An efficient, conservative, time-implicit solver for the fully kinetic arbitrary-species 1D-2V Vlasov-Ampère system

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Abstract

We consider the solution of the fully kinetic (including electrons) Vlasov-Ampère system in a one-dimensional physical space and two-dimensional velocity space (1D-2V) for an arbitrary number of species with a time-implicit Eulerian algorithm. The problem of velocity-space meshing for disparate thermal and bulk velocities is dealt with by an adaptive coordinate transformation of the Vlasov equation for each species, which is then discretized, including the resulting inertial terms. Mass, momentum, and energy are conserved, and Gauss’s law is enforced to within the nonlinear convergence tolerance of the iterative solver for arbitrary discretizations in time, configuration, and velocity space through a set of nonlinear constraint functions. We mitigate the temporal stiffness introduced by, e.g., the plasma frequency through the use of high-order/low-order (HOLO) acceleration of the iterative implicit solver. We present several numerical results for canonical problems of varying degrees of complexity, including the ion-acoustic shock wave, which demonstrate the efficacy, accuracy, and efficiency of the scheme.

Keywords: Conservative discretization, Vlasov-Ampère, adaptive velocity grid, implicit solver, high-order/low-order acceleration, HOLO

1. Introduction

In recent years, it has become apparent that particle long mean-free-path kinetic effects can play a significant role in the evolution of high-energy-density (HED) plasma systems, such as inertial confinement fusion (ICF) capsule implosions [1–5]. To study these systems, radiation-hydrodynamic models are typically used; however, to resolve the long mean-free-path effects it is necessary to employ a kinetic approach. Vlasov-Fokker-Planck codes, such as iFP [6] and FPion [7], have been developed with the goal of resolving ion kinetic effects in weakly collisional regimes with arbitrary Knudsen numbers. However, they continue to treat the electrons as a quasineutral, ambipolar fluid, including only an electron temperature equation. The fluid electron assumption neglects important kinetic plasma effects such as nonlocal electron heat transport, which may be necessary to correctly describe HED plasma phenomena such as shocks and ablation fronts in ICF implosions. This study proposes an efficient and accurate algorithmic solution for simulating the fully kinetic 1D-2V ion-electron system.

There have been attempts to account for nonlocal electron effects within fluid models. A common approach is limiting the electron heat flux to some fraction of the free-streaming flux [8]: another strategy is to spatially convolve the electron heat flux [9]. However, in order to describe electron kinetic effects accurately, it is necessary to solve a fully kinetic model. To this end, the Vlasov-Fokker-Planck(VFP)-Maxwell system of equations may be taken as a first-principles representation of a weakly-coupled plasma. In a one-dimensional spatial system, and assuming an electrostatic field response, this may – without loss of generality – be reduced to a 2D velocity space described by longitudinal (parallel) and perpendicular velocities. This leads to the 1D-2V VFP-Ampère (or VFP-Poisson) system. The 1D Ampère equation describes the evolution of the longitudinal electric field based on the moments of all species’ velocity distribution functions, while the 1D-2V VFP equation describes the evolution of the distribution functions. To simplify the current development and presentation, we explore in this work only the collisionless aspects of the algorithm, i.e., the 1D-2V Vlasov-Ampère system. This in no way compromises our goal of developing a fully kinetic model.
simulation tool for plasmas of arbitrary collisionality, as the numerical details of the Fokker-Planck (FP) collision operator may be considered independently [10, 12].

To solve the Vlasov–Ampère system, there are a variety of possible approaches including temporally implicit or explicit applications of particle-in-cell (PIC) methods [13–16], semi-Lagrangian grid-based methods [17, 19], or Eulerian grid-based approaches [20, 22]. In this work, we apply a temporally fully implicit grid-based Eulerian approach. An implicit approach has significant advantages over explicit schemes, particularly for grid-based approaches wherein the Courant-Friedrichs-Lewy (CFL) time-step limit is determined by the fastest speed on the velocity grid. With a fully-implicit nonlinear iterative solver, highly temporally multiscale problems – in which the system dynamics are driven on time-scales much longer than the fastest supported time-scales – may become much more tractable. A classic collisionless example is the ion-acoustic shock wave, where the dynamic time-scale is roughly 100 times longer than the inverse electron plasma frequency, and may be 1000 times (or more) longer than the explicit time-scale based on the maximum grid velocity [20]. In the current work, the high-order (HO)/low-order (LO) scheme (HOLO) is used so that the LO (moment) system of equations accelerates convergence of the HO (kinetic) system. The LO system consists of the moments of the plasma species’ Vlasov equations coupled to Ampère’s equation, while the HO system consists of the Vlasov equations. HOLO approaches have been used to solve a variety of systems [23], from neutron [24] and thermal radiation transport [25] to BGK gas-kinetics [26]. More importantly, the HOLO approach has been applied to the solution of collisionless [13, 20] and collisional [27] plasma systems. In an earlier study by Taitano and Chácón [20], the HOLO approach was used to accelerate Vlasov–Ampère convergence by using the LO system to efficiently evaluate the electric field with the higher-order moment closure provided by the HO system. In this work, we generalize this study both by applying a non-centered time integration scheme and by considering the adaptive velocity-space strategy proposed in Ref. [11].

When solving the Vlasov–Ampère system, a static velocity mesh may present complications in problems where the species temperatures and bulk velocities may have significant temporal and spatial variations. Specifically, the mesh must be large enough to capture both the shift in the bulk velocity and temperature evolution at the hottest location in space and time (the largest thermal speed), while maintaining a sufficient resolution for the coldest location (the smallest thermal speed) for all species. In contrast, a mesh which dynamically expands/contracts in space and time (the largest thermal speed), while maintaining a sufficient resolution for the coldest location (the velocity-space strategy proposed in Ref. [11].

To preserve the numerical accuracy of long simulations, we desire a discretization scheme for which the continuum symmetries of the governing equations (leading to mass, momentum, and energy conservation) are preserved in the discrete. Without a discrete conservation principle, long-term simulations may produce significant violations of the conservation properties due to accumulated discretization errors, which can manifest as numerical plasma heating or cooling [27], or a departure of the solution from the asymptotic hydrodynamic manifold. Indeed, as we shall demonstrate later, the failure to ensure discrete charge conservation (i.e., enforcing the discrete Gauss’s law) leads to catastrophic failure in simulations, with significant departure from the correct solution. Further, in the case of the Vlasov-Fokker-Planck equation, Taitano et al. [6] showed that even neglecting to ensure discrete momentum and energy conservation relationships only in the Vlasov equation (while enforcing it in the Fokker-Planck collision operator) leads to extremely large numerical errors (∼ O (1)). Thus, discrete conservation is a key for achieving high fidelity and accuracy.

Broadly, we will define two different strategies for achieving discrete conservation. The first, which we term a “passive” approach, relies on specifically chosen discretizations that “passively” preserve the structure of the governing equations. This is a general catch-all for the symplectic and Hamiltonian-preserving techniques for plasma physics systems described by Morrison [29]. Such techniques have also been called “structure-preserving” [29, 30], and are in general very effective at preserving invariants – for the Vlasov-Maxwell system, Shirato et al. [30] demonstrated conservation errors on the order of machine precision. However, from our perspective, there are two significant shortcomings of this approach. The first is that they are generally only possible through central differencing schemes, which are not e.g., monotonic, positivity-preserving, or non-oscillatory (all of which are desirable properties). The second is that, in the case of the velocity-space transformed Vlasov equation used in this work, it is not readily apparent whether such “structure-preserving” discretizations are possible. The second strategy, which we term an “active” approach, is the strategy we employ in this work to achieve discrete conservation. To implement this approach, we introduce Lagrange-multiplier-like constraint functions into the discretized governing equations. These “nonlinear constraint
functions” are defined so as to actively enforce certain continuum symmetries of the governing equations, ensuring conservation of e.g., mass, momentum, and energy in the discretized system. The primary benefit of the “active” strategy is that it permits a choice of arbitrary discretization schemes in both time (e.g., backward Euler, or BDF2) and phase space (e.g., SMART [31] or WENO [32]).

The present approach is similar to the strategies used in Refs. [20] and [28]; however, there are some important differences. In the previous Vlasov-Ampère implementation, the approach relied on a time-centered Crank-Nicolson integrator to achieve energy conservation. The current work uses a BDF2 temporal integration scheme (which is more appropriate for an eventual application to the collisional system), and can in principle be applied to an arbitrary temporal integration scheme. Further, the approach for enforcing discrete conservation with the velocity-space adaptivity (as in Ref. [28]) must be modified because of interaction with the additional constraint functions. Thus, the current work delivers an implicit algorithm for the fully kinetic, arbitrary-species 1D-2V Vlasov-Ampère system, which conserves mass, momentum, and energy to within nonlinear convergence tolerance. The algorithm is adaptive in the velocity space to ease meshing requirements due to temporal and spatial variations in the local bulk velocity and thermal speed of each species, while the nonlinear constraint functions which ensure conservation also allow an arbitrary choice of temporal and advective discretizations for the other discrete operators.

The rest of this paper is organized as follows. Section 2 gives an overview of the governing equations for the Vlasov-Ampère/Poisson system in 1D-2V, its transformation in the velocity space, and the continuum-conservation symmetries of the system. Section 3 describes the discretization of the Vlasov system. Section 4 provides details of our strategy for ensuring the continuum conservation symmetries in the discretized system. In Sec. 5 we present our nonlinear iterative strategy for solving the discretized system implicitly in time using a HOLO acceleration scheme. We present numerical results highlighting the accuracy and performance of the algorithm for several canonical problems of varying difficulty in Sec. 6, and provide concluding remarks in Sec. 7.

2. Vlasov-Ampère system of equations

The Vlasov-Ampère/Poisson system may be regarded as a first-principles representation for a fully ionized electrostatic collisionless plasma. The governing equations are the Vlasov equations for each species \( \alpha \),

\[
\partial_t f_\alpha + \nabla_x \cdot \left( v f_\alpha \right) + \frac{q_\alpha}{m_\alpha} E \cdot \nabla_v \left( f_\alpha \right) = 0,
\]

which describe the evolution in phase space of distribution functions, \( f_\alpha \), and Ampère’s equation,

\[
\epsilon_0 \partial_t E + \sum_\alpha q_\alpha n_{u_\alpha} = 0,
\]

which describes the evolution of the electric field, \( E \). In Eqs. (1) and (2), \( v \) is the particle velocity, and \( q_\alpha \) and \( m_\alpha \) are the particle charge and mass of species \( \alpha \), respectively. The Vlasov-Poisson system instead utilizes Gauss’s law,

\[
\epsilon_0 \nabla_x \cdot E - \sum_\alpha q_\alpha n_{\alpha} = 0,
\]

and the electric potential, \( \Phi \), defined by \( \nabla_x \Phi = -E \), to obtain Poisson’s equation,

\[
\epsilon_0 \nabla_x^2 \Phi + \sum_\alpha q_\alpha n_\alpha = 0.
\]

The Vlasov-Poisson and Vlasov-Ampère systems can be shown to be equivalent through charge conservation, i.e.,

\[
0 = \nabla_x \cdot \left[ \epsilon_0 \partial_t E + \sum_\alpha q_\alpha n_{u_\alpha} \right] = \partial_t \left[ \epsilon_0 \nabla_x \cdot E - \sum_\alpha q_\alpha n_{\alpha} \right] \Rightarrow \partial_t \sum_\alpha q_\alpha n_{\alpha} + \nabla_x \cdot \sum_\alpha q_\alpha n_{u_\alpha} = 0.
\]

In one-dimensional configuration space, Eqs. (1)-(2) may be expressed as

\[
\partial_t f_\alpha + \partial_x \left( v f_\alpha \right) + \frac{q_\alpha}{m_\alpha} E_\parallel \partial_{v_\parallel} \left( f_\alpha \right) = 0,
\]

\[
\epsilon_0 \partial_t E_\parallel + \sum_\alpha q_\alpha n_{u_\parallel,\alpha} = \vec{j}_\parallel.
\]
Note that here we include the spatial average of the current density, \( \bar{J}_\parallel \). This is necessary in the 1D periodic system to preserve Galilean invariance, and is also a solvability constraint \([13][15]\). Without a loss of generality, the velocity-space domain may be reduced to two dimensions by invoking cylindrical symmetry, such that the velocity coordinates reduce from \((v_x, v_y, v_z)\) to \((v_\parallel, v_\perp, \varphi)\), with \(\varphi\) the ignorable azimuthal coordinate angle. In Eqs. \((6)-(7)\), we use the parallel notation to indicate vector components.

2.1. Velocity-space coordinate transformation

We perform a phase-space coordinate transformation of Eq. \((6)\) as was done in Ref. \([28]\). Namely, for each species \(\alpha\) we translate the velocity space by a reference offset velocity \(u_{\parallel,\alpha}^\ast(x, t)\) and then normalize it by a reference speed \(v_\parallel^\ast(x, t)\). These quantities are related to each species bulk-flow velocity and thermal speed, respectively, but are not necessarily equivalent to them. For each species, the velocity coordinate, \(v\), may be thus decomposed as,

\[
v = v_\alpha^\ast(x, t) \hat{v} + v_\alpha^\ast(x, t) \hat{u}_{\parallel,\alpha}^\ast(x, t)e_\parallel,
\]

where \(e_\parallel\) is the unit vector along \(x\) and \(u_{\parallel,\alpha}^\ast = v_\parallel^\ast \hat{u}_{\parallel,\alpha}^\ast\). Thus, the transformed velocity coordinate is defined as

\[
\hat{v} = \frac{v}{v_\alpha^\ast} - \hat{u}_{\parallel,\alpha}^\ast e_\parallel,
\]

where \(\hat{v} = v/v_\alpha^\ast(x, t)\). For full details of the transformation, we refer readers to the work of Taitano et al. \([28]\). The final form of the transformed Vlasov equation is thus

\[
\partial_t \hat{f}_\alpha + \partial_x \left( v_\alpha^\ast \hat{v}_\parallel \hat{f}_\alpha \right) + \frac{q_\alpha}{m_\alpha v_\alpha^\ast} E_\parallel \partial_{\hat{v}_\parallel} \hat{f}_\alpha + \mathbf{\hat{v}} \cdot \nabla \hat{\varphi} \cdot \left\{ \left[ \partial_t \left( \hat{v} v_\alpha^\ast + e_\parallel u_{\parallel,\alpha}^\ast \right) + \partial_x \left( \hat{v} v_\alpha^\ast + e_\parallel u_{\parallel,\alpha}^\ast \right) \right] \hat{f}_\alpha \right\} = 0,
\]

where \(\hat{f}_\alpha = f_\alpha(v_\alpha^\ast)^3\). In what follows, we will use the shorthand notation

\[
\left\langle \Phi \left( \hat{v}_\parallel, \hat{v}_\perp \right) ; \hat{f}_\alpha \left( \hat{v}_\parallel, \hat{v}_\perp \right) \right\rangle_{\hat{v}} \equiv 2\pi \int_{-\infty}^{\infty} d\hat{v}_\parallel \int_{0}^{\infty} \hat{v}_\perp d\hat{v}_\perp \Phi \left( \hat{v}_\parallel, \hat{v}_\perp \right) \hat{f}_\alpha \left( \hat{v}_\parallel, \hat{v}_\perp \right),
\]

to denote the velocity-space moment of a function, \(\hat{f}_\alpha \left( \hat{v}_\parallel, \hat{v}_\perp \right)\), with the weight, \(\Phi \left( \hat{v}_\parallel, \hat{v}_\perp \right)\).

2.2. Summary of key continuum symmetries

Equations \((7)\) and \((9)\) conserve mass, momentum, and energy in the continuum. However, these continuum properties are not automatically preserved when the governing equations are discretized, as we shall see in Sec. \(4\). In what follows, we will highlight particular symmetries of the governing equations that lead to the desired conservation properties. Detailed proofs of the conservation properties including these symmetries can be found in Appendix A.

2.2.1. Symmetries relating to the Vlasov equation velocity-space transformation

For the transformed Vlasov equation, we recall that our independent velocity variables have become \((\hat{v}_\parallel, \hat{v}_\perp)\). However, momentum and energy conservation are still defined in terms of \(v_\parallel\) and \(v_\parallel^2\) (the original velocity) moments of \(f_\alpha\). The important point is that \(v\) moments do not commute with temporal and spatial derivatives in the transformed space, e.g.,

\[
\left\langle m_\alpha v_\parallel, \partial_t \hat{f}_\alpha \right\rangle_{\hat{v}} \neq \left\langle 1, \partial_t \left( m_\alpha v_\parallel \hat{f}_\alpha \right) \right\rangle_{\hat{v}},
\]

\[
\left\langle m_\alpha v_\parallel, \partial_x \left( v_\parallel \hat{f}_\alpha \right) \right\rangle_{\hat{v}} \neq \left\langle 1, \partial_x \left( m_\alpha v_\parallel^2 \hat{f}_\alpha \right) \right\rangle_{\hat{v}}.
\]

Thus, to obtain the momentum conservation theorem for the transformed system, we must utilize integration by parts and the product rule on the temporal and spatial components of the Vlasov equation to obtain the identity:

\[
\left\langle m_\alpha v_\parallel, \partial_t \hat{f}_\alpha \right\rangle_{\hat{v}} + \left\langle m_\alpha v_\parallel, \partial_x \left( v_\parallel \hat{f}_\alpha \right) \right\rangle_{\hat{v}} - \frac{1}{v_\alpha^\ast} \left\langle m_\alpha v_\parallel, \nabla_{\hat{v}} \cdot \left\{ \left[ \partial_t \left( \hat{v} v_\alpha^\ast \right) + \partial_x \left( \hat{v} v_\alpha^\ast \right) \right] \hat{f}_\alpha \right\} \right\rangle_{\hat{v}}
\]

\[
= \left\langle 1, \partial_t \left( m_\alpha v_\parallel \hat{f}_\alpha \right) \right\rangle_{\hat{v}} + \left\langle 1, \partial_x \left( m_\alpha v_\parallel^2 \hat{f}_\alpha \right) \right\rangle_{\hat{v}},
\]

(13)
which must be satisfied locally for each species. Likewise, for the energy conservation theorem we must have the identity:

$$\langle m_\alpha \frac{1}{2} v^2, \partial_t \tilde{f}_\alpha \rangle_{\tilde{\theta}} + \langle m_\alpha \frac{1}{2} v^2, \partial_z (v_i \tilde{f}_\alpha) \rangle_{\tilde{\theta}} - \frac{1}{\nu_\alpha} \langle m_\alpha \frac{1}{2} v^2, \nabla_{\tilde{\theta}} \cdot \left\{ \left[ \partial_t (v) + \partial_z (v_i \tilde{f}_\alpha) \right] \right\}_{\tilde{\theta}}$$

$$= \left\langle 1, \partial_t \left( m_\alpha \frac{1}{2} v^2 \tilde{f}_\alpha \right) \right\rangle_{\tilde{\theta}} + \left\langle 1, \partial_z \left( m_\alpha \frac{1}{2} v^2 v_i \tilde{f}_\alpha \right) \right\rangle_{\tilde{\theta}}.$$  \hspace{1cm} (14)

For an arbitrary discretization, these identities will generally not be satisfied simultaneously or even independently.

### 2.2.2. Symmetries relating to Ampère’s equation

In addition to the preceding symmetries for the velocity-space adaptivity, there are several which must be satisfied for the Vlasov-Ampère system as a whole. The first is the equivalence through charge conservation between Gauss’s law, Ampère’s equation, and the continuity equation:

$$\partial_t \rho_\alpha + \partial_z j_\parallel = \sum_\alpha q_\alpha \left[ \langle 1, \partial_t \tilde{f}_\alpha \rangle_{\tilde{\theta}} + \langle 1, \partial_z (v_i \tilde{f}_\alpha) \rangle_{\tilde{\theta}} \right]. \hspace{1cm} (15)$$

In Eq. (15), we defined $\rho_\alpha \equiv \sum_\alpha q_\alpha n_\alpha$ and $j_\parallel \equiv \sum_\alpha q_\alpha n_\parallel \alpha$, and we further define $\langle 1, \tilde{f}_\alpha \rangle_{\tilde{\theta}} = n_\alpha$ and $\langle v_i \parallel, \tilde{f}_\alpha \rangle_{\tilde{\theta}} = n_\parallel \alpha$. We see that the charge density in Gauss’s law and the current in Ampère’s equation must be proportional to the particle number density and flux in the continuity equation [i.e., the $v^0$ moment of the transformed Vlasov equation, Eq. (1)]. As we will see shortly, the crux is that the current in Ampère’s equation (which drives the electric field $E_\parallel$) must be consistent with Eq. (15), thereby ensuring that $\epsilon_0 \partial_t E_\parallel = \rho_\parallel$ discretely. This equivalence is in some sense a fundamental “zeroth-order” requirement for the Vlasov-Ampère system, and, as we shall see shortly, neglecting it in the discrete will produce catastrophic errors [33–36].

The second requirement is that the $m_\alpha v_\parallel$ moment of the acceleration operator in Eq. (9) must produce a number density $n_\alpha$ which is identical to that which appears in Gauss’s law. If we sum the moment of this term over all species we find

$$\sum_\alpha q_\alpha m_\alpha v_\alpha \langle m_\alpha v_\parallel, \partial_\parallel \tilde{f}_\alpha \rangle_{\tilde{\theta}} = -E_\parallel \sum_\alpha q_\alpha n_\alpha = -\partial_z \left( \epsilon_0 \frac{1}{2} E_\parallel^2 \right). \hspace{1cm} (16)$$

We see that this symmetry introduces the divergence of the electrostatic stress tensor into the momentum equation, which is key to achieving momentum conservation.

To arrive at energy conservation in the Vlasov-Ampère system, we again inspect the acceleration operator. Taking the $m_\alpha \frac{1}{2} v^2$ moment of the acceleration operator we find:

$$\sum_\alpha q_\alpha m_\alpha v_\alpha^2 E_\parallel \langle m_\alpha \frac{1}{2} v^2, \partial_\parallel \tilde{f}_\alpha \rangle_{\tilde{\theta}} = -E_\parallel \sum_\alpha q_\alpha n_\parallel \alpha = E_\parallel \left[ \epsilon_0 \partial_t (E_\parallel) - \tilde{J}_\parallel \right] = \partial_t \left( \epsilon_0 \frac{1}{2} E_\parallel^2 \right) - E_\parallel \tilde{J}_\parallel.$$

Thus, we see that this moment must produce a particle flux density which is consistent with the current which appears in Ampère’s equation. Further, we observe that while the equivalence

$$E_\parallel \partial_t E_\parallel = \partial_t \left( \frac{1}{2} E_\parallel^2 \right)$$

is true in the continuum, it will not be so for an arbitrary temporal discretization.

### 2.3. Strategy for enforcing continuum symmetries in the discrete

To enforce the preceding continuum symmetries in the discretized Vlasov-Ampère system, we introduce a set of nonlinear constraint functions to the discrete representation of Eq. (9). These added nonlinear constraints take the form of Lagrange-multiplier-like coefficients and associated operators. For the symmetries related to the velocity-space adaptivity, we introduce the constraint functions $\gamma_\parallel$ and $\gamma_\perp$, which modify the discretized inertial terms in a manner similar to that of in Refs. [2, 11]. In the discretized form of Eq. (9), these will be highlighted in red. Following a similar approach to Refs. [20, 27] for the Vlasov-Ampère symmetries, we introduce the constraint functions $\xi$, $\phi$, and $\gamma_q$, which appear in their own phase-space advection “pseudo-operators”. We will depict these highlighted in blue.
These constraint functions all act to expose the underlying continuum symmetries of the governing equations and eliminate the truncation errors between different discrete operators, which would break the symmetries. We note that, while having five distinct nonlinear constraint functions ($\xi$, $\phi$, $\gamma_q$, $\gamma_t$, and $\gamma_x$) to enforce only three conservation laws (charge, momentum, and energy conservation) may seem overconstrained, this is not the case. The critical distinction is that we are not directly enforcing the conservation laws themselves, but rather the symmetries that lead to those laws.

3. Numerical implementation

3.1. Discretization of the transformed Vlasov equation

The Vlasov equation, Eq. (9), is discretized using finite differences in the transformed phase space as follows. The discrete cylindrical cell volume in the velocity space for a uniform velocity mesh is

$$\hat{\Omega}_{j,k} \equiv 2\pi \Delta \hat{v}_\parallel \Delta \hat{v}_\perp \hat{v}_\perp,\quad (18)$$

while the total discrete volume including the configuration space on a uniform mesh is

$$\Delta \hat{V}_{i,j,k} = \Delta x \hat{\Omega}_{j,k}.\quad (19)$$

The quantities $\Delta \hat{v}_\parallel$, $\Delta \hat{v}_\perp$, and $\Delta x$ are the mesh spacings for the parallel velocity, perpendicular velocity, and configuration space, respectively. If the domain sizes are defined to be

$$L_x, \bar{L}_\parallel = L_\parallel v_* \alpha, \bar{L}_\perp = L_\perp v_* \alpha,$$

then the mesh spacings are defined as

$$\Delta x = \frac{L_x}{N_x}, \Delta \hat{v}_\parallel = \frac{\bar{L}_\parallel}{N_\parallel}, \Delta \hat{v}_\perp = \frac{\bar{L}_\perp}{N_\perp}.$$

Here, $N_x$, $N_\parallel$, and $N_\perp$ are the numbers of cells along each coordinate. The coordinates $i, j, k$ are defined to be at the cell centers, so that the boundary of the domain in each direction is on cell faces.

Discrete moments in the velocity space are computed via a midpoint quadrature as

$$\langle A, B \rangle_{\delta \hat{v}} \approx \sum_{j=1}^{N_\parallel} \sum_{k=1}^{N_\perp} \hat{\Omega}_{j,k} A_{j,k} B_{j,k}$$

for scalars defined at the cell centers and as

$$\langle 1, A \cdot B \rangle_{\delta \hat{v}} \approx \sum_{j=0}^{N_\parallel} \sum_{k=1}^{N_\perp} \hat{\Omega}_{j+\frac{1}{2},k} A_{\parallel,j+\frac{1}{2},k} B_{\parallel,j+\frac{1}{2},k} + \sum_{j=1}^{N_\parallel} \sum_{k=0}^{N_\perp} \hat{\Omega}_{j,k+\frac{1}{2}} A_{\perp,j,k+\frac{1}{2}} B_{\perp,j,k+\frac{1}{2}}$$

for scalar products of velocity-space vectors defined at the cell faces. Quantities at half-indices (e.g., $j + \frac{1}{2}$) are at the cell faces.
A conservative discretization of the Vlasov equation, Eq. (9), is then given by

\[
\begin{align*}
\delta_t f_{\alpha,i,j,k} + \delta_x \left[ v_{i,j}^p \left( \frac{p+1}{2} \right)_{j,k} \right] + \frac{q_\alpha}{m_\alpha} \frac{E_{\parallel,i,j}^{p+1}}{v_{\alpha,i}} \delta_{\parallel,j} \left[ \left( \frac{p+1}{2} \right)_{i,k} \right] \\
+ \delta_x \left[ \frac{E_{\parallel,i,j}}{\alpha,2} \left( \frac{p+1}{2} \right)_{j,k} \right] + \delta_{\parallel,j} \left[ \phi_{\alpha,i} \left( \frac{p+1}{2} \right)_{i,k} \right] + \delta_{\parallel,j} \left[ \gamma_{q,\alpha,i} \left( \frac{p+1}{2} \right)_{i,k} \right] = 0.
\end{align*}
\]

Here, we define the following notation:

\[
\begin{align*}
\delta_i (F) & \equiv \frac{c^{p+1} F^{p+1} + c^p F^p + c^{p-1} F^{p-1}}{\Delta t^p}, \\
\delta_x F_i & \equiv \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x}, \\
\delta_{\parallel,j} \cdot [F]_{j,k} & \equiv \frac{F_{j+\frac{1}{2},k} - F_{j-\frac{1}{2},k}}{\Delta \parallel_{\perp}} + \frac{\tilde{v}_{\parallel,k,\perp} F_{j,k} + F_{j,k+\perp} - \tilde{v}_{\perp,k,\perp} F_{j,k-\perp}}{v_{\perp} \Delta \parallel_{\perp}}, \\
\hat{v}_{\parallel,\alpha,\perp} |_{i,j} & \equiv \left( \hat{v}_{\parallel,j} + \hat{u}_{\parallel,\alpha,\perp} \right) + \frac{c^{p+1}}{\Delta t^p} \left( \hat{v}_{\parallel,j} + \hat{u}_{\parallel,\alpha,\perp} \right).
\end{align*}
\]

with \(v_{\alpha,i+\frac{1}{2}}^{p+1} = \frac{v_{\alpha,i}^{p+1} + v_{\alpha,i+1}^{p+1}}{2}\) and \(\hat{u}_{\alpha,i+\frac{1}{2}}^{p+1} = \frac{\hat{u}_{\alpha,i}^{p+1} + \hat{u}_{\alpha,i+1}^{p+1}}{2}\). Note that the nonlinear constraint function \(\xi\) is included in \(\hat{v}_{\parallel,\alpha,\perp} |_{i,j}\) (boxed in blue). In Eq. (22), we have utilized a second-order backwards finite difference scheme in time (BDF2), with coefficients \(c^{p+1} = 1.5\), \(c^p = -2\), and \(c^{p-1} = 0.5\). The temporal index is \(p\). For compactness of notation we defined interpolated quantities as

\[
(\Phi)_{\text{face}} = \sum_{i=1}^{N_{\text{face}}} \omega_{\text{face},i'} (a, \phi) \phi_i',
\]

which is an advective interpolation operator acting on a scalar \(\phi\) at a cell face based on an advection coefficient \(a\). In Eq. (27), \(\omega_{\text{face},i'}\) are interpolation weights for the \(i'\) cells surrounding the cell face, and \(\phi_i'\) are the values of the interpolated quantity in those cells. We note here that the cell-center electric field is defined as the interpolation of adjacent cell-face electric fields,

\[
E_{\parallel,i}^{p+1} = \frac{E_{\parallel,i+\frac{1}{2}}^{p+1} + E_{\parallel,i-\frac{1}{2}}^{p+1}}{2}.
\]

Terms (a) and (b) represent the discrete form of the physical configuration-space advection and velocity-space advection due to the acceleration of the electric field, respectively. Terms (c), (d), and (e) (boxed in blue) are the discretized
forms of the ‘pseudo-operators’ arising from the nonlinear constraint coefficients, \( \xi \), \( \phi \), and \( \gamma_q \). Terms \( (f) \) and \( (g) \) are the discretized versions of the inertial terms arising from the respective temporal and spatial gradients in \( v_{\nu}^* \) and \( \hat{u}_e^* \), which also include two nonlinear constraint functions, \( \gamma_\nu \) and \( \gamma_x \), (boxed in red). Note in the velocity-space inertial terms pertaining to \( \gamma_x \), the term \( \hat{v}^{p+1}_{[\alpha,\nu,i,j,k]} \) is boxed in blue to indicate that it also contains the constraint function \( \xi \).

In the present study, we use the SMART scheme \( (31) \) for term \( (a) \) for ions because of its monotonicity- and positivity-preserving properties, as well as for being well-posed for nonlinear iterative methods. For electrons, however, we observed that the switching employed within SMART between upwinding (low-order) and higher-order schemes (e.g., QUICK \( (37) \)) injects numerical noise for certain problems – particularly for the ion-acoustic shock wave multiscale example (discussed shortly). Thus, the WENO5 scheme \( (32) \) – designed to be a high-order and avoid numerical oscillations, particularly near discontinuities – is used for the electron spatial advection. For the physical acceleration term, \( (b) \), we use WENO5 for ions due to increased robustness relative to a central-differencing scheme. We use central differencing for the electrons due to their extreme sensitivity to dissipation in velocity-space for the electrostatic acceleration operator. For robustness, and because as we shall see these terms do not affect the order of accuracy of the scheme, we use an upwind discretization for \( (c) \) and central differencing for \( (d) \) and \( (e) \). For the velocity-space adaptivity inertial terms \( (f) \) and \( (g) \), we use WENO5 for all species.

3.2. Discretization of Ampère’s equation, Eq. (7)

We follow the approach of Ref. \( (20) \) and define the electric field, \( E^0_{[\alpha,i,j,k]} \), at cell-faces. The discrete Ampère equation for the cell-face electric field is thus

\[
\frac{\epsilon_0}{\Delta \nu} \left( E^0_{[\alpha,i,j,k]} + \frac{\Delta \nu}{2} \hat{v}^{p+1}_{[\alpha,i,j,k]} \right) + \frac{N_{sp}}{\sum_{\alpha} q_{\alpha} m_{\nu}^{p+1}_{[\alpha,i,j,k]} = \nu^{p+1}_{[\alpha,i,j,k]}. (28)
\]

The cell-face particle flux density must be defined so as to preserve energy conservation. Thus, instead of being defined based on the “true” momentum moment of \( \hat{f}_{\alpha} \),

\[
\nu^{p+1}_{[\alpha,i,j,k]} = \left( \nu_{[\alpha,i,j,k]} \hat{f}^{p+1}_{[\alpha,i,j,k]} \right)/\delta \nu,
\]

\( \nu^{p+1}_{[\alpha,i,j,k]} \) is defined from the \( \frac{1}{2} m_{\nu} v^2 \) moment of the electrostatic acceleration operator (see the discussion of Eq. \( (17) \) in Sec. \( 2.2 \)).

\[
\nu^{p+1}_{[\alpha,i,j,k]} = -\frac{1}{m_{\nu}} \left( \frac{m_{\nu} (p_{\alpha,i,j,k}^* p_{\alpha,i,j,k})}{2 v_{\nu}^*} \right) \frac{2}{\Delta \nu} \left( \hat{f}^{p+1}_{[\alpha,i,j,k]} \right) \left( \nu_{[\alpha,i,j,k]} \hat{f}^{p+1}_{[\alpha,i,j,k]} \right) \delta \nu,
\]

\[
\nu^{p+1}_{[\alpha,i,j,k]} = \nu^{p+1}_{[\alpha,i,j,k]} + \nu^{p+1}_{[\alpha,i,j,k+1]}.
\]

We note that, while these momenta are equivalent in the continuum, choices of discretization and interpolation for the physical acceleration operator mean this will generally not be so in the discrete. The average current density \( \bar{J}_{\nu}^{p+1} \) must be based on this same particle flux density \( \nu^{p+1}_{[\alpha,i,j,k]} \) and is calculated as

\[
\bar{J}_{\nu}^{p+1} = \sum_{i} \frac{N_{x}}{\Delta x} \left( \sum_{\alpha} q_{\alpha} m_{\nu}^{p+1}_{[\alpha,i,j,k]} \right) / \Delta x.
\]

4. Discrete conservation strategy for charge, momentum, and energy

As we saw in Sec. \( 2.2 \) there are certain symmetries of the continuum equations that must be satisfied in order to conserve charge, momentum, and energy. For an arbitrary discretization, these symmetries will pose conflicting constraints. As a result, it will not generally be possible to satisfy all of them simultaneously unless we design our discretization such that it includes elements that ensure these properties. In the following development, we will present the discrete definitions of the constraints \( (\xi, \alpha, \gamma_q, \gamma_x) \) that will enforce the symmetries discussed in Sec. \( 2.2 \) in the discrete system. For detailed derivations of these constraints, interested readers are referred to Ref. \( (28) \) and Appendix C.
4.1. Discrete definition of $\gamma_t$ and $\gamma_x$

In Sec. 2.2, we saw that there are certain continuum identities [Eqs. (13) and (14)] which must be satisfied regarding the inertial terms coming from the velocity-space transformation. In the discrete, these are used to define the nonlinear constraint functions $\gamma_t$ and $\gamma_x$. From Eq. (13), to obtain discrete momentum conservation, $\gamma_t$ must satisfy

$$\left\{ v^p_{\alpha,i,j,k} \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k} + c^p \tilde{p}_{\alpha,i,j,k} + c^{p-1} \tilde{p}_{\alpha,i,j,k}}{\Delta t^p} \right\}_{\delta \vec{b}} - \left\{ 1, \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k} + c^p \tilde{p}_{\alpha,i,j,k} + c^{p-1} \tilde{p}_{\alpha,i,j,k}}{\Delta t^p} \right\}_{\delta \vec{b}} = 0,$$

while $\gamma_x$ must satisfy

$$\left\{ v^p_{\alpha,i,j} - v^p_{\alpha,i+1,j} \frac{1}{\Delta x} v^p_{\alpha,i+\frac{1}{2},i+\frac{1}{2},j} \eta_{\|,eff} \right\}_{\delta \vec{b}} - \left\{ \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k}}{2v_{\alpha,i}^p} \delta \vec{b} \cdot \left[ \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k}}{2} \delta x (v^p_{i+\frac{1}{2}}) \right]_{\delta \vec{b}} - \left\{ \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k}}{2v_{\alpha,i+1}^p} \delta \vec{b} \cdot \left[ \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k}}{2} \delta x (v^p_{i+1}) \right]_{\delta \vec{b}} = 0. \right.$$ (32)

To obtain discrete energy conservation, according to Eq. (14) $\gamma_t$ must satisfy

$$\left\{ \frac{1}{2} \left( v^p_{\alpha,i,j,k} \right)^2 \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k} + c^p \tilde{p}_{\alpha,i,j,k} + c^{p-1} \tilde{p}_{\alpha,i,j,k}}{\Delta t^p} \right\}_{\delta \vec{b}} - \left\{ 1, \frac{c^{p+1} \tilde{p}_{\alpha,i,j,k} + c^p \tilde{p}_{\alpha,i,j,k} + c^{p-1} \tilde{p}_{\alpha,i,j,k}}{\Delta t^p} \right\}_{\delta \vec{b}} = 0,$$

while $\gamma_x$ must satisfy

$$\left\{ \frac{1}{2} \left( v^p_{\alpha,i,j,k} \right)^2 \frac{1}{\Delta x} v^p_{\alpha,i+\frac{1}{2},i+\frac{1}{2},j} \eta_{\|,eff} \right\}_{\delta \vec{b}} - \left\{ \frac{1}{2} \left( v^p_{\alpha,i,j,k} \right)^2 \frac{1}{2v_{\alpha,i}^p} \delta \vec{b} \cdot \left[ \frac{1}{2} \delta x (v^p_{i+\frac{1}{2}}) \right]_{\delta \vec{b}} - \left\{ \frac{1}{2} \left( v^p_{\alpha,i+1,j,k} \right)^2 \frac{1}{2v_{\alpha,i+1}^p} \delta \vec{b} \cdot \left[ \frac{1}{2} \delta x (v^p_{i+1}) \right]_{\delta \vec{b}} = 0. \right.$$ (34)

The constraint functions $\gamma_t$ and $\gamma_x$ are expanded in velocity-space basis functions (in this work we use a Fourier representation). Equations (13)–(14) are enforced by solving a constrained minimization problem on the Fourier amplitudes of $\gamma_t$ and $\gamma_x$. Details on the approach can be found in Ref. [28]. Note that $\gamma_x$ depends on $\xi$ through $\tilde{v}_{\|,\alpha,eff}$, and so must be calculated after $\xi$ is obtained. Together, these constraint functions ensure that the integration by parts and product rule which produce Eqs. (13)–(14) are upheld discretely.
4.2. Discrete definition of $\xi$, $\phi$, and $\gamma_q$

The constraint function $\xi$ is defined by

$$\xi^{p+1}_{\alpha,i+\frac{1}{2}} = \frac{\eta^{p+1}_{\alpha,i+\frac{1}{2}} - \eta^{p}_{\alpha,i+\frac{1}{2}}}{\Gamma^{p+1}_{\xi,\alpha,i+\frac{1}{2}}}.$$  (36)

The quantity $\eta^{p+1}_{\alpha,i+\frac{1}{2}}$ is defined in Eq. (30), and the discrete moments

$$\eta^{p+1}_{\alpha,i+\frac{1}{2}} = \frac{1}{m_{\alpha}} \left( m_{\alpha} v^{*}_{\alpha,i+\frac{1}{2}} \left( \bar{u}_{\parallel,i+\frac{1}{2}} + \hat{u}^{*}_{\alpha,i+\frac{1}{2}} \right) \left( \bar{p}^{p+1}_{\alpha} \right)_{i+\frac{1}{2},j,k} \right),$$  (37)

$$\Gamma^{p+1}_{\xi,\alpha,i+\frac{1}{2}} = \frac{1}{m_{\alpha}} \left( m_{\alpha} v^{*}_{\alpha,i+\frac{1}{2}} \left( \bar{u}_{\parallel,i+\frac{1}{2}} + \hat{u}^{*}_{\alpha,i+\frac{1}{2}} \right) \left( \bar{p}^{p+1}_{\alpha} \right)_{i+\frac{1}{2},j,k} \right),$$  (38)

are obtained from the fluxes in terms (a) and (c) in Eq. (22). The action of the constraint function $\xi$ is to ensure that Gauss’s law is upheld [see Eq. (15)], and is generally described as the “charge-conserving” constraint.

The constraint functions $\phi$ and $\gamma_q$ are split in velocity space using the following convention:

$$\phi^{p+1}_{\alpha,i,j+\frac{1}{2}} = \begin{cases} \phi^{+p+1}_{\alpha,i} & \text{if } v^{\parallel}_{\alpha,i,j+\frac{1}{2}} \geq 0 \\ 1 & \text{otherwise} \end{cases}$$

$$\gamma^{p+1}_{q,\alpha,i,j+\frac{1}{2}} = \begin{cases} \gamma^{-p+1}_{q,\alpha,i} & \text{if } v^{\parallel}_{\alpha,i,j+\frac{1}{2}} \geq 0 \\ 1 & \text{otherwise} \end{cases}.$$  (39)

The quantities $\phi^{+p+1}_{\alpha,i}$ and $\gamma^{-p+1}_{q,\alpha,i}$ are thus co-defined by the 2 $\times$ 2 linear system

$$\begin{bmatrix} n^{+p+1}_{\alpha,i} & n^{-p+1}_{\alpha,i} \\ u^{+p+1}_{\alpha,i} & u^{-p+1}_{\alpha,i} \end{bmatrix} \begin{bmatrix} \phi^{+p+1}_{\alpha,i} + 1 \\ \gamma^{-p+1}_{q,\alpha,i} + 1 \end{bmatrix} = \begin{bmatrix} \frac{e_{\alpha}}{m_{\alpha} N_{\nu p}} \left( \bar{u}^{p+1}_{\alpha,i} - \bar{m}_{\alpha} \right) \frac{E^{p+1}_{\alpha,i} + u^{p}_{\alpha,i}}{\delta_{d} E^{p+1}_{\alpha,i}} \frac{E^{p+1}_{\alpha,i} + u^{p}_{\alpha,i}}{\delta_{d} (E^{2}_{\alpha,i})} \end{bmatrix},$$  \begin{equation} (40) \end{equation}

which is well-posed (see Appendix E) and may be easily inverted analytically to calculate $\phi$ and $\gamma_q$ independently. In the preceding, we defined the discrete number densities

$$n^{p+1}_{\alpha,i} \equiv \begin{bmatrix} 1, & f^{p+1}_{\alpha,i,k} \end{bmatrix}_{\delta_{d} \bar{u}} \\ \pi^{p+1}_{\alpha,i} \equiv \begin{bmatrix} f^{p}_{\alpha,i,k} \bar{u}^{p}_{\alpha,i,j} \end{bmatrix}_{\delta_{d} \bar{u}} - \begin{bmatrix} f^{p+1}_{\alpha,i,k} \bar{u}^{p+1}_{\alpha,i,j} \end{bmatrix}_{\delta_{d} \bar{u}},$$  \begin{equation} (42) \end{equation}

which come from the direct $f^{0}_{\alpha}$ moment of $\bar{f}_{\alpha}$, and the $v^{p}_{\parallel}$ moment of the electrostatic acceleration operator, respectively. We also defined the “upper” and “lower” densities

$$n^{+p+1}_{\alpha,i,j} = \begin{bmatrix} f^{p+1}_{\alpha,i,j} \bar{u}^{p}_{\alpha,i,j} \end{bmatrix}_{\delta_{d} \bar{u}} \frac{1}{\Delta_{\bar{u}}} \text{central} \begin{bmatrix} \bar{u}^{p+1}_{\alpha,i,j} & \bar{u}^{p+1}_{\alpha,i,j} \end{bmatrix} \Delta \bar{u} \text{ where } v^{\parallel}_{\alpha,i,j+\frac{1}{2}} \geq u^{p}_{\alpha,i},$$  \begin{equation} (43) \end{equation}

$$n^{-p+1}_{\alpha,i,j} = \begin{bmatrix} f^{p+1}_{\alpha,i,j} \bar{u}^{p}_{\alpha,i,j} \end{bmatrix}_{\delta_{d} \bar{u}} \frac{1}{\Delta_{\bar{u}}} \text{central} \begin{bmatrix} \bar{u}^{p+1}_{\alpha,i,j} & \bar{u}^{p+1}_{\alpha,i,j} \end{bmatrix} \Delta \bar{u} \text{ where } v^{\parallel}_{\alpha,i,j+\frac{1}{2}} \leq u^{p}_{\alpha,i},$$  \begin{equation} (44) \end{equation}
which come from the appropriate $m_{\alpha}v_{\parallel}^2$ “half moments” of the pseudo-operators associated with $\phi$ and $\gamma_q$, as well as the upper and lower momenta

$$
\begin{align*}
nu_{\parallel,\alpha,i}^{+,p+1} & \equiv \left( \frac{1}{2} \left( v_{\alpha,i,j,k}^p \right)^2 \right) \left[ \frac{1}{\nu_{\alpha,i}} \frac{1}{\Delta v_{\parallel}} \left( \hat{f}_{\alpha}^{p+1} \right)_{i,j+\frac{1}{2},k} - \left( \hat{f}_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k} \right] \delta \hat{\nu} \quad \text{where } v_{\parallel,\alpha,i,j+\frac{1}{2}} \geq v_{\parallel,\alpha,i}^{p+1}, \\
nu_{\parallel,\alpha,i}^{-,p+1} & \equiv \left( \frac{1}{2} \left( v_{\alpha,i,j,k}^p \right)^2 \right) \left[ \frac{1}{\nu_{\alpha,i}} \frac{1}{\Delta v_{\parallel}} \left( \hat{f}_{\alpha}^{p+1} \right)_{i,j+\frac{1}{2},k} - \left( \hat{f}_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k} \right] \delta \hat{\nu} \quad \text{where } v_{\parallel,\alpha,i,j+\frac{1}{2}} \leq v_{\parallel,\alpha,i}^{p+1},
\end{align*}
$$

(45)

(46)

from the $\frac{1}{2}m_{\alpha}v_{\parallel}^2$ half moments of the same operators. The constraint functions $\phi$ and $\gamma_q$ together act to enforce the symmetries in Eqs. (16) and (17), which produce momentum and energy conservation.

The nonlinear constraint function approach has been employed previously for actively enforcing conservation for the Vlasov-Ampère system \cite{20, 27} with a symplectic time integration scheme as well as for the Vlasov-Fokker-Planck system with a velocity-space adaptive transformation \cite{11, 28}. Here, this approach has been applied to the Vlasov-Ampère system \cite{20, 27} with a symplectic time integration scheme as well as for the Vlasov-Fokker-Planck system \cite{11, 28}. Here, we further point out that all of the constraint functions $(\gamma_t, \gamma_x, \xi, \phi, \gamma_q)$ are calculated locally in configuration space, and are almost entirely independent of one another. The single exception is the dependence of $\gamma_x$ on $\xi$ through the quantity $v_{\parallel,\text{eff}}$, which is satisfied simply by calculating $\xi$ before $\gamma_x$.

5. Solving the discretized Vlasov-Ampère system

To solve the discretized Vlasov-Ampère system, we use the high-order/low-order (HOLO) acceleration strategy \cite{23}. HOLO is an approach for accelerating the nonlinear convergence of the HO Vlasov-Ampère system, which has been successfully used to solve the Vlasov–Ampère and Vlasov-Fokker-Planck–Ampère systems as well as a variety of other problems \cite{13, 20, 23, 27}.

5.1. Formulation, discretization, and solution of the LO system

In our context, the LO equations (moments of the species’ Vlasov equations) are used to provide a well-informed guess for the electric field $E_{\parallel}$, which results in fast nonlinear convergence of the original Vlasov-Ampère system. The LO moment-Ampère system allows for the stiff time-scale, collective physics (e.g., plasma waves) to be efficiently captured on a lower-dimensional system. A key component of the strategy is the enslavement of the discretization error and any missing physics in the LO system through discrete consistency terms. This ensures that the LO and HO moments agree exactly upon numerical convergence.

To obtain the LO quantities and their respective equations, we take the appropriate velocity space moments of the Vlasov equation:

$$
\langle \cdot, \cdot \rangle_{\hat{\phi}} \equiv 2\pi \int_{-\infty}^{\infty} d\hat{v}_{\parallel} \int_{0}^{\infty} \hat{v}_{\perp} d\hat{v}_{\perp} \langle \cdot, \cdot \rangle.
$$

(47)

The evolution of $n_{\alpha}$ and $nu_{\parallel,\alpha}$ are described by the corresponding moments of the Vlasov equation, Eq. (9):

$$
\begin{align*}
\langle 1, Vlasov \rangle_{\hat{\phi}} & = -\partial_t n_{\alpha} + \partial_x \left( nu_{\parallel,\alpha} \right) = 0, \\
\langle v_{\parallel}, Vlasov \rangle_{\hat{\phi}} & = -\partial_t \left( nu_{\parallel,\alpha} \right) + \partial_x S_{\parallel,\alpha}^{(2)} - \frac{q_{\alpha}}{m_{\alpha}} E_{\parallel} = 0.
\end{align*}
$$

(48)

(49)

In Eq. (49), the quantity $S_{\parallel,\alpha}^{(2)}$ is the parallel-parallel component of the total stress tensor (i.e., the $v_{\parallel}^2$ moment of $\hat{f}_{\alpha}$).

Thus, the LO system consists of the moment equations and Ampère’s equation:
moments to the LO system, the density-normalized total stress tensor from the HO system is used, error (and any missing physics) of the LO system to the HO system. Note, that to provide a closure of the higher-order quantities, the discrete consistency terms, \( \eta_{n_{\alpha,i}} \) as definition for the discrete averaged current, \( \nu_{\alpha,i} \) is the density linearly interpolated to cell faces. We note here that for the HOLO system, we use a slightly different configuration space index, \( \alpha \), and electric field, \( E_{\alpha,i}^{\text{LO}} \), at cell faces. The discrete form of the LO system is

\[
R_{n_{\alpha,i}}^l \equiv \frac{c p_{1+1,m_{\alpha,i}^{\text{LO},p+1,l}} + c p_{p_{\alpha,i}^{\text{HO},p}} + c p_{p_{\alpha,i}^{\text{HO},p-1}}}{\Delta t} + \frac{n_{\alpha,i}^{\text{HO},p,l} - n_{\alpha,i}^{\text{LO},p-1}}{\Delta x} \eta_{n_{\alpha,i}} = 0,
\]

\[
R_{n_{\alpha,i}^{\text{HO},p+1,l}}^l \equiv \frac{c p_{1+1,m_{\alpha,i}^{\text{LO},p+1,l}} + c p_{p_{\alpha,i}^{\text{HO},p}} + c p_{p_{\alpha,i}^{\text{HO},p-1}}}{\Delta t} + \frac{n_{\alpha,i}^{\text{HO},p+1,l} - n_{\alpha,i}^{\text{LO},p-1}}{\Delta x} \eta_{n_{\alpha,i}} = 0,
\]

\[
R_{E_{\alpha,i}^{\text{LO},p+1,l}}^l \equiv \frac{c p_{1+1,m_{\alpha,i}^{\text{LO},p+1,l}} + c p_{p_{\alpha,i}^{\text{HO},p}} + c p_{p_{\alpha,i}^{\text{HO},p-1}}}{\Delta t} + \frac{n_{\alpha,i}^{\text{HO},p+1,l} - n_{\alpha,i}^{\text{LO},p-1}}{\Delta x} \eta_{E_{\alpha,i}^{\text{LO},p+1,l}} = 0.
\]

In Eqs. \((51)\) and \((52)\), we have introduced the HO consistency terms, \( \eta_{n_{\alpha,i}}^{\text{HO}} \) and \( \eta_{n_{\alpha,i}}^{\text{HO},p+1,l} \), which enslave the truncation error (and any missing physics) of the LO system to the HO system. Note, that to provide a closure of the higher-order moments to the LO system, the density-normalized total stress tensor from the HO system is used,

\[
\langle \nu_{\alpha,i}^{\text{LO},p+1,l} \rangle_{\text{HO}}^{\text{HO},p+1,l} = \frac{\langle \nu_{\alpha,i}^{\text{LO},p+1,l} \rangle_{\text{HO}}^{\text{HO},p+1,l}}{\langle 1, f_{\alpha} \rangle_{\text{HO}}}.
\]

The corresponding term in Eq. \((52)\) exposes the stiff isothermal wave in the LO system [13, 20].

The LO system of the continuity and momentum conservation equations plus Ampère’s equation is discretized on a staggered finite-difference grid, where we define the density, \( n_{\alpha,i}^{\text{HO},p+1,l} \), at cell centers and the particle number density flux, \( n_{\alpha,i}^{\text{LO},p+1,l} \), and electric field, \( E_{\alpha,i}^{\text{LO},p+1,l} \), at cell faces. The discrete averaged current, \( \nu_{\alpha,i}^{\text{LO},p+1,l} \), is the parallel-parallel component of the cell-center HO density-normalized total stress tensor. We note here that for the HOLO system, we use a slightly different definition for the discrete averaged current, \( \nu_{\alpha,i}^{\text{LO},p+1,l} \), than in Eq. \((31)\), based on the cell-face parallel LO particle flux density:

\[
\nu_{\alpha,i}^{\text{LO},p+1,l} = \sum_{\alpha} \langle \nu_{\alpha,i}^{\text{LO},p+1,l} \rangle_{\text{HO}}^{\text{HO},p+1,l} - \langle 1, f_{\alpha} \rangle_{\text{HO}}^{\text{HO},p+1,l} = 0.
\]

The discrete consistency terms, \( \eta_{n_{\alpha,i}}^{\text{LO},p+1,l} \) and \( \eta_{n_{\alpha,i}^{\text{LO},p+1,l}} \), are defined by introducing HO moments into the LO equations as

\[
\eta_{n_{\alpha,i}}^{\text{LO},p+1,l} = \frac{c p_{1+1,m_{\alpha,i}^{\text{LO},p+1,l}} + c p_{p_{\alpha,i}^{\text{HO},p}} + c p_{p_{\alpha,i}^{\text{HO},p-1}}}{\Delta t} + \frac{n_{\alpha,i}^{\text{HO},p+1,l} - n_{\alpha,i}^{\text{LO},p-1}}{\Delta x} \eta_{n_{\alpha,i}} = 0,
\]
\[
\eta_{nu,u,i+\frac{1}{2}}^l \equiv \frac{c^p + nu_{HO,p+1,l} + c^p nu_{HO,p} + c^p nu_{HO,p-1} + \frac{nu_{HO,p+1,l} S(2)}{\Delta x} - \frac{nu_{HO,p+1,l} E_{LO,p+1,l}}{\Delta x}}{\Delta t^p} - \frac{\frac{q_{\alpha}}{m_{\alpha}} \eta^{HO,p+1,l}_{\alpha,i+\frac{1}{2},i} - \frac{\langle v_{\parallel;i,j}, R^{HO,\alpha}_{\delta v,i} \rangle}{2}}{\eta^{HO,p+1,l}_{\alpha,\alpha,i} - \frac{\langle v_{\parallel;i,j}, R^{HO,\alpha}_{\delta v,i+1} \rangle}{2}} = 0. \quad (59)
\]

The HO quantities are generally defined as the corresponding direct moments of the distribution \( \tilde{f}_{\alpha,i,j,k} \). The exception is the cell-face HO particle flux density used in the LO system, which is taken to be the same as the flux which forms the current for Ampère’s equation,

\[
nu_{\alpha,i} \equiv \eta^{nu}_{\alpha,i+\frac{1}{2}},
\]

where \( \eta^{nu} \) is defined in Eq. (30). This eliminates the need for a HO consistency term in the LO system for Ampère’s equation.

The coupled LO system of fluid moments and Ampère’s equation is solved with Anderson accelerated nonlinear quasi-Newton iteration [38,39]. The system is preconditioned with a direct solution of the linearized moment equations, with continuity, Eq. (54), and Ampère’s equation, Eq. (56), eliminated through substitution into the momentum equation, Eq. (55). The linearized system of equations then becomes

\[
\frac{c^p + \delta n_{\alpha,i} + \delta nu_{\alpha,i+\frac{1}{2}} - \delta nu_{\alpha,i-\frac{1}{2}}}{\Delta t^p} = -R^l_{nu,i}, \quad (60)
\]

\[
\frac{c^p + \delta n_{\alpha,i+\frac{1}{2}}}{\Delta t^p} + \frac{\delta n_{\alpha,i+1}}{\Delta x} = -R^l_{nu,i+\frac{1}{2}}. \quad (61)
\]

After substitution of Eqs. (60) and (62) into Eq. (61) for \( \delta n_{\alpha} \) and \( \delta E \), respectively, the system reduces to a single equation for \( \delta n_{\alpha,i+\frac{1}{2}} \) at cell faces, coupled in space and across species. The resulting linear system is solved with multigrid, with \( \delta n_{\alpha,i} \) and \( \delta E_{\alpha,i+\frac{1}{2}} \) found directly from Eqs. (60) and (62) after obtaining the solution for \( \delta n_{\alpha,i+\frac{1}{2}} \). To further accelerate HOLO convergence, an additional layer of Anderson acceleration wrapped around the outer HOLO iteration is applied to the LO solution similar to what was considered in Ref. [40].

5.2. Discretization and solution of the HO system

The HO system is discretized essentially as presented in Sec. [3] with the result reproduced here to highlight the coupling with the LO system:

\[
R^l_{f,\alpha,i,j,k} \equiv \left\{ \begin{array}{l}
\frac{c^p + \tilde{f}_{\alpha,i,j,k}^p + c^p \tilde{f}_{\alpha,i,j,k}^p + c^p \tilde{f}_{\alpha,i,j,k}^{-1}}{\Delta t^p} + \delta_x \left[ v^p_{\alpha,j,i} \frac{(\tilde{f}_{\alpha,i,j,k})^v_{i,j} v_{i,j}^p}{\Delta t^p} \right] + \frac{q_{\alpha}}{m_{\alpha}} E^{LO,p+1,l}_{\alpha,i} + \frac{q_{\alpha}}{m_{\alpha}} \delta v_{\alpha,i} \left[ \left( f^{p+1,l}_{\alpha,i} - q_{\alpha} E_{\alpha,i} \right) \right] \\
\delta_x \left[ q_{\alpha} \tilde{f}_{\alpha,i,j,k}^p \left( \tilde{f}_{\alpha,i,j,k}^p \right) \right] + \delta_v \left[ \tilde{f}_{\alpha,i,j,k}^p \left( \tilde{f}_{\alpha,i,j,k}^p \right) \right] + \delta_v \left[ \tilde{f}_{\alpha,i,j,k}^p \left( \tilde{f}_{\alpha,i,j,k}^p \right) \right] \\
- \frac{1}{2} \gamma_{\alpha,i,j,k} \tilde{f}_{\alpha,i,j,k}^p \left( \tilde{f}_{\alpha,i,j,k}^p \right) + \frac{1}{2} \gamma_{\alpha,i,j,k} \tilde{f}_{\alpha,i,j,k}^p \left( \tilde{f}_{\alpha,i,j,k}^p \right) \\
- \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) + \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) \\
- \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) + \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) \\
- \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) + \frac{1}{2} \gamma_{\alpha,i,j} \tilde{f}_{\alpha,i,j}^p \left( \tilde{f}_{\alpha,i,j}^p \right) \\
\end{array} \right\} (v^p_{\alpha,i,j,k})^2 \Delta t^p = 0, \quad (63)
\]
Algorithm 1: HOLO solution for VA system

Initialize HOLO iteration index \( (l = 0) \);
Initialize outer HO residual \( (\| R^0 \| \tilde{f}) \);
Initialize consistency terms \( (\gamma^l_{n, \alpha}, \gamma^l_{nu||,\alpha}) \);

while HOLO not converged do
    Solve LO system for \( E^{LO,l} \parallel \) from Eqs. (54)–(56);
    Solve HO system for \( \tilde{f}^l_{\alpha} \) from Eq. (63);
    Compute consistency terms \( (\gamma^l_{n, \alpha}, \gamma^l_{nu||,\alpha}) \) from Eqs. (58)–(59);
    Increment HOLO iteration \( (l = l + 1) \);
    Check HOLO convergence \( (\| R^l \| \tilde{f} < \epsilon) \);
end while

Save \( \tilde{f}^{p+1}_{\alpha}, E^{LO,p+1} \parallel \);

where
\[
\tilde{v}^{p+1,l}_{\parallel, \alpha, i,j} = \left( \tilde{v}_{\parallel,j} + \tilde{v}_{\parallel,i,j}^{*,p} \right) + \xi^{p+1,l}_{\parallel, \alpha,i,j} \left( \tilde{v}_{\parallel,j} + \tilde{v}_{\parallel,i,j}^{*,p} \right).
\]
The quantity \( R^l_{\parallel, \alpha,i,j,k} \) is the HO system residual. Note that we have included the superscript, \( l \), for the HOLO iteration index. Observe that the electric field, \( E_{\parallel, \alpha}^{LO} \), in Eq. (63) is obtained from the solution of the LO system, which effectively Picard linearizes the individual Vlasov equations (HO system) in \( \tilde{f}^l_{\alpha} \) and is a key for effective nonlinear convergence acceleration. However the discretization schemes employed in Eq. (63) may still include significant nonlinearities in the advective terms. Thus, the HO system is also solved with Anderson acceleration. For preconditioning, Eq. (63) is linearized in \( \delta f_{\alpha,i} \), with a linear upwind discretization for all operators. The system is then solved with the multigrid-preconditioned Flexible Generalized Minimal RESiduals (FGMRES) method [41].

5.3. HOLO solution algorithm

Thus, the coupled HOLO system is represented by 1) the HO system, which consists a system of the species’ Vlasov equations, Eqs. (63), and 2) the LO system, which consists of the moment equations for each species’ mass and momentum and Ampère’s equation, Eqs. (54)–(56). Algorithm 1 depicts the algorithm for obtaining the HOLO-accelerated solution for \( \tilde{f}^{p+1}_{\alpha}, E_{\parallel, \alpha}^{LO,p+1} \parallel \) from the HO and LO systems. Convergence is measured through the root-mean-square (rms) of the HO residual vector,

\[
\left| R^l_{\parallel, \alpha,i,j,k} \right|_{\text{rms}} = \left( \frac{1}{N_{\alpha} + N_{x} + N_{y} + N_{z}} \sum_{\alpha=1}^{N_{\alpha}} \sum_{i=1}^{N_{x}} \sum_{j=1}^{N_{y}} \sum_{k=1}^{N_{z}} \left( R^l_{\parallel, \alpha,i,j,k} \right)^2 \right)^{\frac{1}{2}}.
\]

Here, the convergence tolerance, \( \epsilon \), is defined as
\[
\epsilon = \epsilon_a + \epsilon_r \left| R^l_{\parallel, \alpha,i,j,k} \right|_{\text{rms}},
\]
where \( \epsilon_a \) is an absolute tolerance and \( \epsilon_r \) is the relative tolerance.

6. Numerical results

In this section, we demonstrate the accuracy, convergence, and conservation properties of our numerical scheme. We do so using several canonical collisionless problems of increasing complexity, ranging from the linear Landau damping to an ion-acoustic shock wave. Unless specified otherwise, for all the problems presented we normalize the particle mass and charge to the electron mass, \( m_e \), and proton charge, \( q_p \), while normalizing the temperature, density, velocity, and time to the reference temperature, \( T_0 \), density, \( n_0 \), speed, \( v_0 = \sqrt{(T_0/m_e)} \), and time-scale, \( \tau_0 = \omega_{p,e}^{-1} \). The initial velocity distributions for each species, \( \alpha \), are assumed to be normalized Maxwellians.
\[ \dot{f}_{M,\alpha} = \frac{n_\alpha}{\pi^{3/2}} \left( \frac{v_{th,\alpha}^*}{n_\alpha} \right)^3 \exp \left[ -\frac{1}{v_{th,\alpha}^2} \left( \frac{v_{th,\alpha}^*}{v_{th,\alpha}^* + \tilde{u}_{\parallel,\alpha} e_{\parallel}} - u_{\parallel,\alpha} e_{\parallel} \right)^2 \right], \]  

(65)

where \( v_{th,\alpha} = \sqrt{\frac{2T_\alpha}{m_\alpha}} \). The initial electric field, \( E_{\parallel,0} \), is determined from the solution of Poisson’s equation with the initial charge density:

\[ -\epsilon_0 \frac{\partial^2 \Phi_0}{\partial x^2} = \sum_\alpha q_\alpha n_\alpha, \]

\[ E_{\parallel,0} = -\frac{\partial \Phi_0}{\partial x}. \]

A realistic proton-electron mass ratio \( m_i/m_e = 1836 \) is used for all cases. Unless otherwise specified, the relative nonlinear convergence tolerance is \( \epsilon_r = 10^{-4} \), while the absolute tolerance is set to a low value \( \epsilon_a = 10^{-14} \) to avoid interference with the relative convergence (see Sec. 5.3).

6.1. Landau damping

The linear and nonlinear electron Landau damping tests show the ability of the solver to capture fine collisionless features in the phase space. For this problem, the rate of oscillation and decay of the electric field energy is determined by the dispersion relation,

\[ 1 + \frac{1}{k^2} \left[ 1 + \frac{\omega}{\sqrt{2k}} Z \left( \frac{\omega}{\sqrt{2k}} \right) \right] = 0, \]

(66)

which determines the complex frequency \( \omega = \omega_r - i\gamma \) for a given wavenumber \( k \). The function \( Z \) is the plasma dispersion function for a Maxwellian [42].

6.1.1. Linear Landau damping

To initiate the linear Landau damping in an electron-proton plasma, we impose a sinusoidal density perturbation on electrons with wavenumber, \( k\lambda_D = 0.5 \), and amplitude, \( \delta n = 0.01 \). We expect it to decay at a linear rate of \( \gamma = -0.155 \) [20, 43]. Both species have the same initial temperature, \( T_0 = 1 \), bulk velocity, \( u_{\parallel,0} = 0 \), and unperturbed density, \( n_0 = 1 \). The simulation was performed on the mesh \( N_x = 32 \), \( N_{v_\parallel} = 512 \), \( N_{v_\perp} = 32 \), with an average time-step of \( \Delta t = 0.1\omega_{pe}^{-1} \). The velocity-space domain is \( \tilde{v}_\parallel \in [-6, +6], \tilde{v}_\perp \in [0, 5] \). The offset velocity for both species is \( u_{\parallel,0}^* = 0 \), while the species normalization reference speeds are \( v_{e,0}^* = \sqrt{\frac{2T_0}{m_e}}, v_{i,0}^* = \sqrt{\frac{2T_0}{m_i}} \). The configuration space domain size is \( L_x = 4\pi \). From Fig. 1, we see that the rate of decay matches the linear theory well.

Figure 1: Decay (\( \gamma = -0.155 \)) of the electric field energy for the linear Landau damping test.
6.1.2. Numerical convergence of the method

To demonstrate that the discretized governing equations – with the nonlinear constraint functions and pseudo operators that enforce conservation – achieve our desired level of accuracy, we perform a convergence study in time and space. Convergence is measured by computing the \( L^2 \) norm, \( L^E,\Delta \equiv \sqrt{\sum_i (E^\Delta,i - E^\Delta,\text{ref},i)^2} \), of the difference in the electric field for each solution relative to a reference solution \( E^\Delta,\text{ref} \) obtained with a small time-step or a high resolution in the configuration or velocity space.

For the convergence studies, a relative nonlinear convergence tolerance of \( \epsilon_r = 10^{-12} \) was used to resolve the difference in truncation error at small time-steps and fine-grid resolution.

Figure 2 shows convergence with temporal (left, with a reference time-step of \( \Delta t = 3.90625 \times 10^{-3} \)), and a mesh of \( N_x = 32, N_{v_\parallel} = 512, N_{v_\perp} = 32 \), configuration space (center, with a reference mesh of \( N_x = 2048 \), using a time-step \( \Delta t = 0.1 \), with a velocity-space mesh of \( N_{v_\parallel} = 512, N_{v_\perp} = 32 \), and velocity space (right, with a reference mesh of \( N_{v_\parallel} = 4096, N_{v_\perp} = 2048 \), using a time-step of \( \Delta t = 0.1 \), and a configuration-space mesh of \( N_x = 32 \) resolutions). The maximum simulation time was \( t_{\text{max}} = 1 \) for configuration and velocity-space convergence, and \( t_{\text{max}} = 10 \) for the temporal convergence. As can be seen, at least second-order convergence rates are observed for all the independent variables.

6.1.3. Nonlinear Landau damping

To simulate nonlinear (strong) Landau damping, we again chose \( k\lambda_D = 0.5 \), but increased the electron density perturbation magnitude to \( \delta n = 0.5 \). The simulation was performed on a mesh of \( N_x = 256, N_{v_\parallel} = 512, N_{v_\perp} = 32 \), and the initialization was otherwise identical to the linear Landau damping case. According to the literature this should produce an initial decay and a subsequent recurrence with rates of \( \gamma_1 = -0.292 \) and \( \gamma_2 = 0.0815 \), respectively. As we see in Fig. 3, the decay and growth of the electric field energy show excellent agreement with other published results for this problem [17, 20].

6.2. Two-stream instability

The electron-electron two-stream instability simulation [44] is initialized as two relatively cold, counterstreaming Maxwellian electron beams, each with the bulk velocity \( \pm v_b \), and with the thermal speed \( v_{th,b} \ll v_b \), against a neutralizing background of stationary ions. The dispersion relation for this problem is

\[
1 + \frac{\omega_p^2}{k^2 v_{th,b}^2} [2 + \zeta_+ Z (\zeta_+) + \zeta_- Z (\zeta_-)] = 0,
\]

(67)

where

\[
\zeta_{\pm} = \frac{\omega \mp kv_b}{kv_{th,b}},
\]

and \( \omega_p,b \) is the beam plasma frequency. In the limit of \( v_{th,b} \to 0 \), Eq. (67) becomes
The mesh is for thermalized beams (simulations (some critical ratio near 1 γ system to become less unstable (i.e., v
However, for thermalized beams there will be some deviation, and we expect that as the ratio electrons have an initial offset velocity of v

For our simulation, we use electron beam densities of n0 = 0.5, beam velocities vb = ±0.1 and beam thermal velocities vth,b/vb = [0.15, 0.3, 0.5, 0.65, 0.8]. The electron-beam densities are perturbed sinusoidally with wavenumber k = 2π/Lx and magnitude δn = 0.00005. The domain size is Lx = 1. The velocity-space domain is ⃗v∥ ∈ [−4, +4] for vth,b/vb = 0.15, ⃗v∥ ∈ [−5, +5] for vth,b/vb = 0.3, and ⃗v∥ ∈ [−6, +6] for vth,b/vb ≥ 0.5, with ⃗v⊥ ∈ [0, 5]. The electrons have an initial offset velocity of u∥,e = 0 and normalizing speed of v∗,e = [0.083, 0.087, 0.096, 0.10, 0.114]. The mesh is Nx = 128, Ny = 512, Nv = 32. In Fig. 4 we perform a sweep in beam thermal velocity ratio with Δt = 0.25ω−1 pe, while in Fig. 5 we choose vth,b/vb = 0.5 and use Δt = [0.25, 1.0, 2.0]ω−1 pe.

Based on the delta-function dispersion relation, Eq. (68), the growth rate of electric field energy is γ = 0.353ωp,b. However, for thermalized beams there will be some deviation, and we expect that as the ratio vth,b/vb increases the system to become less unstable (i.e., γ will decrease). Indeed, in Fig. 4 we see that if we increase vth,b/vb towards some critical ratio near 1, the growth rate decreases precipitously. As shown in Table 1, growth rates calculated from simulations (γsim) agree very well with the growth rates obtained from a numerical solution of the dispersion relation for thermalized beams (γnum) – details of this analysis may be found in Appendix F. In Fig. 5 we show that there is little change in the simulated electric field growth rate as we vary the time-step size.

### 6.3. Ion-acoustic shock wave

The final test is the ion-acoustic shock wave (IASW [45]). This problem is an excellent test of the scheme because it exhibits strongly nonlinear multi-scale behavior. In this problem, the dynamical time-scale of the system is many times larger than the inverse electron plasma frequency, and so the simulation provides a stringent test of the HOLO algorithm to step over ω−1 pe time-scales, which do not significantly contribute to the system evolution (since the evolution is largely ambipolar)

For this problem, we normalize particle mass to the proton mass, with the electron mass me = 1/1836. We take the Debye length as λD = 1/36, with the system length Lx = 144λD. The problem is initialized with sinusoidally

\[
1 - \frac{1}{(\omega + v_b k)^2} - \frac{1}{(\omega - v_b k)^2} = 0.
\]

(68)

![Figure 3: Initial decay (γ1 = −0.292) and a subsequent recurrence growth (γ2 = 0.0815) of the electric field energy for the nonlinear Landau damping test.](image)

| vth,b/vb | 0.15 | 0.3 | 0.5 | 0.65 | 0.8 |
|----------|------|-----|-----|------|-----|
| γnum/ωpe | 0.3488 | 0.3318 | 0.2734 | 0.1953 | 0.08911 |
| γsim/ωpe | 0.3459 | 0.3291 | 0.2722 | 0.1927 | 0.08745 |
| γsim/γnum | × 100% | −81% | −81% | −44% | −13% | −19% |

Table 1: Numerical solution of two-stream instability growth rate
perturbed ion and electron density profiles

\[ n_{0,i} = 1 + 0.2 \sin(kx), \]

\[ n_{0,e} = 1 + 0.2 \left( 1 - k^2 \lambda_D^2 \right) \sin(kx), \]

and with the same sinusoidal bulk velocity profiles for both species (thus, there is no initial current). The velocity is chosen such that the simulation proceeds in the frame of the shock:

\[ u_{\parallel,0} = -1 + 0.2 \sin(kx). \]

The species temperatures are initially \( T_{0,i} = 0.05, T_{0,e} = 1 \), with the large temperature ratio chosen to avoid electron Landau damping [45]. As a consequence, the ion-acoustic time- and length-scales of the problem are much longer than the inverse plasma frequency \( \omega_{pe}^{-1} \) and the Debye length [14]. The wave number is \( k = \frac{2\pi}{L_x} \). The simulation is performed with a velocity-space domain \( \tilde{v}_\parallel \in [-8, +8], \tilde{v}_\perp \in [0, 5] \), on a mesh of \( N_x = 128, N_{v_\parallel} = 256, N_{v_\perp} = 64 \).

The initial offset velocity of each species is set equal to the bulk velocity, \( u_{\parallel,0} = u_{\parallel,0}^* \), with the initial normalizing speed equal to \( v_{0,i}^* = \sqrt{2T_{0,i}^*}, v_{0,e}^* = \sqrt{2T_{0,e}^*}. \)

The first set of results consider a varying time-step size: \( \Delta t = [1, 10, 100] \omega_{pe}^{-1} \). For this problem, a relative nonlinear convergence tolerance of \( \epsilon_r = 10^{-6} \) was used. At the largest \( \Delta t \) we are stepping over many plasma periods. However, since this problem is not driven by the physics on this time-scale, we do not need to resolve it to correctly capture the solution. Figure 6 shows spatial profiles for the number density of ions and electrons, and the electric field at \( t \approx 5000 \omega_{pe}^{-1} \) for varying time-step sizes. We observe that the solution quality is not significantly affected even at time-steps far larger than the inverse electron plasma frequency (which is itself much larger than the explicit CFL).

Table 2 shows the solver statistics for the simulations at each time-step size (obtained by averaging the number of HOLO iterations for each time-step over the simulation duration), indicating excellent performance even at large \( \Delta t \).

Here we estimate the explicit time-step size as \( \Delta t_{\text{explicit}} = \frac{\Delta x}{v_{\parallel,e,\text{max}}} \). To demonstrate the capabilities of the velocity-space adaptive scheme, we also include in Fig. 6 a contour plot of the ion distribution function integrated over \( v_{\perp} \), \( f_{i,\parallel} \equiv 2\pi \int_{v_{\perp,\text{min}}}^{v_{\perp,\text{max}}} f_i(x, v_{\parallel}, v_{\perp}) v_{\perp} dv_{\perp} \), at \( t \approx 5000 \omega_{pe}^{-1} \) for the case with \( \Delta t = \omega_{pe}^{-1}, \epsilon_r = 10^{-6} \). The velocity-space boundary adapts to variations in the ion bulk velocity, \( u_{\parallel,i} \), and thermal speed, \( v_{th,i} = \sqrt{\frac{2T_{i}}{m_i}} \), as can be clearly seen by the gray background fill of the simulation \( (x, v_{\perp}) \) domain. We can also clearly see the characteristic ‘wave-breaking’ feature of the ion distribution in the velocity space.

In Sec. 4 we discussed the need for enforcing conservation properties in the discrete. Figure 7 shows the error in mass, momentum, and energy conservation and Gauss’s law for the IASW for various time-step sizes. The error is
measured as the absolute value of the difference in a quantity at a given time relative to the initial value,
\[ \left| \frac{\Phi^p - \Phi^0}{\Phi^0} \right|, \]
where \( \Phi \) is the total mass \( \text{TM} \), total momentum \( \text{TP} \), or total energy \( \text{TE} \). Additionally, we calculate the \( L^1 \) norm of the error in the discrete form of Gauss’s law:
\[ |GL|^p = \sum_{i} \epsilon_0 \left( \frac{E^p_{\parallel,i+\frac{1}{2}} - E^p_{\parallel,i-\frac{1}{2}}}{\Delta x_i} \right) - \sum_{\alpha} q_{\alpha} n_{\alpha,i}^p. \]

We see that in all the cases, the conservation error is affected by the different time-step sizes, but is kept well within acceptable levels.

Next, we investigate the effects of the relative nonlinear convergence tolerance, \( \epsilon_r \), on the magnitude of the conservation error. Here, we use a time-step of \( \Delta t = \omega_{pe}^{-1} \), and vary the tolerance: \( \epsilon_r = [10^{-4}, 10^{-6}, 10^{-8}] \). As we can clearly see in Fig. 8, as the tolerance is tightened the level in the conservation error metrics experiences a commensurate decrease. Further decrease in \( \epsilon_r \) will eventually push the conservation error to the machine roundoff.

6.3.1. Importance of discrete conservation

Here, we present IASW simulation results emphasizing the necessity of the developments presented in Sec. 4. In the Vlasov-Ampère system, as we stated previously, the most critical element of the discrete conservation strategy is
Table 2: HOLO solver statistics for the ion-acoustic shock wave at various time-step sizes

| \( \Delta t/\omega_{pe}^{-1} \) | 1   | 10  | 100 |
|-----------------------------------|-----|-----|-----|
| \( \Delta t/\Delta t_{\text{explicit}} \) | 1.01E + 1 | 1.01E + 2 | 1.01E + 3 |
| HOLO iters                        | 3.5 | 6.2 | 11.3 |

Figure 7: Conservation errors for the ion-acoustic shock wave simulations using various time-step sizes for the total mass (top left), total momentum (top right), total energy (bottom left), and charge from Gauss’ law (bottom right).

ensuring that Gauss’ law is satisfied. Here, we compare the case with \( \Delta t = \omega_{pe}^{-1}, \epsilon_r = 10^{-6} \) from Fig. 7 with an identical case wherein the constraint function \( \xi \) (and its associated pseudo-operator) is eliminated from the discretization – the result is shown in Fig. 9. With all constraints except \( \xi \) active, we see that the charge conservation error metric increases monotonically, which is expected. However, we also observe that the momentum and energy conservation metrics also experience significant increase. The reason for this is that violations of charge conservation give rise to (significant) error in the electric field \( E_\parallel \) [33], which results in unphysical acceleration in the Vlasov equation. This, in turn, results in violations of momentum and energy conservation. In Fig. 10 we see the electric field \( E_\parallel \) at \( t \approx 3100\omega_{pe}^{-1} \). The \( E_\parallel \) for the simulation lacking charge conservation has at this stage significantly deviated. Though not shown here, the solutions for the other moment quantities (e.g., number density, temperature) show significant deviation from the case with charge conservation as well.

We also investigate the effect of neglecting the momentum- and energy-conserving constraints (while maintaining the charge conserving constraint \( \xi \)). Here, we again compare the case with \( \Delta t = \omega_{pe}^{-1}, \epsilon_r = 10^{-6} \) from Fig. 7 to a case with the same parameters, but with only the charge-conserving constraint function \( \xi \) active in the discretization (thereby failing to conserve momentum and energy). Figure 11 shows the results, where we see that indeed the simulation fails to conserve momentum and energy (while Gauss’s law is still maintained), although the failure is not as catastrophic as when neglecting charge conservation. However, we emphasize that the methods developed in this work, which explores
only the Vlasov-Ampère system, will ultimately be applied to the arbitrarily collisional Vlasov-Fokker-Planck-Ampère system. As demonstrated in Ref. [6], failing to enforce conservation self-consistently for only the Vlasov portion of the system can lead to extremely large errors in the overall solution.

6.3.2. Importance of keeping the discrete averaged current in Ampère’s equation

In Sec. 2, we presented Ampère’s equation with the spatially-averaged current, \( \bar{j}_\parallel \), which is a necessary solvability constraint to preserve Galilean invariance in a periodic system. In this work, none of the problems presented possess an applied electric field, and thus the spatially averaged electric field, \( \bar{E}_\parallel \), is identically zero at all times. This is clearly seen from the relationship \( \nabla_x \Phi = -E \), which relates the electric field to the electrostatic potential. However, while the average current in the continuum may be zero, we recall that the discrete current, \( j_\parallel \), is based on the particle flux density obtained from the discrete energy moment of the acceleration operator, \( \tilde{n}_\alpha \), which depends, in turn, on the choice of discretization for the acceleration operator for each species. Thus, it is not guaranteed that \( j_\parallel = 0 \) discretely, even if it ought to be so in the continuum (in practice it will be small but finite). In Fig. 12 we compare time traces of the spatially averaged electric field \( \bar{E}_\parallel \),

\[
\bar{E}_\parallel = \frac{N_x}{\sum_i \Delta x} \sum_i \Delta x E_{\parallel, i + \frac{1}{2}},
\]

for two simulations wherein we have either included \( \bar{j}_\parallel \) in Ampère’s equation or neglected it. All other parameters are identical parameters to the \( \Delta t = \omega_{pe}^{-1} \) case in Figs. 6 and 7. We see that there is a significant effect \( \mathcal{O}(10^8) \) on the
value of the discrete average electric field $\langle E_\parallel \rangle$.

7. Conclusions

We have presented a fully conserving, adaptive algorithm for numerically integrating the 1D-2V multi-species Vlasov-Ampère system. The algorithm is applicable for the fully kinetic Vlasov system, with arbitrary species mass ratio, and an arbitrary number of species. The velocity-space adaptivity scheme allows each species’ velocity-space mesh to efficiently capture variations in bulk velocity and temperature. Conservation of the total mass, momentum, and energy, as well as Gauss’s law, are enforced through the introduction of several nonlinear constraint functions, which act to eliminate the truncation error violations of the conservation properties. We emphasize that discrete conservation in our algorithm is achieved with nonlinear discretization operators (e.g., SMART) and BDF2 temporal discretization, and in principle can be used with arbitrary temporal and spatial discretizations. The nonlinear scheme is efficiently solved via a HOLO algorithm, which greatly accelerates the evaluation of the electric field, and exposes stiff time-scales (e.g., the inverse plasma frequency) for effective preconditioning.

The present algorithm was tested with the linear and nonlinear Landau damping, as well as the two-stream instability and ion-acoustic shock wave. For the Landau damping and two-stream instability, we achieved excellent agreement with analytical and previously published numerically obtained rates for growth/decay of the electric field. For the linear Landau damping, we demonstrated that the algorithm achieves second-order convergence in time as well as in the configuration space and the velocity space. For the ion-acoustic shock wave, we demonstrated that the algorithm remains stable when taking time-steps much larger than unimportant fast time-scales (such as the inverse plasma frequency $\omega_{pe}^{-1}$) without affecting the solution and while maintaining a discrete conservation principle. We also
Figure 10: ion-acoustic shock wave solution for electric field $E_\parallel$, at $t \approx 3100\omega_{pe}^{-1}$ for $\Delta t = \omega_{pe}^{-1}$ with (“All”, in blue) and without the charge-conserving nonlinear constraint function $\xi$ active (“no $\xi$”, in red).

demonstrate a commensurate decrease in the discrete conservation metrics when the nonlinear convergence tolerance is tightened – in principle allowing us to reach the limit of machine precision. Further, we demonstrate that without enforcing discrete conservation (particularly for charge conservation), the solution can degrade significantly.

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**Appendix A. Derivation of continuum symmetries for conservation**

**Appendix A.1. Mass & charge conservation**

Mass conservation is demonstrated by taking the $m_\alpha v_0$ moment of Eq. (9):

$$\left\langle m_\alpha, \partial_t \tilde{f}_\alpha \right\rangle_{\tilde{v}} + \left\langle m_\alpha, \partial_x \left( v_\alpha^* \tilde{v} \right) \right\rangle_{\tilde{v}} + \frac{q_\alpha}{m_\alpha v_\alpha^*} E_\parallel \left\langle m_\alpha, \partial_{\tilde{v}} \tilde{f}_\alpha \right\rangle_{\tilde{v}} - \frac{1}{v_\alpha} \left\langle m_\alpha, \nabla_{\tilde{v}} \cdot \left\{ \partial_t (v) + \partial_x (v) v_\alpha^* \right\} \right\rangle_{\tilde{v}} = 0. \quad (A.1)$$

Observing that the first two terms produce the mass density $\left\langle m_\alpha, \tilde{f}_\alpha \right\rangle_{\tilde{v}} = m_\alpha n_\alpha$ and the parallel momentum density $\left\langle m_\alpha, v_\alpha^* \tilde{v} \right\rangle_{\tilde{v}} = m_\alpha n_{\parallel,\alpha}$ while the last two terms are zeros, we obtain the mass conservation equation,

$$m_\alpha \left[ \partial_t n_\alpha + \partial_x n_{\parallel,\alpha} \right] = 0. \quad (A.2)$$

This is straightforward to satisfy in the discrete with appropriate boundary conditions on the distribution $\tilde{f}_\alpha$.

However, we must also be cognizant of the symmetry between Ampère’s and Gauss’s laws and the above statement of mass conservation. If we take Eq. (5) in one dimension we find

$$\partial_t \left( \sum_\alpha \rho_{q,\alpha} \right) + \partial_x \left( \sum_\alpha j_{\parallel,\alpha} \right) = 0, \quad (A.3)$$
where $\rho_{q,\alpha} \equiv q_{\alpha} n_{\alpha}$ and $j_{\parallel,\alpha} \equiv q_{\alpha} n u_{\parallel,\alpha}$. Of course, underlying Eq. (A.3) is simply the summation over all species of Eq. (A.2):

$$\partial_t \left( \sum_{\alpha} \rho_{q,\alpha} \right) + \partial_x \left( \sum_{\alpha} j_{\parallel,\alpha} \right) = \sum_{\alpha} q_{\alpha} \left( \partial_t n_{\alpha} + \partial_x n u_{\parallel,\alpha} \right).$$

Thus, we see that the charge density in Gauss’s law and the current in Ampère’s equation must be proportional to the particle number density and flux in Eq. (A.2).

**Appendix A.2. Momentum conservation**

Momentum conservation is demonstrated by taking the $m_v$ moment of Eq. (9):

$$\left\langle m_{\alpha} v_{\parallel}, \partial_t \tilde{f}_{\alpha} \right\rangle_{\tilde{\varphi}} + \left\langle m_{\alpha} v_{\parallel}, \partial_x \left( v_{\alpha}^* \tilde{v}_{\parallel} \tilde{f}_{\alpha} \right) \right\rangle_{\tilde{\varphi}} + \frac{q_{\alpha}}{m_{\alpha} v_{\alpha}^*} E_{\parallel} \left\langle m_{\alpha} v_{\parallel}, \partial_{\parallel} \tilde{f}_{\alpha} \right\rangle_{\tilde{\varphi}}$$

$$- \frac{1}{v_{\alpha}^*} \left\langle m_{\alpha} v_{\parallel}, \nabla \tilde{\varphi} \cdot \left\{ \left[ \partial_t (v_{\parallel}) + \partial_x (v_{\parallel}) v_{\alpha}^* \right] \tilde{f}_{\alpha} \right\} \right\rangle_{\tilde{\varphi}} = 0.$$
First, we take note of the terms involving temporal derivatives (boxed in blue in Eq. (A.5)), and apply the chain rule with integration by parts (once again applying \( \lim_{\nu \to \pm \infty} f_\alpha = 0 \)):

\[
\left< m_\alpha v_\parallel, \partial_t \tilde{f}_\alpha \right>_{\tilde{\phi}} - \frac{1}{v_\alpha^*} \left< m_\alpha v_\parallel, \nabla_{\tilde{\phi}} \cdot \left\{ \partial_t (v) \tilde{f}_\alpha \right\} \right>_{\tilde{\phi}} = \left< 1, \partial_t \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} \quad \text{with} \quad \left< 1, \partial_t \left( m_\alpha v_\parallel \tilde{f}_\alpha, \partial_t v_\parallel \right) \right>_{\tilde{\phi}} = \frac{1}{v_\alpha^*} \left< 1, m_\alpha \partial_t (v) \tilde{f}_\alpha \cdot \nabla_{\tilde{\phi}} v_\parallel \right>_{\tilde{\phi}}.
\]

(A.6)

In a similar manner, we may inspect the terms in Eq. (A.5) involving spatial derivatives (boxed in red)

\[
\left< m_\alpha v_\parallel, \partial_x \left( v_\alpha^* \tilde{v} \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} - \frac{1}{v_\alpha^*} \left< m_\alpha v_\parallel, \nabla_{\tilde{\phi}} \cdot \left\{ \partial_x (v) \tilde{f}_\alpha \right\} \right>_{\tilde{\phi}} = \left< 1, \partial_x \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} - \left< 1, \partial_x \left( m_\alpha v_\parallel, \partial_x v_\parallel \right) \right>_{\tilde{\phi}} = \frac{1}{v_\alpha^*} \left< 1, m_\alpha \partial_x (v) \tilde{f}_\alpha \cdot \nabla_{\tilde{\phi}} v_\parallel \right>_{\tilde{\phi}}.
\]

(A.7)

Observing that \( \nabla_{\tilde{\phi}} v_\parallel = v_\alpha^* e_\parallel \), we see that the last two terms cancel in both Eq. (A.6) and Eq. (A.7). Together these equations become

\[
\left< m_\alpha v_\parallel, \partial_t \tilde{f}_\alpha \right>_{\tilde{\phi}} + \left< m_\alpha v_\parallel, \partial_x \left( v_\alpha^* \tilde{v} \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} - \frac{1}{v_\alpha^*} \left< m_\alpha v_\parallel, \nabla_{\tilde{\phi}} \cdot \left\{ \partial_t (v) + \partial_x (v) \tilde{v} v_\alpha^* \tilde{f}_\alpha \right\} \right>_{\tilde{\phi}} = \left< 1, \partial_t \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} + \left< 1, \partial_x \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}}.
\]

(A.8)

If we inspect the acceleration term in Eq. (A.5) and observe that \( \partial_{\tilde{\phi}} v_\parallel = v_\alpha^* \), we find

\[
\frac{q_\alpha}{m_\alpha v_\alpha^*} E_\parallel \left< m_\alpha v_\parallel, \partial_t \tilde{f}_\alpha \right>_{\tilde{\phi}} - \frac{q_\alpha}{m_\alpha v_\alpha^*} E_\parallel \left< m_\alpha v_\parallel, \partial_t v_\parallel \tilde{f}_\alpha \right>_{\tilde{\phi}} = -\frac{q_\alpha}{m_\alpha} E_\parallel \left< 1, m_\alpha \tilde{f}_\alpha \right>_{\tilde{\phi}}.
\]

(A.9)

Thus, if we sum over all species, Eq. (A.5) becomes

\[
\sum_\alpha \left[ \left< 1, \partial_t \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} + \left< 1, \partial_x \left( m_\alpha v_\parallel \tilde{f}_\alpha \right) \right>_{\tilde{\phi}} - \frac{q_\alpha}{m_\alpha} E_\parallel \left< 1, m_\alpha \tilde{f}_\alpha \right>_{\tilde{\phi}} \right] = 0.
\]

(A.10)

We may now define \( \left< 1, m_\alpha v_\parallel^2 \tilde{f}_\alpha \right>_{\tilde{\phi}} = S_{2,\parallel,\alpha} \). If we recall Gauss’s law, Eq. (3), we may make a substitution in the acceleration term:

\[
\partial_t P_\parallel + \partial_x S_{2,\parallel} - E_\parallel \epsilon_0 \partial_x E_\parallel = \partial_t P_\parallel + \partial_x \left[ S_{2,\parallel} - \frac{1}{2} \epsilon_0 E_\parallel^2 \right] = 0.
\]

(A.11)
where \( P_\parallel = \sum_\alpha m_\alpha n\|_\alpha \) is the total (parallel) momentum density, \( S_{2,\|} \) is the total (fluid) stress and \( 1/2 \varepsilon_0 E_\|^2 \) is the electrostatic stress. Equation (A.11) is a succinct statement of total momentum conservation – when we integrate over a periodic domain \( L \int_0^L dx \) to obtain the total system momentum we obtain
\[
\partial_t \mathcal{P}_{\|} = 0, 
\]
where \( \mathcal{P}_{\|} = \int_0^L P_{\|} dx \). The key symmetries here are 1) the equivalences in Eqs. (A.6) and (A.7), and 2) the equivalence in Eq. (A.9) of the density arising from the acceleration term to that which appears in the temporal term – i.e., through Gauss’s law in Eq. (A.5). In general, none of these symmetries are guaranteed in the discrete system. Indeed, we see that the second symmetry here involving Gauss’s law and the acceleration operator may directly contradict the charge-conservation requirement leading to Eq. (A.3).

Appendix A.3. Energy conservation

Energy conservation is demonstrated by taking the \( m_\alpha \nu^2 / 2 \) moment of Eq. (9):
\[
\left\langle m_\alpha \frac{1}{2} \nu^2, \partial_t \tilde{f}_\alpha \right\rangle - \frac{1}{v_\alpha} \left\langle \frac{1}{2} \nu^2, \nabla_{\tilde{\nu}} \cdot \{ \partial_t (\nu) \tilde{f}_\alpha \} \right\rangle = \int_1 \partial_t \left( \frac{1}{2} \nu^2 \tilde{f}_\alpha \right) \left\rangle_{\tilde{\nu}} - \left\langle m_\alpha \nu \tilde{f}_\alpha, \partial_t \left( \frac{1}{2} \nu^2 \right) \right\rangle_{\tilde{\nu}} + \frac{1}{v_\alpha} \left\langle 1, m_\alpha \partial_t (\nu) \tilde{f}_\alpha \cdot \nabla_{\tilde{\nu}} \left( \frac{1}{2} \nu^2 \right) \right\rangle_{\tilde{\nu}}, \tag{A.12}
\]
and for the spatial terms:
\[
\left\langle m_\alpha \frac{1}{2} \nu^2, \partial_x (\nu \tilde{f}_\alpha) \right\rangle - \frac{1}{v_\alpha} \left\langle \frac{1}{2} \nu^2, \nabla_{\tilde{\nu}} \cdot \{ \partial_x (\nu) \nu \tilde{f}_\alpha \} \right\rangle = \int_1 \partial_x \left( \frac{1}{2} \nu^2 \tilde{f}_\alpha \right) \left\rangle_{\tilde{\nu}} - \left\langle m_\alpha \nu \tilde{f}_\alpha, \partial_x \left( \frac{1}{2} \nu^2 \right) \right\rangle_{\tilde{\nu}} + \frac{1}{v_\alpha} \left\langle 1, m_\alpha \partial_x (\nu) \nu \tilde{f}_\alpha \cdot \nabla_{\tilde{\nu}} \left( \frac{1}{2} \nu^2 \right) \right\rangle_{\tilde{\nu}}. \tag{A.14}
\]
Here, we observe that \( \nabla_{\tilde{\nu}} \left( \frac{1}{2} \nu^2 \right) = \nu \nabla_{\tilde{\nu}} \), \( \partial_x \left( \frac{1}{2} \nu^2 \right) = \nu \cdot \partial_x \nu \), and \( \partial_t \left( \frac{1}{2} \nu^2 \right) = \nu \cdot \partial_t \nu \). Thus, the last two terms on the right-hand sides of Eqs. (A.13) and (A.14) cancel, and together these equations become
\[
\left\langle m_\alpha \frac{1}{2} \nu^2, \partial_t \tilde{f}_\alpha \right\rangle + \left\langle m_\alpha \frac{1}{2} \nu^2, \partial_x (\nu \tilde{f}_\alpha) \right\rangle - \frac{1}{v_\alpha} \left\langle \frac{1}{2} \nu^2, \nabla_{\tilde{\nu}} \cdot \{ \partial_t (\nu) + \partial_x (\nu) \nu \} \tilde{f}_\alpha \right\rangle = \int_1 \partial_t \left( \frac{1}{2} \nu^2 \tilde{f}_\alpha \right) \left\rangle_{\tilde{\nu}} + \left\langle 1, \partial_x \left( \frac{1}{2} \nu^2 \tilde{f}_\alpha \right) \right\rangle_{\tilde{\nu}} \tag{A.15}
\]
Returning to the acceleration term in Eq. (A.12) and integrating by parts gives
\[
\frac{q_\alpha}{m_\alpha v_\alpha} E_\parallel \left\langle m_\alpha \frac{1}{2} \nu^2, \partial_t \tilde{f}_\alpha \right\rangle = - \frac{q_\alpha}{m_\alpha v_\alpha} E_\parallel \left\langle m_\alpha \nu \tilde{f}_\alpha, \partial_t \nu \left( \frac{1}{2} \nu^2 \right) \right\rangle_{\tilde{\nu}} = - \frac{q_\alpha}{m_\alpha} E_\parallel \left\langle 1, m_\alpha \nu \tilde{f}_\alpha \right\rangle_{\tilde{\nu}} \tag{A.16}
\]
where we utilized the relationship \( \partial_t \nu \left( \frac{1}{2} \nu^2 \right) = v_\nu v_\nu ^\alpha \).

Combining the preceding results and summing over all species \( \alpha \), Eq. (A.12) becomes
\[
\sum_\alpha \left[ \int_1 \partial_t \left( m_\alpha \frac{1}{2} \nu^2 \tilde{f}_\alpha \right) \left\rangle_{\tilde{\nu}} + \int_1 \partial_x m_\alpha \nu \tilde{f}_\alpha \left\rangle_{\tilde{\nu}} - \frac{q_\alpha}{m_\alpha} E_\parallel \left\langle 1, m_\alpha \nu \tilde{f}_\alpha \right\rangle_{\tilde{\nu}} \right] = 0. \tag{A.17}
\]
We note the definitions \( \langle 1, m_\alpha \frac{1}{2} v^2 f_\alpha \rangle_\phi = \epsilon_\alpha \) and \( \langle 1, m_\alpha \frac{1}{2} v^2 v_\parallel f_\alpha \rangle_\phi = S_{3,\parallel,\alpha} \) and, recalling Ampère’s equation, we introduce it in the acceleration term to find

\[
\partial_t U + \partial_z S_{3,\parallel} + E_\parallel \epsilon_0 \partial_t E_\parallel = \partial_x \left[ U + \frac{1}{2} \epsilon_0 E_\parallel^2 \right] + \partial_x S_{3,\parallel} - E_\parallel \pi J_\parallel = 0. \tag{A.18}
\]

Here, \( U \) is the total (fluid) energy density, \( \frac{1}{2} \epsilon_0 E_\parallel^2 \) is the electrostatic energy density, and \( S_{3,\parallel} \) is the total energy flux. Equation (A.18) expresses conservation of the total energy density of the system. Integrating over the periodic domain gives the total energy conservation:

\[
\partial_t U_{\text{tot}} - \pi E_\parallel J_\parallel = \partial_t U_{\text{tot}} = 0.
\]

The \( \pi E_\parallel J_\parallel \) term vanishes in a periodic system with no external electric field. Again, the symmetry of the temporal/spatial inertial terms is a key point. We also note that, in the discrete, the requirements for energy conservation with the inertial terms are not guaranteed to be compatible with those for momentum conservation. Further, we again observe that the second moment of the acceleration term must correspond to the current in Ampère’s equation, which, as we saw in Appendix A.1 must also correspond to the zeroth moment of the advective flux. This once again presents apparently conflicting requirements for discrete conservation.

**Appendix B. Detailed definitions of discrete fluxes**

As we saw in section 3, the transformed Vlasov equation is discretized conservatively as

\[
\delta_t f_{\alpha,i,j,k} + \delta_x \left[ v_{\alpha,i,j}^p \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{j,k} + \frac{q_\alpha}{m_\alpha} E_{\parallel,i,p} \delta_{\parallel,i} \left[ \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{i,j,k} + \delta_{\parallel,j} \left[ \phi_{\alpha,i,j} \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{i,k} + \delta_{\parallel,k} \left[ \gamma_{\alpha,i,j} \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{i,j} = 0. \tag{B.1}
\]

The various fluxes in Eq. (B.1) are defined as follows. The physical configuration-space advection, \( (a) \), is defined as

\[
\delta_x \left[ v_{\alpha,i,j}^p \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{j,k} = v_{\alpha,i,j}^{p,p} \left( v_{\alpha,i,j}^{p,p} + \frac{1}{2} \right) \left( \tilde{v}_{\alpha,i,j} + \frac{1}{2} \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \text{Interp} \left( \tilde{v}_{\alpha,i,j} + \frac{1}{2} \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} , \tilde{f}_{\alpha,i,j} \right)_{i,j,k}. \tag{B.2}
\]

Term \( (b) \) – the velocity-space advection operator due to electric field acceleration – is defined as

\[
\delta_{\parallel,i} \left[ \phi_{\alpha,i,j} \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{j,k} = \frac{q_\alpha}{m_\alpha} E_{\parallel,i,p} \text{Interp} \left( q_\alpha E_{\parallel,i,p} \tilde{f}_{\alpha,i,j} \right)_{i,j,k}. \tag{B.3}
\]

The various fluxes in Eq. (B.1) are defined as follows. The physical configuration-space advection, \( (a) \), is defined as

\[
\delta_x \left[ v_{\alpha,i,j}^p \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{j,k} = v_{\alpha,i,j}^{p,p} \left( v_{\alpha,i,j}^{p,p} + \frac{1}{2} \right) \left( \tilde{v}_{\alpha,i,j} + \frac{1}{2} \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \text{Interp} \left( \tilde{v}_{\alpha,i,j} + \frac{1}{2} \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} , \tilde{f}_{\alpha,i,j} \right)_{i,j,k}. \tag{B.2}
\]

Term \( (b) \) – the velocity-space advection operator due to electric field acceleration – is defined as

\[
\delta_{\parallel,i} \left[ \phi_{\alpha,i,j} \left( \frac{p_{\alpha,i,j} + 1}{p_{\alpha,i,j}} \right) \right]_{j,k} = \frac{q_\alpha}{m_\alpha} E_{\parallel,i,p} \text{Interp} \left( q_\alpha E_{\parallel,i,p} \tilde{f}_{\alpha,i,j} \right)_{i,j,k}. \tag{B.3}
\]
Terms \((c), (d),\) and \((e)\) are the ‘pseudo-operators’ introduced by the inclusion of nonlinear constraint functions, \(\xi_\alpha,\phi_\alpha,\) and \(\gamma_{q,\alpha},\) which act to enforce the conservation symmetries discussed in Sec. 2.2 (see Ref. [20]). Here, we will only discuss their discrete appearance in the numerical implementation of the governing equation. The nature and definitions of these constraint functions and their respective pseudo-operators are discussed Appendix D and Sec. 4. Term \((c)\) is the pseudo-advection operator arising due to the discrete nonlinear constraint function \(\xi_\alpha\) and is defined to be

\[
\left[ \frac{\phi_{\alpha,i}^{p+1}}{\Delta t} + \frac{\psi_{\alpha,j}^{p+1}}{\Delta x} \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} \right]_{i+\frac{1}{2},j,k} = \phi_{\alpha,i}^{p} \left( \frac{\tilde{f}_\alpha^{p+1}}{\Delta t} \right)_{i,j,k} + \psi_{\alpha,j}^{p} \left( \frac{\tilde{f}_\alpha^{p+1}}{\Delta x} \right)_{i,j,k}.
\]

where \(\text{Upw}\) denotes the use of straightforward upwinding based on the sign of \(\tilde{f}_\alpha^{p+1}\). The discretization of terms \((d)\) and \((e)\) is given as

\[
\left[ \gamma_{q,\alpha,i}^{p+1} \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} \right]_{i+\frac{1}{2},j,k} = \gamma_{q,\alpha,i}^{p} \left( \frac{\tilde{f}_\alpha^{p+1}}{\Delta t} \right)_{i,j,k} + \gamma_{x,\alpha,i}^{p} \left( \frac{\tilde{f}_\alpha^{p+1}}{\Delta x} \right)_{i,j,k},
\]

with straightforward central differencing of \(\tilde{f}_\alpha^{p+1} / \mathbf{v}_j\). Recall that \(\phi_\alpha\) and \(\gamma_{q,\alpha}\) have a dependence on the parallel velocity space; the details of this dependence are given in Sec. 4.

The inertial terms \((f)\) and \((g)\) arise due to the velocity-coordinate transformation. Similar to terms \((c), (d),\) and \((e)\), they contain additional nonlinear constraint functions \(\gamma_t\) and \(\gamma_x,\) which also act so as to enforce the continuum conservation symmetries discussed previously. The specific definitions and action of \(\gamma_t,\alpha\) and \(\gamma_{x,\alpha}\) are discussed in more detail in Sec. 4 Appendix C and Ref. [28]. The parallel-velocity flux of the temporal inertial term, \((f)\), is defined as

\[
- \left[ \gamma_{t,\alpha,i}^{p+1} \delta_t \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} \right]_{i+\frac{1}{2},j,k} = \gamma_{t,\alpha,i}^{p} \delta_t \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} + \gamma_{x,\alpha,i}^{p} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k}.
\]

The perpendicular-velocity flux of the temporal inertial term is defined similarly:

\[
- \left[ \gamma_{x,\alpha,i}^{p+1} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} \right]_{i+\frac{1}{2},j,k} = \gamma_{x,\alpha,i}^{p} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} + \gamma_{x,\alpha,i}^{p} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k}.
\]

For the spatial inertial terms, \((g),\) the parallel-velocity flux is defined by

\[
- \left[ \gamma_{x,\alpha,i}^{p+1} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} \right]_{i+\frac{1}{2},j,k} = \gamma_{x,\alpha,i}^{p} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k} + \gamma_{x,\alpha,i}^{p} \delta_x \left( \mathbf{v}_i^{p} \right) \left( \tilde{f}_\alpha^{p+1} \right)_{i,j,k}.
\]

Here, we note the pseud-flux involving the nonlinear constraint function \(\xi_{\alpha,i}^{p+1}\) appears through \(\mathbf{v}_i^{p+1}\).
Similarly, the perpendicular-velocity flux is defined by

\[
\rho \frac{\partial v_{\perp,i,j,k}}{\partial t} = -\left[ \rho \frac{\partial p_{\perp,i,j,k}}{\partial i} \right]_{t} - \gamma_{x,\alpha,i+\frac{1}{2},j,k+\frac{1}{2}} \frac{\partial p_{\perp,i+\frac{1}{2},j,k}}{\partial i} + \frac{1}{\rho} \frac{\partial \rho_{\alpha,i,j}}{\partial i} + \rho_{\alpha,i,j+\frac{1}{2}} \frac{\partial p_{\perp,i,j+\frac{1}{2}}}{\partial i} \right]
\]

We note here that to evolve the normalizing speed \(v_{\alpha}^{*}\) and offset velocity \(u_{\alpha}^{*}\) in space and time we use the same strategies as in Ref. [28].

Appendix C. Derivation of constraint definitions for \(\gamma_{t}\) and \(\gamma_{x}\)

Appendix C.1. Discrete momentum conservation

First, we observe that Eqs. (A.6) and (A.7) may be discretely represented as

\[
\left\langle v_{\alpha,i,j}^{p} \delta t \tilde{\Omega}_{\alpha,i,j,k} \right\rangle \delta \tilde{\Theta} - \left\langle v_{\alpha,i,j}^{p} \delta t \left[ \gamma_{x,\alpha,i+\frac{1}{2},j,k} \frac{v_{\alpha,i+\frac{1}{2},j,k}}{\delta x_{\alpha,i+\frac{1}{2}}} \right]_{j,k} \right\rangle_{\delta \tilde{\Theta}} = \left\langle 1, \frac{c_{p} v_{\alpha,i,j}^{p} \tilde{p}_{\alpha,i,j,k}^{p+1}}{\Delta t} + \frac{c_{p} v_{\alpha,i,j}^{p-1} \tilde{p}_{\alpha,i,j,k}^{p-1}}{\Delta t} \right\rangle_{\delta \tilde{\Theta}}
\]

and

\[
\left\langle v_{\alpha,i,j}^{p} \delta t \tilde{\Omega}_{\alpha,i,j,k} \right\rangle \delta \tilde{\Theta} - \left\langle v_{\alpha,i,j}^{p} \delta t \left[ \gamma_{x,\alpha,i+\frac{1}{2},j,k} \frac{v_{\alpha,i+\frac{1}{2},j,k}}{\delta x_{\alpha,i+\frac{1}{2}}} \right]_{j,k} \right\rangle_{\delta \tilde{\Theta}} = \left\langle 1, \delta x_{\alpha,i,j} \left\langle \tilde{p}_{\alpha,i,j,k}^{p+1} \right\rangle_{j,k} \right\rangle_{\delta \tilde{\Theta}} + \left\langle 1, \delta x_{\alpha,i,j} \left\langle \tilde{p}_{\alpha,i,j,k}^{p} \right\rangle_{j,k} \right\rangle_{\delta \tilde{\Theta}}
\]

respectively.

If we expand the discretized form of Eq. (C.1), we find

\[
\left\langle v_{\alpha,i,j}^{p} \frac{c_{p} \tilde{p}_{\alpha,i,j,k}^{p+1} + c_{p} \tilde{p}_{\alpha,i,j,k}^{p} + c_{p} \tilde{p}_{\alpha,i,j,k}^{p-1}}{\Delta t} \right\rangle_{\delta \tilde{\Theta}} = 0
\]

which is a concise representation of the first discrete constraint on the definition of the nonlinear constraint function \(\gamma_{t}\).
To enforce Eq. (C.2), we observe that by integrating through configuration-space (i.e., sum over \( N_x \Delta x \)), the right-hand side of Eq. (C.2) vanishes with periodic boundaries. Thus, expanding the individual flux terms, we find

\[
\sum_{i}^{N_x} \Delta x \left\{ \left\langle v_{\|,\alpha,i,j}^{p} \right\rangle_{\delta_0} \right\} = 0. \tag{C.4}
\]

Recall we have defined the effective velocity

\[
v_{\|,\alpha,i,j}^{p+1} \equiv \left( \begin{array}{c}
\bar{\nu}_{\|,\alpha,i,j} + \frac{\Delta p^{+1}_{\|,\alpha,i,i,j}}{2} \left( \bar{f}_{\|,\alpha,i,j}^{p+1} \right)_{i+\frac{1}{2},j,k}
\end{array} \right).
\]

Note that in the case of \( \bar{\nu}_{\|,\alpha,i,j}^{p+1} \equiv \left( \begin{array}{c}
\bar{f}_{\|,\alpha,i,j}^{p+1} \end{array} \right)_{i+\frac{1}{2},j,k} \) in the first term of Eq. (C.4), this is simply a shorthand for the summation of the individually interpolated fluxes \( \left\langle \bar{f}_{\|,\alpha,i,j}^{p+1} \right\rangle_{i+\frac{1}{2},j,k} \) in configuration-space, we find

\[
\sum_{i}^{N_x} \Delta x \left\{ \left\langle v_{\|,\alpha,i,j}^{p} \right\rangle_{\delta_0} \right\} = 0. \tag{C.5}
\]

where the discrete constraint on \( \gamma_{x,\alpha} \) is found by enforcing that

\[
\left\langle v_{\|,\alpha,i,j}^{p} - v_{\|,\alpha,i+1,j}^{p} \right\rangle_{\delta_0} = 0. \tag{C.6}
\]

is zero for each cell-face \( i + \frac{1}{2} \).

**Appendix C.2. Discrete energy conservation**

We first observe that Eqs. (A.13) and (A.14) may be discretely represented as

\[
\left\langle m_{\alpha} \frac{1}{2} \left( \va_{\|,\alpha,i,j,k} \right)^{2} \right\rangle_{\delta_0} - \left\langle m_{\alpha} \frac{1}{2} \left( \va_{\|,\alpha,i,j,k} \right)^{2} \right\rangle_{\delta_0} = \left\langle m_{\alpha} \frac{1}{2} \left( \va_{\|,\alpha,i,j,k} \right)^{2} \right\rangle_{\delta_0} - \left\langle m_{\alpha} \frac{1}{2} \left( \va_{\|,\alpha,i,j,k} \right)^{2} \right\rangle_{\delta_0} \triangleq 0. \tag{C.7}
\]
and

\[
\left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \delta_x \left[ \mathbf{v}_{\parallel,\alpha,j}^p \left( \mathbf{f}_{\alpha,j}^{p+1} \right)^{\parallel}_{j,k} \right] \right\rangle + m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 \delta_x \left[ \mathbf{v}_{\parallel,\alpha,j}^p \right| \left( \mathbf{f}_{\alpha,j}^{p+1} \right)^{\xi}_{j,k} \right]_{i/\delta t} \\
+ \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{\mathbf{J}_{x,i,j}^+ + \mathbf{J}_{x,i,j}^-}{\Delta t} \right\rangle_{i/\delta t} \\
- m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 \left[ \frac{1}{2} \mathbf{f}_{\alpha,i,j,k} + m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^{p+1} \right)^2 \mathbf{f}_{\alpha,i,j,k} + c_0^{p+1} \mathbf{f}_{\alpha,i,j,k} + c_0^{p-1} \mathbf{f}_{\alpha,i,j,k} \right]_{\Delta t} \\
- \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{1}{2} \mathbf{f}_{\alpha,i,j,k} \delta_\xi \left[ \mathbf{v}_{\alpha,i,j,k} \right| \mathbf{f}_{\alpha,j}^{p+1} \right\rangle_{j,k/\delta t} = 0, \quad (C.8)
\]

If we expand Eq. \( (C.7) \), we find

\[
\left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{c_0^{p+1} \mathbf{f}_{\alpha,i,j,k} + c_0^{p-1} \mathbf{f}_{\alpha,i,j,k} + \mathbf{f}_{\alpha,i,j,k}}{\Delta t} \right\rangle_{\delta t} \\
- \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{c_0^{p+1} \mathbf{f}_{\alpha,i,j,k} + c_0^{p-1} \mathbf{f}_{\alpha,i,j,k} + \mathbf{f}_{\alpha,i,j,k}}{\Delta t} \right\rangle_{\delta t} \\
- \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{1}{2} \mathbf{f}_{\alpha,i,j,k} \delta_\xi \left[ \mathbf{v}_{\alpha,i,j,k} \right| \mathbf{f}_{\alpha,j}^{p+1} \right\rangle_{j,k/\delta t} = 0, \quad (C.9)
\]

which is a concise representation of the final discrete constraint on the definition of the nonlinear constraint function \( \gamma \).

As in the case of momentum conservation, Eq. \( (C.8) \) must be enforced more carefully. Once again we will integrate through configuration-space and assume periodic boundaries, whereupon we arrive at

\[
\sum_{i} N_x \left\{ \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{\mathbf{v}_{\alpha,i,j,k}^{p+1}}{2} \right\rangle_{i/\Delta t} \right\} \\
- \left\langle m_0 \frac{1}{2} \left( \mathbf{v}_{\alpha,i,j,k}^p \right)^2 , \frac{1}{2} \mathbf{f}_{\alpha,i,j,k} \delta_\xi \left[ \mathbf{v}_{\alpha,i,j,k} \right| \mathbf{f}_{\alpha,j}^{p+1} \right\rangle_{j,k/\delta t} = 0. \quad (C.10)
\]
Again telescoping the summation in configuration-space and equating the quantity inside braces to zero, we find

\[
\left\langle \left( \frac{\nu^p_{\alpha,i,j,k}}{2} \right)^2 - \left( \frac{\nu^p_{\alpha,i+1,j,k}}{2} \right)^2, \frac{1}{\Delta x} \right\rangle \left( \tilde{\nu}^{p+1}_{\alpha,i+\frac{1}{2},\text{eff},\alpha,i+\frac{1}{2},j,k} \left( \tilde{\nu}^{p+1}_{\alpha} \right)_{i+\frac{1}{2},j,k} \right) - \left\langle \left( \frac{\nu^p_{\alpha,i,j,k}}{2} \right)^2, \frac{1}{2\nu^p_{\alpha,i}} \delta_\theta \right\rangle \left[ \gamma^{p+1}_{N,\alpha,i+\frac{1}{2}} \nu^p_{\alpha,i+\frac{1}{2},\text{eff},i+\frac{1}{2},j,k} \tilde{\nu}^p \left( \nu^p \right)_{i+\frac{1}{2},j,k} \right] = 0, \tag{C.11}
\]

which is the final discrete constraint on \( \gamma_{i,j,k} \).

Appendix D. Derivation of constraint definitions for \( \xi, \phi, \) and \( \gamma_q \)

Appendix D.1. Discrete charge & mass conservation

To demonstrate a discrete mass conservation, we apply to Eq. (22) the discrete moment \( \left\langle m_\alpha, \cdots \right\rangle_{\delta_\theta} \). First, we observe that with appropriate discrete boundary conditions (i.e., zero mass flux in the velocity space and periodic boundaries in the configuration space), all velocity-space divergence terms vanish under the discrete moment (as in the continuum case). Thus, we are left with

\[
\left\langle m_\alpha, \delta_\theta \tilde{f}_{\alpha,i,j,k} \right\rangle_{\delta_\theta} + \left\langle m_\alpha, \delta_\theta \left[ \nu^p_{\alpha,i,j} \left( \tilde{f}^{p+1}_{\alpha} \right)_{j,k,i} \right] \right\rangle_{\delta_\theta} + \left\langle m_\alpha, \delta_\theta \left[ \frac{\varepsilon^{p+1}}{\xi_{i,j,k}} \nu^p_{\alpha,i,j} \left( \tilde{f}^{p+1}_{\alpha} \right)_{j,k,i} \right] \right\rangle_{\delta_\theta} = 0. \tag{D.1}
\]

Clearly, if we sum over all species \( \alpha \) and integrate over the configuration space, \( \sum_{\alpha=1}^{N_\alpha} \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} m_\alpha \left\langle \tilde{f}^{p+1}_{\alpha} \right\rangle_{\nu,i,j,k} \), we will obtain the proper discrete mass conservation (assuming a periodic domain in the configuration space):

\[
\delta_\theta M_{\text{tot}} = \frac{c^{p+1} M_{\text{tot}}^{p+1} + c^p M_{\text{tot}}^p + c^{p-1} M_{\text{tot}}^{p-1}}{\Delta t^p},
\]

where \( M_{\text{tot}}^p \equiv \sum_{\alpha=1}^{N_\alpha} \sum_{i=1}^{N_i} m_\alpha n_{\alpha,i}^p = \sum_{\alpha=1}^{N_\alpha} \sum_{i=1}^{N_i} m_\alpha \left\langle \tilde{f}^p_{\alpha,i,j,k} \right\rangle_{\nu,i,j,k} \). Defining the discrete moments

\[
\nu^{p+1}_{\alpha,i,j,k} \equiv \left\langle 1, \tilde{f}^{p+1}_{\alpha,i,j,k} \right\rangle_{\delta_\theta}, \tag{D.2}
\]

\[
\tilde{\nu}^{p+1}_{\alpha,i+\frac{1}{2},\text{eff},i+\frac{1}{2},j,k} \equiv \left\langle 1, \nu^{p+1}_{\alpha,i+\frac{1}{2}} \left( \tilde{u}^{p+1}_{\alpha,i+\frac{1}{2},j,k} \right)_{\delta_\theta} \right\rangle_{\delta_\theta}, \tag{D.3}
\]

\[
\Gamma^{p+1}_{\alpha,i+\frac{1}{2},\text{eff},i+\frac{1}{2},j,k} \equiv \left\langle 1, \nu^{p+1}_{\alpha,i+\frac{1}{2}} \left( \tilde{u}^{p+1}_{\alpha,i+\frac{1}{2},j,k} \right)_{\delta_\theta} \right\rangle_{\delta_\theta}, \tag{D.4}
\]

we may further express Eq. (D.1) in terms of discrete moment quantities:

\[
m_\alpha \left( \frac{c^{p+1} \nu^{p+1}_{\alpha,i} + c^p \nu^p_{\alpha,i} + c^{p-1} \nu^{p-1}_{\alpha,i}}{\Delta t^p} \right)
+ m_\alpha \left( \frac{\nu^{p+1}_{\alpha,i+\frac{1}{2}} - \nu^{p+1}_{\alpha,i-\frac{1}{2}}}{\Delta x} + \frac{\nu^{p+1}_{\alpha,i+\frac{1}{2}} - \nu^{p+1}_{\alpha,i-\frac{1}{2}}}{\nu^{p+1}_{\alpha,i+\frac{1}{2}} - \nu^{p+1}_{\alpha,i-\frac{1}{2}}} \right) = 0. \tag{D.5}
\]
If we recall Sec. Appendix A.1, we know that the species particle flux density density that forms the current in Ampère’s equation must be identical to the momentum density that appears in the continuity equation. We observe that the discrete flux density forming the current in Ampère’s equation, \( \tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}}^{p+1} \), must therefore be

\[
\tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}}^{p+1} = \tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}}^{p+1} + \xi_{\alpha,i+\frac{1}{2}}^{p+1} \Gamma_{\alpha,i+\frac{1}{2}}^{p+1} .
\]

Thus, the purpose of the nonlinear constraint function \( \xi \) is to enforce that the truncation error between the discrete representations of particle flux density, \( \tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}} \) and \( \tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}}^{p+1} \), vanishes. The precise discrete definition of \( \tilde{n}\! \tilde{u}_{\alpha,i+\frac{1}{2}}^{p+1} \) is given in Appendix D.3. The constraint function \( \xi \) and its ‘pseudo-advection’ operator are critical to enforcing charge conservation, as we will see in Sec. 6.3.

Appendix D.2. Discrete momentum conservation

To demonstrate a discrete momentum conservation, we apply to Eq. (22) the discrete moment \( \left\langle m_{\alpha} v_{\alpha,i,j}^{p} \delta_{\beta} \right\rangle \), and note that \( v_{\alpha,i,j,k}^{p} = v_{\alpha,i}^{p} \left( \vec{v}_{j,k} + M_{\alpha,i,j} \right) \), i.e., \( v_{\alpha,i,j}^{p} = v_{\alpha,i}^{p} \left( \vec{v}_{j} + \vec{u}_{\alpha,i}^{p} \right) \) and \( v_{\perp,\alpha,i,k}^{p} = v_{\alpha,i}^{p} \vec{v}_{\perp,k} \). Employing the discrete number density in the configuration space, we find

\[
m_{\alpha} \sum_{i} \Delta x \left( \frac{c^{p+1} u_{\alpha,i}^{p+1} + c^{p} u_{\alpha,i}^{p} + c^{p-1} u_{\alpha,i}^{p-1}}{\Delta t} + \frac{q_{\alpha} E_{\alpha,i}^{p+1}}{m_{\alpha} v_{\alpha,i}^{p}} \delta \phi_{i,k}^{\alpha} + \frac{q_{\alpha} E_{\alpha,i}^{p+1}}{m_{\alpha} v_{\alpha,i}^{p}} \delta \phi_{i,k}^{\alpha} \right) = 0,
\]

where we have defined

\[
n_{\alpha,i}^{p+1} \equiv \left\langle 1, v_{\alpha,i}^{p}, \tilde{p}_{\alpha,i}^{p+1} \right\rangle \delta \phi .
\]

Expanding the individual flux operators and defining the discrete number density based on the moment of the acceleration operator,

\[
\vec{p}_{\alpha,i}^{p+1} \equiv - \left\langle v_{\alpha,i,j}^{p}, \frac{c^{p+1} u_{\alpha,i}^{p+1} + c^{p} u_{\alpha,i}^{p} + c^{p-1} u_{\alpha,i}^{p-1}}{\Delta t} \right\rangle \delta \phi \frac{q_{\alpha} E_{\alpha,i}^{p+1}}{m_{\alpha} v_{\alpha,i}^{p}}
\]

we find

\[
m_{\alpha} \sum_{i} \Delta x \left( \frac{c^{p+1} u_{\alpha,i}^{p+1} + c^{p} u_{\alpha,i}^{p} + c^{p-1} u_{\alpha,i}^{p-1}}{\Delta t} - \frac{q_{\alpha} E_{\alpha,i}^{p+1}}{m_{\alpha} v_{\alpha,i}^{p}} \delta \phi_{i,k}^{\alpha} \right) \delta \phi_{i,k}^{\alpha} = 0,
\]

Here, we defined \( \phi \) and \( \gamma \) to be split in \( v_{\alpha,i} \)-space as

\[
\phi_{\alpha,i,j+\frac{1}{2}}^{p+1} = \begin{cases} \phi_{\alpha,i,j+\frac{1}{2}}^{p+1} & \text{if } v_{\alpha,i,j+\frac{1}{2}}^{p+1} \geq u_{\alpha,i}^{p} , \\ 1 & \text{otherwise} \end{cases},
\]

\[
\gamma_{\alpha,i,j+\frac{1}{2}}^{p+1} = \begin{cases} \gamma_{\alpha,i,j+\frac{1}{2}}^{p+1} & \text{if } v_{\alpha,i,j+\frac{1}{2}}^{p+1} \geq u_{\alpha,i}^{p} , \\ 1 & \text{otherwise} \end{cases},
\]

where the definitions for \( \phi_{\alpha,i,j+\frac{1}{2}}^{p+1} \) and \( \gamma_{\alpha,i,j+\frac{1}{2}}^{p+1} \) will be determined shortly. The rationale for splitting \( \phi \) and \( \gamma \) in this way is, as shall be seen in Sec. Appendix D.3 for solvability of the resulting \( 2 \times 2 \) linear system from which \( \phi \) and \( \gamma \)
are calculated. From this splitting, we define the “upper” and “lower” densities as

$$
n^{+1}_{\alpha,i} = \left( v_{\alpha,i,j}^p \right)^2 \pi_{\alpha,i}^{p+1} \frac{q_{\alpha,i}}{m_{\alpha}} \left( \phi_{\alpha,i}^{p+1} + 1 \right) n^{+1}_{\alpha,i} + \left( \gamma_{q,\alpha,i}^{p+1} - 1 \right) n^{-p+1}_{\alpha,i} \right) \equiv \delta \tilde{\nu} \text{ where } v_{\alpha,i,j+\frac{1}{2}} \geq n^0_{\alpha,i}, \quad \text{(D.11)}$$

$$
n^{-p+1}_{\alpha,i} = \left( v_{\alpha,i,j}^p \right)^2 \pi_{\alpha,i}^{p+1} \frac{q_{\alpha,i}}{m_{\alpha}} \left( \phi_{\alpha,i}^{p+1} + 1 \right) n^{+1}_{\alpha,i} + \left( \gamma_{q,\alpha,i}^{p+1} - 1 \right) n^{-p+1}_{\alpha,i} \right) \equiv \delta \tilde{\nu} \text{ where } v_{\alpha,i,j+\frac{1}{2}} < n^0_{\alpha,i}. \quad \text{(D.12)}$$

If we then sum Eq. (D.9) over all species \( \alpha \), we find

$$
\delta_t P_{\text{total}} = \sum_{\alpha} m_{\alpha} \sum_i \Delta x \left\{ \pi_{\alpha,i}^{p+1} E_{\alpha,i}^{p+1} \frac{q_{\alpha,i}}{m_{\alpha}} + \left( \phi_{\alpha,i}^{p+1} + 1 \right) n^{+1}_{\alpha,i} + \left( \gamma_{q,\alpha,i}^{p+1} + 1 \right) n^{-p+1}_{\alpha,i} \right\} = 0. \quad \text{(D.13)}$$

where

$$
\delta_t P_{\text{total}} = \sum_{\alpha} m_{\alpha} \sum_i \Delta x \frac{c_{\alpha,i}^{p+1} n u_{\alpha,i}^{p+1} + c_{\alpha}^{p} n u_{\alpha,i}^{p} + c_{\alpha}^{p-1} n u_{\alpha,i}^{p-1}}{\Delta t} = 0. \quad \text{(D.14)}$$

is the discrete time derivative of the total momentum of the system. Recalling the symmetry with Gauss’ law in Eq. (A.10), we realize that Eq. (D.13) must become

$$
\delta_t P_{\text{total}} = \sum_{\alpha} m_{\alpha} \sum_i \Delta x \left\{ \pi_{\alpha,i}^{p+1} E_{\alpha,i}^{p+1} \frac{q_{\alpha,i}}{m_{\alpha}} \right\} = \delta_t P_{\text{total}} = \sum_{\alpha} m_{\alpha} \sum_i \Delta x \left\{ \epsilon_0 E_{\alpha,i}^{p+1} \right\} = 0. \quad \text{(D.14)}$$

where the final summation vanishes – assuming periodic boundaries – when we recall that \( E_{\alpha,i}^{p+1} \) is the average of adjacent cell-face values. Thus we achieve \( \delta_t P_{\text{total}} = 0 \), which is a discrete statement of momentum conservation. The equivalence between Eqs. (D.13) and (D.14) provides us the first discrete constraint for the nonlinear constraint functions \( \phi_{\alpha,i} \) and \( \gamma_{q,\alpha,i} \):

$$
\left( \phi_{\alpha,i}^{p+1} + 1 \right) n^{+1}_{\alpha,i} + \left( \gamma_{q,\alpha,i}^{p+1} + 1 \right) n^{-p+1}_{\alpha,i} = \left( n^{+1}_{\alpha,i} - \pi_{\alpha,i}^{p+1} \right) E_{\alpha,i}^{p+1} \frac{q_{\alpha,i}}{m_{\alpha}}. \quad \text{(D.15)}$$

Thus, \( \phi \) and \( \gamma_q \) act in concert to enforce that the truncation error between the two discrete representations of density, \( n_{\alpha,i} \) and \( \pi_{\alpha,i} \), vanishes.

**Appendix D.3. Discrete energy conservation**

To demonstrate discrete energy conservation, we apply the discrete moment \( \left( m_{\alpha} \frac{1}{2} \left( v_{\alpha,i,j,k}^p \right)^2 \right) \) to Eq. (22), where \( \frac{1}{2} \left( v_{\alpha,i,j,k}^p \right)^2 = \frac{1}{2} \left[ \left( v_{\alpha,i,j}^p \right)^2 + \left( v_{\alpha,i,k}^p \right)^2 \right] \). Utilizing the preceding developments and evaluating the discrete moment in the configuration space while summing over all species, we find

$$
\delta_t U_{\text{fluid}} + \sum_{\alpha} \sum_i \sum_k \Delta x \left\{ \left( m_{\alpha} \frac{1}{2} \left( v_{\alpha,i,j,k}^p \right)^2 \right) \right\} \frac{q_{\alpha,i}}{m_{\alpha}} \left( \phi_{\alpha,i}^{p+1} \right) \frac{\pi_{\alpha,i}^{p+1}}{E_{\alpha,i}^{p+1}} \frac{E_{\alpha,i}^{p+1}}{\delta \tilde{\nu} E_{\alpha,i}^{p+1}} \right\} \right\} = 0. \quad \text{(D.16)}$$
where we defined the quantities

\[ \delta_{\alpha} U_{\text{fluid}}^{+} \equiv \sum_{\alpha} \sum_{i} N_{\alpha} \Delta x \frac{c^{p+1} \varepsilon_{\alpha,i}^{p+1} + c^{P} \varepsilon_{\alpha,i}^{P} + c^{P+1} \varepsilon_{\alpha,i}^{P+1}}{\Delta P}, \]

and

\[ \varepsilon_{\alpha,i}^{p+1} \equiv \left( 1, m_{\alpha} \frac{1}{2} \left( \left( f_{\alpha}^{p+1} \right)_{i,j,k}^{\text{central}} - \left( f_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k}^{\text{central}} \right) \right) v_{j,k}^{p+1}. \]

Again, expanding the individual flux operators and defining the discrete particle flux density obtained from the moment of the acceleration operator,

\[ m_{\alpha,i}^{p+1} \equiv - \left( \frac{v_{\alpha,i,j,k}}{2}, \frac{\left( f_{\alpha}^{p+1} \right)_{i,j+\frac{1}{2},k}^{\text{central}} - \left( f_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k}^{\text{central}}}{\Delta \bar{v}} \right) \delta \bar{b}, \]

we obtain

\[ \delta_{\alpha} U_{\text{fluid}}^{+} = \sum_{\alpha} \sum_{i} N_{\alpha} \Delta x \left\{ q_{\alpha} E_{\alpha,i}^{p+1} m_{\alpha,i}^{p+1} + m_{\alpha} \left( \phi_{\alpha,i}^{p+1} + 1 \right) n_{\alpha,i}^{+} + m_{\alpha} \left( \gamma_{\alpha,i}^{p+1} + 1 \right) n_{\alpha,i}^{-} \right\} = 0. \tag{D.17} \]

Here, as before, we defined the “upper” and “lower” momenta as

\[ n_{\alpha,i}^{+} \equiv \left( 1, 2 \left( v_{\alpha,i,j,k}^{p} \right)^{2}, \frac{1}{2}, \frac{\left( f_{\alpha}^{p+1} \right)_{i,j+\frac{1}{2},k}^{\text{central}} - \left( f_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k}^{\text{central}}}{\Delta \bar{v}} \right) \delta \bar{b} \text{ where } v_{\alpha,i,j,k}^{p} \geq u_{\alpha,i}^{p}, \tag{D.18} \]

\[ n_{\alpha,i}^{-} \equiv \left( 1, 2 \left( v_{\alpha,i,j,k}^{p} \right)^{2}, \frac{1}{2}, \frac{\left( f_{\alpha}^{p+1} \right)_{i,j+\frac{1}{2},k}^{\text{central}} - \left( f_{\alpha}^{p+1} \right)_{i,j-\frac{1}{2},k}^{\text{central}}}{\Delta \bar{v}} \right) \delta \bar{b} \text{ where } v_{\alpha,i,j,k}^{p} < u_{\alpha,i}^{p}. \tag{D.19} \]

Thus we see Eq. \[ (D.17) \] is the discrete time derivative of the total fluid energy of the system, including the total thermal and kinetic energy of the plasma. Recalling the definition of \( E_{\alpha,i}^{p+1} \), we may rearrange the summation in Eq. \[ (D.17) \], which gives us

\[ \delta_{\alpha} U_{\text{fluid}}^{+} = \sum_{\alpha} \sum_{i} N_{\alpha} \Delta x \left\{ m_{\alpha} \frac{E_{\alpha,i}^{p+1}}{\Delta x} q_{\alpha} \right\} - \sum_{\alpha} m_{\alpha} \sum_{i} N_{\alpha} \Delta x \left\{ \phi_{\alpha,i}^{p+1} + 1 \right\} n_{\alpha,i}^{+} + \left( \gamma_{\alpha,i}^{p+1} + 1 \right) n_{\alpha,i}^{-} = 0. \tag{D.20} \]

where we defined

\[ m_{\alpha,i}^{p+1} \equiv m_{\alpha,i}^{p+1} + m_{\alpha,i}^{p+1}. \tag{D.21} \]

Next, we recall the symmetry with Ampère’s equation in Eq. \[ (A.17) \] and define

\[ m_{\alpha,i}^{p+1} \equiv m_{\alpha,i}^{p+1}, \tag{D.22} \]

to enforce particle fluxes in the current in Ampère’s equation that come from the energy moment of the acceleration operator. Thus, we find that the nonlinear constraint function \( \xi_{\alpha,i}^{p+1} \) is completely determined by requiring

\[ \xi_{\alpha,i}^{p+1} = \frac{m_{\alpha,i}^{p+1} - m_{\alpha,i}^{p+1}}{\xi_{\alpha,i}^{p+1}}. \tag{D.23} \]
We now observe that Eq. (D.20) must become

\[
\delta_t U_{\text{fluid}} + \sum_i \Delta x \left\{ \epsilon_0 E_{\|,i+\frac{1}{2}}^p \delta_t E_{\|,i+\frac{1}{2}} - E_{\|,i+\frac{1}{2}}^p \right\}
- \sum_i \Delta x \left\{ \sum_{\alpha} m_{\alpha} \left[ (\phi_{\alpha,i}^{+,p+1} + 1) n_{\alpha,i}^{+,p+1} + (\gamma_{q,\alpha,i}^{-,p+1} + 1) n_{\alpha,i}^{-,p+1} \right] \right\} = 0. \tag{D.24}
\]

In a previous implementation of this method, as was done in Refs. [20, 27], the use of a Crank-Nicolson integration scheme ensured the equivalence

\[
E_{\|,i+\frac{1}{2}}^{p+1} \delta_t E_{\|,i+\frac{1}{2}} = \frac{1}{2} \delta_t \left( E_{\|,i+\frac{1}{2}}^2 \right)
\]

in the discrete. However, BDF2 in the current development does not ensure this relation. Thus, the second purpose of the quantities \( \phi \) and \( \gamma_q \) is to enforce the equivalence of Eq. (D.24) to the equation

\[
\delta_t U_{\text{fluid}} + \sum_i \Delta x \left\{ \delta_t \left( \frac{1}{2} E_{\|,i+\frac{1}{2}}^2 \right) - E_{\|,i+\frac{1}{2}}^{p+1} \right\}
= \delta_t U_{\text{fluid}} + \delta_t U_{\text{E1}} - E_{\|,i+\frac{1}{2}}^{p+1} \delta t = \delta_t U_{\text{total}} - E_{\|,i+\frac{1}{2}}^{p+1} = 0. \tag{D.25}
\]

Note, that in the absence of an external electric field, \( E_{\|,i+\frac{1}{2}}^{p+1} \) vanishes discretely, preserving the discrete conservation principle. The final constraint on \( \phi \) and \( \gamma_q \) is thus

\[
\left( \phi_{\alpha,i}^{+,p+1} + 1 \right) n_{\alpha,i}^{+,p+1} + \left( \gamma_{q,\alpha,i}^{-,p+1} + 1 \right) n_{\alpha,i}^{-,p+1} = \frac{1}{m_q N_{sp}} \left\{ \epsilon_0 \left[ E_{\|,i+\frac{1}{2}}^{p+1} \delta_t E_{\|,i+\frac{1}{2}} - \delta_t \left( \frac{1}{2} E_{\|,i+\frac{1}{2}}^2 \right) \right] \right\}, \tag{D.26}
\]

where we have pulled the temporal derivatives into the species summation by dividing by the number of species, \( N_{sp} \).

We see from Eqs. (D.15) and (D.26) that \( \phi \) and \( \gamma_q \) are determined for each species and locally at each point in the configuration space by a simple \( 2 \times 2 \) linear system of equations:

\[
\begin{bmatrix}
n_{\alpha,i}^{+,p+1} & n_{\alpha,i}^{-,p+1} \\
n_{\alpha,i}^{+,p+1} & n_{\alpha,i}^{-,p+1}
\end{bmatrix}
\begin{bmatrix}
\phi_{\alpha,i}^{+,p+1} + 1 \\
\gamma_{q,\alpha,i}^{-,p+1} + 1
\end{bmatrix}
= \frac{1}{m_q N_{sp}} \left\{ \epsilon_0 \left[ E_{\|,i+\frac{1}{2}}^{p+1} \delta_t E_{\|,i+\frac{1}{2}} - \delta_t \left( \frac{1}{2} E_{\|,i+\frac{1}{2}}^2 \right) \right] \right\}. \tag{D.27}
\]

To ensure solvability of Eq. (D.27), the determinant of the system

\[
\text{Det} \begin{bmatrix}
n_{\alpha,i}^{+,p+1} & n_{\alpha,i}^{-,p+1} \\
n_{\alpha,i}^{+,p+1} & n_{\alpha,i}^{-,p+1}
\end{bmatrix}
= n_{\alpha,i}^{+,p+1} n_{\alpha,i}^{-,p+1} - n_{\alpha,i}^{-,p+1} n_{\alpha,i}^{+,p+1},
\]

must be strictly finite. It can be shown that if the splitting velocity for Eq. (D.10) is within the discrete bounds of \( v_{\|,\alpha,i,j}^{p+1} \), then the system in Eq. (D.27) is well-posed (see Appendix E). To reduce nonlinearity of the algorithm we use \( u_{\|,\alpha,i}^{p+1} \) as the splitting velocity, which is sufficiently close to \( v_{\|,\alpha,i,j}^{p+1} \) for the constraint functions \( \phi \) and \( \gamma_q \) to remain well-behaved.

**Appendix E. Well-posedness of 2 × 2 system for \( \phi^+ \) and \( \gamma^- \)**

In Sec. 4 we presented a \( 2 \times 2 \) linear system to be solved (locally, for each species) for \( \phi_{\alpha,i}^{+,p+1} \) and \( \gamma_{q,\alpha,i}^{-,p+1} \). This may be expressed in simpler notation as

\[
\begin{bmatrix}
n^+ & n^- \\
n^+ & n^-
\end{bmatrix}
\begin{bmatrix}
(\phi^+ + 1) \\
(\gamma^- + 1)
\end{bmatrix}
= \begin{bmatrix}
R_1 \\
R_2
\end{bmatrix}. \tag{E.1}
\]

To be well-posed, the determinant

\[
\text{Det} \begin{bmatrix}
n^+ & n^- \\
n^+ & n^-
\end{bmatrix} = n^+ n^- - n^- n^+ \tag{E.2}
\]

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must be strictly non-zero. To show when this is the case, we will for simplicity consider a 1D-1V system, with moments \( n \) and \( nu \) defined as

\[
 n = \int_{-\infty}^{\infty} f(v) dv, \quad (E.3)
\]

\[
 nu = \int_{-\infty}^{\infty} vf(v) dv. \quad (E.4)
\]

We define the bulk velocity \( u \equiv \frac{nu}{n} \), and the split quantities \( n^+/− \) and \( nu^+/− \) by

\[
 n− = \int_{u∗}^{−\infty} f(v) dv, \quad (E.5)
\]

\[
 n+ = \int_{u∗}^{\infty} f(v) dv, \quad (E.6)
\]

\[
 nu− = \int_{u∗}^{−\infty} vf(v) dv, \quad (E.7)
\]

\[
 nu+ = \int_{u∗}^{\infty} vf(v) dv. \quad (E.8)
\]

We may then perform a coordinate transformation \( v′ = v − u∗ \) of the integration for Eqs. (E.7) and (E.8):

\[
 nu− = \int_{0}^{∞} (v′ + u∗) f(v′) dv′ = \int_{0}^{∞} v′ f(v′) dv′ + n− u∗, \quad (E.9)
\]

\[
 nu+ = \int_{0}^{∞} (v′ + u∗) f(v′) dv′ = \int_{0}^{∞} v′ f(v′) dv′ + n+ u∗. \quad (E.10)
\]

If we define

\[
 (nw)− = \int_{0}^{∞} v′ f(v′) dv′, \quad (E.11)
\]

\[
 (nw)+ = \int_{0}^{∞} v′ f(v′) dv′, \quad (E.12)
\]

we see that \( (nw)− \) is negative definite and \( (nw)+ \) is positive definite. Equation \( (E.2) \) now becomes

\[
 n+ \left[ (nw)− + n− u∗ \right] − n− \left[ (nw)+ + n+ u∗ \right] = n+ (nw)− − n− (nw)+ + n− n+ (u∗ − u∗), \quad (E.13)
\]

which is negative definite. Thus, we find that Eq. \( (F.1) \) is well-posed for arbitrary \((finite)\) \( u∗ \). We note that in the discrete system \( u_{\alpha,i}^∗ \) must lie within the discrete bounds of \( v_{\parallel}^\alpha \) for the given species \( \alpha \) at configuration-space index \( i \).

In practice any choice near \( u_{\parallel,\alpha,i}^{p+1} \) should be suitable.

**Appendix F. Two-stream instability for cold Maxwellian beams**

Recall that the general dispersion relation for the electron-electron two stream instability \[44\] is

\[
 1 + \frac{\omega_{p,b}^2}{k^2 v_{th,b}^2} \left[ 2 + \zeta_\pm Z (\zeta_\pm) + \zeta_\mp Z (\zeta_\mp) \right] = 0, \quad (F.1)
\]

where

\[
 \zeta_\pm \equiv \frac{\omega \mp k v_b}{k v_{th,b}},
\]

and \( \omega_{p,b} \) is the beam plasma frequency. Recall also that if the electron beams are delta functions \((i.e. \text{ in the limit } v_{th,b} \to 0)\) Eq. \( (F.1) \) becomes
\[ 1 - \frac{1}{(\omega + v_b k)^2} - \frac{1}{(\omega - v_b k)^2} = 0. \]  \hfill (F.2)

Based on the delta-function dispersion relation, Eq. (F.2), the growth rate of electric field energy is \( \gamma = 0.353 \omega p,b. \) However, as we mentioned in Sec. (6.2), for thermalized beams there will be some deviation, and we expect that as the ratio \( v_{th,b}/v_b \) increases that the system will become more stable (i.e. \( \gamma \) will decrease). Figure 4 indeed shows that if we increase \( v_{th,b}/v_b \) towards some critical ratio near 1, the growth rate decreases precipitously. Here we present a semi-analytic analysis of the generalized two-stream dispersion relation in Eq. (F.1).

First, we will rearrange Eq. (F.1):

\[ k^2 \lambda_D^2 + 2 + \zeta Z(\zeta) + \zeta - Z(\zeta) = 0, \]  \hfill (F.3)

where \( \lambda_D^2 \equiv \frac{v_{th,b}^2}{\omega_{p,b}}. \) For convenience we then recast \( \zeta \pm \) in terms of dimensionless quantities:

\[ \zeta \pm = \left( \frac{\beta_r}{\delta} \pm \alpha \right) + i \left( -\frac{\beta}{\delta} \right), \]  \hfill (F.4)

where

\[
\begin{align*}
\omega &\equiv \omega_r - i\gamma, \alpha \equiv \frac{v_b}{v_{th,b}}, \\
\beta_r &\equiv \frac{\omega_r}{\omega_{p,b}}, \beta &\equiv \frac{\gamma}{\omega_{p,b}}, \\
\delta &\equiv k\lambda_D.
\end{align*}
\]

We next observe that the plasma dispersion function \( Z(\zeta) \) is given as

\[ Z(\zeta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-z^2} e^{-z(\zeta)} dz, \]  \hfill (F.5)

which may be expressed in terms of the complex error function \( \text{erf}(z) \) as \[42\]

\[ Z(\zeta) = i\sqrt{\pi} e^{-\zeta^2} [1 + \text{erf}(i\zeta)]. \]  \hfill (F.6)

Thus, combining Eqs. (F.4) and (F.6) with Eq. (F.3), we obtain

\[ \delta^2 + 2 + i\sqrt{\pi} \zeta_+ e^{-[(\frac{\beta_r}{\delta} - \alpha) + i(-\frac{\beta}{\delta})]^2} \left[ 1 + \text{erf} \left( i \left( \frac{\beta_r}{\delta} - \alpha \right) - \left( -\frac{\beta}{\delta} \right) \right) \right] \\
+ i\sqrt{\pi} \zeta_- e^{-[(\frac{\beta_r}{\delta} + \alpha) + i(-\frac{\beta}{\delta})]^2} \left[ 1 + \text{erf} \left( i \left( \frac{\beta_r}{\delta} + \alpha \right) - \left( -\frac{\beta}{\delta} \right) \right) \right] = 0. \]  \hfill (F.7)

Equation (F.7) may be separated into its real and imaginary components, and for a given \( \alpha \) and \( \delta \) (i.e., given the beam velocity \( v_b \), beam thermal speed \( v_{th,b} \), wavenumber \( k \), and Debye length \( \lambda_D \)), we may solve for the instability growth rate \( \beta \) (as well as the oscillatory component \( \beta_r \)).

For the case in Sec. (6.2) we have \( v_{th,b}/v_b = [0.15, 0.3, 0.5, 0.65, 0.8] \) and \( k = 2\pi \). For this case, we have \( \omega_{p,b} = \omega_{p,e} = 1 \), defined using the total electron density, which with a fixed \( |v_b| = 0.1 \), will give us \( \delta = 2\pi \times [0.015, 0.03, 0.05, 0.065, 0.08] \). As we saw in Table 1 this will produce

\[ \beta = [0.3488, 0.3318, 0.2734, 0.1953, 0.08911]. \]

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