwise adopted. However, the field equations are solved using PETSc, and the field solver is fully parallelized. While the atomic operations, such as ‘MPI_ACCUMULATE’ on the shared memory are supported by MPI-3, the communication cost is still inefficient for marker-field projection and thus, the projection operation in TRIMEG-GKX is performed by binning the markers according to which part of the memory they are to be written to, as shown in figure 1. Since the computational cost is mainly in the calculation of the basis function values at the marker location, the additional cost in determining whether it is the turn to put data in memory is negligible.

4. Simulation setup and results

The toroidicity induced Alfvén eigenmode driven by EPs are simulated using the parameters defined by the International Tokamak Physics Activity (ITPA) group [8]. The major radius $R_0 = 10$ m, minor radius $a = 1$ m, on-axis magnetic field $B_0 = 3$ T, and the safety factor profile $q(r) = 1.71 + 0.16 r^2$. The electron density is consistent with $n_{e0} = 2.0 \times 10^{19}$ m$^{-3}$, $T_e = 1$ keV. The ratio of the electron pressure to the magnetic pressure is $\beta_e \approx 9 \times 10^{-4}$. The Larmor radius of the thermal ions is $r_L = cm_n q_n / (eB_{\parallel}) = 0.00152$ m. The ratio between the adiabatic part ($\delta A_A/d_0^2$) and the non-adiabatic part ($\nabla_\perp^2 \delta A^b$) in the left hand side of Ampère’s equation is $1/(d_0^2 k_0^2) \approx \beta_e / (k_0^2 n_0^2) \approx (m_n T_n/m_e T_e) \approx 1.622 \times 10^3$, where $k_0 \approx n q / r = 6 \times 1.75 / 0.5 = 21$. The ITPA-TAE case is featured with a small electron skin depth ($d_e \approx 1.182 \times 10^{-3}$ m) and suffers from the ‘cancellation problem’ if the pullback scheme is not adopted.

The EP density profile is given by

$$n_{\text{EP}}(r) = n_{\text{EP},0} c_3 \exp \left( - \frac{c_2}{c_1} \tan^2 r - c_0 \right),$$

where $n_{\text{EP},0} = 1.44131 \times 10^{21}$ m$^{-3}$, the subscript ‘EP’ indicates EPs (energetic particles), $c_0 = 0.49123$, $c_1 = 0.298228$, $c_2 = 0.198739$, $c_3 = 0.521298$. The EP temperature is 400 keV for the base case. The $n = 6$ mode is simulated with four dominant harmonics ($m = 9, 10, 11, 12$) included.

4.1. Numerical verification

The base case of the EP driven TAE ($T_{\text{EP}} = 400$ keV) is used for the convergence studies. First, we need to identify the time step size and know its maximum acceptable value in the following studies. In this work, we simulate the $n = 6$ TAE and only take 1/6 of the torus in the toroidal direction. Since using eight grid points per wavelength is sufficient, we take $N_\theta = 8$. Since the frequency is mainly determined by non-resonant particles, while the growth rate is mainly determined by resonant EPs, the growth rate usually requires better resolution, and we only show the convergence with respect to the growth rate. For a typical grid size $(N_r, N_\theta, N_z) = (64, 128, 8)$, we choose the marker number $N_{\text{marker}} = 4 \times 10^3$ for each species. The growth rate for various time step size is shown in the left frame of figure 2. The growth rate starts to converge for $\Delta t/T_A \lesssim 0.05$, where $T_A$ is the TAE period estimated at $r_c = 0.5$, i.e. $T_A = 4 \pi q(r = r_c) R_0 / v_A$, where $q(r = r_c) = q_c = 1.75$. For the convergence test related to the marker number, we choose $\Delta t/T_A = 0.05$ and the result is shown in the right frame of figure 2. Good convergence is achieved for $N_{\text{marker}} > 2 \times 10^5$.

The iterative Ampère solver in equation (38) is crucial for the accurate calculation of $\delta A^b$ and for the mitigation of the ‘cancellation’ problem. We show the convergence of the iterative Ampère solver of a typical nonlinear run in figure 3. Good convergence is observed for the base case ($T_{\text{EP}} = 400$ keV). The EP driven TAE is excited and reaches saturation after $t/T_A \approx 10$. The correction in $\delta A^b$ is smaller as the number of iterations increases. In the initial state, the convergence is better than at later times since the marker distribution deviates away from the Maxwell distribution due to the finite orbit width effect and mirror force, which leads to a larger discrepancy of the $\delta A^b$ from the rigorous solution $\sum_{p=0,1,2} \delta A^b_p$. Nevertheless, the convergence is good in the whole simulation, and the correction to $\delta A^b$ is suppressed to be lower than 1% in only four iterations.

4.2. Linear $\delta f$ simulations of EP driven TAEs

The EP driven TAE is simulated with various EP temperatures for the benchmark with other codes in the previous work [8]. To make the model in TRIMEG-GKX similar to
other codes, the $\delta f$ scheme is applied to thermal ions, EPs and electrons. Since we focus on the linear solution, the linear gyrokinetic equations are solved with markers pushed along the unperturbed trajectory but the marker weight evolving over time. We only compare with ORB5 and GYGLES results since the models are more similar to ours. The growth rate of EP driven TAE is shown in figure 4. Good agreement is achieved, for the model without a finite Larmor radius effect.

The radial mode structures of the poloidal harmonics for $T_{\text{EP}} = 400$ keV are shown in figure 5. The mode width is comparable to that from ORB5/GYGLES [8]. The magnitude of the $m = 10$ harmonics is significantly higher than that of the $m = 11$ harmonics, which is also consistent with the results of GYGLES/ORB5 as shown in the previous work [8].

### 4.3. Nonlinear $\delta f$ and full $f$ EP simulations

Nonlinear simulations are performed using the $\delta f$ scheme and the mixed-full-$f$-EPs-$\delta f$-electrons/thermal-ions scheme separately. Note that in the mixed full $f-\delta f$ scheme, the full $f$ scheme is only applied to EPs, but electrons and thermal ions are always treated using the $\delta f$ scheme. To estimate the minimum marker number for proper treatment of TAE, it is noticed that $\delta n \sim \delta \phi (k_B T_e)^{1/2} / \rho_i$, $\delta j \sim \delta \phi (\beta m_i / m_e) / \rho_i^2 \sim 6.2 \times 10^{-4} \delta \phi$ where $\delta n$ and $\delta j$ are normalized using electron equilibrium density and electron thermal velocity. At the saturation level, $\delta \phi \sim 1$, $\delta \phi_{\parallel} \sim 1$. If the full $f$ is adopted for all species, the noise level in density and current should be much lower than $\delta n$ and $\delta j$ which yields that the marker number per degree of freedom (the product of the cell number and the Fourier mode number) $N_{\text{mark, DOF}} \gg 10^4$ for density and $N_{\text{mark, DOF}} \gg 2.6 \times 10^6$ for the current. In order to reduce the marker number but keep the capability of treating EPs using the full $f$ scheme, in this work we adopt the $\delta f$ scheme for electrons and thermal ions. Thus, the main noise is from the full $f$ EPs. Since the EP density is less than 1% of the electron density, the criteria for the marker number is relaxed to that of the marker number per cell or per Fourier mode $N_{\text{mark, DOF}} \gg 10^2$ for the density and $N_{\text{mark, DOF}} \gg 2.6 \times 10^5 \sqrt{T_{\text{EP}} m_e / (T_{\text{MEP}})} \sim 0.86 \times 10^2$ for the current.

The time evolution of the field energy is shown in figure 6. In these single $n$ nonlinear simulations, the saturation is due to the nonlinear interaction between the particles and the single-$n$ mode, as reported in previous work [16]. The wave-particle interaction causes a flattening of the EP distribution at specific phase space locations. The noise level is controlled by the marker numbers $N_e = 2.5 \times 10^3$, $N_i = 2.5 \times 10^3$, $N_{\text{EP}} = 16 \times 10^4$ in the full $f$ simulations. In the $\delta f$ simulation, $N_e = 2.5 \times 10^3$, $N_i = 2.5 \times 10^5$, $N_{\text{EP}} = 2.5 \times 10^5$. The main computational consumption is for the operations related to markers, namely, the interpolation of the field at the marker location, the calculation of the density and the current using markers, and the calculation of the marker trajectories.
Figure 4. The growth rate of EP-driven TAEs for different values of EP temperature for models without finite Larmor radius (FLR) effect.

Figure 5. The radial structure of poloidal harmonics for EP driven TAE, with EP temperature $T_{EP} = 400$ keV. The four dominant harmonics are plotted ($m = 9, 10, 11, 12$).

The full $f$ case is about 20 times more expensive than the $\delta f$ case, which is consistent with the marker numbers $16.5 \times 10^6$ in the full $f$ case and $0.75 \times 10^6$ in the $\delta f$ case. A clear linear growth stage and mode saturation is observed. The mode structure of the linear stage is in good agreement with the $\delta f$ simulations. As far as we know, this mixed scheme with full $f$ EPs and $\delta f$ thermal ions and electrons have not been reported before. In our study, this method has been validated to be practical and suitable for studying EP-related physics. We estimate that the simulation time is reduced to $(n_{EP}/n_e)^2 \sim 10^{-4}$ of that if the full $f$ scheme is applied to electrons and ions.

The linear growth rate and saturation level of the full $f$ simulation is relatively smaller by $\sim 40\%$ than those of the $\delta f$ simulation, due to the weaker driving strength caused by the EP profile relaxation. Note that in both the full $f$ and the $\delta f$ simulations, the same particle refilling scheme has been applied, namely, the lost particles are refilled at the poloidal location $\theta_{p,\text{refill}} = -\theta_{p,\text{loss}}$, and at the toroidal location $\phi_{p,\text{refill}} = \phi_{p,\text{loss}} - 2q(r_{p,\text{loss}})/v_{\parallel}$, where $r_{p,\text{loss}}$ indicates the radial location of the lost particles. The EP profile relaxation comes from the marker loading process. The local Maxwellian distribution is not a steady state solution in tokamak geometry, namely, the distribution function relaxes in a few particle transit periods ($\sim 2\pi q R_0/v_{\parallel}$). The EP profile relaxation in the full $f$ scheme should be treated rigorously by adopting the EP distribution in constant of motion space, in order to eliminate artificial ingredients for the benchmark with different codes and for interpreting experimental observations. As the EP relaxation occurs, the symmetry breaking in $v_{\parallel}$ direction of the distribution also occurs and can be closely linked to the asymmetric properties of the TAE mode. The two-dimensional mode structure is tilted more significantly in the full $f$ simulation than that in the $\delta f$ one, as indicated in the lower frame of figure 6. More dedicated studies will be needed in the future to identify the features and the causes/consequences of the symmetry-breaking properties of the TAE mode related to toroidal rotation and current generation [17–22].

4.4. Full $f$ simulation using canonical Maxwellian distribution

While the full $f$ simulations using a local Maxwellian distribution are a well-defined problem and can be used as a benchmark case for full $f$ studies, it is important to adopt a kinetic equilibrium based on the constants of motion (canonical
Maxwellian distribution) and to identify the differences between simulations using the canonical Maxwellian distribution and a local one. The EP profile relaxation is shown in figure 7 for cases using the local Maxwellian distribution and the canonical Maxwellian distribution. The logarithmic EP gradient decreases by ~40% in 1–2 EP transit period for the local Maxwellian distribution (left frame) but stays almost the same for the canonical distribution (right frame) ($T_{\text{trans,EP}}/T_A \sim 1$ for the base case with $T_{\text{EP}} = 400$ keV). However, the canonical distribution should be adjusted to match the analytical radial distribution since the EP distribution function using the shifted canonical toroidal momentum $\psi_{\text{can}}$ describes the distribution of the EP orbit center. Note that the density flattening is more significant for larger values of the EP finite orbit width and the initial value of $d\ln n/dr$; thus in the inner and outer regions ($r \leq 0.3$ and $r \geq 0.7$), the density flattening is less significant as shown in the left frame of figure 7.

While the EP guiding center distribution is given by equation (80), the conversion between the EP guiding center and the EP orbit center can be obtained theoretically by applying the push-forward and pull-back transformation between the guiding center and the orbit center. In this work, we show that the matching procedure can be performed numerically. Several cases with canonical EP distribution featured by different values of $c_0, c_1, c_2, c_3$ are run and adapted so that the density profile of the guiding center matches that in equation (80). A good match is obtained when we choose $(c_0, c_1, c_2, c_3)_{\text{can}} = (0.46623, 0.17042, 0.11357, 0.521298)$ as the coefficients in the canonical EP distribution in equation (46)

\[
n(\psi_{\text{can}}) = n(r_{\text{can}}) = n_{\text{EP}} \exp \left( \frac{c_2_{\text{can}}}{c_1_{\text{can}}} \tanh \frac{r - c_0_{\text{can}}}{c_2_{\text{can}}} \right).
\]

For the full $f$ case, the marker numbers $N_c = 2.5 \times 10^5, N_f = 2.5 \times 10^5, N_{\text{EP}} = 64 \times 10^6$. The guiding center profile of this matched case is shown in the left frame of figure 8. The equation is very close to the nominal profile described by the ITPA-TAE case in equation (80). Note that the Maxwellian distribution and the canonical Maxwellian distribution are intrinsically different and as long as we match these two, differences would appear anyway. Our goal is to match the maximum value of $d\ln n/dr$ between the local Maxwellian and the canonical one, while still maintaining the density profiles in equations (80) and (82), respectively. More precise matching can be achieved in principle by representing the EP profile using the finite element method in constant of motion space, but this is beyond the scope of this work. In addition, artificial relaxation is avoided. In the right frame, the time evolution of the full $f$ scheme agrees with that of the $\delta f$ scheme. The difference in growth rate is still observed but is only by ~8%, since the detailed structure of the distributions in full $f$ and $\delta f$ and the related wave-particle interactions can be different. Nevertheless, the application of the canonical EP distribution is shown to be a practical way to avoid the large EP profile relaxation and to match the EP density profile in the full $f$ simulations. For the ITPA-TAE case, the EP density perturbation is small $\delta n/n_0 < 1\%$ and the $\delta f$ scheme is still applicable, thus, it is suitable to compare the full $f$ and the $\delta f$ schemes. For longer timescale simulations and intermittent and transient plasmas, the EP profile can vary more significantly, and the full $f$ EP scheme provides a natural way due to its capability of describing the arbitrary distribution and its time evolution in phase space directly but the $\delta f$ may lose its advantage in noise reduction due to the larger $\delta f/f_0$ and the consequently enhanced noise level. In principle, the $\delta f$ scheme can also simulate large evolution of plasma profiles and distribution functions using many markers, similar to what full $f$ does. More simulations with a more significant time evolution of the EP distribution will be our future work.
5. Conclusions

In this work, the full $f$ and $\delta f$ gyrokinetic particle models are formulated and implemented on the same footing and applied to the simulation of toroidicity-induced Alfvén eigenmode driven by EPs. The mixed full $f$-$\delta f$ scheme has been proposed for the studies of Alfvén waves and EP physics. The mixed variables have been adopted in the formulation, and the pullback scheme is implemented in TRIMEMG-GKX code. Excellent performance has been demonstrated for the simulation of the electromagnetic problem and the cancellation problem is mitigated even for the ITPA-TAE case for which the electron skin depth is small. Good agreement with previous results from other codes is observed in terms of the linear growth rate of EP-driven TAEs and mode structures.

Important physics properties of the EPs have been demonstrated by the full $f$ (EP) simulations. Due to the high energy of EPs, the finite orbit width is large, and the local Maxwell distribution is not a good approximation of the steady-state EP distribution. Using the Maxwell EP distribution in the full $f$ simulations, the EP distribution deviates from the initial one in a few transit periods, leading to an EP profile relaxation featured by a weakened EP density gradient. Consequently, the full $f$ EP simulations give a linear growth rate smaller than the $\delta f$ simulations by 40% for $T_{\text{EP}} = 400$ keV using the ITPA-TAE parameters, which suggests that the EP profile relaxation in the full $f$ scheme should be treated properly. The shifted canonical toroidal moment, the particle energy, and the magnetic momentum are adopted in this work as the constants of motion of EPs and the EP distribution defined in these coordinates gives a more rigorous description of the EP steady state, without suffering from artificial density relaxation. In addition, a matching scheme has been introduced to demonstrate the pullback transition from the shifted canonical toroidal momentum coordinate to the EP guiding center coordinate, showing the essence of the EP properties due to the finite orbit width effect. The mixed-full-$f$-\$\delta f$ scheme developed in this work makes the kinetic simulations of the background electrons and thermal ions computationally economical and meanwhile brings in a flexible description for EPs, which allows a large variation of EP profiles and distributions in velocity space. This provides a powerful tool for kinetic studies using realistic experimental EP distributions related to intermittent and transient plasma activity.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Appendix A. Ad-hoc equilibrium

For the tokamak geometry, the coordinates $(r, \phi, \theta)$ are adopted and the magnetic field is represented as $\mathbf{B} = \nabla \psi \times \nabla \phi + F \nabla \phi$ and $\mathbf{b} = \mathbf{B}/B$ is the unit vector along the field lines. An ad-hoc equilibrium has been adopted, featured with concentric
circular magnetic flux surfaces and constant $F$. The poloidal flux
\[ \psi(r) = \frac{B_0}{2\delta_0} \ln \left(1 + \frac{q_2^2}{q_1^2} r^2\right), \]
where $q(r) = q_0 + q_2 r^2$, $q_2 = \delta_{\text{edge}} - q_0$. The function of the safety factor
\[ q(r) = \frac{q}{\sqrt{1 - (r/R_o)^2}}. \]
The curl of the magnetic field direction
\[ (\nabla \times \mathbf{b}) \cdot \hat{r} = \frac{R_0 \sin \theta}{R \sqrt{r^2/q_1^2 + R_0^2}}. \quad \text{(A.1)} \]
\[ (\nabla \times \mathbf{b}) \cdot \hat{\theta} = \frac{\cos \theta}{R} - \frac{R_0 (q_0 - q_2 r^2)}{q_1 (r^2/q_1^2 + R_0^2)^{3/2}}. \quad \text{(A.2)} \]
\[ (\nabla \times \mathbf{b}) \cdot \hat{\phi} = \frac{-2 R_0^2 q_0}{q_1 (r^2/q_1^2 + R_0^2)^{3/2}}. \quad \text{(A.3)} \]

Appendix B. Guiding center equations of motion in ad-hoc equilibrium

In this section, all variables such as $v$, $\mu$, $m$, $q$, and $\delta G$ are normalized. The equilibrium part of the motion is as follows,
\[ \frac{dv}{dt} = \frac{b_z^*}{r} v \]