An adaptive, conservative 0D-2V multispecies Rosenbluth-Fokker-Planck solver for arbitrarily disparate mass and temperature regimes

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Abstract

In this study, we propose an *adaptive* velocity-space discretization scheme for the multi-species, multidimensional Rosenbluth-Fokker-Planck (RFP) equation, which is exactly mass-, momentum-, and energy-conserving. Unlike most earlier studies, our approach normalizes the velocity-space coordinate to the temporally varying individual plasma species' local-thermal velocity, $v_{th}(t)$, and explicitly considers the resulting inertial terms in the Fokker-Planck equation. Our conservation strategy employs nonlinear constraints to enforce discretely the conservation properties of these inertial terms and the Fokker-Planck collision operator. To deal with situations of extreme thermal velocity disparities among different species, we employ an asymptotic v_{th} -ratio-based expansion of the Rosenbluth potentials that only requires the computation of several velocity-space integrals. Numerical examples demonstrate the favorable efficiency and accuracy properties of the scheme. In particular, we show that the combined use of the velocity-grid adaptivity and asymptotic expansions delivers many orders-of-magnitude savings in mesh resolution requirements compared to a single, static uniform mesh.

Keywords: Conservative discretization, thermal velocity based adaptive grid, Fokker-Planck, Rosenbluth potentials, asymptotics

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1. Introduction

The Rosenbluth-Fokker-Planck (RFP) collision operator describes the local collisional relaxation process of particle distribution functions in plasmas under the assumption of binary, grazing-angle collisions [1, 2, 3, 4, 5, 6, 7]. This operator, when employed in the kinetic equations for plasma species that are coupled to Maxwell's equations, is regarded as a first-principles physical model for describing weakly coupled plasmas in all collisionality regimes, and accordingly, has a wide range of applications in laboratory (e.g., magnetic and inertial thermonuclear fusion), space (e.g., Earth's magnetosphere), and astrophysical (e.g., stellar mass ejections) plasmas.

The system of RFP equations for various plasma species supports disparate length and time scales, which makes it particularly challenging to solve with grid-based approaches. The thermal speed, $v_{th} = \sqrt{2T/m}$, which provides the characteristic width of the plasma species distribution function in the velocity space, is a function of the plasma temperature, T , and particle species mass, m . In many practical applications of interest, v_{th} separation among species can span several orders of magnitude, either because of large temperature variations or because of large mass disparities. For instance, for protons in thermal equilibrium with electrons, $v_{th,e}/v_{th,p} \sim 42$. The separation can be much stronger when heating is applied preferentially

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to one species (e.g, RF heating in tokamaks or shock compression in inertial confinement fusion, ICF) and v_{th} evolves dynamically. Since the velocity-space domain size is determined by the hottest species, and the velocity-grid spacing must resolve the coldest one, velocity-space discretizations with uniform Cartesian grids in such scenarios may lead to impractical grid resolution requirements.

Several studies recognized and tried to address these challenges [8, 9, 10, 11]. In Ref. [9], the velocity-space domain was evolved for multiple ion species based on the local *average* v_{th} (over the ion species) and hydrodynamic velocity of the plasma. This powerful strategy enabled the fully kinetic implosion simulations of inertial confinement fusion (ICF) capsules [9, 12, 13]. However, the implementation was based on grid remapping, and did not conserve mass, momentum, or energy. Moreover, by employing a single reference thermal velocity, the approach loses effectiveness for moderate mass ratios or temperature disparities among ions. In Ref. [8], the concept of multiple velocity-space grids was introduced to model the α -particle distribution function in terms of the cold thermal component and the hot suprathermal component. The velocity-space grid domains were chosen based on the thermal spread of each component ($v_{th,h} \gg v_{th,c}$) and, together with the average v_{th} adaptive velocity-space grid for the fuel species, enabled, to our knowledge, the first kinetic ICF implosion calculations with α heating [11]. Similar ideas have been employed in Ref. [10] to adapt the velocity-space domain in terms of a **spatially dependent** v_{th} using a block-structured adaptive grids for tokamak gyrokinetic simulations.

Despite the enabling nature of the adaptive velocity-space methods described above, none of these strategies can be effectively applied to intermediate mass-ratio regimes (i.e. $10 \leq m_\alpha/m_\beta \leq 100$), which arises for example in ICF pusher-fuel mix or in Tokamak impurity transport. In Omega ICF capsules, the pusher species typically contains Carbon (plastic ablator [14]), or Silicon and Oxygen (glass-micro balloon [15]) with recent experiments including Titanium tracers [16], whereas the fuel is typically comprised of Hydrogen and/or Helium isotopes. Recent and future experiments at the National Ignition Facility (NIF) consider capsules with multiple layers of doped materials such as Copper-doped Beryllium [17, 18]. These configurations feature mass ratios that are not always amenable to an asymptotic treatment of the kind proposed in Ref. [8], but are large enough to challenge the single- v_{th} normalization approach of Ref. [9].

In this study, we consider a conservative, multiple- v_{th} dynamic velocity-space adaptive strategy, in which each species employs its own temporally varying thermal velocity to normalize its velocity-space domain. (In the general case, v_{th} will be a function of time and space, but in this study we only consider its temporal evolution.) This ensures that each species' distribution function is always well resolved regardless of temperature and mass. The treatment of like-particle collisions only needs to know about that species domain, and is therefore relatively straightforward. The treatment of unlike-particle collisions, however, is complicated significantly by the fact that different species are represented in different domains, particularly in the case of very disparate thermal velocity ratios. For this scenario, we use Taylor and multipole expansion strategies to derive suitable approximations of the corresponding Rosenbluth potentials. As a result, our approach is able to effectively address the above-mentioned issues with intermediate mass ratios and species out of thermal equilibrium. Instead of remapping the distribution function at each time-step, we perform an analytical transformation of the Fokker-Planck equation by considering the velocity variable normalized to the (in general, spatially and temporally varying) local v_{th} . This transformation introduces additional inertial terms in the Fokker-Planck equation, which avoid remapping and can be shown to preserve conservation properties in the continuum. These conservation properties are then enforced discretely by introducing suitable nonlinear constraints, in the same spirit as was proposed for the collision operator in Ref. [19].

The rest of the paper is organized as follows. Section 2 introduces the RFP equation and discusses its main properties. We present the v_{th} normalization and corresponding transformation of the RFP equation along with the resulting inertial term in Sec. 3. We follow by discussing the asymptotic approximation of the cross-species Rosenbluth potentials in Sec. 4. In Sec. 5, we provide a detailed discussion on the implementation of the proposed schemes in the following order: 1) discretization of the Fokker-Planck collision

operator and the inertial term, 2) numerical treatment of the Rosenbluth potentials and collisional fluxes for the multiple grid approach with and without asymptotics, 3) discrete enforcement of the conservation symmetries for the inertial terms, and 4) the temporal evolution of v_{th} . The numerical performance of the scheme is demonstrated with various multi-species tests of varying degrees of difficulty in Sec. 6. Finally, we conclude in Sec. 7.

2. The multi-species Rosenbluth-Fokker-Planck equation

Collisional relaxation in a spatially homogeneous multi-species plasma is described by a system of the Fokker-Planck equations for the particle distribution functions, $f_\alpha(\mathbf{v}, t)$, in velocity space, $\mathbf{v}$:

$$\frac{\partial f_\alpha}{\partial t} = \sum_{\beta}^{N_s} C_{\alpha\beta}, \quad (2.1)$$

where N_s is the total number of plasma species α in the system, and $C_{\alpha\beta}$ is the Fokker-Planck collision operator for species α colliding with species β :

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\overset{\leftrightarrow}{D}_\beta \cdot \nabla_v f_\alpha - \frac{m_\alpha}{m_\beta} \mathbf{A}_\beta f_\alpha \right]. \quad (2.2)$$

Here, $\Gamma_{\alpha\beta} = \frac{2\pi Z_\alpha^2 Z_\beta^2 e^4 \Lambda_{\alpha\beta}}{m_\alpha^2}$, $\overset{\leftrightarrow}{D}_\beta$ and $\mathbf{A}_\beta$ are the tensor-diffusion and friction coefficients for species β , m_α and m_β are the masses of species α and β , Z_α and Z_β are the ionization states of species α and β , e is the proton charge, and $\Lambda_{\alpha\beta}$ is the Coulomb logarithm ($\Lambda_{\alpha\beta} = 10$ is assumed in this study for all species for simplicity).

In the Rosenbluth-Fokker-Planck formulation, which uses the Fokker-Planck equation with the Rosenbluth form [1, 2] of the Coulomb binary collision operator, the velocity-space-transport coefficients are computed from the Rosenbluth potentials G_β, H_β as:

$$\overset{\leftrightarrow}{D}_\beta = \nabla_v \nabla_v G_\beta, \quad (2.3)$$

$$\mathbf{A}_\beta = \nabla_v H_\beta, \quad (2.4)$$

and the Rosenbluth potentials are in turn computed from the distribution function of species β as:

$$\nabla_v^2 H_\beta = -8\pi f_\beta, \quad (2.5)$$

$$\nabla_v^2 G_\beta = H_\beta. \quad (2.6)$$

The collision operator (Eq. 2.2) preserves the positivity of f , and conserves mass, momentum, and energy. These conservation properties stem from the following symmetries [20]:

$$\langle 1, C_{\alpha\beta} \rangle_v = 0, \quad (2.7)$$

$$m_\alpha \langle \mathbf{v}, C_{\alpha\beta} \rangle_v = -m_\beta \langle \mathbf{v}, C_{\beta\alpha} \rangle_v, \quad (2.8)$$

$$m_\alpha \left\langle \frac{v^2}{2}, C_{\alpha\beta} \right\rangle_v = -m_\beta \left\langle \frac{v^2}{2}, C_{\beta\alpha} \right\rangle_v, \quad (2.9)$$

where the inner product is defined as $\langle A, B \rangle_v = 2\pi \int_{-\infty}^{\infty} dv_{||} \int_0^{\infty} dv_{\perp} v_{\perp} A(\mathbf{v}) B(\mathbf{v})$ for the cylindrically symmetric coordinate system in the velocity space employed herein. The collision operator also satisfies the so-called H-theorem, which states that the total entropy of the system, $S = -\sum_{\alpha} \langle \ln |f_\alpha|, f_\alpha \rangle_v$, increases monotonically with time, unless all f_α are Maxwellians with common temperature and flow velocity. These symmetries are enforced in the discrete following the procedure discussed in Ref. [19].

Figure 3.1: Illustration of the velocity distribution functions for fast and slow species.

3. Normalization of the RFP equation to the local thermal velocity

The Fokker-Planck equation is very challenging to solve numerically due to its nonlinear, integro-differential character. In the multispecies case, additional challenges arise when different species feature disparate thermal velocities (e.g., ion-electron and DT- α interactions in fusion plasmas). A sketch of such a situation is presented in Fig. 3.1. These challenges arise since the velocity-space domain size is determined by the fast species, and the velocity-grid spacing must resolve the slow one. The natural resolution of this issue is to adapt the velocity-space mesh to each species' characteristic thermal velocity, v_{th} . This idea is not new, with practitioners using velocity-space remapping and/or discontinuous velocity-space meshes across spatial mesh points [10, 21], breaking the structured nature of the mesh. In this study, we explore an analytical transformation of the Fokker-Planck equation that preserves the structured nature of the underlying logical mesh. A key requirement in our approach is the exact preservation of physical invariants such as mass, momentum, and energy.

3.1. Normalization of the Fokker-Planck collision operator

We normalize all velocity-space dependent quantities for a species α to its thermal velocity, $v_{th,\alpha}$, as follows:

$$\hat{\mathbf{v}}_\alpha = \frac{\mathbf{v}}{v_{th,\alpha}}, \quad \hat{\nabla}_{v,\alpha} = v_{th,\alpha} \nabla_v, \quad \hat{f}_\alpha = v_{th,\alpha}^3 f_\alpha. \quad (3.1)$$

In general, v_{th} is a function of time and space, but here we only consider its temporal evolution. Here and elsewhere, the over-hat denotes normalized (dimensionless) quantities.

We begin by normalizing the Rosenbluth potentials equations, for which one must consider separately the like-particle potentials (a species colliding with itself, with the potentials in the same domain as the distribution function) and the unlike-particle potentials (a species α colliding with another species β). Consider the β -species colliding with itself. The corresponding normalized like-particle H -potential equation, represented in the β velocity space, reads:

$$\hat{\nabla}_{v,\beta}^2 (H_\beta v_{th,\beta}) = -8\pi \hat{f}_\beta (\hat{v}_\beta).$$

This leads to the definition of the normalized like-particle H_β Rosenbluth potential as:

$$\hat{H}_{\beta\beta} = H_\beta v_{th,\beta}. \quad (3.2)$$

Similarly, the normalized like-particle G_β Rosenbluth potential equation reads:

$$v_{th,\beta}^{-2} \widehat{\nabla}_{v,\beta}^2 G_\beta = v_{th,\beta}^{-1} \widehat{H}_{\beta\beta},$$

leading to the definition:

$$\widehat{G}_{\beta\beta} = v_{th,\beta}^{-1} G_\beta. \quad (3.3)$$

Now consider unlike-particle collisions. The normalized H -potential equation for the β species in the α -species velocity space reads:

$$v_{th,\alpha}^{-2} \widehat{\nabla}_{v,\alpha}^2 H_\beta = -8\pi v_{th,\beta}^{-3} \widehat{f}_\beta,$$

which, using Eq. 3.2, leads to the definition of the normalized unlike-particle H Rosenbluth potential as:

$$\widehat{H}_{\alpha\beta} = \widehat{H}_{\beta\beta} \left(\frac{v_{th,\beta}}{v_{th,\alpha}} \right)^2, \quad (3.4)$$

with the corresponding governing equation:

$$\widehat{\nabla}_{v,\alpha}^2 \widehat{H}_{\alpha\beta} = -8\pi \widehat{f}_\beta \left(\widehat{v}_\beta = \widehat{v}_\alpha \frac{v_{th,\alpha}}{v_{th,\beta}} \right). \quad (3.5)$$

Note that the source term must in principle be interpolated from its original representation β -velocity space. Similarly, for the unlike-particle G potentials, we obtain:

$$\widehat{G}_{\alpha\beta} = \widehat{G}_{\beta\beta} \left(\frac{v_{th,\beta}}{v_{th,\alpha}} \right)^4, \quad (3.6)$$

with the corresponding governing equation:

$$\widehat{\nabla}_{v,\alpha}^2 \widehat{G}_{\alpha\beta} = \widehat{H}_{\alpha\beta}. \quad (3.7)$$

The unlike-particle collision operator can then be expressed in normalized form as:

$$\widehat{C}_{\alpha\beta} = v_{th,\alpha}^3 C_{\alpha\beta} = \Gamma_{\alpha\beta} v_{th,\beta}^{-3} \widehat{\nabla}_{v,\alpha} \cdot \left[\widehat{\nabla}_{v,\alpha} \widehat{\nabla}_{v,\alpha} \widehat{G}_{\alpha\beta} \cdot \widehat{\nabla}_{v,\alpha} \widehat{f}_\alpha - \frac{m_\alpha}{m_\beta} \widehat{f}_\alpha \widehat{\nabla}_{v,\alpha} \widehat{H}_{\alpha\beta} \right]. \quad (3.8)$$

The normalized like-particle collision operator is obtained from this expression by replacing β with α .

3.2. Temporal update term

Multiple velocity-space grids normalized to the species' v_{th} allow one to address the v_{th} disparity between species. However, time-dependent temperatures introduce inertial terms in the temporal update term, $\partial_t f_\alpha$. To find this term, we transform the velocity coordinates:

$$\mathbf{v} = v_{th,\alpha}(t) \widehat{\mathbf{v}}.$$

The total derivative of $\widehat{f}_\alpha(t, \widehat{\mathbf{v}})$ **keeping $\mathbf{v}$ constant** yields:

$$\partial_t \widehat{f}_\alpha|_{\mathbf{v}} = \partial_t \widehat{f}_\alpha|_{\widehat{\mathbf{v}}} + \frac{d\widehat{\mathbf{v}}}{dt} \cdot \frac{\partial \widehat{f}_\alpha}{\partial \widehat{\mathbf{v}}}. \quad (3.9)$$

But $\frac{d\widehat{\mathbf{v}}}{dt}$ can be expressed as:

$$\frac{d\hat{\mathbf{v}}}{dt} = -\hat{\mathbf{v}} \frac{1}{v_{th,\alpha}} \frac{dv_{th,\alpha}}{dt}. \quad (3.10)$$

There results:

$$\partial_t \hat{f}_\alpha|_{\mathbf{v}} = \partial_t \hat{f}_\alpha|_{\hat{\mathbf{v}}} - v_{th,\alpha}^{-1} \frac{dv_{th,\alpha}}{dt} \hat{\mathbf{v}} \cdot \hat{\nabla}_v \hat{f}_\alpha. \quad (3.11)$$

On the other hand, we have:

$$\partial_t f_\alpha|_{\mathbf{v}} = \partial_t \left(\frac{\hat{f}_\alpha}{v_{th,\alpha}^3} \right) \Big|_{\mathbf{v}} = \frac{\partial_t \hat{f}_\alpha|_{\mathbf{v}}}{v_{th,\alpha}^3} + \hat{f}_\alpha \partial_t (v_{th,\alpha}^{-3}) = \frac{1}{v_{th,\alpha}^3} \left[\partial_t \hat{f}_\alpha|_{\hat{\mathbf{v}}} - v_{th,\alpha}^{-1} \frac{dv_{th,\alpha}}{dt} (\hat{\mathbf{v}} \cdot \hat{\nabla}_v \hat{f}_\alpha + 3\hat{f}_\alpha) \right]. \quad (3.12)$$

But $\hat{\nabla}_v \cdot \hat{\mathbf{v}} = 3$, and therefore:

$$\partial_t f_\alpha|_{\mathbf{v}} = \frac{1}{v_{th,\alpha}^3} \left[\partial_t \hat{f}_\alpha|_{\hat{\mathbf{v}}} - v_{th,\alpha}^{-1} \frac{dv_{th,\alpha}}{dt} \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \right] = \sum_{\beta} C_{\alpha\beta}. \quad (3.13)$$

There results the following transformed transport equation for $\hat{f}_\alpha(\hat{\mathbf{v}}, t)$:

$$\partial_t \hat{f}_\alpha - v_{th,\alpha}^{-1} \frac{dv_{th,\alpha}}{dt} \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) = v_{th,\alpha}^3 \sum_{\beta} C_{\alpha\beta} = \sum_{\beta} \hat{C}_{\alpha\beta}, \quad (3.14)$$

where we have used Eq. 3.8.

4. Asymptotic expansion of cross-species Rosenbluth potentials for disparate thermal velocities

As pointed out in Sec. 3.1, the computation of unlike-particle normalized Rosenbluth potentials requires the mapping of the target species distribution function to the colliding species domain. However, for sufficiently large disparity in the v_{th} ratio, the resulting disparity in velocity mesh cell sizes makes the interpolation step either inaccurate or impossible. (The limiting situation can be envisioned where the complete slow (s) domain fits in a single cell in the fast (f) domain.) In this study, we address this issue by deriving an asymptotic formulation of the Rosenbluth potentials in the limit of $v_{th,f}/v_{th,s} \gg 1$ for both the slow-on-fast and fast-on-slow interactions, which only requires the evaluation of moments of the distribution function.

Disparate thermal velocities arise either when $T_f \sim T_s$ and $m_f \ll m_s$, as in collisions between ions and electrons; or when $T_f \gg T_s$ and $m_f \sim m_s$, as in collisions between energetic α -particles and the deuterium-tritium plasma. Here, T_s , T_f , m_s and m_f are temperatures and masses of the slow and fast particles. We will assume small slow-to-fast thermal velocity ratio, $v_{th,s}/v_{th,f} \ll 1$, but allow the ratio m_f/m_s to be arbitrary.

4.1. Asymptotic slow-on-fast collisions

In general, the Fokker-Planck collision operator C_{sf} for slow particles colliding with fast particles, which is analogous to ion-electron collision operator, can be written in the Landau form as:

$$C_{sf} = \Gamma_{sf} \nabla_v \cdot \left[\int d^3 v' \nabla_g \nabla_g g \cdot \left(f'_f \nabla_v f_s - \frac{m_s}{m_f} f_s \nabla_{v'} f'_f \right) \right], \quad (4.1)$$

where $f_s \equiv f_s(\mathbf{v})$; $f'_f \equiv f'_f(\mathbf{v}')$; $\mathbf{g} \equiv \mathbf{v} - \mathbf{v}'$ and $g \equiv |\mathbf{g}|$; $\nabla_v \equiv \partial/\partial \mathbf{v}$ etc. Taylor-expanding in $v/v' \sim v_{th,s}/v_{th,f} \ll 1$,

$$\nabla_g \nabla_g g = \nabla_{v'} \nabla_{v'} |\mathbf{v}' - \mathbf{v}| = \nabla_{v'} \nabla_{v'} v' - \mathbf{v} \cdot \nabla_{v'} \nabla_{v'} \nabla_{v'} v' + \dots, \quad (4.2)$$

and keeping three expansion terms in the first integral on the right-hand side of Eq. 4.1, and four expansion terms in the second integral, gives:

$$C_{sf} = \Gamma_{sf} \nabla_v \cdot \left[\nabla_v \nabla_v G_f \cdot \nabla_v f_s - \frac{m_s}{m_f} f_s \nabla_v H_f \right] \quad (4.3)$$

with

$$G_f = \frac{1}{2} \mathbf{v} \mathbf{v} : \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} v' \right) - \frac{1}{6} \mathbf{v} \mathbf{v} \mathbf{v} : \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) + \frac{1}{24} \mathbf{v} \mathbf{v} \mathbf{v} \mathbf{v} : \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) + \dots, \quad (4.4)$$

$$H_f = 2 \mathbf{v} \cdot \left(\int d^3 v' f'_f \frac{\mathbf{v}'}{v'^3} \right) + \mathbf{v} \mathbf{v} : \left[\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] - \frac{1}{3} \mathbf{v} \mathbf{v} \mathbf{v} : \left[\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] + \frac{1}{12} \mathbf{v} \mathbf{v} \mathbf{v} \mathbf{v} : \left[\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] + \dots. \quad (4.5)$$

Explicit expressions for these integrals are given in AppendixA.

4.2. Asymptotic fast-on-slow collisions

The general form of the collision operator for fast species colliding with slow species, which is analogous to electron-ion collision operator, is given by Eq. (4.1) but with f and s interchanged. Taylor-expanding in $v'/v = v_{th,s}/v_{th,f} \ll 1$ and retaining three expansion terms of $\nabla_g \nabla_g g$ in both the first and second integrals on the right-hand side of thus modified Eq. (4.1) gives:

$$C_{fs} = \Gamma_{fs} \nabla_v \cdot \left[\nabla_v \nabla_v G_s \cdot \nabla_v f_f - \frac{m_f}{m_s} f_f \nabla_v H_s \right] \quad (4.6)$$

with:

$$G_s = n_s v - \frac{n_s \mathbf{V}_s \cdot \mathbf{v}}{v} + \nabla_v \nabla_v v : \left(\frac{1}{2} \int d^3 v' f'_s \mathbf{v}' \mathbf{v}' \right) + \dots, \quad (4.7)$$

$$H_s = 2 \frac{n_s}{v} + 2 \frac{n_s \mathbf{V}_s \cdot \mathbf{v}}{v^3} + \frac{3 \mathbf{v} \mathbf{v} - \overset{\leftrightarrow}{I} v^2}{v^5} : \left(\int d^3 v' f'_s \mathbf{v}' \mathbf{v}' \right) + \dots. \quad (4.8)$$

Here,

$$\nabla_v \nabla_v v : \left(\frac{1}{2} \int d^3 v' f'_s \mathbf{v}' \mathbf{v}' \right) = \frac{1}{v} \left(\int d^3 v' f'_s \frac{v'^2}{2} \right) + \frac{v_\perp^2}{2v^3} \left[\int d^3 v' f'_s \left(v_{\parallel}^2 - \frac{1}{2} v_\perp^2 \right) \right] \quad (4.9)$$

and

$$\frac{3 \mathbf{v} \mathbf{v} - \overset{\leftrightarrow}{I} v^2}{v^5} : \left(\int d^3 v' f'_s \mathbf{v}' \mathbf{v}' \right) = \frac{v_\parallel^2 - \frac{1}{2} v_\perp^2}{v^5} \int d^3 v' f'_s \left(v_{\parallel}^2 - \frac{1}{2} v_\perp^2 \right). \quad (4.10)$$

These expressions are equivalent to the first few terms of a multipole expansion, and are accurate to less than 1% with respect to the exact solution for $v_{th,s}/v_{th,f} < 0.5$, and feature negligible error for $v_{th,s}/v_{th,f} < 0.1$. The asymptotic expressions for the potentials are checked against known results and explicitly shown in AppendixB. The conservation properties of the asymptotic formulation of the slow-on-fast and fast-on-slow collision operators are analyzed in AppendixC, where we conclude that both energy and momentum are conserved to at least $\mathcal{O}[(v_{th,s}/v_{th,f})^2] \ll 1$. This small conservation error can be absorbed in the numerical conservation constraints, as described in Ref. [19] and in AppendixD. In Sec. 5.2.1, we discuss the regularization procedure of singularities in Eqs. 4.7 and 4.8.

Figure 5.1: 0D2V cylindrical velocity-space grid with azimuthal symmetry.

5. Numerical implementation

5.1. Discretization of the Fokker-Planck collision operator

In this manuscript, we consider a finite-volume approach to discretize the Fokker-Planck collision operator. We consider a 2V cylindrical velocity space ($v_{||}$ and $v_{\perp}$) with azimuthal symmetry (Fig. 5.1). The discrete volume for cell (j,k) is computed as:

$$\Delta V_{j,k} = 2\pi v_{\perp,k} \Delta v_{||,j} \Delta v_{\perp,k},$$

where $\Delta v_{||,j}$ and $\Delta v_{\perp,k}$ are the discrete velocity-space cell sizes in the parallel and perpendicular directions, respectively. For a uniform mesh, we have:

$$\Delta v_{||} = \frac{L_{||}}{N_{||}}, \quad \Delta v_{\perp} = \frac{L_{\perp}}{N_{\perp}},$$

where $L_{||}$ and $L_{\perp}$ are the parallel and perpendicular velocity-space domain sizes, and $N_{||}$ and $N_{\perp}$ are the number of cells in the respective directions. The mesh is arranged such that cell faces map to the domain boundary (and therefore outermost cell centers are half a mesh-spacing away from the boundary). The distribution function f and the Rosenbluth potentials H , G are defined at cell centers. Velocity-space inner products are approximated via a mid-point quadrature rule as:

$$\langle A, B \rangle_v \approx 2\pi \sum_{j=1}^{N_{||}} \sum_{k=1}^{N_{\perp}} v_{\perp,k} \Delta v_{||,j} \Delta v_{\perp,k} A_{j,k} B_{j,k}. \quad (5.1)$$

The Fokker-Planck operator can be written as

$$C_{\alpha\beta} = \nabla_v \cdot \mathbf{J}_{\alpha\beta}, \quad (5.2)$$

where:

$$\mathbf{J}_{\alpha\beta} = \Gamma_{\alpha\beta} \left[\mathbf{J}_{G,\alpha\beta} - \frac{m_{\alpha}}{m_{\beta}} \mathbf{J}_{H,\alpha\beta} \right],$$

is the Fokker-Planck flux, and

$$\mathbf{J}_{G,\alpha\beta} = \overleftrightarrow{D}_{\beta} \cdot \nabla_v f_{\alpha} \quad (5.3)$$

$$\mathbf{J}_{H,\alpha\beta} = \mathbf{A}_{\beta} f_{\alpha} \quad (5.4)$$

Figure 5.2: Illustration of flux on 2D velocity-space cell faces in terms of parallel ($\parallel$) and perpendicular ($\perp$) components.

are the collisional inter-species diffusion and friction fluxes, respectively. We discretize Eq. 5.2 in flux-form in a cylindrical velocity space as (Fig. 5.2):

$$C_{\alpha\beta,j,k} = \frac{J_{||,\alpha\beta,j+1/2,k} - J_{||,\alpha\beta,j-1/2,k}}{\Delta v_{||,j}} + \frac{v_{\perp,k+1/2} J_{\perp,\alpha\beta,j,k+1/2} - v_{\perp,k-1/2} J_{\perp,\alpha\beta,j,k-1/2}}{v_{\perp,k} \Delta v_{\perp,k}}.$$

Fluxes at cell faces are given by:

$$J_{||,G,\alpha\beta,j+\frac{1}{2},k} = \left(D_{||\parallel,\beta} \partial_{v_{||}} f_{\alpha} + D_{||\perp,\beta} \partial_{v_{\perp}} f_{\alpha} \right)_{j+\frac{1}{2},k}, \quad (5.5)$$

$$J_{\perp,G,\alpha\beta,j,k+\frac{1}{2}} = \left(D_{\perp\parallel,\beta} \partial_{v_{||}} f_{\alpha} + D_{\perp\perp,\beta} \partial_{v_{\perp}} f_{\alpha} \right)_{j,k+\frac{1}{2}}, \quad (5.6)$$

$$J_{||,H,\alpha\beta,j+\frac{1}{2},k} = A_{||,\beta,j+\frac{1}{2},k} f_{\alpha,j+\frac{1}{2},k}, \quad (5.7)$$

$$J_{\perp,H,\alpha\beta,j,k+\frac{1}{2}} = A_{\perp,\beta,j,k+\frac{1}{2}} f_{\alpha,j,k+\frac{1}{2}}. \quad (5.8)$$

We discretize the friction flux using SMART [22] and the tensor diffusion flux using an MC limiter [23], as was described in Ref. [19].

5.2. Numerical treatment of Rosenbluth potentials

We describe next the numerical treatment of the Rosenbluth potentials in the case of unlike-particle collisions, which requires interpolation between different meshes, see Fig. 5.3. For like-particle collisions, the Rosenbluth potentials and the distribution function are on the same mesh, and the treatment has been mostly addressed in Ref. [19]. **In the current study, instead of resorting to far-field evaluation of the ghost-cell boundary values of the Rosenbluth Potentials for Poisson solves (as in Ref. [19]), we use the multipole expansions in Sec. 4.2 (as was also proposed in Ref. [24]).**

5.2.1. Fast-on-slow collisions

In the case of a fast species colliding with a slower species ($v_{th,\alpha} > v_{th,\beta}$), the *primary (target) grid domain* (Ω_f) is larger than the *secondary (slave) grid domain* (Ω_s). It follows that the Rosenbluth potentials of the slower species cannot be interpolated everywhere in the fast-species domain, and must be *reconstructed* in areas not overlapping with the slow-species one. In this study, when the thermal velocity disparity is not too large, we proceed by interpolating the Rosenbluth potentials from the slow to the overlapping fast

Figure 5.3: Illustration of the multiple grid concept. The black and red grids represent the fast and slow grids, respectively.

Figure 5.4: Coarse-graining transfer of the slow-species potentials onto the fast-species velocity-space grid for a case of moderate thermal velocity disparity. The black grid corresponds to the fast-species grid, the red to the slow-species one, and the blue to the coarse-grained region ($\delta\Omega_{f,j,k}$).

species domain, and then fill the outer void region ($\Omega_f \cap \Omega_s = 0$) using the multipole expansion. We refer to this procedure as the *transfer procedure*. For large thermal velocity disparities, the interpolation is inaccurate, and we perform a direct coarse graining of the fast-on-slow collisional flux in the slow-species domain. We refer to this procedure as the *asymptotic procedure*. The ratio of v_{th} at which the switching occurs is determined by accuracy considerations of the asymptotic expansions, and will be discussed in Sec. 5.2.2. We provide details next.

Fast-on-slow transfer procedure for moderate thermal-velocity disparities. The slow potentials, $(H, G)_s$, are transferred to the fast domain via the following coarse-graining procedure. Consider only a portion of the slow mesh on the fast domain as shown in Fig. 5.4 with a blue-shaded region. We first construct a subgrid within a fast species cell where the overlapping exists (i.e. $\Omega_f \cap \Omega_s$) with the number of subgrid mesh cells $N_{sg,||}$, $N_{sg,\perp}$ and cell sizes $\Delta v_{sg,||}$, $\Delta v_{sg,\perp}$ defined in terms of the fast grid cell sizes as:

$$\Delta v_{sg,||} = \Delta v_{f,||} / N_{sg,||} ; \Delta v_{sg,\perp} = \Delta v_{f,\perp} / N_{sg,\perp}. \quad (5.9)$$

In this study, we employ:

$$N_{sg,||} = N_{sg,\perp} = \begin{cases} \min(N_{v,\perp}, \text{floor}[v_{th,f}/v_{th,s}]) & \text{if } \delta\Omega_{f,j,k} \cap \Omega_s \neq 0 \\ 3 & \text{else} \end{cases}.$$

Figure 5.5: A scenario of $v_{th,f}/v_{th,s} \gg 1$ leading to the lack of velocity-space resolution in the fast velocity space.

We use different resolutions for the subgrid because, in the overlap region, small-scale structures exist which require finer resolution, while away from the overlap region structures are smoother. We remark that we set $N_{sg} = 3$ in the non-overlap region to guarantee smoothness in the transition of the potentials.

We interpolate $(H, G)_s$ onto this subgrid using spline reconstruction and then average within this cell:

$$(H, G)_{fs,j,k} = \frac{\int_{\delta\Omega_{f,j,k}} (H, G)_s d^3v}{\int_{\delta\Omega_{f,j,k}} d^3v} \approx \frac{\sum_{j'=1}^{N_{sg,||}} \sum_{k'=1}^{N_{sg,\perp}} v_{sg,\perp,k'} \Delta v_{sg,||,j'} \Delta v_{sg,\perp,k'} (H, G)_{s,j',k'}}{\sum_{j'=1}^{N_{sg,||}} \sum_{k'=1}^{N_{sg,\perp}} v_{sg,\perp,k'} \Delta v_{sg,||,j'} \Delta v_{sg,\perp,k'}}, \quad (5.10)$$

where $\delta\Omega_{f,j,k}$ is the fast-domain cell and $v_{sg,\perp,k'}$ is the subgrid perpendicular velocity, defined as:

$$v_{sg,\perp,k'} = v_{f,\perp,k-1/2} + \left(k' - \frac{1}{2}\right) \Delta v_{sg,\perp,k'}. \quad (5.11)$$

Once the slow-species potentials are interpolated onto the fast grid in the overlapping region, we fill the non-overlapping regions using the multipole fast-on-slow expansion as discussed in Section 4.2. Finally, the cross-species transport coefficients are computed as:

$$\overleftrightarrow{D}_{fs} = \nabla_v \nabla_v G_{fs}, \quad (5.12)$$

$$\mathbf{A}_{fs} = \nabla_v H_{fs}. \quad (5.13)$$

Fast-on-slow asymptotic treatment for large thermal velocity disparity. For large v_{th} disparities, a special treatment must be provided near the origin, $v = 0$, where the majority of the slow species distribution function is concentrated and the Rosenbluth potentials vary quickly. For sufficiently large thermal velocity disparity, these sharply varying structures may all be contained in a single cell (Fig. 5.5). **If a low-order finite difference discretization is used to compute the collisional flux within this cell, a significant numerical error will be introduced since the slow potentials will be severely under resolved.** To compute the flux accurately in these situations, we again employ a coarse-graining technique:

$$\langle \mathbf{J}_{G/H,fs} \rangle_{j,k} = \frac{[\int d^3v \mathbf{J}_{G/H,fs}]_{j,k}}{[\int d^3v]_{j,k}}. \quad (5.14)$$

The computation of this flux requires one to discriminate between regions of full overlap between slow and fast grids, and regions where partial or no overlap exists; refer to Fig. 5.6. In full overlap regions, the underlying slow species potentials are used for the flux coarse-graining; in no-overlap regions, the asymptotic

Figure 5.6: Illustration of the coarse graining procedure for a case of large thermal velocity disparity. The red grid represents the slow grid and the black grid represents the fast grid. The purple region denotes the region of no overlap (where asymptotic potentials are used), while the red region uses the potentials interpolated from the slow grid.

potentials are used instead. In partial overlap regions, both slow and asymptotic potentials are used for the coarse-graining of the flux.

The coarse graining of the *cell-centered* flux is performed in a similar fashion to the coarse-graining of the slow potentials (Eq. 5.10):

$$\langle \mathbf{J}_{G/H,fs} \rangle_{j,k} \approx \frac{\sum_{j'=1}^{N_{sg,\parallel}} \sum_{k'=1}^{N_{sg,\perp}} v_{sg,\perp,k'} \Delta v_{sg,\parallel,j'} \Delta v_{sg,\perp,k'} \mathbf{J}_{G/H,fs,j',k'}}{\sum_{j'=1}^{N_{sg,\parallel}} \sum_{k'=1}^{N_{sg,\perp}} v_{sg,\perp,k'} \Delta v_{sg,\parallel,j'} \Delta v_{sg,\perp,k'}} \quad (5.15)$$

with the collision fluxes given by:

$$\mathbf{J}_{G,fs} = \overleftrightarrow{D}_{fs} \cdot \nabla_v f_f, \quad \mathbf{J}_{H,fs} = \mathbf{A}_{fs} f_f.$$

Subgrid sizes for coarse graining are chosen as before. As stated above, the transport coefficients $\overleftrightarrow{D}_{fs}$ and $\mathbf{A}_{fs}$ are computed differently depending on whether a given cell in the sum in Eq. 5.15 lies in the overlapping region or not:

$$\overleftrightarrow{D}_{fs} = \begin{cases} \overleftrightarrow{D}_{ss,asy} & \text{if } \mathbf{v}_f \notin \Omega_s \\ \overleftrightarrow{D}_{ss} & \text{else} \end{cases} \quad (5.16)$$

and

$$\mathbf{A}_{fs} = \begin{cases} \mathbf{A}_{ss,asy} & \text{if } \mathbf{v}_f \notin \Omega_s \\ \mathbf{A}_{ss} & \text{else} \end{cases}. \quad (5.17)$$

The local values of f_f and $\nabla_v f_f$, required to reconstruct the fluxes in the coarse-graining integrals, are obtained from a quadratic spline reconstruction of the fast distribution function in its native mesh.

The final step in the coarse-graining procedure is to estimate a face-centered flux from the cell-centered coarse-grained ones as:

$$\langle \mathbf{J}_{\parallel,G/H,fs} \rangle_{j+1/2,k} = \frac{1}{2} \left[\langle \mathbf{J}_{\parallel,G/H,fs} \rangle_{j+1,k} + \langle \mathbf{J}_{\parallel,G/H,fs} \rangle_{j,k} \right] \quad (5.18)$$

and:

$$\langle J_{\perp, G/H, fs} \rangle_{j, k+1/2} = \frac{\Delta v_{f, \perp, k+1} v_{f, \perp, k+1} \langle J_{\perp, G/H, fs} \rangle_{j, k+1} + \Delta v_{f, \perp, k} v_{f, \perp, k} \langle J_{\perp, G/H, fs} \rangle_{j, k}}{\Delta v_{f, \perp, k+1} v_{f, \perp, k+1} + \Delta v_{f, \perp, k} v_{f, \perp, k}}. \quad (5.19)$$

5.2.2. Slow-on-fast collisions

Slow-on-fast transfer procedure for moderate thermal velocity disparities. In slow-on-fast interactions, the *primary grid domain*, Ω_s , is fully contained by the *secondary grid domain*, Ω_f . For small and moderate thermal velocity disparities, given their smoothness, the potentials H_{sf} and G_{sf} can be directly interpolated from the fast species grid onto the slow species grid (here, we use a quadratic spline interpolation).

Slow-on-fast asymptotic treatment for large thermal velocity disparities. The slow-on-fast asymptotic formulas for the potentials require $v_{th,s}/v_{th,f} \ll 1$. The accuracy of the asymptotic expansion depends on smallness of the expansion parameter. In order to ensure an accurate expansion of fast potentials in the slow domain (of size $L_{v,s}$) in the limit $v_{th,s}/v_{th,f} \ll 1$, we must ensure that the slow domain size $L_{v,s}$ is small enough with respect to the fast thermal velocity. In practice, this means that:

$$\frac{L_{v,s}}{v_{th,f}} \equiv \widehat{L}_v \frac{v_{th,s}}{v_{th,f}} \leq \epsilon_{asy}, \quad (5.20)$$

where we have used that $L_{v,s} = v_{th,s} \widehat{L}_v$, and ϵ_{asy} is a tolerance, which depends on the order of accuracy of the asymptotic expansion (here, we have used a fourth-order Taylor expansion, which allows $\epsilon_{asy} \sim 0.5$ before we lose asymptotic accuracy). **From Eq. 5.20, it follows that:**

$$\frac{v_{th,s}}{v_{th,f}} \leq \frac{\epsilon_{asy}}{\widehat{L}_v}, \quad (5.21)$$

which is the threshold that determines whether an asymptotic treatment is warranted.

In addition, Eq. 5.20 implies a minimum velocity-space resolution for accuracy. The argument is as follows. Let n_{min} be the minimum number of fast-domain velocity-space cells spanned by the slow domain allowed before one transitions to the asymptotic formula treatment, i.e.:

$$n_{min} \Delta v_f \leq L_{v,s}.$$

Recognizing that $\Delta v_f = v_{th,f} \Delta \widehat{v}$, and $\Delta \widehat{v} = \frac{\widehat{L}_v}{N_v}$ (with N_v the number of velocity-space mesh points per dimension) gives then:

$$n_{min} v_{th,f} \frac{\widehat{L}_v}{N_v} \leq v_{th,s} \widehat{L}_v.$$

Rearranging and using Eq. 5.20, we obtain:

$$\frac{n_{min}}{N_v} \leq \frac{v_{th,s}}{v_{th,f}} \leq \frac{\epsilon_{asy}}{\widehat{L}_v}$$

which gives a condition for the minimum velocity-space resolution:

$$N_v \geq \frac{n_{min} \widehat{L}_v}{\epsilon_{asy}}.$$

This expression highlights the need to maximize ϵ_{asy} (i.e., to use a high-order Taylor expansion) to minimize N_v . For $\widehat{L}_v \sim 5$, $\epsilon_{asy} \sim 0.5$, and $n_{min} \sim 10$, we find $N_v \sim 100$ and (from Eq. 5.20) **$v_{th,f}/v_{th,s} \geq 10$ for the asymptotic expansion to be accurate. Smaller values of the thermal-velocity ratio, in particular for the slow-on-fast expansion, will result in incorrect curvatures of the Rosenbluth potentials near the velocity-space boundary, leading to unphysical results.**

5.3. Discretization of the inertial component: exact conservation properties

We discuss next the enforcement of exact conservation properties of the Fokker-Planck equation with velocity-space adaptivity. The original approach of enforcing discrete conservation in the collision operator [19] has been improved for the multiple-grid approach and is discussed in AppendixD. We focus the discussion in this section on the inertial terms of the temporal update term (the left-hand side of Eq. 3.14). We begin by developing independent mass, momentum, and energy conserving schemes, then combine mass and momentum conservation, and finally combine all conservation properties.

5.3.1. Exact Mass Conservation

We show that mass conservation is trivially enforced by the left-hand side of Eq. 3.14 for a 0D case. Taking the zeroth moment of the left-hand side of Eq. 3.14, we find in the continuum:

$$\frac{\partial \langle 1, \hat{f}_\alpha \rangle_{\hat{v}}}{\partial t} - v_{th,\alpha}^{-1} \frac{\partial_t v_{th,\alpha}}{2} \langle 1, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_{\hat{v}} = \frac{\partial n_\alpha}{\partial t} = 0, \quad (5.22)$$

where $n_\alpha = \langle 1, \hat{f}_\alpha \rangle_{\hat{v}}$ is the number density of species α . Here, we have used that $\langle 1, \hat{f} \rangle_{\hat{v}} = \langle 1, f \rangle_v = n$, and that $\langle 1, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_{\hat{v}} = 0$ in both continuum and discrete representations because it is in conservative form.

5.3.2. Exact Momentum Conservation

We derive the exact momentum conservation scheme for the left-hand side of Eq. 3.14 for a 0D case. We rewrite the left-hand side of Eq. 3.14 (by multiplying with $v_{th,\alpha}$) as:

$$\partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} [\hat{f}_\alpha + \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha)] = 0. \quad (5.23)$$

Momentum conservation can be shown by taking the first velocity moment of the above equation, to find:

$$\partial_t (v_{th,\alpha} \langle \hat{\mathbf{v}}, \hat{f}_\alpha \rangle_{\hat{v}}) - \partial_t v_{th,\alpha} [\langle \hat{\mathbf{v}}, \hat{f}_\alpha \rangle_{\hat{v}} + \langle \hat{\mathbf{v}}, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_{\hat{v}}] = \partial_t (n \mathbf{u}_\alpha) = 0,$$

where $n \mathbf{u}_\alpha = v_{th,\alpha} \langle \hat{\mathbf{v}}, \hat{f}_\alpha \rangle_{\hat{v}}$ is the number density flux of species α (for momentum density, we simply multiply by the mass of the species). Here, we have used that, in the continuum:

$$\langle \hat{\mathbf{v}}, \hat{f}_\alpha \rangle_{\hat{v}} + \langle \hat{\mathbf{v}}, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_{\hat{v}} = 0. \quad (5.24)$$

However, this identity is not satisfied discretely in general due to discretization error. We follow the concepts introduced in Ref. [19], and introduce a dyad $\overleftrightarrow{\mathcal{R}}_{t,\alpha}$ into Eq. 5.22:

$$\partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} [\hat{f}_\alpha + \hat{\nabla}_v \cdot (\overleftrightarrow{\mathcal{R}}_{t,\alpha} \cdot \hat{\mathbf{v}} \hat{f}_\alpha)] = 0, \quad (5.25)$$

such that the cancellation in Eq. 5.24 be strictly enforced. This is accomplished with $\overleftrightarrow{\mathcal{R}}_{t,\alpha}$ defined as:

$$\overleftrightarrow{\mathcal{R}}_{t,\alpha} \cdot = \begin{bmatrix} \Upsilon_{t,\alpha,\parallel} & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} -\frac{\langle v_{\parallel}, \hat{f}_\alpha \rangle_v}{\langle v_{\parallel}, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_v} & 0 \\ 0 & 1 \end{bmatrix}. \quad (5.26)$$

However, care must be taken since $\langle v_{\parallel}, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \rangle_{\hat{v}}$ can vanish. To address this issue, we split the $v_{\parallel}$ domain of integration into two subdomains:

$$\langle \hat{v}_{\parallel}, \partial_{\parallel} \Upsilon_{t,\alpha,\parallel} \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{v}} = \Upsilon_{t,\alpha,\parallel}^+ \langle v_{\parallel}, \partial_{\parallel} \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{v}} \Big|_{\hat{u}_{\alpha,\parallel}}^{\infty} + \Upsilon_{t,\alpha,\parallel}^- \langle v_{\parallel}, \partial_{\parallel} \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{v}} \Big|_{-\infty}^{\hat{u}_{\alpha,\parallel}},$$

with $\hat{u}_{\alpha,\parallel}$ the normalized parallel bulk flow of the α species and $\langle v_{\parallel}, (\cdot) \rangle_{\hat{v}} \Big|_a^b \equiv \int_0^\infty v_{\perp} dv_{\perp} \int_a^b (\cdot) dv_{\parallel}$. By setting $\Upsilon_{t,\alpha,\parallel}^+ = 1$ without loss of generality, and performing an integration by parts, we find $\Upsilon_{t,\alpha,\parallel}$ as:

$$\Upsilon_{t,\alpha,\parallel} = \begin{cases} \frac{\langle \hat{v}_{\parallel}, f_{\alpha} \rangle_{\hat{v}} - \langle 1, \hat{v}_{\parallel} \hat{f}_{\alpha} \rangle_{\hat{v}} \Big|_{\hat{u}_{\alpha}}^{\infty}}{\langle 1, \hat{v}_{\parallel} \hat{f}_{\alpha} \rangle_{\hat{v}} \Big|_{-\infty}^{\hat{u}_{\alpha}}}, & \hat{v}_{\parallel} < \hat{u}_{\alpha,\parallel}, \\ 1 & \hat{v}_{\parallel} > \hat{u}_{\alpha,\parallel} \end{cases}, \quad (5.27)$$

which is well posed.

5.3.3. Exact Energy Conservation

We derive an exact energy conservation scheme by first multiplying the left-hand side of Eq. 3.14 by $v_{th,\alpha}^2$:

$$v_{th,\alpha}^2 \frac{\partial \hat{f}_{\alpha}}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) = 0. \quad (5.28)$$

Using the chain rule, we obtain:

$$\partial_t (v_{th,\alpha}^2 \hat{f}_{\alpha}) - \partial_t v_{th,\alpha}^2 \left[\hat{f}_{\alpha} + \frac{\hat{\nabla}_v}{2} \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) \right] = 0. \quad (5.29)$$

Energy conservation can be shown in the continuum by evaluating the second velocity moment of the above equation:

$$\partial_t \left(v_{th,\alpha}^2 \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{v}} \right) - \partial_t v_{th,\alpha}^2 \left[\left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{v}} + \left\langle \frac{\hat{v}^2}{2}, \frac{\hat{\nabla}_v}{2} \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) \right\rangle_{\hat{v}} \right] = \partial_t U_{\alpha}^* = 0,$$

where $U_{\alpha}^* = v_{th,\alpha}^2 \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{v}}$ is the total specific energy density of species α (for total energy density, we simply multiply by the mass of the species) and we have used that

$$\left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{v}} + \left\langle \frac{\hat{v}^2}{2}, \frac{\hat{\nabla}_v}{2} \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) \right\rangle_{\hat{v}} = 0. \quad (5.30)$$

To enforce this identity discretely, we modify Eq. 5.29 as:

$$\partial_t (v_{th,\alpha}^2 \hat{f}_{\alpha}) - \partial_t v_{th,\alpha}^2 \left[\hat{f}_{\alpha} + \frac{\gamma_{t,\alpha}}{2} \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) \right] = 0. \quad (5.31)$$

Here, $\gamma_{t,\alpha}$ is the constraint coefficient that enforces Eq. 5.30, and is given by:

$$\gamma_{t,\alpha} = - \frac{2 \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{v}}}{\left\langle \frac{\hat{v}^2}{2}, \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_{\alpha}) \right\rangle_{\hat{v}}}. \quad (5.32)$$

5.3.4. Exact Mass and Momentum Conservation

We now extend the discretization scheme to enforce mass and momentum conservation simultaneously. In the development of the momentum-conserving scheme, we begin by multiplying Eq. 5.23 by $v_{th,\alpha}$ and taking the zeroth velocity moment to find:

$$v_{th,\alpha} [\partial_t (v_{th,\alpha} n_{\alpha}) - n_{\alpha} \partial_t v_{th,\alpha}] = 0. \quad (5.33)$$

In the continuum, we can perform the following manipulation,

$$\partial_t (v_{th,\alpha} n_\alpha) = v_{th,\alpha} \partial_t n_\alpha + n_\alpha \partial_t v_{th,\alpha} \quad (5.34)$$

to find $\partial_t n_\alpha = 0$, which is precisely the statement of mass conservation. However, in order to arrive at mass conservation from the momentum-conserving formulation, we require the chain rule to hold. This is achieved by reformulating Eq. 5.25 as:

$$v_{th,\alpha} \left\{ \partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \hat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \hat{\mathbf{v}} \hat{f}_\alpha \right) \right] \right\} + \eta_{t,\alpha} = 0, \quad (5.35)$$

where, as before:

$$\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} = \begin{bmatrix} \Upsilon_{t,\alpha,\parallel} & 0 \\ 0 & 1 \end{bmatrix}. \quad (5.36)$$

In Eq. 5.35, $\eta_{t,\alpha}$ is a discrete consistency source in velocity space defined as:

$$\eta_{t,\alpha}(\hat{\mathbf{v}}) = \left\{ v_{th,\alpha}^2 \partial_t \hat{f}_\alpha - \partial_t v_{th,\alpha}^2 \frac{\hat{\nabla}_v}{2} \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \right\} - v_{th,\alpha} \left\{ \partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \right] \right\}, \quad (5.37)$$

which vanishes identically in the continuum, and enforces the chain rule discretely. Introducing the definition of $\eta_{t,\alpha}$ in Eq. 5.35, we obtain:

$$\begin{aligned} & v_{th,\alpha} \left\{ \partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \hat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \hat{\mathbf{v}} \hat{f}_\alpha \right) \right] \right\} \\ & + \left\{ v_{th,\alpha}^2 \partial_t \hat{f}_\alpha - \partial_t v_{th,\alpha}^2 \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \right\} \\ & - v_{th,\alpha} \left\{ \partial_t (v_{th,\alpha} \hat{f}_\alpha) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) \right] \right\} \\ & = v_{th,\alpha}^2 \partial_t \hat{f}_\alpha - \partial_t v_{th,\alpha}^2 \hat{\nabla}_v \cdot (\hat{\mathbf{v}} \hat{f}_\alpha) - v_{th,\alpha} \partial_t v_{th,\alpha} \hat{\nabla}_v \cdot \left[\left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} - \overset{\leftrightarrow}{I} \right) \cdot \hat{\mathbf{v}} \hat{f}_\alpha \right], \end{aligned} \quad (5.38)$$

which is in conservative form in velocity space.

In order to enforce momentum conservation, we redefine $\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha}$ to absorb the new truncation error arising from $\eta_{t,\alpha}$ as:

$$\Upsilon_{t,\alpha,\parallel} = \begin{cases} \frac{v_{th,\alpha} \partial_t v_{th,\alpha} \left[\langle \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{\mathbf{v}}} - \langle 1, \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{\mathbf{v}}} |_{\hat{u}_{\alpha,\parallel}}^{\infty} \right] - \langle \hat{v}_{\parallel}, \eta_{t,\alpha} \rangle_{\hat{\mathbf{v}}}}{v_{th,\alpha} \partial_t v_{th,\alpha} \langle 1, \hat{v}_{\parallel} \hat{f}_\alpha \rangle_{\hat{\mathbf{v}}} |_{-\infty}^{\hat{u}_{\alpha,\parallel}}}, & \hat{v}_{\parallel} < \hat{u}_{\alpha,\parallel} \\ 1 & \hat{v}_{\parallel} > \hat{u}_{\alpha,\parallel} \end{cases}. \quad (5.39)$$

We show next that Eq. 5.35 (or equivalently Eq. 5.38) enforces exact mass and momentum conservation discretely. Mass conservation follows from the conservative form of Eq. 5.38. Momentum conservation follows from taking the first parallel velocity moment of Eq. 5.35, we find:

$$v_{th,\alpha} \partial_t (v_{th,\alpha} n \hat{u}_{\alpha,\parallel}) = v_{th,\alpha} \partial_t v_{th,\alpha} \int d\hat{\mathbf{v}} \hat{v}_{\parallel} \left[\hat{f}_\alpha + \hat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \hat{\mathbf{v}} \hat{f}_\alpha \right) \right] - \int d\hat{\mathbf{v}} \hat{v}_{\parallel} \eta_{t,\alpha} = 0,$$

where the last equality is justified by the definition of $\Upsilon_{t,\alpha}$.

5.3.5. Exact Mass, Momentum, and Energy Conservation

Following the same template, we finally extend the scheme to enforce mass, momentum, and energy conservation simultaneously. We perform a recursive enslavement of the mass and momentum conserving

equation (Eq. 5.35) into the energy conserving equation (Eq. 5.31) by introducing a discrete consistency source, $\xi_{t,\alpha}$:

$$\partial_t \left(v_{th,\alpha}^2 \hat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\hat{f}_\alpha + \gamma_{t,\alpha} \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] + \xi_{t,\alpha} = 0 \quad (5.40)$$

with

$$\begin{aligned} \xi_{t,\alpha} = & v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \hat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] \right\} \\ & - \left\{ \partial_t \left(v_{th,\alpha}^2 \hat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\hat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] \right\} + \eta_{t,\alpha}, \end{aligned} \quad (5.41)$$

$\gamma_{t,\alpha}$ redefined to take into account $\xi_{t,\alpha}$ as

$$\gamma_{t,\alpha} = \frac{-\partial_t v_{th,\alpha}^2 \left\langle \frac{\widehat{v}^2}{2}, \hat{f}_\alpha \right\rangle_{\widehat{\mathbf{v}}} + \left\langle \frac{\widehat{v}^2}{2}, \xi_{t,\alpha} \right\rangle_{\widehat{\mathbf{v}}}}{\partial_t v_{th,\alpha}^2 \left\langle \frac{\widehat{v}^2}{2}, \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right\rangle_{\widehat{\mathbf{v}}}}, \quad (5.42)$$

$\eta_{t,\alpha}$ defined in Eq. 5.37, and as before $\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha}$ defined as:

$$\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} = \begin{bmatrix} \Upsilon_{t,\parallel,\alpha} & 0 \\ 0 & 1 \end{bmatrix},$$

with,

$$\Upsilon_{t,\alpha,\parallel} = \begin{cases} \frac{v_{th,\alpha} \partial_t v_{th,\alpha} \left[\left\langle \widehat{v}_{\parallel}, \hat{f}_\alpha \right\rangle_{\widehat{\mathbf{v}}} - \left\langle 1, \widehat{v}_{\parallel} \hat{f}_\alpha \right\rangle_{\widehat{\mathbf{v}}} \right]_{\widehat{u}_{\alpha,\parallel}}^\infty - \left\langle \widehat{v}_{\parallel}, \eta_{t,\alpha} \right\rangle_{\widehat{\mathbf{v}}} - \partial_t v_{th,\alpha}^2 (\gamma_{t,\alpha} - 1) \left\langle 1, \frac{\widehat{v}_{\parallel} \hat{f}_\alpha}{2} \right\rangle_{\widehat{\mathbf{v}}}}{v_{th,\alpha} \partial_t v_{th,\alpha} \left\langle 1, \widehat{v}_{\parallel} \hat{f}_\alpha \right\rangle_{\widehat{\mathbf{v}}} \Big|_{-\infty}^{\widehat{u}_{\alpha,\parallel}}}, & \widehat{v}_{\parallel} \leq \widehat{u}_{\alpha,\parallel} \\ 1 & \widehat{v}_{\parallel} > \widehat{u}_{\alpha,\parallel} \end{cases} \quad (5.43)$$

We show next that Eq. 5.40 preserves mass, momentum, and energy exactly. We begin by taking the second moment of Eq. 5.40 to find:

$$\partial_t U_\alpha^* = \partial_t v_{th,\alpha}^2 \left[\left\langle \frac{\widehat{v}^2}{2}, \hat{f}_\alpha \right\rangle_{\widehat{\mathbf{v}}} + \gamma_{t,\alpha} \left\langle \frac{\widehat{v}^2}{2}, \widehat{\nabla}_v \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right\rangle_{\widehat{\mathbf{v}}} \right] - \left\langle \frac{\widehat{v}^2}{2}, \xi_{t,\alpha} \right\rangle_{\widehat{\mathbf{v}}} = 0,$$

where for the last equality we have used Eq. 5.41. To prove momentum conservation, we substitute Eq. 5.41 into Eq. 5.40, to find:

$$v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \hat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\hat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] \right\} + \eta_{t,\alpha} - \frac{(\gamma_{t,\alpha} - 1)}{2} \partial_t v_{th,\alpha}^2 \left[\widehat{\nabla}_v \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] = 0.$$

Taking the first moment of this equation yields:

$$v_{th,\alpha} \partial_t (v_{th,\alpha} n \widehat{\mathbf{u}}_\alpha) = v_{th,\alpha} \partial_t v_{th,\alpha} \int d\widehat{\mathbf{v}} \widehat{\mathbf{v}} \left[\hat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} \cdot \widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] - \int d\widehat{\mathbf{v}} \widehat{\mathbf{v}} \left[\eta_{t,\alpha} - \frac{(\gamma_{t,\alpha} - 1)}{2} \partial_t v_{th,\alpha}^2 \widehat{\nabla}_v \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] = 0$$

by Eq. 5.43. Finally, mass conservation follows by substituting Eq. 5.37 and 5.41 into Eq. 5.40 to find:

$$v_{th,\alpha}^2 \partial_t \hat{f}_\alpha - \partial_t v_{th,\alpha}^2 \left[\frac{(\gamma_{t,\alpha} - 1)}{2} \widehat{\nabla}_v \cdot \left(\widehat{\mathbf{v}} \hat{f}_\alpha \right) \right] - v_{th,\alpha} \partial_t v_{th,\alpha} \widehat{\nabla}_v \cdot \left[\left(\overset{\leftrightarrow}{\mathcal{R}}_{t,\alpha} - \overset{\leftrightarrow}{I} \right) \cdot \widehat{\mathbf{v}} \hat{f}_\alpha \right] = 0,$$

which is conservative in velocity space, and thus ensures mass conservation.

The final form of the 0D2V Fokker-Planck equation to be solved numerically in this study is:

$$\partial_t \left(v_{th,\alpha}^2 \hat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\hat{f}_\alpha + \gamma_{t,\alpha} \frac{\hat{\mathbf{v}}_v}{2} \cdot \left(\hat{\mathbf{v}} \hat{f}_\alpha \right) \right] + \xi_{t,\alpha} [\Upsilon_{t,\alpha,||}] = v_{th,\alpha}^2 \sum_{\beta} \hat{C}_{\alpha\beta},$$

where we have stressed that $\xi_{t,\alpha}$ is a (linear) function of $\Upsilon_{t,\alpha,||}$. The evaluation of this equation in residual form (e.g., for a Jacobian-free Newton-Krylov solver) requires computing two moment constraints, $\Upsilon_{t,\alpha,||}$ and $\gamma_{t,\alpha}$, which in turn requires solving a 2×2 linear set of equations involving moments of $\hat{f}$. The details are given in AppendixE.

6. Numerical results

In this section, we demonstrate the properties of our numerical implementation, both in terms of conservation and order of accuracy, with various examples of varying degrees of complexity. We also provide evidence of the impact of velocity-space adaptivity in the efficiency of the scheme. For all problems, the mass, charge, temperature, density, velocity, and time are normalized with respect to the proton mass, proton charge, a reference temperature T_0 , density, n_0 , thermal velocity, $v_{th,0}$, and time-scale, τ_0 , respectively. Here, τ_0 is the inverse collision frequency computed from m_0 , q_0 , n_0 , and T_0 and is a dependent quantity. We note that, throughout this section, we employ the same solver strategy as documented in Ref. [19], except as indicated in AppendixD. We also note that when electrons are not explicitly included in the calculation, quasineutrality is assumed. In all cases, the plasma distribution function is initialized as a Maxwellian with a specified density, n , fluid velocity, u , and temperature, T .

Before we consider the numerical results, a word is in order about our temporal evolution strategy for v_{th} . The normalization of the Fokker-Planck equation with respect to the thermal velocity v_{th} ensures optimal resolution of the corresponding distribution function at all times, provided that the thermal velocity evolves in time consistently with the temperature of the distribution function itself. However, one must use care in the practical implementation of this strategy. Firstly, we avoid additional nonlinearity in our equation set by normalizing all quantities at time-level $k+1$ with the time-level k thermal velocity, $v_{th,\alpha}^k$, i.e. $\hat{f}_\alpha^{k+1} = (v_{th,\alpha}^k)^3 f_\alpha^{k+1}$. As we will show later in this section, this choice does not spoil second-order accuracy in time. The reason is that the normalization with v_{th} is a numerical trick, not a fundamental physical principle, and, when implemented correctly and consistently (particularly in the computation of its temporal derivatives), it does not change the temporal accuracy properties of the solution. Secondly, care must be taken in the definition of v_{th} . Here, we use the prescription $v_{th,\alpha}^k = v_{th,\alpha}^0 \sqrt{T_\alpha^k / T_\alpha^{k=0}}$ instead of the more intuitive definition $v_{th,\alpha}^k = \sqrt{2T_\alpha^k / m_\alpha}$. The motivation behind this choice is the better accuracy performance of the former vs. the latter. More details are given in AppendixF.

6.1. Two species temperature and momentum equilibration

We begin by considering time equilibration of two species with different initial flow velocities and temperatures. This is the same case as considered in Sec. 5.4 of Ref. [19]. The purpose of this case is to demonstrate that the adaptive-grid approach with transfer of cross-species potentials produces results equivalent to a single-grid approach in accuracy, but with much improved efficiency. It will also allow us to quantify the overhead impact of transfer operations in the adaptive case.

Specific setup parameters are masses $m_1 = 2$, $m_2 = 4$, charges $Z_1 = 1$, $Z_2 = 2$, densities $n_1 = n_2 = 1$, temperatures $T_1 = 1$, $T_2 = 25$, drifts $u_{||,1} = -3\sqrt{2}$, $u_{||,2} = 3\sqrt{2}$, a normalized velocity-space domain of $\hat{v}_{||} \in [-9, 6]$ and $\hat{v}_\perp \in [0, 6]$, and a mesh of $N_v = N_{||} \times N_\perp = 128 \times 64$. The correct equilibrium values for temperature and momentum can be computed from total energy and momentum conservation:

Figure 6.1: Two-species temperature and momentum equilibration: comparison of the adaptive-grid approach vs. the single-grid (SG) approach [19].

$$\sum_{\alpha} U_{\alpha}^0 \equiv \sum_{\alpha} \left(\frac{3}{2} n_{\alpha} T_{\alpha} + \frac{m_{\alpha} n_{\alpha} u_{\alpha}^2}{2} \right)^0 = \sum_{\alpha} \left(\frac{3}{2} n_{\alpha} T_{\alpha} + \frac{m_{\alpha} n_{\alpha} u_{\alpha}^2}{2} \right)^n,$$

$$\sum_{\alpha} I_{\alpha}^0 \equiv \sum_{\alpha} (m_{\alpha} n_{\alpha} u_{||,\alpha})^0 = \sum_{\alpha} (m_{\alpha} n_{\alpha} u_{||,\alpha})^n,$$

where superscripts denote the time-level. The initial total momentum and energy are $I^0 = 8.49$ and $U^0 = 93$. From momentum conservation, $u_1^{\infty} = u_2^{\infty} = 1.41$ and from energy conservation, $T_1^{\infty} = T_2^{\infty} = 29$.

The time history of temperatures and flow velocities for both single-grid [19] and adaptive-grid approaches are plotted in Fig. 6.1. Excellent agreement is found between both approaches, and the correct equilibrium values are achieved. The time history of relative errors in conserved quantities, namely, the discrete mass,

$$\Delta M^n = \frac{|M^n - M^0|}{|M^0|},$$

parallel momentum,

$$\Delta I^n = \frac{|I^n - I^0|}{|I^0|},$$

and energy,

$$\Delta U^n = \frac{|U^n - U^0|}{|U^0|},$$

are depicted in Fig. 6.2 as functions of time for varying nonlinear solver tolerances, ε_r (for details, refer to Ref. [19]). Here, $M^n = \sum_{\alpha}^{N_s} m_{\alpha} \langle 1, \hat{f}_{\alpha}^n \rangle_{\hat{v}}$, $I^n = \sum_{\alpha}^{N_s} m_{\alpha} v_{th,\alpha}^{n-1} \langle \hat{v}_{||}, \hat{f}_{\alpha}^n \rangle_{\hat{v}}$ and $U^n = \sum_{\alpha}^{N_s} \frac{m_{\alpha} (v_{th,\alpha}^{n-1})^2}{2} \langle \hat{v}^2, \hat{f}_{\alpha}^n \rangle_{\hat{v}}$ are the total mass, momentum, and energy of the system. Owing to the conservation constraints in both the collision operator and the inertial term, the conservation properties are enforced down to the nonlinear convergence tolerance level, as expected. The comparison of conservation errors with and without the nonlinear conservation constraints in the inertial operator (but still keeping them in the collision operator) is shown in Fig. 6.3. As can be seen, without enforcing strict conservation properties, conservation errors are

Figure 6.2: Two-species temperature and momentum equilibration: conservation errors as functions of time and nonlinear tolerance.

Figure 6.3: Two-species temperature and momentum equilibration: conservation errors with (dashed) and without (solid) exact conservation in the inertial term.

four to five orders of magnitude larger, becoming of order 0.1% at the end of the simulation.

We demonstrate next using this test example that our proposed scheme is second-order accurate in both space and time. We remark that, owing to the velocity-space adaptivity, it is difficult to use the L_2 -norm of the distribution function,

$$L_2 = \sum_{\alpha=1}^{N_s} \sqrt{\int dv \left(f_{\alpha} - f_{\alpha}^{ref} \right)^2},$$

to quantify the error, because $f_{\alpha}^{\Delta t} = \left(v_{th,\alpha}^{\Delta t} \right)^{-3} \hat{f} \left(v_{th,\alpha}^{\Delta t} \hat{v} \right)$ and $f_{\alpha}^{\Delta t,ref} = \left(v_{th,\alpha}^{\Delta t,ref} \right)^{-3} \hat{f} \left(v_{th,\alpha}^{\Delta t,ref} \hat{v} \right)$ live on *different* meshes. We recall that this difference in the mesh stems from the fact that the velocity space is normalized by v_{th} , which is lagged by a time-step. As a proxy measure of the numerical error, much simpler to compute and independent of normalization choice, we consider the temperature. We demonstrate second-order-accurate velocity-space convergence of our discretization by computing the relative difference in the temperature against a reference solution,

$$\mathcal{E}_T^{\Delta \hat{v}} = \sum_{\alpha=1}^{N_s} \frac{\left| T_{\alpha}^{\Delta \hat{v},ref} - T_{\alpha}^{\Delta \hat{v}} \right|}{T_{\alpha}^{\Delta \hat{v},ref}}. \quad (6.1)$$

Here, $T^{\Delta \hat{v},ref}$ is the reference temperature solution obtained using a reference cell size $\Delta \hat{v}_{\perp} = 1.12 \times 10^{-2}$ ($N_v^{ref} = 1024 \times 512$). For all cases, we use a time-step size, $\Delta t = 10^{-3}$, with a final time of $t_{max} = 5 \times 10^{-3}$ with uniform grid refinement performed in both velocity-space directions. Fig. 6.4 confirms second-order convergence with $\Delta \hat{v}$ refinement.

Figure 6.4: Two-species temperature and momentum equilibration: Demonstration of second-order convergence with velocity-space refinement.

Figure 6.5: Two-species temperature and momentum equilibration: Demonstration of second-order convergence of the BDF2 scheme.

To demonstrate second-order temporal convergence of the BDF2 scheme, we use a similar approach and compute the relative difference in temperature against a reference solution,

$$\mathcal{E}_T^{\Delta t} = \sum_{\alpha=1}^{N_s} \frac{|T_{\alpha}^{\Delta t, ref} - T_{\alpha}^{\Delta t}|}{T_{\alpha}^{\Delta t, ref}}. \quad (6.2)$$

Here, $T^{\Delta t, ref}$ is the reference temperature solution obtained using a reference time-step size ($\Delta t_{ref} = 10^{-4}$) with a final time of $t_{max} = 2 \times 10^{-2}$. For all cases, we use a grid size of $N_v = 128 \times 64$. Fig. 6.5 confirms the expected order of accuracy with Δt refinement.

Finally, we use this test case to compare the efficiency between the adaptive and single-grid approaches, and to estimate the impact of the computational overhead of the former vs. the latter (the adaptive scheme requires additional operations compared to the single-grid approach, namely, *transfer* operations for the potentials, evaluation of additional inertial terms, etc.). We perform the comparison in terms of the time per nonlinear residual evaluation (which accounts for all the additional operations). The average time spent for the solver per nonlinear function evaluation for a single grid of resolution $N_v = 256 \times 128$ is 13.4 seconds,

Figure 6.6: Proton-electron thermalization: Temperature as a function of time with (left) and without (right) enforced discrete conservation of the collision operator. The solid and dashed lines represent the numerical solution while the solid and open circles represent the Braginskii solution.

vs. 3.7 seconds for the adaptive approach with resolution $N_v = 128 \times 64$. These timings were averaged over 30 nonlinear function evaluations. Thus, the multiple grid provides a computational speed-up of 3.6 vs. the optimal value of 4.0, which implies a 90% efficiency even for this very moderate grid reduction of a factor of 4. We show in subsequent examples that the adaptive strategy is in fact able to provide orders-of-magnitude larger mesh savings for problems of practical interest.

6.2. Proton-electron thermalization

We consider next thermalization of two species with strongly disparate masses. In such a case, a v_{th} disparity exists regardless of the species achieving thermal equilibrium or not. It is in such scenarios that the asymptotic formulation of the Rosenbluth potentials is particularly effective in affording significant computational savings, as we shall see.

The parameters are chosen as follows: $m_p = 1, m_e = 1/1836, Z_p = 1, Z_e = -1, n_p = n_e = 1, u_{||,p} = u_{||,e} = 0, T_p = 1, T_e = 2$, and a normalized velocity-space domain of $\hat{v}_{||} \in [-6, 6]$ and $\hat{v}_{\perp} \in [0, 6]$ are considered with a very coarse mesh of $N_v = 128 \times 64$. Fig. 6.6 depicts the temperature equilibration history, with and without enforcing conservation properties in the collision operator (conservation is enforced in the inertial terms in all cases). We also compare against the semi-analytical solution derived by Braginskii [20]. As can be seen, good agreement between theory and the numerical solution is achieved *only* when one enforces the collisional conservation symmetries [19]. We note that both the accurate asymptotic formulation of the Rosenbluth potentials and the careful coarse-graining of the fast-on-slow flux are responsible for the quality of this comparison despite the coarseness of the velocity-space mesh considered.

Next, we estimate the mesh savings attained by our asymptotic formulation for this example. The required resolution for the uniform-, single-grid approach can be estimated as:

$$N_{v,unif} = 2 \left(\frac{v_{th,f}}{v_{th,s}} n_{min} \hat{L}_{v,\perp} \right)^2. \quad (6.3)$$

Here, we assumed n_{min} velocity-space mesh points per v_{th} , and used $\hat{L}_{v,||} = 2\hat{L}_{v,\perp}$. The factor of $\frac{v_{th,f}}{v_{th,s}}$ originates in the fact that the velocity-space domain is determined by the fast species, but the resolution is determined by the slow one. For this example, $v_{th,f}/v_{th,s} \sim 60$ and $n_{min} \sim 10$ (as in the adaptive computation), and therefore the uniform-mesh approach would have required a mesh of $N_{v,unif} \sim 7200 \times 3600$. Therefore, our asymptotic approach has resulted in mesh resolution savings of about $N_{v,unif}/N_v \sim 3200$.

Figure 6.7: Proton-proton disparate temperature equilibration: Temperature as a function of time.

Figure 6.8: Proton-proton disparate temperature equilibration: Normalized hot proton distribution functions at time $t = 0$ (left) and $t = 1.39$ (right). As can be seen, at early time, a *pinching* of the hot proton distribution function occurs, significantly deviating it from a Maxwellian. Physically, this is caused by the friction between hot and cold species.

6.3. Proton-proton disparate temperature equilibration

For comparable masses, disparate v_{th} can only be supported by temperature disparity. This poses a unique challenge, since both the asymptotic treatment and v_{th} -based adaptivity are required to deliver significant velocity-space mesh resolution savings.

We consider a two-species (hot and cold) proton thermalization case with the following parameters: $m_h = m_c = 1$, $Z_h = Z_c = 1$, $u_{||,h} = u_{||,c} = 0$, $T_h = 450$, $T_c = 0.5$. We perform the calculation on a normalized velocity-space domain of $\hat{v}_{||} \in [-6, 6]$ and $\hat{v}_{\perp} \in [0, 6]$ with a mesh of $N_v = 128 \times 64$. We show the temperature of the two species as a function of time in Fig. 6.7. As can be seen, the solution equilibrates to the correct temperature of $T^{\infty} = 225.25$. We note that, for this case, the hot species distribution deviates significantly from a Maxwellian due to pinching caused by friction (see Fig. 6.8), and therefore the semi-analytical Braginskii solution is not a very accurate approximation to the dynamics.

This test is a good showcase for the importance of a positivity-preserving velocity-space discretization for both the friction and diffusion terms in the Fokker-Planck collision operator [19]. The friction pinching in velocity space generates sharp gradients, which in turn challenge the discrete formulation. Fig. 6.9 depicts the hot-species distribution function at early times with and without positivity preservation. The non-

Figure 6.9: Proton-proton disparate temperature equilibration: Early time distribution function of hot species with (left) and without (right) SMART and tensor-diffusion MC discretization. As can be seen, without positivity preserving discretization, the maximum negative value of the distribution function can be on the order $\sim 1\%$ of the the bulk distribution, leading to a catastrophic failure in the simulation.

positivity-preserving discretization fails catastrophically in the pinched region by producing a large negative value of the PDF, while the positivity-preserving discretization succeeds in keeping the PDF positive.

The required uniform-mesh resolution for this example can be estimated from Eq. 6.3 with $\frac{v_{th,f}}{v_{th,s}}$ computed at a point in time with maximum temperature disparity ($t = 0$). For this case, we have $v_{th,h}^0/v_{th,c}^0 = 30$, $\hat{L}_v = 6$ and $n_{min} = 10$, and therefore a uniform mesh of $N_{v,unif} \sim 3600 \times 1800$ would be required. The adaptive grid provides a mesh savings of $N_{v,unif}/N_v \sim 800$.

6.4. Proton-proton disparate temperature and momentum equilibration

We consider a case similar to the previous problem with two (hot and cold) proton species, but with a large initial drift velocity disparity. This problem challenges the conservation scheme of the collision operator proposed in Ref. [19], as the large initial drift between the two species introduces considerable asymmetry in the evolution of the solution and the approach of enforcing the conservation discussed in Ref. [19] becomes ill behaved. We have devised an improved method of enforcing the momentum collisional symmetry, which is discussed in AppendixD.

The problem is initialized as follows: $m_h = m_c = 1$, $Z_h = Z_c = 1$, $n_h = n_c = 1$, $u_{||,h} = 42.4264$, $u_{||,c} = -1.4142$, $T_h = 900$, $T_c = 1$. The calculation is done on a normalized velocity-space domain of $\hat{v}_{||} \in [-6, 6]$ and $\hat{v}_{\perp} \in [0, 6]$, with a mesh of $N_v = 128 \times 64$. Fig. 6.10 shows the temporal evolution of temperature and the fluid velocity of the two species. As can be seen, the solution equilibrates to the correct final temperature of $T^\infty = 610.7$ and fluid velocity of $u_{||}^\infty = 20.5$. The quality of the conserved quantities as a function of the nonlinear tolerance ϵ_r is illustrated in Fig. 6.11, again demonstrating that it improves with tighter nonlinear tolerances. Finally, Fig. 6.12 depicts the hot-species distribution function at different times, illustrating the significant asymmetry that develops at the cold species location ($\hat{v}_{||,h} = u_{||,c}/v_{th,h} \sim 0$), which challenged the original momentum-conserving approach of Ref. [19], and motivated the new development in AppendixD.

6.5. Three-species (D-electron- α) thermal equilibration

As the final example, we consider a three-species (D-electron- α) temperature equilibration problem. This is a case of certain interest in fusion plasmas where hot α particles from fusion reactions will first exchange energy with the electrons (of comparable v_{th}), and later thermalize with the fuel ions (deuterium here). The problem is initialized as follows: $m_D = 2$, $m_e = 1/1836$, $m_\alpha = 4$, $Z_D = 1$, $Z_e = -1$, $Z_\alpha = 2$,

Figure 6.10: Proton-proton disparate temperature and momentum equilibration: Temperature and fluid velocity as a function of time.

Figure 6.11: Proton-proton disparate temperature and momentum equilibration: Conservation errors as functions of time.

Figure 6.12: Proton-proton disparate temperature and momentum equilibration: The hot species distribution function at (a) initial time, (b) early time, (c) mid time, and (d) later time.

Figure 6.13: Deuterium-electron- α thermal equilibration: Temperature of the three species as a function of time (left) and of the deuterium and electron at early time (right).

$n_D = n_\alpha = 1$ and $n_e = 3$, $u_{||,D} = u_{||,e} = u_{||,\alpha} = 0$, $T_D = T_e = 1$, $T_\alpha = 1750$. At early times, $v_{th,e}/v_{th,\alpha} \sim \mathcal{O}(1)$, and fluid electron models cannot be justified for this case.

The computation is performed with a grid of $N_v = 128 \times 64$ on a normalized velocity-space domain of $\hat{v}_{||} \in [-6, 6]$ and $\hat{v}_\perp \in [0, 6]$. We initialize all species as Maxwellians with the above-mentioned density, drift velocity, and temperature. For these conditions, $v_{th,e} \approx 60$, $v_{th,\alpha} \approx 30$, $v_{th,D} = 1$.

Fig. 6.13 shows the temporal history of all the temperatures as a function of time. As expected, at early time, electrons heat up more rapidly than the deuterium. However, as electrons and D quickly heat up and α particles cool down, the preferential interaction switches to one between α and D , which eventually thermalize together, and then both with the electrons producing the expected equilibrium temperature of $T_\infty = 350.8$. We note that, given the Maxwellian initial condition, the behavior reported here is qualitatively related, but differs in the details, to the usual case of quasi-monoenergetic α born in thermonuclear D-T fusion reactions. Mesh requirements for a static uniform single grid are determined by the initial D temperature and the final electron temperature, and can be estimated from Eq. 6.3 with $v_{th,s} \equiv v_{th,D}^0 = 1$, $v_{th,f} \equiv v_{th,e}^\infty = 1135$, $n_{min} = 10$, and $\hat{L}_v = 6$, yielding $N_{v,unif} \sim 140000 \times 70000$. Therefore, mesh savings of $N_{v,unif}/N_v \sim 1.2 \times 10^6$ are realized.

7. Conclusion

In this study, we have developed and demonstrated for the first time, a fully conservative, optimal grid adaptation strategy for the multi-species, multidimensional Rosenbluth–Fokker–Planck equations. The algorithm features exact (in practice, up to nonlinear tolerance) mass, momentum, and energy conservation and allows for an arbitrary temperature and mass disparity. Unlike earlier studies, our approach is based on analytically adapting *each species'* velocity-space grid by normalizing the velocity space to its thermal velocity, v_{th} (i.e., we consider multiple velocity-space grids). The analytical formulation allows us to expose the continuum conservation symmetries in the inertial term, which are then enforced discretely by the use of nonlinear constraints, as explored in earlier studies [25, 19].

In order to deal with arbitrarily large mass and temperature ratios, we have expanded the cross-species Rosenbluth potentials in the limits of large and small v_{th} ratios, and provided suitable coarse graining strategies to regularize multipole expansions. We have verified our multiple-grid approach with several challenging problems with varying initial conditions. We have demonstrated that our approach is positivity preserving and second-order accurate temporally and in terms of the velocity-space discretization. We have

also demonstrated that our implementation is able to transition smoothly and robustly between asymptotic and non-asymptotic regimes. For one example, the three species D-e- α thermalization case, we have demonstrated resolution savings of more than six orders of magnitude, thus underscoring the enabling potential of the approach for multiscale simulation of multispecies plasmas.

The real impact of the proposed approach will require its extension to spatially inhomogeneous plasmas. This has been already worked out by the authors (including all conservation properties), and will be discussed in a future publication. We finally remark that the present approach cannot handle well situations where the bulk velocity can be much larger than the thermal velocity of the plasma. In these situations, one must *shift* the velocity space by the bulk velocity as was done in Ref. [9]. This will give rise to an additional inertial term, which will be considered in future work.

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Appendix A. Singular integrals in asymptotic fast-on-slow Rosenbluth potentials

The integrals from Eqs. 4.4, 4.5 are given as follows:

$$\begin{aligned}
2\mathbf{v} \cdot \left(\int d^3v' f'_f \frac{\mathbf{v}'}{v'^3} \right) &= 2v_{\parallel} \left(\int d^3v' f'_f \frac{v'_{\parallel}}{v'^3} \right), \\
\frac{1}{2}\mathbf{vv} : \left(\int d^3v' f'_f \nabla_{v'} \nabla_{v'} v' \right) &= \frac{1}{2}v^2 \left[\int d^3v' f'_f \left(\frac{2v'^2 - v'^2_{\perp}}{2v'^3} \right) \right] + \frac{1}{2}v_{\parallel}^2 \left[\int d^3v' f'_f \left(\frac{v'^2_{\perp} - 2v'^2_{\parallel}}{2v'^3} \right) \right], \\
\frac{1}{6}\mathbf{vvv} : \left(\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) &= \frac{1}{2}v_{\parallel}^3 \int d^3v' f'_f \left(\frac{v'^3_{\parallel} - \frac{3}{2}v'_{\parallel}v'^2_{\perp}}{v'^5} \right) + \frac{3}{2}v_{\parallel}v^2 \int d^3v' f'_f \frac{v'_{\parallel}(v'^2_{\perp} - \frac{2}{3}v'^2)}{2v'^5}.
\end{aligned}$$

To obtain these expressions we have assumed f'_f to be isotropic in the azimuthal angle, and we have used:

$$\begin{aligned}
\nabla_{v'} \nabla_{v'} v' &= (v'^2 \overset{\leftrightarrow}{I} - \mathbf{v}' \mathbf{v}')/v'^3, \\
(\nabla_{v'} \nabla_{v'} \nabla_{v'} v')_{ijk} &= 3v'_i v'_j v'_k / v'^5 - (v'_i \delta_{jk} + v'_j \delta_{ik} + v'_k \delta_{ij})/v'^3, \\
\langle \mathbf{v}' \rangle &= v'_{\parallel} \hat{\mathbf{r}}, \\
\langle \mathbf{v}' \mathbf{v}' \rangle &= v_{\parallel}^2 \hat{\mathbf{r}} \hat{\mathbf{r}} + \frac{1}{2}v_{\perp}^2 (\overset{\leftrightarrow}{I} - \hat{\mathbf{r}} \hat{\mathbf{r}}), \\
\langle \mathbf{v}' \mathbf{v}' \mathbf{v}' \rangle_{ijk} &= (v_{\parallel}^3 - \frac{3}{2}v'_{\parallel}v_{\perp}^2) \hat{r}_i \hat{r}_j \hat{r}_k + \frac{1}{2}v'_{\parallel}v_{\perp}^2 (\hat{r}_i \delta_{jk} + \hat{r}_j \delta_{ik} + \hat{r}_k \delta_{ij}),
\end{aligned}$$

where $\langle \dots \rangle$ denotes the average in the azimuthal angle, $\hat{\mathbf{r}}$ is the unit vector in the axial direction of the cylindrical velocity coordinate system, $\overset{\leftrightarrow}{I}$ is the unit dyad, and δ_{ij} is the Kronecker delta symbol.

The remaining integrals in Eqs. 4.4, 4.5 are given as follows.

$$\begin{aligned}
\mathbf{vv} : \left[\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] &= -\mathbf{vv} : \left[\int d^3v' (\nabla_{v'} f'_f) \nabla_{v'} \left(\frac{1}{v'} \right) \right] = \\
&v_{\parallel}^2 \left(\int d^3v' \frac{\partial f'_f}{\partial v'_{\parallel}} \frac{v'_{\parallel}}{v'^3} \right) + v_{\perp}^2 \left(\int d^3v' \frac{\partial f'_f}{\partial v'_{\perp}} \frac{v'_{\perp}}{2v'^3} \right), \tag{A.1}
\end{aligned}$$

where we used $\nabla_{v'} f'_f = (\partial f'_f / \partial v'_{\parallel}) \hat{\mathbf{r}} + (\partial f'_f / \partial v'_{\perp}) (\mathbf{v}'_{\perp} / v'_{\perp})$, $\nabla_{v'} (1/v') = -\mathbf{v}'/v'^3$, and $\langle \mathbf{v}' \nabla_{v'} f'_f \rangle = v'_{\parallel} (\partial f'_f / \partial v'_{\parallel}) \hat{\mathbf{r}} \hat{\mathbf{r}} +$

$\frac{v'_\perp}{2}(\partial f'_f/\partial v'_\perp)(\hat{l} - \hat{r}\hat{r})$. Similarly,

$$\begin{aligned} \frac{1}{24}\mathbf{vvvv} : \left(\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) &= -\frac{1}{24}\mathbf{vvvv} : \left[\int d^3v' (\nabla_{v'} f'_f) \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right] = \\ &= -\frac{1}{8}v_\parallel^4 \left\{ \int d^3v' \frac{1}{v'^5} \left[\frac{\partial f'_f}{\partial v'_\parallel} \left(v_\parallel^3 - \frac{3}{2}v'_\parallel v_\perp'^2 \right) + \frac{\partial f'_f}{\partial v'_\perp} \left(\frac{3}{8}v_\perp'^3 - \frac{3}{2}v'_\parallel v_\perp'^2 \right) \right] \right\} \\ &- \frac{1}{8}v_\parallel^2 v_\perp'^2 \left\{ \int d^3v' \frac{1}{v'^5} \left[\frac{\partial f'_f}{\partial v'_\parallel} \left(\frac{3}{2}v'_\parallel v_\perp'^2 - v'_\parallel v_\perp'^2 \right) + \frac{\partial f'_f}{\partial v'_\perp} \left(-\frac{3}{4}v_\perp'^3 + \frac{3}{2}v'_\parallel v_\perp'^2 + \frac{1}{2}v'_\perp v_\perp'^2 \right) \right] \right\} \\ &- \frac{1}{8}v_\perp'^4 \left[\int d^3v' \frac{1}{v'^5} \frac{\partial f'_f}{\partial v'_\perp} \left(\frac{3}{8}v_\perp'^3 - \frac{1}{2}v'_\perp v_\perp'^2 \right) \right], \end{aligned} \quad (\text{A.2})$$

where we employed $\langle \mathbf{v}' \mathbf{v}' \mathbf{v}' \mathbf{v}' \rangle_{ijkl} = (v_\parallel^4 - 3v_\parallel^2 v_\perp'^2 + \frac{3}{8}v_\perp'^4) \hat{r}_i \hat{r}_j \hat{r}_k \hat{r}_l + \frac{1}{8}v_\perp'^4 (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + (\frac{1}{2}v_\parallel^2 v_\perp'^2 - \frac{1}{8}v_\perp'^4) (\delta_{ij} \hat{r}_k \hat{r}_l + \delta_{ik} \hat{r}_j \hat{r}_l + \delta_{il} \hat{r}_j \hat{r}_k + \delta_{jk} \hat{r}_i \hat{r}_l + \delta_{jl} \hat{r}_i \hat{r}_k + \delta_{kl} \hat{r}_i \hat{r}_j)$. In the same fashion we can obtain

$$\begin{aligned} -\frac{1}{3}\mathbf{vvv} : \left[\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] &= \frac{1}{3}v_\parallel^3 \int d^3v' \frac{1}{v'} \frac{\partial^3 f'_f}{\partial v_\parallel'^3} \\ &+ \frac{1}{2}v_\parallel v_\perp'^2 \int d^3v' \frac{1}{v'} \frac{\partial}{\partial v'_\parallel} \left(\frac{\partial^2 f'_f}{\partial v_\perp'^2} + \frac{1}{v'_\perp} \frac{\partial f'_f}{\partial v'_\perp} \right) \end{aligned} \quad (\text{A.3})$$

and

$$\begin{aligned} \frac{1}{12}\mathbf{vvvv} : \left[\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] &= \frac{1}{12}v_\parallel^4 \int d^3v' \frac{v'_\parallel}{v'^3} \frac{\partial^3 f'_f}{\partial v_\parallel'^3} \\ &+ \frac{1}{8}v_\parallel^2 v_\perp'^2 \left[\int d^3v' \frac{v'_\perp}{v'^3} \frac{\partial^3 f'_f}{\partial v_\parallel'^2 \partial v'_\perp} + \int d^3v' \frac{1}{v'} \frac{\partial^2}{\partial v_\parallel'^2} \left(\frac{\partial^2 f'_f}{\partial v_\perp'^2} + \frac{1}{v'_\perp} \frac{\partial f'_f}{\partial v'_\perp} \right) \right] \\ &+ \frac{1}{32}v_\perp'^4 \int d^3v' \frac{1}{v'} \left(\frac{\partial^2}{\partial v_\perp'^2} + \frac{1}{v'_\perp} \frac{\partial}{\partial v'_\perp} \right) \left(\frac{\partial^2 f'_f}{\partial v_\perp'^2} + \frac{1}{v'_\perp} \frac{\partial f'_f}{\partial v'_\perp} \right). \end{aligned} \quad (\text{A.4})$$

Appendix B. Comparing the asymptotic limit expressions for the Rosenbluth potentials against known results

To check our asymptotic expressions for G_f and H_f (Eqs. 4.4 and 4.5), as well as for G_s and H_s (Eqs. 4.7 and 4.8), we can evaluate the velocity-space integrals using $f' = f'_M$, to find

$$\begin{aligned} G_f &= \frac{2}{3\sqrt{\pi}} \frac{n_f v^2}{v_{th,f}} - \frac{1}{15\sqrt{\pi}} \frac{n_f v^4}{v_{th,f}^3}, \\ H_f &= -\frac{4}{3\sqrt{\pi}} \frac{n_f v^2}{v_{th,f}^3} + \frac{2}{5\sqrt{\pi}} \frac{n_f v^4}{v_{th,f}^5}, \end{aligned} \quad (\text{B.1})$$

and

$$\begin{aligned} G_s &= n_s \left(v + \frac{v_{th,s}^2}{2v} \right), \\ H_s &= 2 \frac{n_s}{v}, \end{aligned} \quad (\text{B.2})$$

where we neglected the $\mathbf{V}_s$ contributions to Eq. B.2. These results should be compared against the well-known expressions for the Rosenbluth potentials for the Maxwellian [26],

$$\begin{aligned} G_M &= n'v \left[\left(1 + \frac{1}{2x^2} \right) \text{erf}(x) + \frac{\exp(-x^2)}{\sqrt{\pi}x} \right], \\ H_M &= 2 \frac{n'}{v} \text{erf}(x), \end{aligned} \quad (\text{B.3})$$

where $x = v/v'_{th}$. Taking the limit of $x \ll 1$, which corresponds to evaluating the fast potentials, gives

$$\begin{aligned} G_{Mf} &= \frac{2}{\sqrt{\pi}} n_f v_{th,f} + \frac{2}{3\sqrt{\pi}} \frac{n_f v^2}{v_{th,f}} - \frac{1}{15\sqrt{\pi}} \frac{n_f v^4}{v_{th,f}^3} + n_f v_{th,f} O\left(\frac{v^6}{v_{th,f}^6}\right), \\ H_{Mf} &= \frac{4}{\sqrt{\pi}} \frac{n_f}{v_{th,f}} - \frac{4}{3\sqrt{\pi}} \frac{n_f v^2}{v_{th,f}^3} + \frac{2}{5\sqrt{\pi}} \frac{n_f v^4}{v_{th,f}^5} + \frac{n_f}{v_{th,f}} O\left(\frac{v^6}{v_{th,f}^6}\right), \end{aligned} \quad (\text{B.4})$$

which agrees with Eq. B.1 up to constants. Taking, in turn, the limit of $x \gg 1$, which corresponds to evaluating the slow potentials, gives

$$\begin{aligned} G_{Ms} &= n_s \left(v + \frac{v_{th,s}^2}{2v} \right) + n_s v_{th,s} O\left(\exp^{-v^2/v_{th,s}^2}\right), \\ H_{Ms} &= 2 \frac{n_s}{v} + \frac{n_s}{v_{th,s}} O\left(\exp^{-v^2/v_{th,s}^2}\right), \end{aligned}$$

which also agrees with Eq. B.2, as expected.

Appendix C. Conservation properties of the asymptotic formulation of collision operators

One can show that energy and momentum conservation properties of the Fokker-Planck collision operators in the Rosenbluth form for collisions between particles α and β can be expressed as

$$\begin{aligned} \int d^3v_\alpha \mathbf{v}_\alpha \cdot \nabla_{v_\alpha} \nabla_{v_\alpha} G_\beta \cdot \nabla_{v_\alpha} f_\alpha &= \int d^3v_\beta f_\beta \mathbf{v}_\beta \cdot \nabla_{v_\beta} H_\alpha, \\ \int d^3v_\beta \mathbf{v}_\beta \cdot \nabla_{v_\beta} \nabla_{v_\beta} G_\alpha \cdot \nabla_{v_\beta} f_\beta &= \int d^3v_\alpha f_\alpha \mathbf{v}_\alpha \cdot \nabla_{v_\alpha} H_\beta \end{aligned} \quad (\text{C.1})$$

for energy and

$$\begin{aligned} \int d^3v_\alpha \nabla_{v_\alpha} \nabla_{v_\alpha} G_\beta \cdot \nabla_{v_\alpha} f_\alpha &= \int d^3v_\beta f_\beta \nabla_{v_\beta} H_\alpha, \\ \int d^3v_\beta \nabla_{v_\beta} \nabla_{v_\beta} G_\alpha \cdot \nabla_{v_\beta} f_\beta &= \int d^3v_\alpha f_\alpha \nabla_{v_\alpha} H_\beta \end{aligned} \quad (\text{C.2})$$

for momentum. The above symmetries can be derived from the Landau formulation and is also discussed in Ref. [19]. Next, we will use our expressions for G_f , H_f , G_s , and H_s to check that these properties are

satisfied. Employing Eqs. (4.5) and (4.8) gives

$$\begin{aligned}
\nabla_v \nabla_v G_f &= \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} v' \right) - \mathbf{v} \cdot \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) \\
&\quad + \frac{1}{2} \mathbf{v} \mathbf{v} : \left(\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right), \\
\nabla_v H_f &= 2 \left(\int d^3 v' f'_f \frac{\mathbf{v}'}{v'^3} \right) + 2 \mathbf{v} \cdot \left[\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] + \frac{n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right), \\
\nabla_v \nabla_v G_s &= n_s \nabla_v \nabla_v v - n_s \mathbf{V}_s \cdot \nabla_v \nabla_v \nabla_v v + \left(\frac{1}{2} \int d^3 v' f'_s \mathbf{v}' \mathbf{v}' \right) : \nabla_v \nabla_v \nabla_v \nabla_v v, \\
\nabla_v H_s &= 2 n_s \nabla_v \left(\frac{1}{v} \right) - 2 n_s \mathbf{V}_s \cdot \nabla_v \nabla_v \left(\frac{1}{v} \right) + \frac{n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right). \tag{C.3}
\end{aligned}$$

Then, considering the first of the energy conservation constraints gives

$$\begin{aligned}
\int d^3 v \mathbf{v} \cdot \nabla_v \nabla_v G_f \cdot \nabla_v f_s &= -2 n_s \left(\int d^3 v' f'_f \frac{1}{v'} \right) - 4 n_s \mathbf{V}_s \cdot \left(\int d^3 v' f'_f \frac{\mathbf{v}'}{v'^3} \right) \\
&\quad - 3 \left(\int d^3 v f_s \mathbf{v} \mathbf{v} \right) : \left[\int d^3 v' f'_f \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right], \tag{C.4}
\end{aligned}$$

where the last term on the right-hand side is a factor of $(v_{th,s}/v_{th,f})^2 \ll 1$ smaller than the first term. Similarly

$$\int d^3 v f_f \mathbf{v} \cdot \nabla_v H_s = -2 n_s \left(\int d^3 v f_f \frac{1}{v} \right) - 4 n_s \mathbf{V}_s \cdot \left(\int d^3 v f_f \frac{\mathbf{v}}{v^3} \right) + \frac{n_s n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right), \tag{C.5}$$

so that

$$\int d^3 v \mathbf{v} \cdot \nabla_v \nabla_v G_f \cdot \nabla_v f_s = \int d^3 v f_f \mathbf{v} \cdot \nabla_v H_s + \frac{n_s n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right), \tag{C.6}$$

as required. Considering the first of the momentum conservation constraints gives

$$\int d^3 v \nabla_v \nabla_v G_f \cdot \nabla_v f_s = -2 n_s \left(\int d^3 v f_f \frac{\mathbf{v}}{v^3} \right) - 2 n_s \mathbf{V}_s \cdot \left[\int d^3 v f_f \nabla_v \nabla_v \left(\frac{1}{v} \right) \right] \tag{C.7}$$

and

$$\int d^3 v f_f \nabla_v H_s = -2 n_s \left(\int d^3 v f_f \frac{\mathbf{v}}{v^3} \right) - 2 n_s \mathbf{V}_s \cdot \left[\int d^3 v f_f \nabla_v \nabla_v \left(\frac{1}{v} \right) \right] + \frac{n_s n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right) \tag{C.8}$$

where the third term in Eq. C.8 is a factor of $v_{th,s}^2/v_{th,f}^2 \ll 1$ smaller than the first term. Therefore momentum and energy conservation is ensured to $O(v_{th,s}^2/v_{th,f}^2)$ in the continuum. This error (which is commensurate with numerical truncation errors for typical velocity-space meshes employed in this study) is absorbed in the nonlinear conservation constraints of our method, and thus does not spoil the conservation properties of the method.

Considering the other pair of the constraints gives

$$\int d^3v \mathbf{v} \cdot \nabla_v \nabla_v G_s \cdot \nabla_v f_f = 2n_s \mathbf{V}_s \cdot \left(\int d^3v f_f \frac{\mathbf{v}}{v^3} \right) + 2 \left(\int d^3v' f'_s \mathbf{v}' \mathbf{v}' \right) : \left[\int d^3v f_f \nabla_v \nabla_v \left(\frac{1}{v} \right) \right], \quad (\text{C.9})$$

$$\int d^3v f_s \mathbf{v} \cdot \nabla_v H_f = 2n_s \mathbf{V}_s \cdot \left(\int d^3v f_f \frac{\mathbf{v}}{v^3} \right) + 2 \left(\int d^3v' f'_s \mathbf{v}' \mathbf{v}' \right) : \left[\int d^3v f_f \nabla_v \nabla_v \left(\frac{1}{v} \right) \right] + \frac{n_s n_f v_{th,s}}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right), \quad (\text{C.10})$$

$$\int d^3v \nabla_v \nabla_v G_s \cdot \nabla_v f_f = 2n_s \left(\int d^3v f_f \frac{\mathbf{v}}{v^3} \right) + 2n_s \mathbf{V}_s \cdot \left[\int d^3v f_f \nabla_v \nabla_v \left(\frac{1}{v} \right) \right] \quad (\text{C.11})$$

$$- \left(\int d^3v' f'_s \mathbf{v}' \mathbf{v}' \right) : \left[\int d^3v f_f \nabla_v \nabla_v \nabla_v \left(\frac{1}{v} \right) \right] \quad (\text{C.12})$$

and

$$\int d^3v f_s \nabla_v H_f = 2n_s \left(\int d^3v' f'_f \frac{\mathbf{v}'}{v'^3} \right) + 2n_s \mathbf{V}_s \cdot \left[\int d^3v' f'_f \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] + \frac{n_s n_f}{v_{th,f}^2} O \left(\frac{v_{th,s}^2}{v_{th,f}^2} \right). \quad (\text{C.13})$$

Since the third terms on the right-hand side of Eq. (C.12) and Eq. (C.13) are a factor of $(v_{th,s}/v_{th,f})^2 \ll 1$ smaller than the first terms, the required constraints are satisfied up to such small terms.

For purposes of a numerical evaluation, it is helpful to rewrite the last two equations in Eq. C.3 as follows:

$$\begin{aligned} \nabla_v \nabla_v G_s &= n_s \frac{v^2 \overset{\leftrightarrow}{I} - \mathbf{v} \mathbf{v}}{v^3} + n_s \left[\frac{\mathbf{v} \mathbf{V}_s + \mathbf{V}_s \mathbf{v}}{v^3} + (\mathbf{v} \cdot \mathbf{V}_s) \frac{v^2 \overset{\leftrightarrow}{I} - 3\mathbf{v} \mathbf{v}}{v^5} \right] \\ &+ \frac{3}{4} n_s v_{th,s}^2 \frac{3\mathbf{v} \mathbf{v} - v^2 \overset{\leftrightarrow}{I}}{v^5} + 6 \frac{\mathbf{v}(\mathbf{v} \cdot \overset{\leftrightarrow}{M}) + (\mathbf{v} \cdot \overset{\leftrightarrow}{M})\mathbf{v}}{v^5} - \frac{2 \overset{\leftrightarrow}{M}}{v^3} + (\mathbf{v} \cdot \overset{\leftrightarrow}{M} \cdot \mathbf{v}) \frac{3v^2 \overset{\leftrightarrow}{I} - 15\mathbf{v} \mathbf{v}}{v^7}, \\ \nabla_v H_s &= 2n_s \frac{\mathbf{V}_s - \mathbf{v}}{v^3} - 6n_s (\mathbf{v} \cdot \mathbf{V}_s) \frac{\mathbf{v}}{v^5}, \end{aligned} \quad (\text{C.14})$$

where $\overset{\leftrightarrow}{M} \equiv \frac{1}{2} \int d^3v' f'_s \mathbf{v}' \mathbf{v}'$.

AppendixD. Robust discrete conservation approach for the collision operator in the presence of multiple velocity-space meshes

In Ref. [19], a conserving scheme was developed for a multi-dimensional, single-grid, multi-species Rosenbluth-Fokker-Planck collision operator. In the reference, the authors identified the continuum integral symmetries of the collision operator and introduced a nonlinear consistency dyad to enforce them in the discrete. The integral symmetries are

$$\langle 1, J_{\alpha\beta,G,||} \rangle_v = \langle 1, J_{\beta\alpha,H,||} \rangle_v \quad (\text{D.1})$$

and

$$\langle \mathbf{v}, \mathbf{J}_{\alpha\beta,G} \rangle_v = \langle \mathbf{v}, \mathbf{J}_{\beta\alpha,H} \rangle_v. \quad (\text{D.2})$$

Discretely, these symmetries are generally enforced only down to some numerical error. Exact enforcement can be achieved by introducing a consistency dyad $\overset{\leftrightarrow}{\eta}_{\alpha\beta}$ into the collision operator:

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\overset{\leftrightarrow}{\eta}_{\alpha\beta} \cdot \mathbf{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \mathbf{J}_{\alpha\beta,H} \right]$$

such that

$$\langle 1, \eta_{\alpha\beta,||} J_{\alpha\beta,G,||} \rangle_v = \langle 1, J_{\beta\alpha,H,||} \rangle_v$$

and

$$\langle \mathbf{v}, \overset{\leftrightarrow}{\eta}_{\alpha\beta} \cdot \mathbf{J}_{\alpha\beta,G} \rangle_v = \langle \mathbf{v}, \mathbf{J}_{\beta\alpha,H} \rangle_v.$$

Here, $\overset{\leftrightarrow}{\eta}_{\alpha\beta}$ is given by,

$$\overset{\leftrightarrow}{\eta}_{\alpha\beta} = \begin{bmatrix} \gamma_{\alpha\beta} + \varepsilon_{\alpha\beta} & 0 \\ 0 & \gamma_{\alpha\beta} \end{bmatrix},$$

with $\gamma_{\alpha\beta} = 1 + \mathcal{O}(\Delta)$ and $\varepsilon_{\alpha\beta} = \mathcal{O}(\Delta)$, and Δ the measure of the truncation of error associated with the discretization of the flux.

In the reference, $\overset{\leftrightarrow}{\eta}_{\alpha\beta}$ was defined in terms of quadratures over the whole velocity space, and the approach did not discriminate between *fast* and *slow* species when multiple velocity-space meshes are present. Furthermore, $\overset{\leftrightarrow}{\eta}_{\alpha\beta}$ was applied to the flux globally and did not take advantage of the fact that the majority of conservation error was caused by the bulk structure of the distribution function where sharp gradients were present. In the particular case when $v_{th,f}/v_{th,s} \gg 1$ (as considered in this manuscript), we have a situation as illustrated in Fig. 5.5 where only a few fast domain cells overlap with the slow grid, and the discretization truncation error is concentrated there. If $\overset{\leftrightarrow}{\eta}_{fs}$ is applied to the entire velocity space (as considered in Ref. [19]), it will affect the entire fast-on-slow flux by a large truncation error factor. Thus, it is advantageous for a scheme to recognize where the truncation errors are concentrated and appropriately enslave them to the flux.

We propose an improvement to the collisional conservation scheme of Ref. [19] that does this by modifying the collision operator *only* for the *fast-on-slow* term as:

$$C_{fs} = \Gamma_{fs} \nabla_v \cdot \left[(1 + \eta_{fs,G}) \mathbf{J}_{fs,G} - \frac{m_f}{m_s} (1 + \eta_{fs,H}) \mathbf{J}_{fs,H} \right]$$

where

$$\eta_{fs}(v_{||}) = c_{fs,0} + c_{fs,1} \mathcal{P}_v(v_{||}).$$

Here, $c_{fs,0}$ and $c_{fs,1}$ are coefficients of $\mathcal{O}(\Delta)$ that enforce the conservation symmetries, and $\mathcal{P}_v$ is a weighting function, which for this study is chosen as:

$$\mathcal{P}_v(v_{||}) = \begin{cases} 1 + \beta (v_{||} - u_{s,||}) & \text{if } \mathbf{v} \in \Omega_{\eta,fs} \text{ and } v_{||} \geq u_{||,s} \\ -1 + \beta (v_{||} - u_{s,||}) & \text{elseif } \mathbf{v} \in \Omega_{\eta,fs} \text{ and } v_{||} < u_{||,s} \\ 0 & \text{else} \end{cases}.$$

Here $\eta_{fs} \in \Omega_{\eta,fs} = [L_{\eta,||} \times L_{\eta,\perp}]$, $L_{\eta,||} \in [-(L_{s,||} + \Delta v_{||,f}) + u_{s,||}, (L_{s,||} + \Delta v_{||,f}) + u_{s,||}]$, $L_{\eta,\perp} \in [0, L_{s,\perp} + \Delta v_{\perp,f}]$,

$$\beta = -\frac{1}{L_{s,||} + \Delta v_{||,f}}.$$

Refer to Fig. D.1 for a graphical relationship of $\Omega_{\eta,fs}$, with Ω_f and Ω_s , and Fig. D.2 for $\mathcal{P}_v$. The domain of $\Omega_{\eta,fs}$ includes a buffer layer Δv_f to ensure that more than one cell face is used to ensure two constraints.

Figure D.1: Domain for η_{fs} , $\Omega_{\eta,fs}$, and relation to Ω_f and Ω_s .

Figure D.2: Graphical illustration of $\mathcal{P}_v$.

Otherwise, if one considers the limiting case of $v_{th,f}/v_{th,s} \rightarrow \infty$, only one cell face will be available to enforce two constraints, leading to an ill-defined system. The weighting function is chosen in such a way that the truncation error correction vanishes as one moves away from the main slow PDF structure. Unlike the original approach, η_{fs} is applied to both the diffusion and friction terms of the fast-on-slow fluxes (in the original approach, it was applied on the diffusion fluxes of all species). This is in an attempt to enslave the coarse, less accurate fast-on-slow representation to the more accurate slow-on-fast representation.

The conservation coefficients $c_{fs,0}$ and $c_{fs,1}$ are computed similarly to the original approach by solving a simple 2×2 linear system from the following constraint equations obtained from the corresponding collision-operator symmetries:

$$c_{fs,G,0} \langle 1, J_{fs,G,||} \rangle_{v \in \Omega_{\eta,fs}} + c_{fs,G,1} \langle 1, \mathcal{P}_v J_{fs,G,||} \rangle_{v \in \Omega_{\eta,fs}} = \langle 1, J_{sf,H,||} \rangle_v - \langle 1, J_{fs,G,||} \rangle_v \quad (D.3)$$

$$c_{fs,G,0} \langle \mathbf{v}, \mathbf{J}_{fs,G} \rangle_{v \in \Omega_{\eta,fs}} + c_{fs,G,1} \langle \mathbf{v}, \mathcal{P}_v \mathbf{J}_{fs,G} \rangle_{v \in \Omega_{\eta,fs}} = \langle \mathbf{v}, \mathbf{J}_{sf,H} \rangle_v - \langle \mathbf{v}, \mathbf{J}_{fs,G} \rangle_v \quad (D.4)$$

and

$$c_{fs,H,0} \langle 1, J_{fs,H,||} \rangle_{v \in \Omega_{\eta,fs}} + c_{fs,H,1} \langle 1, \mathcal{P}_v J_{fs,H,||} \rangle_{v \in \Omega_{\eta,fs}} = \langle 1, J_{sf,G,||} \rangle_v - \langle 1, J_{fs,H,||} \rangle_v \quad (D.5)$$

$$c_{fs,H,0} \langle \mathbf{v}, \mathbf{J}_{fs,H} \rangle_{v \in \Omega_{\eta,fs}} + c_{fs,H,1} \langle \mathbf{v}, \mathcal{P}_v \mathbf{J}_{fs,H} \rangle_{v \in \Omega_{\eta,fs}} = \langle \mathbf{v}, \mathbf{J}_{sf,G} \rangle_v - \langle \mathbf{v}, \mathbf{J}_{fs,H} \rangle_v, \quad (D.6)$$

where

$$\langle v^l, (\cdot) \rangle_{v \in \Omega_{\eta,fs}} = \int_{\Omega_{\eta,fs}} d\mathbf{v} v^l (\cdot).$$

This approach ensures that, in the limit of $v_{th,f}/v_{th,s} \gg 1$, the fluxes are modified only in the regions where the truncation error is large. We note that this approach to enforcing conservation symmetries is highly flexible, and that a careful physics-based insight can make a profound impact on its robustness.

Appendix E. Practical solution procedure for the moment constraints

From a practical implementation standpoint, it is critical to minimize the computational effort in computing the coefficients, $\eta_{t,\alpha}$, $\xi_{t,\alpha}$, $\gamma_{t,\alpha}$, and $\Upsilon_{t,\alpha,||}^-$ in Eqs. 5.37, 5.41, 5.42 and 5.43. From the definitions of the coefficients, one can easily obtain the following linear system (for a given $\hat{f}_\alpha$) for the coefficients:

$$\begin{bmatrix} a_{\eta\eta} & 0 & 0 & 0 \\ a_{\xi\eta} & a_{\xi\xi} & 0 & a_{\xi\Upsilon} \\ 0 & a_{\gamma\xi} & a_{\gamma\gamma} & 0 \\ a_{\Upsilon\eta} & 0 & a_{\Upsilon\gamma} & a_{\Upsilon\Upsilon} \end{bmatrix} \begin{bmatrix} \eta_{t,\alpha} \\ \xi_{t,\alpha} \\ \gamma_{t,\alpha} \\ \Upsilon_{t,\alpha,||}^- \end{bmatrix} = \begin{bmatrix} b_\eta \\ b_\xi \\ b_\gamma \\ b_\Upsilon \end{bmatrix}. \quad (E.1)$$

Since evaluating $\eta_{t,\alpha}$ is trivial, the effective linear system size can be reduced to:

$$\begin{bmatrix} a_{\xi\xi} & 0 & a_{\xi\Upsilon} \\ a_{\gamma\xi} & a_{\gamma\gamma} & 0 \\ 0 & a_{\Upsilon\gamma} & a_{\Upsilon\Upsilon} \end{bmatrix} \begin{bmatrix} \xi_{t,\alpha} \\ \gamma_{t,\alpha} \\ \Upsilon_{t,\alpha,||}^- \end{bmatrix} = \begin{bmatrix} b_\xi - a_{\xi\eta} \eta_{t,\alpha} \\ b_\gamma \\ b_\Upsilon - a_{\Upsilon\eta} \eta_{t,\alpha} \end{bmatrix} = \begin{bmatrix} b_\xi^* \\ b_\gamma \\ b_\Upsilon^* \end{bmatrix}. \quad (E.2)$$

One may attempt to solve the linear system shown above and quickly realize that since $\xi_{t,\alpha}$ is function of the velocity space, the linear system size is not a 3×3 , but rather, a $(N_v + 2) \times (N_v + 2)$, where N_v is the

number of velocity-space cell. In order to get around this problem, we will reduce the linear system further by eliminating $\xi_{t,\alpha}$. Substituting the definition of $\xi_{t,\alpha}$ from Eq. 5.41 into $\Upsilon_{t,\alpha,\parallel}^-$ from Eq. 5.42 gives:

$$\begin{bmatrix} a_{\gamma\gamma} & a_{\gamma\parallel} \\ a_{\Upsilon_{\parallel}\gamma} & a_{\Upsilon_{\parallel}\Upsilon_{\parallel}} \end{bmatrix} \begin{bmatrix} \gamma_{t,\alpha} \\ \Upsilon_{t,\alpha,\parallel}^- \end{bmatrix} = \begin{bmatrix} b_{\gamma}^* \\ b_{\Upsilon_{\parallel}}^* \end{bmatrix}, \quad (\text{E.3})$$

which is a 2×2 system which can be solved for $\gamma_{t,\alpha}$ and $\Upsilon_{t,\alpha,\parallel}^-$ by:

$$\begin{bmatrix} \gamma_{t,\alpha} \\ \Upsilon_{t,\alpha,\parallel}^- \end{bmatrix} = \frac{1}{a_{\gamma\gamma}a_{\Upsilon_{\parallel}\Upsilon_{\parallel}} - a_{\gamma\Upsilon_{\parallel}}a_{\Upsilon_{\parallel}\gamma}} \begin{bmatrix} a_{\Upsilon_{\parallel}\Upsilon_{\parallel}} & -a_{\gamma\Upsilon_{\parallel}} \\ -a_{\Upsilon_{\parallel}\gamma} & a_{\gamma\gamma} \end{bmatrix} \begin{bmatrix} b_{\gamma}^* \\ b_{\Upsilon_{\parallel}}^* \end{bmatrix}. \quad (\text{E.4})$$

Here, the coefficients a and b for each element are given as:

$$a_{\gamma\gamma} = \frac{\partial_t v_{th,\alpha}^2}{2} \left\langle \hat{\mathbf{v}}, \hat{\mathbf{v}} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \quad (\text{E.5})$$

$$a_{\gamma\Upsilon_{\parallel}} = v_{th,\alpha} \partial_t v_{th,\alpha} \left\langle \hat{v}_{\parallel}, \hat{v}_{\parallel} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \Big|_{-\infty}^{\hat{u}_{\alpha,\parallel}}, \quad (\text{E.6})$$

$$a_{\Upsilon_{\parallel}\Upsilon_{\parallel}} = v_{th,\alpha} \partial_t v_{th,\alpha} \left\langle 1, \hat{v}_{\parallel} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \Big|_{-\infty}^{\hat{u}_{\alpha,\parallel}}, \quad (\text{E.7})$$

$$a_{\Upsilon_{\parallel}\gamma} = \partial_t v_{th,\alpha}^2 \left\langle 1, \frac{\hat{v}_{\parallel} \hat{f}_{\alpha}}{2} \right\rangle_{\hat{\mathbf{v}}}, \quad (\text{E.8})$$

$$\begin{aligned} b_{\gamma}^* &= \partial_t v_{th,\alpha}^2 \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} - v_{th,\alpha} \left\langle \frac{\hat{v}^2}{2}, \partial_t (v_{th,\alpha} \hat{f}_{\alpha}) \right\rangle_{\hat{\mathbf{v}}} + v_{th,\alpha} \partial_t v_{th,\alpha} \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} - \\ &v_{th,\alpha} \partial_t v_{th,\alpha} \left[\left\langle \hat{v}_{\parallel}, \hat{v}_{\parallel} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \Big|_{-\infty}^{\hat{u}_{\alpha,\parallel}} + \left\langle \hat{v}_{\perp}, \hat{v}_{\perp} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \right] - \left\langle \frac{\hat{v}^2}{2}, \eta_{t,\alpha} \right\rangle_{\hat{\mathbf{v}}} + \left\langle \frac{\hat{v}^2}{2}, \partial_t (v_{th,\alpha}^2 \hat{f}_{\alpha}) \right\rangle_{\hat{\mathbf{v}}} - \\ &\partial_t v_{th,\alpha}^2 \left\langle \frac{\hat{v}^2}{2}, \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} + \partial_t v_{th,\alpha}^2 \left\langle \hat{\mathbf{v}}, \frac{\hat{\mathbf{v}} \hat{f}_{\alpha}}{2} \right\rangle_{\hat{\mathbf{v}}}, \quad (\text{E.9}) \end{aligned}$$

$$b_{\Upsilon_{\parallel}}^* = -\left\langle \hat{v}_{\parallel}, \eta_{t,\alpha} \right\rangle_{\hat{\mathbf{v}}} + \partial_t v_{th,\alpha}^2 \left\langle 1, \frac{\hat{v}_{\parallel} \hat{f}_{\alpha}}{2} \right\rangle_{\hat{\mathbf{v}}} + v_{th,\alpha} \partial_t v_{th,\alpha} \left[\left\langle \hat{v}_{\parallel}, \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} - \left\langle 1, \hat{v}_{\parallel} \hat{f}_{\alpha} \right\rangle_{\hat{\mathbf{v}}} \Big|_{-\infty}^{\hat{u}_{\alpha,\parallel}} \right]. \quad (\text{E.10})$$

AppendixF. Temporal evolution equation for v_{th}

We motivate in this section the temporal update strategy for v_{th} chosen in this study. Since only past time values of v_{th} are needed for the normalization of the current-time PDF, we can compute $v_{th,\alpha}^k$ directly from known values of the temperature, T_{α}^k , which is found from $v_{th,\alpha}^{k-1}$ and $\hat{f}_{\alpha}^k$ as:

$$T_{\alpha}^k = \frac{m_{\alpha}}{2} \left(v_{th,\alpha}^{k-1} \right)^2 \hat{T}_{\alpha}^k \quad (\text{F.1})$$

where

$$\hat{T}_\alpha^k = \frac{2}{3} \frac{\langle (\hat{\mathbf{v}} - \hat{\mathbf{u}}_\alpha^k)^2, \hat{f}_\alpha^k \rangle_{\hat{\mathbf{v}}}}{\langle 1, \hat{f}_\alpha^k \rangle_{\hat{\mathbf{v}}}}$$

and

$$\hat{\mathbf{u}}_\alpha^k = \frac{\langle \hat{\mathbf{v}}, \hat{f}_\alpha^k \rangle_{\hat{\mathbf{v}}}}{\langle 1, \hat{f}_\alpha^k \rangle_{\hat{\mathbf{v}}}}.$$

Here, $\hat{T}$ is the normalized temperature and $\hat{\mathbf{u}}$ the normalized bulk fluid velocity.

Let us consider the standard definition of $v_{th,\alpha}$ from T_α :

$$v_{th,\alpha}^k = \sqrt{\frac{2T_\alpha^k}{m_\alpha}} = v_{th,\alpha}^{k-1} \sqrt{\hat{T}_\alpha^k}. \quad (\text{F.2})$$

It follows by induction that:

$$v_{th,\alpha}^k = v_{th,\alpha}^{k-2} \sqrt{\hat{T}_\alpha^k \hat{T}_\alpha^{k-1}} = \dots = v_{th,\alpha}^0 \sqrt{\prod_{j=1}^k \hat{T}_\alpha^j}.$$

However, this definition is not optimal numerically, because it can propagate velocity-space quadrature errors. This is easiest to see in the case of a non-drifting Maxwellian equilibrium with thermal velocity $v_{th,\alpha}$. The exact normalized temperature for this case is $\hat{T}_\alpha = 1$. Since it is an equilibrium, neither $\hat{T}_\alpha$ nor $v_{th,\alpha}^k$ should evolve in time. However, numerical quadrature errors will give a normalized temperature value slightly different from unity, $\hat{T}_\alpha^k = 1 + \varepsilon_k$. As a result, after k time steps, the thermal velocity can drift from unity according to:

$$v_{th,\alpha}^k = v_{th,\alpha}^0 \sqrt{\prod_{j=1}^k (1 + \varepsilon_j)} \neq v_{th,\alpha}^0.$$

In our scheme, this drift is ultimately nonlinearly controlled by the exact conservation of energy. However, much improved accuracy of v_{th} is obtained when one computes $v_{th,\alpha}^k$ relative to the initial temperature and thermal velocity as:

$$v_{th,\alpha}^k = v_{th,\alpha}^0 \sqrt{\frac{T_\alpha^k}{T_\alpha^{k=0}}}. \quad (\text{F.3})$$

It is straightforward to show that, in an equilibrium configuration, $v_{th,\alpha}^k$ will not evolve in time as long as both T_α^k and $T_\alpha^{k=0}$ are computed using the same quadrature rule.