Structure-Preserving Numerical Methods for Collision Operators in Plasma Physics

Sandra Jeyakumar

A thesis submitted for the degree of

Doctor of Philosophy

The Australian National University

Mathematical Sciences Institute

September 2024

Disclaimer

I hereby declare that the work undertaken in this thesis has been conducted by me alone, except where indicated in the text. I conducted this work between January 2021 and September 2024, during which period I was a PhD student at the Australian National University and the University of Western Australia. This thesis, in whole or any part of it, has not been submitted to this or any other university for a degree.

Sandra Jeyakumar

2 September 2024

Acknowledgements

I would like to start by thanking my supervisors, Matthew Hole and David Pfefferlé, for their support throughout the length of this PhD. I would also like to acknowledge Zhisong Qu, who gave me (and many others) invaluable advice and spared time whenever we needed it. Finally, I must thank Michael Kraus, without whose collaboration this work would not have been possible in any way.

To my family — Mom, Dad, Steve, Peter and Laurelle – thank you for always being there, no matter what. You guys are the best cheer squad. To all friends near and far, you made the hardest things bearable and it wouldn't have been possible to do it without you.

Finally, to my fiancé Dean, who was always there despite his own thesis and stresses — we made it.

Abstract

In this thesis, we present two new families of structure-preserving particle methods for collision operators in plasma physics. Many advances have been made in recent years for modelling ideal kinetics, such as the Vlasov–Poisson or Vlasov–Maxwell systems, in a structure-preserving manner. The problem of treating dissipation, or collisions specifically, in this way has been more recently studied, since collision operators do not fit straightforwardly into a geometric framework in the same manner as the ideal dynamics. Though there has now been some work on this topic, many existing methods are grid-based approaches and do not lend themselves to being coupled to the particle methods which are used to solve the ideal problem, such as the Particle-In-Cell method. Thus, it is of interest to consider structure-preserving particle methods for such operators. The two operators considered in this thesis are the Lenard-Bernstein and Landau collision operators.

A deterministic particle method approach is taken to discretise a conservative version of the Lenard-Bernstein operator. An L^2 projection is used to construct a second representation of the distribution function, which has sufficient regularity for computation of the collision operator. The obtained semi-discretisation is shown to preserve mass, momentum and energy automatically. The implicit midpoint method is shown to preserve these properties in time as well. The method is implemented in the one-dimensional case with a cubic spline basis, and various examples are constructed to demonstrate the method's behaviour and conservation properties. Preservation of the invariants is demonstrated to machine precision, and entropy is shown to be monotonically dissipated in time as well.

The Landau operator is discretised using the metriplectic approach of Morrison (1986). Two separate discretisations are constructed, and both make use of the projection approach introduced in the Lenard-Bernstein case. The first method is obtained by directly discretising the metric bracket for the Landau operator by the particle distribution function, with the projected representation being used for evaluation of the entropy only. The semi-discretisation is shown to preserve mass, momentum, and energy, and the method of discrete gradients is shown to preserve these quantities in time as well. However, the method is shown to have a computational cost of $\mathcal{O}(N^2)$, where N is the number of particles. A second discretisation is constructed also via the metriplectic approach, but where the metric bracket is discretised via a two-step approach. First, the bracket is restricted to finite-element type functions, leading to a similar bracket as that of Kraus & Hirvijoki (2017). Then, the bracket is further restricted to those finite-element functions that are obtained by the projection of a particle solution. This leads to a method with a much

improved cost of $\mathcal{O}(NM^2)$, where M is the number of basis functions. There are, however, some unresolved challenges in implementing these methods, and the work is concluded with a discussion of these.

Contents

Chapter 0

Introduction

Structure-preserving methods are a family of numerical approaches that aim to retain, at the discrete level, the underlying mathematical structures and properties of the equations to which they are applied. Examples include Hamiltonian or Poisson structure, conservation laws, symmetries, and so on. Preserving these properties can be crucial to obtaining physically valid discrete solutions, and can also produce better behaved numerical simulations (both in terms of accuracy and robustness), especially over long times when compared to the timescales of the problem (Hairer & Wanner 2006).

These methods are extremely useful in the field of plasma physics. Here, at a fundamental level, we are interested in the behaviour of charged particles under the influence of an electromagnetic field, to which they are also contributing. The Vlasov–Maxwell system of equations, which attempts to model exactly this behaviour, possesses Hamiltonian structure and preserving this can be key to obtaining discretisations with desirable qualities. Examples of recent works where this has been studied in the context of the Vlasov–Maxwell system, or related kinetic equations in plasma physics, includes Chen *et al.* (2011); Markidis & Lapenta (2011); Squire *et al.* (2012); Evstatiev & Shadwick (2013); Qin *et al.* (2016); Burby (2017); Kraus *et al.* (2017); Zhang & Gamba (2017); Campos Pinto *et al.* (2022). For a review of the use of structure-preserving methods in the overarching field of plasma physics, we refer to Morrison (2017).

The Vlasov–Maxwell system, or ideal kinetic models in plasma physics in general, is collision-less and does not include dissipative effects. Though these effects are weak in plasmas, it can be important to include them in long-time simulations to obtain physically correct results. Moreover, not including any dissipation in kinetic simulations can result in the formation of small-scale structures that are not resolvable at the level of the computational grid; this is a well-known issue in the Vlasov equation. Often, these structures are unphysical and can destroy the quality of the discrete solution. As such, it can be useful to consider the addition of

dissipation to such systems from the perspective of aiding numerical robustness as well.

Adding collisions to the Vlasov–Maxwell system, however, does complicate the structure of the equations, as dissipation in general does not fit into a Hamiltonian framework. Thus, works that consider the addition of collisions in a structure-preserving manner are more recent, and primarily consist of grid-based approaches. These include Yoon & Chang (2014); Taitano *et al.* (2015); Hirvijoki & Adams (2017); Kraus & Hirvijoki (2017); Shiroto & Sentoku (2019).

However, it is of interest to consider structure-preserving *particle* methods for modelling dissipation, as one of the primary tools for solving the Vlasov–Maxwell system are Particle-In-Cell, or PIC, methods. This family of methods treats the particle distribution function as a sum of Dirac delta functions, and so it is necessary to consider methods for treating collisions in a similar manner such that the ideal and dissipative parts can be coupled together. This is not straightforward, however, as collision operators are usually second-order differential operators, and so are not directly amenable to being discretised by particles.

Nevertheless, there have been some recent works which have considered structure-preserving particle methods for collisions. Hirvijoki *et al.* (2018) discretise the collision operator using marker particles, but consider varying their weights in time instead of their velocities. The works of Carrillo *et al.* (2020) and Hirvijoki (2021) consider regularising their particle solutions by convolution with finite-sized cutoff functions. Work by Bailo *et al.* (2024) extends this approach to consider the full system with both ideal and dissipative dynamics.

Alternative approaches to modelling dissipation include Monte Carlo methods, which treat collisions as a stochastic process and effectively model their underlying microscopic behaviour (see for e.g. Boozer & Kuo-Petravic (1981)). This is, most often, the method that is favoured for implementation in production codes due to its relatively cheaper complexity compared to many of the previously mentioned methods. However, it does not preserve the intrinsic structure of the collision operator, such as the dissipation of entropy or the conservation of invariants. More recent versions of such an approach are structure-preserving stochastic methods for collision operators, including the Landau operator (Tyranowski 2021*a*,*b*). Schnake *et al.* (2024) considers a sparse-grid discontinuous Galerkin approach to the Vlasov–Poisson–Lenard–Bernstein equations, which considers both a sparse grid for the entire phase space, as well as a hybrid grid which only uses a sparse grid in velocity space. Finally, the work of Laidin & Pareschi (2024) considers a constrained polynomial based approach to solving collisional equations while conserving the required

moments, such as momentum and energy.

In this thesis, we will present two new families of approaches for constructing structure-preserving particle methods for collision operators. The underpinning idea of both sets of approaches is regularisation using L^2 projection onto a chosen basis, rather than a convolution approach as currently exists in the literature. The first method, which is based on a deterministic particle approach, will be applied to the Lenard-Bernstein collision operator. The second approach is based on the metriplectic framework of Morrison (1986), and we will construct two separate structure-preserving discretisations of the Landau operator under this framework.

0.1 Thesis Outline

In Chapter 1, we introduce the theoretical background material that underpins the work presented in this thesis. Hamiltonian systems are first introduced in the finite-dimensional context, and then extended to infinite dimensional systems. The metriplectic formulation of Morrison (1986) is then presented, as a means of coupling such Hamiltonian systems to dissipative dynamics in a geometric way. The Vlasov–Maxwell equations and related systems are introduced, as well as the respective collision operators that are studied in later chapters – the Lenard-Bernstein and Landau operators. The structure and conservation properties of these operators are discussed.

In Chapter 2, the numerical techniques utilised in this thesis are introduced. This includes the basics of finite-element discretisations, as well as deterministic particle methods. Regularisation methods for particle methods are discussed, and projection methods are introduced. Finally, the relevant time integration schemes used in this thesis are discussed as well.

In Chapter 3, a structure-preserving particle method for the Lenard-Bernstein operator is derived, from a deterministic particle method approach. Conservation properties are demonstrated for the semi-discretisation, as well as the fully-discrete case. Numerical results are presented for a one-dimensional case.

In Chapter 4, three different semi-discretisations are derived for the Landau collision operator. One is derived based on the deterministic particle method approach used for the Lenard-Bernstein operator, while two separate discretisations are derived under the metriplectic formulation of the Landau operator. Conservation properties in each case are presented, and the advantages and/or disadvantages of each approach are discussed. Finally, the implementation challenges of these approaches are discussed.

Chapter 1

Theoretical Background

In this chapter, we present the foundations of plasma theory that are relevant to the thesis. In Section 1.1 we present the foundations of Hamiltonian systems, building up to the infinite-dimensional case that will be required to describe the Vlasov–Maxwell equations. In Section 1.2, we present the metriplectic formulation of Morrison (1986) as a means of combining Hamiltonian and dissipative (collisional) dynamics in a geometric manner. Then, we introduce the Vlasov–Maxwell system and detail its Hamiltonian structure in Section 1.3. Finally we discuss the two collision operators that are studied in this thesis — the Lenard–Bernstein operator in Section 1.4 and the Landau operator in 1.5. The discussion of the Landau operator is concluded by considering its combined metriplectic structure, together with the Vlasov–Maxwell equations.

1.1 Hamiltonian systems

In this section, we present the fundamentals of finite-dimensional Hamiltonian systems, as may be familiar to many readers, and then extend to the infinite-dimensional case that is required to describe partial differential equations.

1.1.1 Finite-dimensional Hamiltonian systems

First, let us briefly introduce Hamilton's equations. Let $\{q_1, \ldots, q_d\} \in \mathbb{R}^d$ represent the position coordinates of our system, and $\{p_1, \ldots, p_d\} \in \mathbb{R}^d$ the conjugate momentum coordinates, where d is the number of degrees of freedom. The Hamiltonian function $H(q_1, \ldots, q_d, p_1, \ldots, p_d) : \mathbb{R}^{2d} \to \mathbb{R}$ typically represents the total energy of the system. Then, Hamilton's equations are as follows:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad \dot{q}_i = \frac{\partial H}{\partial p_i}, \tag{1.1}$$

a set of $2d$ coupled first-order ordinary differential equations, which govern the evolution of the position and momentum variables in time.

An example of a system that can be described in this way is the mathematical pendulum. Here, the Hamiltonian function is as follows:

$$H(q,p) = \frac{1}{2}p^2 - \cos q + 1, \tag{1.2}$$

where we have set all physical constants to unity. From Hamilton's equations (1.1), we obtain the following equations of motion:

$$\dot{p} = -\sin q, \qquad \dot{q} = p, \tag{1.3}$$

which is as expected. Many $2d$-dimensional systems can be described in this canonical way through Hamilton's equations, however, it is possible to generalise this in a way that can be applied to more general systems (including ones which are odd dimensional). To do this, we first define the canonical Poisson bracket on functions of the coordinates:

$$[g,h]_c = \sum_{i=1}^{d} \left(\frac{\partial g}{\partial q_i}\frac{\partial h}{\partial p_i} - \frac{\partial g}{\partial p_i}\frac{\partial h}{\partial q_i} \right). \tag{1.4}$$

Using this bracket, Hamilton's equations of (1.1) can be recast as follows:

$$\dot{p}_i = [p_i, H]_c, \qquad \dot{q}_i = [q_i, H]_c. \tag{1.5}$$

There are, however, Hamiltonian systems whose dynamical equations are not generated specifically by the canonical Poisson bracket. An example of this is any odd-dimensional Hamiltonian system. Let us thus define a Poisson bracket in general.

Let M be a smooth manifold, and take smooth functions $A, B, C, D \in C^\infty(M)$. The Poisson bracket $[\cdot,\cdot] : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$ is an operation which is defined by the following properties:

1. It is bilinear:

$$\begin{aligned} [A + C, B] &= [A, B] + [C, B], \\ [A, B + D] &= [A, B] + [A, D]. \end{aligned} \tag{1.6}$$

2. It is antisymmetric:

$$[A, B] = -[B, A]. \tag{1.7}$$

3. It satisfies the Jacobi identity:

$$[A,[B,C]]+[B,[C,A]]+[C,[A,B]]=0. \tag{1.8}$$

4. It satisfies the Leibniz rule:

$$[AB,C]=A[B,C]+B[A,C]. \tag{1.9}$$

Together with the Hamiltonian function H, the dynamical equations for a given smooth function A of the coordinates can then be generated through a corresponding Poisson bracket in the following way:

$$\dot{A}=[A,H]. \tag{1.10}$$

In the case where a bracket $[\cdot,\cdot]$ is different to (1.4), it is referred to as a non-canonical Poisson bracket. From this description, we can also see that the Hamiltonian is always a conserved quantity of such a system:

$$\begin{aligned}\frac{d}{dt}H&=[H,H],\\&=\frac{1}{2}[H,H]+\frac{1}{2}[H,H],\\&=\frac{1}{2}[H,H]-\frac{1}{2}[H,H]=0,\end{aligned} \tag{1.11}$$

where the second line follows from bilinearity of the bracket, and the third from its antisymmetry.

We now introduce two important concepts in this framework — Casimir invariants and momentum maps. A Casimir invariant of a given Poisson bracket $[\cdot,\cdot]$ is a function C that satisfies the following condition:

$$[C,A]=0, \tag{1.12}$$

for all smooth functions A. By contrast, a momentum map is a function I which is associated with a symmetry of the Hamiltonian function. Specifically, it is a function under whose action the Hamiltonian is constant, i.e. it satisfies:

$$[H,I]=0. \tag{1.13}$$

By the anti-symmetry of the bracket, we can then see that the momentum map is

an invariant of the Hamiltonian system:

$$\frac{d}{dt}I = [I, H] = -[H, I] = 0. \tag{1.14}$$

Describing Hamiltonian systems through such Poisson brackets is much more general than Hamilton's equations of (1.1). An example of a system that cannot be obtained by (1.1) but can be formulated via a non-canonical approach is the rigid body. The equations that describe the motion of a rigid body rotating about its center of mass are as follows:

$$\begin{aligned} I_1\dot{\Omega}_1 &= (I_2 - I_3)\Omega_2\Omega_3, \\ I_2\dot{\Omega}_2 &= (I_3 - I_1)\Omega_3\Omega_1, \\ I_3\dot{\Omega}_3 &= (I_1 - I_2)\Omega_1\Omega_2, \end{aligned} \tag{1.15}$$

where $\Omega = [\Omega_1, \Omega_2, \Omega_3]^T$ is the angular velocity vector in the body frame, and I_1, I_2, I_3 are the moments of inertia of the rigid body. To cast this in the Hamiltonian form of (1.10), we introduce the angular momenta:

$$\Pi_i = I_i\Omega_i, \qquad i = 1, 2, 3. \tag{1.16}$$

Under this coordinate transformation, the rigid body's equations of motion in (1.15) become:

$$\begin{aligned} \dot{\Pi}_1 &= \frac{I_2 - I_3}{I_2 I_3}\Pi_2\Pi_3, \\ \dot{\Pi}_2 &= \frac{I_3 - I_1}{I_3 I_1}\Pi_3\Pi_1, \\ \dot{\Pi}_3 &= \frac{I_1 - I_2}{I_1 I_2}\Pi_1\Pi_2. \end{aligned} \tag{1.17}$$

Let us denote the angular momentum vector $\Pi = [\Pi_1, \Pi_2, \Pi_3]^T$. The above set of equations then becomes:

$$\dot{\Pi} = \Pi \times \Omega. \tag{1.18}$$

These equations can be derived by (1.10) with the following Hamiltonian function:

$$H_{RB} = \frac{1}{2}\left(\frac{\Pi_1^2}{I_1} + \frac{\Pi_2^2}{I_2} + \frac{\Pi_3^2}{I_3}\right), \tag{1.19}$$

and a non-canonical Poisson bracket as follows:

$$[A, B]_{RB}(\Pi) = -\Pi \cdot (\nabla F \times \nabla G). \tag{1.20}$$

Thus, the equations of motion for the rigid body (1.17) can be obtained using a Poisson bracket as follows:

$$\dot{\Pi}_i = [\Pi_i, H_{RB}]_{RB}. \tag{1.21}$$

The rigid body bracket of (1.20) has a special property, namely that the total angular momentum

$$C(\Pi) = \frac{1}{2}(\Pi_1^2 + \Pi_2^2 + \Pi_3^2), \tag{1.22}$$

is conserved regardless of the Hamiltonian function, i.e. it is a Casimir invariant.

1.1.2 Infinite-dimensional Hamiltonian systems

Thus far, we have considered systems that are given by ordinary differential equations. Our objective, however, is to study PDEs in a Hamiltonian setting, and so it is necessary to generalise to infinite-dimensional Hamiltonian systems.

In the finite-dimensional case, we considered the evolution of our coordinates, for e.g. (q_i, p_i) in the canonical case, or the angular momentum vector Π in the case of the rigid body. In the case of PDEs, however, we are interested in the evolution of field variables, which are *functions* of the underlying coordinates.

Let us denote the coordinates $z \in \Omega \subset \mathbb{R}^d$, and time $t \in \mathcal{T} = [0, \infty)$. Then, we can denote the field variables as $u(t,z) = (u^1(t,z),\, u^2(t,z),\, ...,\, u^m(t,z))^T$. The Hamiltonian depends on the dynamical quantities, which in this case are the field variables. As such, it is a *functional*, and correspondingly we require a Poisson bracket on functionals as well.

In such case, the Poisson bracket takes the following form on functionals $\mathcal{A}, \mathcal{B}$ of the field variables u (Morrison 1998):

$$\{\mathcal{A}, \mathcal{B}\} = \int_\Omega \frac{\delta \mathcal{A}}{\delta u^i} \mathcal{J}_{ij}(u) \frac{\delta \mathcal{B}}{\delta u^j}, \tag{1.23}$$

where $\delta\mathcal{A}/\delta u^i$ denotes the functional derivative of $\mathcal{A}$ with respect to the dynamical variable u^i, defined as follows:

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{A}\left[u^1, \ldots, u^i + \epsilon v^i, \ldots, u^m\right]\big|_{\epsilon=0} = \int_\Omega \frac{\delta \mathcal{A}}{\delta u^i}\, v^i \mathrm{d}z. \tag{1.24}$$

The infinite-dimensional Poisson bracket satisfies the same properties (1.6)–(1.9), as in the finite-dimensional case. In this form, the properties of the kernel $\mathcal{J}(u)$ ensure that the resultant Poisson bracket satisfies the requisite properties.

The notion of Casimirs and momentum maps are defined analogously to the finite-dimensional case. The nullspace of $\mathcal{J}(u)$ plays an important role as if it is non-empty, then there must exist Casimir invariants.

The equations of motion for a Hamiltonian PDE system can be obtained by:

$$\dot{\mathcal{A}} = \{\mathcal{A}, \mathcal{H}\}, \tag{1.25}$$

where $\mathcal{A}$ is a given functional of the dynamical variables, and $\mathcal{H}$ is the Hamiltonian functional. Examples of systems that can be described in this way include many equations from fluid dynamics, and as we will see later in this chapter, the Vlasov–Maxwell equations in plasma physics.

1.2 The Metriplectic Formulation

The metriplectic framework (Morrison 1986; Kaufman & Morrison 1982; Kaufman 1984; Morrison 1984*a*,*b*; Grmela 1984*a*,*b*, 1985; Morrison & Updike 2023) provides a convenient way to express dynamical systems which consist of two parts: a conservative, Hamiltonian part and a dissipative part, which are compatible with the laws of thermodynamics. The ideal dynamics are described via a Hamiltonian functional and a Poisson bracket, and the dissipative dynamics through a symmetric metric bracket and a functional representing the dissipated quantity, usually the entropy.

In this section, we give an overview of the metriplectic framework.

1.2.1 General Framework

As before, let us denote by $u(t, z) = (u^1(t, z), u^2(t, z), ..., u^m(t, z))^T$ the field variables of our dynamical system, defined over the domain Ω with coordinates z, and let $\mathcal{A}$ be an arbitrary functional of the field variables u. In the metriplectic framework, the evolution of any functional $\mathcal{A}$ of the dynamical variables is given by:

$$\dot{\mathcal{A}} = \{\mathcal{A}, \mathcal{F}\} + (\mathcal{A}, \mathcal{F}), \tag{1.26}$$

where $\mathcal{F} = \mathcal{H} - \mathcal{S}$ is the free energy, i.e., the difference between the Hamiltonian functional $\mathcal{H}$ and the entropy functional $\mathcal{S}$. The Poisson bracket $\{\cdot, \cdot\}$, as defined in (1.23), describes the conservative or Hamiltonian part of the dynamics.

The metric bracket $(\cdot, \cdot)$ describes the dissipative part of the dynamics. It is a bilinear operation and is defined by the following properties for all functionals $\mathcal{A}$.

1. It is positive semi-definite:
$$(\mathcal{A}, \mathcal{A}) \geq 0. \tag{1.27}$$

2. It is symmetric in its arguments:
$$(\mathcal{A}, \mathcal{B}) = (\mathcal{B}, \mathcal{A}). \tag{1.28}$$

3. It satisfies the Leibniz rule, i.e. for a functional $\mathcal{C}$:
$$(\mathcal{A}\mathcal{B}, \mathcal{C}) = \mathcal{B}(\mathcal{A}, \mathcal{C}) + \mathcal{A}(\mathcal{B}, \mathcal{C}) \tag{1.29}$$

With the sign convention chosen here, entropy is always dissipated. The bracket can be formulated in a similar way to the infinite-dimensional Poisson bracket (1.23), as follows:
$$(\mathcal{A}, \mathcal{B}) = \int \frac{\delta \mathcal{A}}{\delta u^i} \mathcal{G}_{ij}(u) \frac{\delta \mathcal{B}}{\delta u^j}. \tag{1.30}$$
Here, $\mathcal{G}(u)$ is a self-adjoint operator (as opposed to the anti-self-adjoint kernel $\mathcal{J}(u)$ in the Poisson bracket) to ensure that the metric bracket is positive semi-definite. The nullspace of $\mathcal{G}(u)$ also determines the Casimir invariants of the metric bracket.

The two brackets have to satisfy certain compatibility conditions which ultimately guarantee compliance with the laws of thermodynamics. The entropy functional is usually chosen to be a Casimir invariant of the Poisson bracket.

The metric bracket is constructed to ensure that the Hamiltonian and other physically relevant invariants $\mathcal{I}$ of the conservative system (Casimir invariants or momentum maps) are Casimir invariants of the metric bracket. This is with the exception of the entropy itself, as the metric bracket is constructed to dissipate this quantity. Thus, the evolution equation of (1.26) becomes:
$$\begin{aligned} \dot{\mathcal{A}} &= \{\mathcal{A}, \mathcal{F}\} + (\mathcal{A}, \mathcal{F}) \\ &= \{\mathcal{A}, \mathcal{H}\} - \cancelto{0}{\{\mathcal{A}, \mathcal{S}\}} + \cancelto{0}{(\mathcal{A}, \mathcal{H})} - (\mathcal{A}, \mathcal{S}) \\ &= \{\mathcal{A}, \mathcal{H}\} - (\mathcal{A}, \mathcal{S}). \end{aligned} \tag{1.31}$$

The compatibility conditions ensure a separation of the conservative and dissipative dynamics, as the Hamiltonian dynamics do not affect the entropy, and the dissipative dynamics do not affect the Hamiltonian or any other physically relevant invariant of the ideal dynamics. It is desirable to also preserve this property in the course of discretisation.

1.2.2 H-Theorem and Energy-Casimir principle

With the aforementioned requirements that (i) $\mathcal{H}$ is a Casimir of the metric bracket, (ii) $\mathcal{S}$ is a Casimir of the Poisson bracket, and that (iii) the metric bracket is positive semi-definite, the metriplectic framework automatically reproduces the First and Second Law of Thermodynamics:

$$\frac{d\mathcal{H}}{dt} = \{\mathcal{H}, \mathcal{H}\} - (\mathcal{H}, \mathcal{S}) = 0, \tag{1.32a}$$

$$\frac{d\mathcal{S}}{dt} = \{\mathcal{S}, \mathcal{H}\} - (\mathcal{S}, \mathcal{S}) = -(\mathcal{S}, \mathcal{S}) \leq 0. \tag{1.32b}$$

When a metriplectic system possesses no Casimir invariants, its equilibrium state, u_{eq}, is determined fully by an energy principle, $\delta\mathcal{F}[u_{eq}] = 0$. Additionally, this state is stable given the second variation satisfies $\delta^2\mathcal{F}[u_{eq}] > 0$. When there are Casimir invariants, however, the equilibrium condition must be modified to account for the degeneracies in the state of the system (Morrison 1998). In this case, the equilibrium state must satisfy an energy-Casimir principle as follows:

$$\left[\delta\mathcal{F} + \sum_i \lambda_i \delta\mathcal{C}_i\right]\Bigg|_{u=u_{eq}} = 0, \tag{1.33}$$

where $\mathcal{C}_i$ are the Casimir invariants, and λ_i are corresponding Lagrange multipliers which are determined by the initial conditions of the system.

1.3 Vlasov-Maxwell and Vlasov-Poisson systems

The Vlasov-Maxwell system can be considered one of the most fundamental ways of describing the dynamics in a plasma, which is comprised of charged particles under the influence of electromagnetic fields to which they also contribute through their motion. We begin by defining the system.

Let the spatial domain be given by $\Omega \subset \mathbb{R}^3$, and the corresponding phase space coordinates be denoted $(x, v) \in \Omega \times \mathbb{R}^3$ with position x and velocity v. Let the time $t \in \mathcal{T} = [0, \infty)$ as before. Then, the Vlasov equation for a given particle species is:

$$\partial_t f_s + v \cdot \nabla_x f_s + \frac{q_s}{m_s}(E + v \times B) \cdot \nabla_v f_s = 0, \tag{1.34}$$

where the quantities q_s and m_s are the charge and mass of the species under consideration, respectively. This equation describes the evolution of the distribution

function of species s, $f_s(x, v, t) : \Omega \times \mathbb{R}^3 \times \mathcal{T} \to [0, \infty)$, a non-negative scalar function. The system possesses such a distribution function for each species, and each f_s satisfies its own Vlasov equation. Each distribution function satisfies the following normalisation condition:

$$\int_{\mathbb{R}^3} \int_{\Omega} f_s(x, v, t) \mathrm{d}x \mathrm{d}v = 1, \tag{1.35}$$

and so, it is a probability density function for the position and velocity of the charged particles at any given time t.

The Vlasov equation is coupled to Maxwell's equations for electromagnetic fields via the electric field E and magnetic field B. Maxwell's equations are as follows:

$$\frac{1}{c^2}\frac{\partial E}{\partial t} = \text{curl } B - \mu_0 j, \tag{1.36}$$

$$\frac{\partial B}{\partial t} = -\text{curl } E, \tag{1.37}$$

$$\text{div } E = \frac{\rho}{\varepsilon_0}, \tag{1.38}$$

$$\text{div } B = 0, \tag{1.39}$$

where the electric and magnetic fields are given by $E(x, t) : \mathbb{R}^3 \times \mathcal{T} \to \mathbb{R}^3$ and $B(x, t) : \mathbb{R}^3 \times \mathcal{T} \to \mathbb{R}^3$, respectively. The quantities $\mu_0, \varepsilon_0 \in \mathbb{R}$ are both physical constants, namely the vacuum magnetic permeability and vacuum electric permittivity. The charge and current densities are denoted by ρ and j respectively, and they are defined in terms of the distribution functions f_s:

$$\rho = \sum_s q_s \int_{\mathbb{R}^3} f_s \, \mathrm{d}v, \quad j = \sum_s q_s \int_{\mathbb{R}^3} v f_s \, \mathrm{d}v, \tag{1.40}$$

thus coupling Maxwell's equations to the Vlasov equations for each species.

Equations (1.36) and (1.37) are known as Ampère's law and Faraday's law respectively, while Equation (1.38) is known as Gauss' law. Equation (1.39) is Gauss' law for magnetism, and is often referred to as the "div B" constraint. It should be noted that Equations (1.38)–(1.39) are constraints that are satisfied by solutions to the Vlasov–Maxwell system for all time, given that they are satisfied by the chosen initial conditions.

In Appendix A, we detail the derivation of the Vlasov equation from its statistical mechanics origins.

The Vlasov-Poisson system

The Vlasov-Poisson system is an approximation of the Vlasov–Maxwell equations, in the limit of a non-magnetised plasma. In the equations, this limit is obtained by considering $c \to \infty$. Typically, the Vlasov–Poisson equations consider only the distribution function f for the electrons, and treat the ions as a fixed background species. The equations are as follows:

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m} E \cdot \nabla_v f = 0, \tag{1.41}$$

$$-\nabla^2 \phi = \rho, \tag{1.42}$$

where ϕ is an electrostatic potential, defined as $-\nabla\phi = E$, and ρ is the charge density defined as:

$$\rho = q \int f \mathrm{d}v - \rho_i, \tag{1.43}$$

where ρ_i is the density of the background ions. These equations are commonly used in the study of several plasma phenomena, such as Landau damping, and form the basis of cold plasma theory.

1.3.1 Hamiltonian description

The Vlasov–Maxwell system possesses an infinite-dimensional Hamiltonian structure, as demonstrated by Morrison (1980) and Marsden & Weinstein (1982). Namely, the equations of motion (for both the distribution function and fields, which are collectively the dynamic variables) shown above can be derived through the use of a Hamiltonian functional and a Poisson bracket as in (1.25).

The Hamiltonian functional for the Vlasov–Maxwell system is:

$$\mathcal{H}[f, E, B] = \int \frac{1}{2}|v|^2 f \mathrm{d}x\mathrm{d}v + \int \frac{1}{2}\left(|E|^2 + |B|^2\right) \mathrm{d}x. \tag{1.44}$$

To define the Poisson structure, we require the following space of functions (Marsden & Weinstein 1982):

$$MV = \left\{ (f, E, B) \,\middle|\, \mathrm{div}B = 0,\ \mathrm{div}E = \int f(x, v)\mathrm{d}v \right\}. \tag{1.45}$$

The Poisson bracket is then defined on functionals $\mathcal{A} : MV \to \mathbb{R}$.

The full Vlasov–Maxwell Poisson bracket derived by Marsden & Weinstein (1982)

is then as follows:

$$\begin{aligned}\{\mathcal{A},\mathcal{B}\} = &\int f\left[\frac{\delta\mathcal{A}}{\delta f},\frac{\delta\mathcal{B}}{\delta f}\right]\mathrm{d}x\mathrm{d}v + \int\left(\frac{\delta\mathcal{A}}{\delta\mathbf{E}}\cdot\mathrm{curl}\frac{\delta\mathcal{B}}{\delta\mathbf{B}} - \frac{\delta\mathcal{B}}{\delta\mathbf{E}}\cdot\mathrm{curl}\frac{\delta\mathcal{A}}{\delta\mathbf{B}}\right)\mathrm{d}x \\ &+\int\left(\frac{\delta\mathcal{A}}{\delta\mathbf{E}}\cdot\frac{\delta f}{\delta\mathbf{v}}\frac{\delta\mathcal{B}}{\delta f} - \frac{\delta\mathcal{B}}{\delta\mathbf{E}}\cdot\frac{\delta f}{\delta\mathbf{v}}\frac{\delta\mathcal{A}}{\delta f}\right)\mathrm{d}x\mathrm{d}v \\ &+\int f\mathbf{B}\cdot\left(\frac{\partial}{\partial\mathbf{v}}\frac{\delta\mathcal{A}}{\delta f}\times\frac{\partial}{\partial\mathbf{v}}\frac{\delta\mathcal{B}}{\delta f}\right)\mathrm{d}x\mathrm{d}v,\end{aligned} \tag{1.46}$$

where $[\cdot,\cdot]$ is the Poisson bracket on functions of Equation (1.4), and $\delta/\delta f$ denotes the Fréchet or functional derivative as defined in (1.24). For a detailed exposition on the derivation of this bracket, we refer the reader to Marsden & Weinstein (1982).

Finally, with our Hamiltonian functional and the Poisson bracket on functionals, we can express the equations of motion for any functional of the dynamical quantities as follows:

$$\dot{\mathcal{A}} = \{\mathcal{A},\mathcal{H}\}. \tag{1.47}$$

This is a very useful result from the point of view of discretisation, as knowledge of the Hamiltonian / Poisson structure of the problem gives us valuable insight on the structure that should then be preserved by the discretised problem. Furthermore, it informs the approach to discretisation itself, as the bracket is what will be discretised, which together with a discrete Hamiltonian will produce the discrete equations of motion.

1.3.2 Final notes on the Vlasov–Maxwell system

The Vlasov equation is derived from the Liouville equation through a series of assumptions and simplifications, the details of which are discussed in Appendix A. Chief among these is the assumption that the plasma is correlation-less, and so is free of collisions. While this assumption is mostly satisfied as plasmas have very low density, there are instances where collisions have an important contribution to the plasma dynamics. For such cases, a collision operator is added to the Vlasov equation as follows:

$$\partial_t f + v\cdot\nabla_x f + \frac{q}{m}(E + v\times B)\cdot\nabla_v f = C[f], \tag{1.48}$$

where the right-hand side now consists of an additional term, $C[f]$. Here, the notation $[f]$ denotes that the collision operator is a functional of the particle distribution function f. In general, collision operators are only functions of velocity, and act locally in space. The following sections present two such operators which form the

subject of this thesis.

1.4 The Lenard-Bernstein operator

The Lenard-Bernstein collision operator (Lenard & Bernstein 1958) is given by the following equation:

$$C[f] = \nu \frac{\partial}{\partial v} \cdot \left(\frac{\partial f}{\partial v} + vf \right), \tag{1.49}$$

where f is the single-species distribution function, $v \in \mathbb{R}^d$ is the velocity and ν is the collision frequency, which is assumed to be constant in time. This operator preserves mass (or particle number), but not momentum or energy.

The Lenard-Bernstein operator is applicable in velocity dimensions $d = 1, 2, 3$, though collision operators which describe more physics effects, such as the Landau operator, may be preferred in two and three-dimensions in order to allow, for example, interchange of momentum between different components. The steady-state solution to $\partial_t f = C[f]$ for this operator is an d-dimensional standard Normal distribution, with mean $\mu = 0$ and variance $\sigma^2 = 1$.

This operator is often paired with the Vlasov–Poisson equations in order to study one-dimensional plasma dynamics with the effect of collisions.

The Lenard-Bernstein operator (1.49) preserves mass density, the zeroth moment of the distribution function f. However, it does not preserve momentum density or energy density, which are the first and second moments of the distribution function in velocity, respectively, and whose conservation is crucial for obtaining physically correct results in numerical simulations. In the following section, we detail the derivation of a modified Lenard-Bernstein operator that is energy and momentum preserving.

1.4.1 Construction of the conservative operator

In order to enforce conservation of energy and momentum, we follow Kraus (2013) (see also Filbet & Sonnendrücker (2003)) and modify the operator through an expansion as follows,

$$C[f] = \nu \frac{\partial}{\partial v} \cdot \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right). \tag{1.50}$$

We will consider solving the following differential equation:

$$\partial_t f = C[f], \tag{1.51}$$

with the coefficients A_1, A_2 being obtained as detailed in the following discussion.

In the following, we will see that the coefficients A_m are functions of the moments of the distribution function f. In general, preserving k moments of the distribution function will require an expansion including k terms in the operator. The coefficients are then computed by requiring Equation (1.51) to obey the respective conservation laws, which here are for momentum and energy. Specifically, conservation of the k-th moment requires the following condition to hold:

$$\int v^k C[f] \mathrm{d}v = \nu \int v^k \left[\frac{\partial}{\partial v} \cdot \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right) \right] \mathrm{d}v = 0. \tag{1.52}$$

Integrating this by parts, we obtain the following condition:

$$\nu \left[v^k \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right) \right]_{-\infty}^{+\infty} - k\nu \int v^{k-1} \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right) \mathrm{d}v = 0. \tag{1.53}$$

Without loss of generality, we assume that f and $\partial f / \partial v$ approach zero as $|v| \to \infty$, so that the first term in Equation (1.53) is zero and we obtain the following condition:

$$\int v^{k-1} \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right) \mathrm{d}v = 0, \tag{1.54}$$

for $k = 1, 2$. Integrating the first term by parts once again, this equation becomes:

$$\int \left[(k-1) v^{k-2} - A_1 v^{k-1} - A_2 v^k \right] f \mathrm{d}v = 0, \tag{1.55}$$

where the assumption that f approaches zero as $|v|$ tends to infinity has been utilised once more. Writing the moments as $M_m[f] = \int v^m f \mathrm{d}v$, we obtain the following conditions:

$$(k-1) M_{k-2} = A_1 M_{k-1} + A_2 M_k, \quad k = 1, 2. \tag{1.56}$$

These conditions provide a linear system of equations that can be solved for the coefficients A_1, A_2:

$$\begin{aligned} A_1 M_0 + A_2 M_1 &= 0, \\ A_1 M_1 + A_2 M_2 &= M_0. \end{aligned} \tag{1.57}$$

The solution to the system of equations in (1.57) is:

$$A_1 = \frac{M_0 M_1}{M_0 M_2 - M_1^2} = \frac{-u}{\varepsilon - u^2}, \tag{1.58}$$

$$A_2 = \frac{-M_0^2}{M_0 M_2 - M_1^2} = \frac{1}{\varepsilon - u^2}, \tag{1.59}$$

where nu and $n\varepsilon$ are the momentum and energy density, respectively, and are related to the moments as follows:

$$n = M_0 = \int f \mathrm{d}v, \quad nu = M_1 = \int v f \mathrm{d}v, \quad n\varepsilon = M_2 = \int v^2 f \mathrm{d}v. \tag{1.60}$$

Let us note that here, n, u, and ε are just constants. However, in the general Vlasov-case, these quantities have a spatial dependency. Upon inserting the expressions for A_1, A_2 into (1.50), we obtain the following operator:

$$C[f] = \nu \frac{\partial}{\partial v} \cdot \left(\frac{\partial f}{\partial v} + \frac{v - u}{\varepsilon - u^2} f \right), \tag{1.61}$$

which can be seen as a conservative version of the Lenard-Bernstein operator (1.49). This is the same operator as the one obtained by Filbet & Sonnendrücker (2003) and is closely related to the operator studied in Hakim *et al.* (2020).

This operator preserves mass, momentum and energy by construction, which is as desired. However, to our knowledge, there is no proof in the literature of whether this modified operator satisfies a H-theorem. In the following section, we demonstrate that this is indeed the case.

1.4.2 H-theorem

We follow a similar strategy to Hakim *et al.* (2020) to demonstrate that the continuous operator satisfies the H-theorem. Let us denote the collisional flux by

$$F[f] = \frac{\partial f}{\partial v} + A_1 f + A_2 v f, \tag{1.62}$$

so that

$$\frac{\partial f}{\partial t} = C[f] = \nu \frac{\partial}{\partial v} \cdot F[f]. \tag{1.63}$$

The change in entropy is then

$$\begin{aligned}\frac{dS}{dt} &= \frac{d}{dt}\int f\log f\mathrm{d}v = \int(1+\log f)\frac{\partial f}{\partial t}\mathrm{d}v = \nu\int(1+\log f)\frac{\partial}{\partial v}\cdot F\mathrm{d}v,\\ &= -\nu\int\frac{1}{f}\frac{\partial f}{\partial v}\cdot F\mathrm{d}v = -\nu\int\frac{1}{f}|F|^2\mathrm{d}v + \int(A_1+A_2v)F\mathrm{d}v, \end{aligned} \tag{1.64}$$

where integration by parts, the assumption that F goes to zero as $|v|\to\infty$ and the substitution $\partial f/\partial v = F - A_1 f - A_2 v f$ were used. By Equation (1.54), the second term in the last expression is designed to vanish, namely

$$\int(A_1+A_2v)F\mathrm{d}v = 0.$$

Hence, the entropy is monotonically dissipated (provided that f is non-negative):

$$\frac{dS}{dt} = -\int\frac{1}{f}F^2\mathrm{d}v \le 0. \tag{1.65}$$

The entropy is stationary when $F[f_{eq}] = 0$, that is when f_{eq} solves the PDE

$$\frac{\partial f_{eq}}{\partial v} = -\frac{v-u}{\varepsilon-u^2}f_{eq}. \tag{1.66}$$

The (unique) solution with conditions $f \overset{|v|\to\infty}{\longrightarrow} 0$ and $\int f\mathrm{d}v = n$ is a d-dimensional shifted Gaussian distribution with mean u and variance $\varepsilon - u^2$,

$$f_{eq}(v) = \frac{n}{(2\pi(\varepsilon-u^2))^{d/2}}\,e^{-\frac{1}{2}(v-u)^2/(\varepsilon-u^2)}. \tag{1.67}$$

Thus, the continuous operator of (1.61) satisfies the H-theorem.

1.5 The Landau operator

The Landau operator is described by the following equation:

$$C[f] = \nu\frac{\partial}{\partial v}\cdot\int U(v,v')\left(f(v')\frac{\partial f}{\partial v} - f(v)\frac{\partial f}{\partial v'}\right)\mathrm{d}v', \tag{1.68}$$

where f is again the single-particle distribution function of the Vlasov equation, $v\in\mathbb{R}^d$ is the velocity, and $\nu\in\mathbb{R}$ is the collision frequency.[1] The tensor U :

[1] We note that the position dependency of f has been suppressed in the equation as the collision operator acts purely in velocity-space, and we will use this notation throughout the thesis.

$\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is defined through its components in the following way:

$$U_{ij}(v, v') = \frac{1}{|v - v'|}\left(\delta_{ij} - \frac{(v_i - v_i')(v_j - v_j')}{|v - v'|^2}\right). \tag{1.69}$$

The tensor $U(v, v')$ is a scaled orthogonal projector onto the subspace orthogonal to the vector $v - v'$, i.e. it satisfies:

$$U(v, v')(v - v') = 0. \tag{1.70}$$

As a projector, it is also symmetric and positive definite, and these properties are important in ensuring the conservative properties of the Landau operator, which preserves mass, momentum, and energy. The operator also satisfies an H-theorem.

It should also be noted that the Landau operator is valid for dimensions $d = 2, 3$, but not when $d = 1$. Thus, it is often of interest as a means of adding dissipation to the Vlasov–Maxwell system.

First, we consider purely the dissipative dynamics described by the collision operator, that is

$$\partial_t f = C[f], \tag{1.71}$$

omitting the Hamiltonian part of the system. In the metriplectic framework, the collision operator $C[f]$ can be described as

$$C[f] = -(f, \mathcal{S}), \tag{1.72}$$

where the entropy functional $\mathcal{S}$ is given by:

$$\mathcal{S} = -\int f \log f \mathrm{d}v. \tag{1.73}$$

The metric bracket for the Landau collision operator is given by

$$(\mathcal{A}, \mathcal{B}) = \frac{1}{2}\int\int \left(\frac{\partial \mathcal{A}_f}{\partial v} - \frac{\partial \mathcal{A}_{f'}}{\partial v'}\right) f(v) U(v, v') f(v') \left(\frac{\partial \mathcal{B}_f}{\partial v} - \frac{\partial \mathcal{B}_{f'}}{\partial v'}\right) \mathrm{d}v\mathrm{d}v', \tag{1.74}$$

with $\mathcal{A}, \mathcal{B}$ functionals, and $\mathcal{A}_f$ and $\mathcal{A}_{f'}$ denoting the functional derivatives of $\mathcal{A}$ with respect to $f(v)$ and $f(v')$, respectively. The tensor $U(v, v')$ is as defined in (1.69). By the chosen sign conventions for the entropy $\mathcal{S}$ and the bracket, entropy is dissipated in time:

$$\frac{d}{dt}\mathcal{S} = -(\mathcal{S}, \mathcal{S}) \leq 0. \tag{1.75}$$

There are three physically important invariants in the Vlasov system that we wish

to also conserve in the metric bracket – mass, momentum, and energy:

$$\mathcal{M} = m\int f \mathrm{d}v, \qquad \mathcal{P} = m\int v f \mathrm{d}v, \qquad \mathcal{E} = \frac{1}{2}m\int |v|^2 f \mathrm{d}v. \tag{1.76}$$

We note that in the case of the full Vlasov–Maxwell–Landau system, the conserved quantities shown above will be augmented to take the electromagnetic contributions into account.

The quantities in (1.76) are Casimir invariants of the metric bracket, i.e. they satisfy:

$$(\mathcal{A}, \mathcal{M}) = 0, \qquad (\mathcal{A}, \mathcal{P}) = 0, \qquad (\mathcal{A}, \mathcal{E}) = 0, \tag{1.77}$$

for any functional $\mathcal{A}$.

The equilibrium state of the system can then be obtained by applying the energy-Casimir principle (1.33). Here, the equilibrium state must satisfy:

$$\left[\frac{\delta \mathcal{S}}{\delta f} + \lambda_{\mathcal{M}}\frac{\delta \mathcal{M}}{\delta f} + \lambda_{\mathcal{P}} \cdot \frac{\delta \mathcal{P}}{\delta f} + \lambda_{\mathcal{E}}\frac{\delta \mathcal{E}}{\delta f}\right]\Bigg|_{f=f_{eq}} = 0. \tag{1.78}$$

Using Equations (1.73) and (1.76), the above condition becomes:

$$-(1 + \log f_{eq}) + \lambda_{\mathcal{M}} m + \lambda_{\mathcal{P}} \cdot mv + \lambda_{\mathcal{E}} m|v|^2 = 0, \tag{1.79}$$

and so equilibrium distribution functions are of the form:

$$f_{eq} = \exp\big(-(\lambda_M m + 2\lambda_P \cdot mv + \lambda_E m|v|^2)\big). \tag{1.80}$$

Thus, we have that equilibrium distribution functions of the Landau operator are Maxwellians, with mean, standard deviation, and normalisation determined by initial conditions.

Now that we have described how the Landau operator can be described in the metriplectic framework, we can consider the full Vlasov–Maxwell–Landau system.

1.5.1 The Vlasov–Maxwell–Landau system

The Vlasov–Maxwell–Landau system is obtained by taking the Vlasov–Maxwell system of Equations (1.34), (1.36)-(1.39), and adding the Landau operator (1.68) to the right-hand side of the Vlasov equation:

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m}(E + v \times B) \cdot \nabla_v f = C[f], \tag{1.81}$$

$$C[f] = \frac{\partial}{\partial v} \cdot \int U(v - v') \left(f(v') \frac{\partial f}{\partial v} - f(v) \frac{\partial f}{\partial v'} \right) \mathrm{d}v', \tag{1.82}$$

$$\frac{1}{c^2} \frac{\partial E}{\partial t} = \text{curl } B - \mu_0 q \int v f \mathrm{d}v, \tag{1.83}$$

$$\frac{\partial B}{\partial t} = -\text{curl } E. \tag{1.84}$$

$$\text{div } E = \frac{q}{\varepsilon_0} \int f \mathrm{d}v, \tag{1.85}$$

$$\text{div } B = 0. \tag{1.86}$$

In the metriplectic framework, using the Poisson bracket defined in Equation (1.46) and the metric bracket of Equation (1.74), we can represent this system as follows:

$$\dot{\mathcal{A}} = \{\mathcal{A}, \mathcal{H}\} - (\mathcal{A}, \mathcal{S}), \tag{1.87}$$

where $\mathcal{A} \in \{f, E, B\}$, and the Hamiltonian and entropy functionals are:

$$\mathcal{H} = \int \frac{1}{2} |v|^2 f \mathrm{d}x\mathrm{d}v + \int \frac{1}{2} \left(|E|^2 + |B|^2 \right) \mathrm{d}x, \tag{1.88}$$

$$\mathcal{S} = -\int f \log f \mathrm{d}v. \tag{1.89}$$

It should be noted that Gauss's law and the div-B constraint (1.85)-(1.86) arise as Casimir invariants of the Hamiltonian part of the system.

The total mass $\mathcal{M}$ remains a Casimir of the full system:

$$\mathcal{M} = \int f \mathrm{d}x\mathrm{d}v. \tag{1.90}$$

The total momentum is as follows:

$$\mathcal{P} = \int v f \mathrm{d}x\mathrm{d}v + \int E \times B \mathrm{d}x, \tag{1.91}$$

and is a momentum map of the Poisson bracket. It is, however, also in the nullspace of the metric bracket and so is conserved by the full system. The Hamiltonian $\mathcal{H}$ (or total energy) is also a conserved quantity of the full system.

Finally, there is now a modified energy-Casimir principle which determines the equi-

librium state of the system:

$$\delta\mathcal{F} + \lambda\delta\mathcal{M} = \left(\frac{\delta\mathcal{H}}{\delta f} - \frac{\delta\mathcal{S}}{\delta f} + \lambda\frac{\delta\mathcal{M}}{\delta f}\right)\delta f_{eq} + \frac{\delta\mathcal{H}}{\delta E}\cdot\delta E_{eq} + \frac{\delta\mathcal{B}}{\delta B}\cdot\delta B_{eq} = 0. \qquad (1.92)$$

The benefit of the metriplectic description of the Vlasov–Maxwell–Landau system is two-fold. Firstly, it allows us to focus on the discretisation of the problem in two separate pieces – Hamiltonian and dissipative – as long as the discretisation of each maintains the compatibility conditions between the two. Hence, the focus in Chapter 4 will be purely on methods for discretising the metric (dissipative) part, as there are several existing methods in the literature for handling the Hamiltonian part in an appropriate manner as mentioned in the introduction.

Secondly, the metriplectic formulation actually provides us with a geometric structure for the dissipation operator, and this is key when designing the discretisation as it actually tells us what structure we should be preserving in our methods. Again, this idea will be explored in deeper detail in Chapter 4.

Chapter 2

Numerical Methods

In this chapter, we introduce a number of fundamental and advanced numerical techniques that are used in this thesis. We first begin with a brief discussion of finite element methods, before moving on to the fundamentals of deterministic particle methods. We briefly touch on regularisation approaches, and then describe projection methods and their advantages. Finally, we discuss the two time integration schemes that will be used in this thesis.

2.1 Finite Element Methods

In this section, we provide a brief introduction to finite element methods, as these techniques will underpin the approach that is taken in the latter parts of this thesis.

Finite element methods (FEM) are a commonly used numerical method for solving partial differential equations. They are a subset of a family known as Galerkin methods. We introduce the fundamental ideas behind FEM via the d-dimensional Poisson equation:

$$-\nabla^2 u = f, \text{ on } \Omega, \tag{2.1}$$

where $\Omega \subset \mathbb{R}^d$, $u : \Omega \to \mathbb{R}$ is the solution, and $f : \Omega \to \mathbb{R}$ is a source term. We will also need a boundary condition for the solution to be fully defined, so let us consider a homogeneous Dirichlet boundary condition:

$$u = 0, \text{ on } \partial\Omega, \tag{2.2}$$

where $\partial\Omega$ is the boundary of the domain Ω. The finite element methods seeks numerical approximations to the *weak* solutions of PDEs, and so let us state the weak form of the Poisson equation:

$$-\int_\Omega v\nabla^2 u \mathrm{d}x = \int_\Omega v f \mathrm{d}x, \tag{2.3}$$

where v is known as the test function, and is taken to be in the same space as the solution (importantly, it satisfies the same boundary conditions). Using integration by parts on the left-hand side, this equation can be simplified to the following:

$$\int_\Omega \nabla v \cdot \nabla u \mathrm{d}x = \int_\Omega v f \mathrm{d}x, \tag{2.4}$$

where we have used the homogeneous boundary condition of v to cancel the boundary term that arises from integration. From this equation, we can consider the function spaces that are required for each function in the weak form. Let us define the two main function spaces that will be required in this case.

Let Ω be a bounded open subset of $\mathbb{R}^n$, and let $f : \Omega \to \mathbb{R}$ be a measurable function. Then $f \in L^2(\Omega)$, i.e. is square-integrable, if

$$\|f\|_2^2 := \int_\Omega |f(x)|^2 \mathrm{d}x < \infty, \tag{2.5}$$

where we identify functions f which agree almost everywhere. The L^2 inner product for two functions $f, g \in L^2(\Omega)$ is defined as follows:

$$(f, g)_{L^2} = \int_\Omega f(x) g(x) \mathrm{d}x, \tag{2.6}$$

and the operation $\|\cdot\|_2$ is the norm on this space.

We also define the Sobolev space of once-weakly differentiable functions, $H^1(\Omega)$. For Ω and f as before, $f \in H^1(\Omega)$ if f is square-integrable (i.e. $f \in L^2(\Omega)$) and there exist functions $g_1, \ldots, g_n \in L^2(\Omega)$ such that the following is satisfied:

$$\int_\Omega f \frac{\partial \varphi}{\partial x_i} \mathrm{d}x = -\int_\Omega g_i \varphi \mathrm{d}x \qquad \forall \varphi \in C_c^\infty(\Omega), \tag{2.7}$$

where $C_c^\infty(\Omega)$ is the space of infinitely differentiable, or smooth, functions with compact support. We will primarily make use of the subspace $H_0^1(\Omega)$, which is the closure of the space $C_c^\infty(\Omega)$ in $H^1(\Omega)$. The functions of this subspace can be considered as functions in $H^1(\Omega)$ which vanish on the boundary $\partial\Omega$, making this the natural space of interest for Dirichlet problems.

Now, let us consider the weak form of the Poisson equation as given in (2.4). As only the first derivative of the solution appears in this equation (after the integration by parts), and we have homogeneous Dirichlet boundary conditions, it is sufficient to consider $u \in H_0^1(\Omega)$. The same is the case for the test functions $v \in H_0^1(\Omega)$.

The main principle of the finite element method is to construct an approximation

to the solution of (2.4) by constructing finite function spaces that approximate the solution and test function spaces, and obtaining the solution by solving the resulting system of algebraic equations.

In the case of the Poisson equation, let us denote the approximation space for the discrete solution, u_h, as $X_N \subset H_0^1(\Omega)$ with a spanning basis set $\{\phi_1, \ldots, \phi_N\} \in X_N$. Thus, a function in this space, $g_h \in X_N$, can be expressed as follows:

$$g_h(x) = \sum_{j=1}^{N} g_j \phi_j(x). \tag{2.8}$$

Let us also define the approximate test function space as X_N, so that $v_h \in X_N$.[1] Then, the finite element approximation of the problem can be formulated as

$$\int_\Omega \nabla v_h \cdot \nabla u_h \mathrm{d}x = \int_\Omega v_h f \mathrm{d}x, \text{ for all } v_h \in X_N. \tag{2.9}$$

As we let the discrete solution $u_h \in X_N$ and take test functions $v_h \in X_N$, these functions take the form of (2.8), and so Equation (2.9) becomes:

$$\int_\Omega \nabla \left(\sum_{i=1}^{N} v_i \phi_i(x) \right) \cdot \nabla \left(\sum_{i=1}^{N} u_i \phi_i(x) \right) \mathrm{d}x = \int_\Omega \sum_{i=1}^{N} v_i \phi_i(x) f(x) \mathrm{d}x. \tag{2.10}$$

Denote the coefficient vectors as $\hat{u} = [u_1, \ldots, u_N]^T$, and let $b_i = \int \phi_i(x) f(x) \mathrm{d}x$ be the integral of the i-th basis function against the right-hand side function $f(x)$. The above equation then becomes the following linear algebra problem for the vector of unknowns $\hat{u}$:

$$\hat{v}^T \mathbb{A} \hat{u} = \hat{v}^T \hat{b}, \text{ for all } \hat{v} \in \mathbb{R}^N, \tag{2.11}$$

where the matrix $\mathbb{A}$ has entries $\mathbb{A}_{ij} = \int \nabla \phi_i(x) \cdot \nabla \phi_j(x) \mathrm{d}x$, and $\hat{b} = [b_1, \ldots, b_N]^T$. Since Equation (2.11) must hold for all test coefficient vectors $\hat{v} \in \mathbb{R}^N$, we can equivalently solve the linear system:

$$\mathbb{A} \hat{u} = \hat{b}, \tag{2.12}$$

for the coefficients $\hat{u}$, with the discrete solution then being given by $u_h(x) = \sum_j u_j \phi_j(x)$.

While we have introduced finite elements in the context of a time-independent prob-

[1] It should be noted that it is not necessary for the space of test functions to be the same as that of the approximate solution. Different choices of approximation spaces can be used to produce different discretisations, where some may be more advantageous for certain problems.

lem, they can also be applied to time dependent PDEs. In this case, the finite element approximation of (2.8) becomes

$$g_h(x,t) = \sum_{j=1}^{N} g_j(t)\phi_j(x), \tag{2.13}$$

with the time dependence of the discrete solution being captured in the coefficients $\hat{g}$. This approximation, with an appropriately chosen function space for the basis functions $\{\phi_j\}$, can be applied to discretise the PDE in space to obtain a semi-discretisation, that is a system of ODEs in time only. Time discretisation techniques that are suited to the particular problem being considered can then be applied to the semi-discretisation, to obtain a full discretisation in both space and time. We will discuss some time integration techniques used in thesis at the end of this chapter.

In general, the finite element method falls into a category of grid-based schemes, along with other techniques such as finite-difference and finite-volume methods. Also known as Eulerian approaches, these methods can be highly accurate for a wide range of problems. In some cases, however, most often when considering hyperbolic PDEs (such as transport problems), Eulerian approaches can be subject to stability issues due to grid-scale oscillations. Ameliorating such issues can result in either high computational cost (to obtain good accuracy) or a loss in accuracy (if resolution becomes limited by computational cost). Additionally, in problems such as kinetics (e.g. in the Vlasov equation), the high dimensionality of the problem can result in large computational costs for Eulerian approaches. In such cases, particle methods can provide a viable alternative.

2.2 (Deterministic) Particle Methods

Particle methods are another approach to finding numerical solutions to partial differential equations. The basic idea behind a particle method is that we wish to represent the discrete solution to our problem as a sum of Dirac delta functions, i.e.

$$u_h(x,t) = \sum_{i=1}^{N} w_i(t)\delta(x - x_i(t)), \tag{2.14}$$

where $\{w_i(t)\}_{i=1}^N$ are the weights, and $\{x_i(t)\}_{i=1}^N$ are the particle positions. Together, these quantities are the degrees of freedom of the discrete problem, and are evolved in time by a system of ODEs that are typically determined from the weak form of the underlying PDE.

Following Chertock (2017), let us use the example of the linear transport equation to describe the basic principles of a particle method. In divergence form, the homogeneous transport equation is as follows:

$$\partial_t u + \nabla \cdot (au) + a_0 u = 0, \tag{2.15}$$

where $x \in \mathbb{R}^d$ and $t \in [0, T]$ for some $T > 0$. Here, $u : \mathbb{R}^d \times [0, T] \to \mathbb{R}$ is the unknown scalar field, and $a(x, t) = [a_1(x, t), \ldots, a_d(x, t)]^T$ is known as the velocity vector. The functions $a_1, \ldots, a_d$ must be given for the problem to be fully defined, along with the coefficient $a_0(x, t)$ and the initial conditions:

$$u_0(x) := u(x, 0). \tag{2.16}$$

As mentioned before, the time evolution of the particles is constructed through considering the weak form of the PDE. Thus, let us define a weak form of this particular problem. A function u is a weak solution to (2.15), (2.16), if it satisfies the following:

$$\begin{aligned} -\int_{\mathbb{R}^d} u_0(x)\varphi(x, 0)\mathrm{d}x - \int_0^T \int_{\mathbb{R}^d} u(x, t) \left[\partial_t \varphi(x, t) + a(x, t) \cdot \nabla\varphi(x, t)\right] \mathrm{d}x\mathrm{d}t \\ + \int_0^T \int_{\mathbb{R}^d} a_0(x, t)u(x, t)\varphi(x, t)\mathrm{d}x\mathrm{d}t = 0, \end{aligned} \tag{2.17}$$

for any test function $\varphi \in C_c^1(\mathbb{R}^d \times [0, T))$. Here, the weak solution u lies in the space dual to $C_c^1(\mathbb{R}^d \times [0, T))$, which is the space of measures on $\mathbb{R}^d \times [0, T)$.

Then, the particle solution to this problem, with initial weights $w_i(0)$ and particle positions $x_i(0)$, is given by (2.14) where the positions and weights solve the following ODEs:

$$\frac{dx_i(t)}{dt} = a(x_i(t), t), \tag{2.18}$$

$$\frac{dw_i(t)}{dt} + a_0(x_i(t), t)w_i(t) = 0, \tag{2.19}$$

for $i = 1, \ldots, N$.

For the full proof of this statement, we refer the reader to Chertock (2017). Let us, however, give a sketch of the proof here.

First, we substitute the form of the particle solution (2.14) into the weak form of

the PDE (2.17), as follows

$$-\sum_{i=0}^{N} w_i(0)\varphi(x_i(0),0) - \sum_{i=0}^{N}\int_0^T w_i(t)[\partial_t\varphi(x_i(t),t) + a(x_i(t),t)\cdot\nabla\varphi(x_i(t),t)]\mathrm{d}t + \sum_{i=0}^{N}\int_0^T w_i(t)a_0(x_i(t),t)\varphi(x_i(t),t)\mathrm{d}t = 0. \quad (2.20)$$

Using integration by parts, and the fact that the convective derivative of the test function φ is given by

$$\frac{d\varphi(x_i(t),t)}{dt} = \partial_t\varphi(x_i(t),t) + \frac{dx_i(t)}{dt}\cdot\nabla\varphi(x_i(t),t), \quad (2.21)$$

we can finally arrive at the following:

$$\sum_{i=0}^{N}\int_0^T w_i(t)\left[\frac{dx_i(t)}{dt} - a(x_i(t),t)\right]\cdot\nabla\varphi(x_i(t),t)\mathrm{d}t + \sum_{i=0}^{N}\int_0^T\left[\frac{dw_i(t)}{dt} + a_0(x_i(t),t)w_i(t)\right]\varphi(x_i(t),t)\mathrm{d}t = 0. \quad (2.22)$$

As the above holds for all test functions $\varphi \in C_c^1(\mathbb{R}^d\times[0,T)$, we have that the particle solution with particles and weights evolved by (2.18), (2.19) is a weak solution, as required.

Finally, we observe from Equation (2.19) that we can consider the particle weights to be constant in time for a problem where $a_0 = 0$.

2.2.1 Regularisation approaches

We have now seen how a discrete particle solution in the form of (2.14) can be obtained via a deterministic particle method approach. In some cases, however, it may be desirable to have a smoother representation of the solution, either for evaluation of the solution point-wise or if the PDE in question requires higher-order regularity than that of the particle solution. In such instances, a common technique is to adopt a convolution-based regularisation approach.

Here, the particle solution is modified as follows:

$$u_h^\varepsilon(x,t) := (u_h(\cdot,t) * \zeta_\varepsilon(\cdot))(x) = \sum_{i=1}^{N} w_i(t)\zeta_\varepsilon(x - x_i(t)), \quad (2.23)$$

where $*$ represents convolution, $u_h(x,t)$ is the particle solution of (2.14), and $\zeta_\varepsilon(x)$,

referred to as the mollifier, satisfies the following properties:

$$\zeta_\varepsilon(x) = \frac{1}{\varepsilon^d}\zeta\left(\frac{x}{\varepsilon}\right), \qquad \int_{\mathbb{R}^d} \zeta(x)\mathrm{d}x = 1. \tag{2.24}$$

Here, ε acts as a parameter that controls the size of the mollifier.

Such regularisation methods are often used when considering particle methods for PDEs that require high-order regularity, including collision operators. The work of Carrillo *et al.* (2020) uses exactly this principle to smooth the particle solution, in order to be able to compute the required derivatives for the Landau collision operator.

While mollification in this manner is a very natural extension of the particle method, there are some drawbacks to this type of regularisation as well. Primarily, the cost of computing the mollifier, and detecting where particles overlap, can be very high. There can be challenges from the point of view of implementation as well.

An alternative approach to regularisation is that of projection methods, which will be the type of regularisation used in this thesis, as computing a collision operator always requires a distribution function that is at least once-weakly differentiable. We now introduce projections in the context of regularising particle solutions.

2.2.2 Projection methods

Let us introduce projections directly in the context of collision operators, namely where we are considering a PDE as follows:

$$\partial_t f = C[f], \tag{2.25}$$

where $f(v,t)$ is the single-particle distribution function, and $C[f]$ is some collision operator (e.g. the Lenard-Bernstein or Landau operator, as introduced in Chapter 1). Importantly, let us consider an operator $C[f]$ that is a second-order differential operator in f, where we require a solution $f \in H^1$. In this case, a particle solution will not have sufficient regularity and some form of regularisation will be necessary.

Let us define our particle distribution function analogously to the particle solution in (2.14):

$$f_p(v,t) = \sum_{\alpha=1}^{N} w_\alpha \delta(v - v_\alpha(t)), \tag{2.26}$$

where $\{w_\alpha\}$ are the weights[2] and $\{v_\alpha(t)\}$ the particle velocities.

We introduce a second representation for the distribution function, mirroring a finite element solution as in (2.8):

$$f_s(v,t) = \sum_{j=1}^{M} f_j(t)\varphi_j(v), \tag{2.27}$$

where $\hat{f}(t) = [f_1(t), \cdots, f_M(t)]^T$ are the coefficients in this representation, and the basis $\{\varphi_j\}_{j=1}^M$ is chosen to have sufficient regularity for the collision operator $C[f]$ to be computed.

The key step in the projection method is then as follows. To obtain the coefficients $\hat{f}$, we relate the two representations of the distribution function by L^2 projection onto the basis $\{\varphi_j\}$, requiring weak equality as follows:

$$\langle f_s, \varphi_j \rangle = \langle f_p, \varphi_j \rangle, \quad j = 1, \ldots, M, \tag{2.28}$$

where

$$\begin{aligned}
\langle f_s, \varphi_j \rangle &= \int f_s(v,t)\varphi_j(v)dv = \sum_{i=1}^{M} \mathbb{M}_{ji} f_i, \\
\langle f_p, \varphi_j \rangle &= \int f_p(v,t)\varphi_j(v)dv = \sum_{\alpha : v_\alpha \in \Omega_{\varphi_j}} w_\alpha \varphi_j(v_\alpha),
\end{aligned}$$

and $\mathbb{M}_{ij} = \int \varphi_i(v)\varphi_j(v)\mathrm{d}v$ are the elements of the mass matrix $\mathbb{M}$ of the basis. Here, the notation $\sum_{\alpha : v_\alpha \in \Omega_{\varphi_j}}$ signifies that we only sum over the particles which are in the support of the basis function φ_j. Thus, the coefficients of the projected distribution function are computed as follows:

$$f_i(v_1(t), \ldots, v_N(t)) = \sum_{k=1}^{M} \mathbb{M}^{-1}_{ik} \sum_{\alpha : v_\alpha \in \Omega_{\varphi_k}} w_\alpha \varphi_k(v_\alpha). \tag{2.29}$$

Here, it is important to note that these coefficients $\hat{f}$ are *not* independent degrees of freedom but instead, they are computed from the particle velocities themselves. As functions of the particle velocities, the coefficients can be differentiated with respect

[2] In all the work in this thesis, we will consider weights that stay constant in time.

to individual particle velocities, v_β:

$$\frac{\partial f_i}{\partial v_\beta} = \sum_{k:v_\beta \in \Omega_{\varphi_k}} \mathbb{M}^{-1}_{ik} w_\beta \nabla \varphi_k(v_\beta). \tag{2.30}$$

There are several advantages to this approach to regularising a particle solution. The first is that the number of coefficients in the projected representation (2.27) is usually significantly smaller than the number of particles, i.e. $M \ll N$. Secondly, the projection itself is fairly cheap to compute as it only requires the solution of a linear system of equations. Additionally, the matrix is time independent (as it is simply the mass matrix for the chosen basis) and so does not require re-computation in different timesteps. The projected solution can also be evaluated anywhere in the domain.

As mentioned, in the case of time-dependent PDEs, the described methods can be used to produce a spatial, or semi-, discretisation – a system of ODEs that is discrete in space but remains continuous in time. These ODEs can then be integrated in time with an appropriate choice of time integration methods. In the following section, we introduce the two main methods that will be used for this purpose in this thesis.

2.3 Time Integrators

In this section, we introduce two methods — the implicit midpoint method, and discrete gradients. The implicit midpoint scheme will be used in Chapter 3 to discretise the Lenard-Bernstein operator, while discrete gradients will be used to obtain time discretisations of the Landau operator in Chapter 4.

2.3.1 Implicit Midpoint

Let us consider an ODE of the form:

$$\dot{z}(t) = f(t, z), \qquad z(t_0) = z_0, \tag{2.31}$$

where $\dot{z} = dz/dt$, t_0 is the initial time, and z_0 the initial condition. Denote the step-size by h, the n-th timestep by $t_n = t_0 + nh$, and the computed solution at time t_n by z_n. The implicit midpoint scheme is then given by:

$$z_{n+1} = z_n + hf\left(t_n + \frac{h}{2}, \frac{z_n + z_{n+1}}{2}\right), \tag{2.32}$$

where $n = 0, 1, 2, \ldots$. The point $t_{n+1/2} = t_n + h/2$ is referred to as the midpoint.

The method is derived by considering an approximation of the time derivative as follows:

$$\frac{z(t+h) - z(t)}{h} = \dot{z}\left(t + \frac{h}{2}\right), \tag{2.33}$$

which combined with (2.31) becomes:

$$\frac{z(t+h) - z(t)}{h} = f\left(t + \frac{h}{2}, z\left(t + \frac{h}{2}\right)\right). \tag{2.34}$$

The final step to obtain the scheme is to approximate $z(t + h/2)$:

$$z\left(t + \frac{h}{2}\right) \approx \frac{z(t) + z(t+h)}{2}, \tag{2.35}$$

which is the midpoint of the line connecting $z(t)$ and $z(t + h)$. Together with the above equation, this gives us the implicit midpoint update rule in (2.32). The implicit midpoint method is a special case of a Gauss–Legendre Runge–Kutta method.

2.3.2 Discrete gradients

Another method for integrating ODEs is the discrete gradient method (Quispel & Turner 1996; McLachlan *et al.* 1999). It is an integral preserving technique, initially developed for Hamiltonian systems and others with first integrals, which can also be adopted to dissipative systems as shown below.

To illustrate, we begin with a system of ODEs in gradient form,

$$\dot{z} = G(z)\nabla S(z), \tag{2.36}$$

where $z \in \mathbb{R}^n$. Here, $G(z)$ can be a skew-symmetric matrix in the case of a Hamiltonian system, or a negative semi-definite symmetric matrix in the case of a dissipative one. In the case of a Hamiltonian system, or one with preserved first integrals in general, $S(z)$ is the preserved integral quantity. In the dissipative case, $S(z)$ is the dissipated quantity. The system of ODEs is then approximately solved by the following equation:

$$\frac{z_{n+1} - z_n}{h} = \tilde{G}(z_n, z_{n+1})\bar{\nabla} S(z_n, z_{n+1}), \tag{2.37}$$

where $\bar{\nabla} S(z_n, z_{n+1})$ is known as the discrete gradient, and $\tilde{G}(z_n, z_{n+1})$ is a matrix

such that $\tilde{G}(z_n, z_{n+1}) \to G(z_n)$ in the limit $z_{n+1} \to z_n$ as $h \to 0$. The discrete gradient, $\bar{\nabla} S(z_n, z_{n+1})$, satisfies the following two properties:

$$(z_{n+1} - z_n) \cdot \bar{\nabla} S(z_n, z_{n+1}) = S(z_{n+1}) - S(z_n), \tag{2.38a}$$

$$\bar{\nabla} S(z_n, z_n) = \nabla S(z_n). \tag{2.38b}$$

One such discrete gradient is the one by Gonzalez (1996), also known as the midpoint discrete gradient:

$$\begin{aligned} \bar{\nabla} S(z_n, z_{n+1}) = \nabla S(z_{n+1/2}) \\ + (z_{n+1} - z_n) \frac{S(z_{n+1}) - S(z_n) - (z_{n+1} - z_n) \cdot \nabla S(z_{n+1/2})}{|z_{n+1} - z_n|^2}, \end{aligned} \tag{2.39}$$

where $z_{n+1/2} = (z_n + z_{n+1})/2$ is the midpoint. The extra terms in this expression, compared to the implicit midpoint method, ensure the energy conservation / entropy dissipation properties of this scheme.

We can demonstrate the conserving properties of discrete gradients straightforwardly. From Equation (2.38), we have that:

$$S(z_{n+1}) - S(z_n) = (z_{n+1} - z_n) \cdot \bar{\nabla} S(z_n, z_{n+1}). \tag{2.40}$$

Using the discrete gradient update rule (2.37), this becomes:

$$S(z_{n+1}) - S(z_n) = h \bar{\nabla} S(z_n, z_{n+1}) \tilde{G}(z_n, z_{n+1}) \bar{\nabla} S(z_n, z_{n+1}). \tag{2.41}$$

As the matrix $\tilde{G}$ is antisymmetric if G is antisymmetric (for an energy conserving system), we have:

$$S(z_{n+1}) - S(z_n) = 0. \tag{2.42}$$

Alternatively, for a dissipative system, we have that $\tilde{G}$ is negative (or positive) semi-definite and so we have:

$$S(z_{n+1}) - S(z_n) \leq 0, \tag{2.43}$$

i.e. S is monotonically dissipated in time by construction.

Chapter 3

Discretisation of the Lenard-Bernstein operator

In this chapter, a discretisation of the conservative Lenard-Bernstein collision operator (1.50) is constructed based on a deterministic particle method approach. A projection method is used to regularise the particle solution. The scheme is shown to satisfy energy and momentum conservation semi-discretely, and in time using the implicit midpoint scheme. Numerical results are shown in 1D to demonstrate the aforementioned properties and the validity of the method. This section is based on our published article in the Journal of Plasma Physics, "A structure-preserving particle discretisation for the Lenard-Bernstein collision operator" (Jeyakumar *et al.* 2024*a*).

3.1 Semi-discrete operator

In order to discretise the conservative Lenard-Bernstein operator in velocity-space, we need to introduce a second representation of the distribution function. The particle-representation with Dirac delta distributions, which is usually used to solve the ideal part, is not differentiable and thus cannot be used to evaluate the collisional part. Previous works regularised the collision operator by using finite sized particles (Carrillo *et al.* (2020); Hirvijoki (2021)). Here, we explore a different approach based on finite element or spline spaces of sufficient regularity, following the projection methods discussed in Section 2.2.2.

The particle distribution function is given by

$$f_p(v,t) = \sum_\alpha w_\alpha \delta(v - v_\alpha(t)), \tag{3.1}$$

where $\{v_\alpha(t)\}_{\alpha=1}^N$ are the particle velocities which evolve over time, where N is the number of particles. As the particle distribution function f_p is non-differentiable,

we use an L^2 projection of f_p onto a set of differentiable basis functions $\{\varphi_j\}_{j=1}^M$ for $M \ll N$ as follows:

$$f_s(v,t) = \sum_i \varphi_i(v) f_i(t) = \sum_{i,j} \varphi_i(v)\, \mathbb{M}_{ij}^{-1} \sum_\alpha w_\alpha \varphi_j(v_\alpha(t)), \tag{3.2}$$

where $\{f_i(t)\}$ are the coefficients of the projected distribution function, f_s, expressed in the basis $\{\varphi_i\}$, and $\mathbb{M}_{ij} = \int \varphi_i \varphi_j \mathrm{d}x$ are the elements of the corresponding mass matrix $\mathbb{M}$. The projected representation of the distribution function, $f_s(v)$, will be used as an auxiliary representation for the evaluation of the collision operator where differentiability is required. This type of projection also offers the benefit of smoothing the solution for appropriately-chosen basis functions $\{\varphi_j\}$. We note that Equation (3.1) remains the primary representation of the distribution function in our method, and that Equation (3.2) is only used in order to satisfy the differentiability requirements of the collision operator.

To construct the semi-discretisation of the conservative Lenard-Bernstein operator, we return to its form in Equation (1.50). We will discretise this equation first, and then derive the discrete coefficients A_1 and A_2 in terms of the discrete momentum and energy densities.

To discretise the conservative collisional dynamics,

$$\frac{\partial f}{\partial t} = \nu \frac{\partial}{\partial v} \cdot \left(\frac{\partial f}{\partial v} + A_1 f + A_2 v f \right), \tag{3.3}$$

we apply a deterministic particle method (as introduced in Section 2.2). Typically, deterministic particle methods are formulated for first order transport-type problems. They can, however, be adapted to the context of diffusion problems as shown by Degond & Mustieles (1990). Following this approach, we rewrite Equation (3.3):

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial v}\left(a(v,f) f\right) = 0, \quad a(v,f) = -\nu \left(\frac{1}{f} \frac{\partial f}{\partial v} + A_1 + A_2 v \right). \tag{3.4}$$

This equation is approximately solved in terms of the particle distribution function (3.1), where the particle velocities $\{v_\alpha\}$ satisfy the following ordinary differential equations:

$$\dot{v}_\alpha = a(v_\alpha, f) = -\nu \left(\frac{1}{f(v_\alpha)} \frac{\partial f}{\partial v}(v_\alpha) + A_1 + A_2 v_\alpha \right). \tag{3.5}$$

Let us note that the first term on the right-hand side is not well defined if the

distribution function f is replaced by its particle representation f_p. Therefore, we will use the projection shown in Equation (3.2) instead and replace both instances of the distribution function f with the projected distribution function f_s to arrive at the following equation:

$$\dot{v}_\alpha = a(v_\alpha, f_s) = -\nu \left(\frac{1}{f_s(v_\alpha)} \frac{\partial f_s}{\partial v}(v_\alpha) + A_1 + A_2 v_\alpha \right). \tag{3.6}$$

The final step in obtaining the semi-discrete system of equations is to compute the coefficients A_1 and A_2. In analogy to the continuous case as described in Section 1.4.1, A_1 and A_2 are determined by requiring conservation of the discrete momentum and energy[1]:

$$\frac{d}{dt} \sum_\alpha w_\alpha v_\alpha = -\nu \sum_\alpha w_\alpha \left[\frac{1}{f_s(v_\alpha)} \frac{\partial f_s}{\partial v}(v_\alpha) + A_1 + A_2 v_\alpha \right] = 0, \tag{3.7}$$

$$\frac{1}{2} \frac{d}{dt} \sum_\alpha w_\alpha v_\alpha^2 = -\nu \sum_\alpha w_\alpha \left[\frac{v_\alpha}{f_s(v_\alpha)} \frac{\partial f_s}{\partial v}(v_\alpha) + A_1 v_\alpha + A_2 v_\alpha^2 \right] = 0. \tag{3.8}$$

Upon introduction of the discrete mass, momentum, and energy densities,

$$n_h(v_\alpha) = \sum_\alpha w_\alpha, \quad n_h u_h(v_\alpha) = \sum_\alpha w_\alpha v_\alpha, \quad n_h \varepsilon_h(v_\alpha) = \sum_\alpha w_\alpha v_\alpha^2, \tag{3.9}$$

we obtain a linear system of equations which can be solved to find the discrete A_1, A_2:

$$\begin{aligned} A_1 n_h + A_2 n_h u_h &= -\sum_\alpha w_\alpha \frac{f_s'(v_\alpha)}{f_s(v_\alpha)}, \\ A_1 n_h u_h + A_2 n_h \varepsilon_h &= -\sum_\alpha w_\alpha v_\alpha \frac{f_s'(v_\alpha)}{f_s(v_\alpha)}. \end{aligned} \tag{3.10}$$

The solution to this linear system is as follows:

$$\begin{aligned} A_1 &= \frac{1}{n_h \varepsilon_h - n_h u_h^2} \sum_\alpha w_\alpha (u_h v_\alpha - \varepsilon_h) \frac{f_s'(v_\alpha)}{f_s(v_\alpha)}, \\ A_2 &= \frac{1}{n_h \varepsilon_h - n_h u_h^2} \sum_\alpha w_\alpha (u_h - v_\alpha) \frac{f_s'(v_\alpha)}{f_s(v_\alpha)}. \end{aligned} \tag{3.11}$$

We note that these quantities implicitly depend on time through their dependence on the particle velocities $\{v_\alpha(t)\}$, and so must be recomputed at every timestep.

[1]Here, we have chosen to preserve the discrete moments in the particle basis but it is also possible to derive a different scheme by imposing the conservation conditions on the projected moments.

We also note that in order for the projection to preserve the moments of the distribution function, it is sufficient that the functions $\{1, v, v^2\}$ are contained in $span\{\varphi_j\}$. This can be demonstrated by considering the example of conservation of mass, which requires:

$$\int 1 f_p \mathrm{d}v = \int 1 f_s \mathrm{d}v. \tag{3.12}$$

To show this holds, we begin from the condition used to construct the projection:

$$\int \varphi_j f_p \mathrm{d}v = \int \varphi_j f_s \mathrm{d}v, \quad \forall j \in 1, \ldots, M. \tag{3.13}$$

Let $1 \in span\{\varphi_j\}$. Then, there exists a set of coefficients $\{c_j\}$ such that $1 = \sum_j c_j \varphi_j$. Multiplying both sides of (3.13) with the corresponding c_j and summing over j, we have:

$$\sum_j c_j \int \varphi_j f_p \mathrm{d}v = \sum_j c_j \int \varphi_j f_s \mathrm{d}v, \tag{3.14}$$

which by linearity of the integral becomes:

$$\int \sum_j c_j \varphi_j f_p \mathrm{d}v = \int \sum_j c_j \varphi_j f_s \mathrm{d}v. \tag{3.15}$$

Since we have that $1 = \sum_j c_j \varphi_j$, we then have that

$$\int 1 f_p \mathrm{d}v = \int 1 f_s \mathrm{d}v, \tag{3.16}$$

which is the required condition for mass conservation. Momentum and energy conservation follow similarly from requiring the functions v and v^2 to be in the span of basis $\{\varphi_j\}$. We note that the spline basis chosen in the numerical implementation, as detailed in Section 3.3, satisfies this property since it is a cubic basis.

We remark that at this time, a proof of monotonic entropy dissipation for the semi-discrete Lenard-Bernstein operator remains elusive. We have, however, numerically demonstrated that our discretisation maintains this property in Section 3.3.

3.2 Time discretisation

In this chapter, we describe the temporal discretisation of the system of ODEs (3.6) by the implicit midpoint scheme (as introduced in Section 2.3), which is a possible choice for a method that maintains the discrete conservation laws exactly (up to machine-precision). Let us start by introducing some notation. Denote by h a single timestep, by $t_n = t_0 + nh$ the time after the n-th timestep, and by $v_\alpha^n \approx v_\alpha(t_n)$

the corresponding particle velocity. Further, let $v_\alpha^{n+1/2} = (v_\alpha^n + v_\alpha^{n+1})/2$ be the particle velocity at the midpoint and, following Equation (3.2), denote the spline representation of the distribution function at the midpoint by

$$f_s^{n+1/2}(v) = \sum_{i,j} \varphi_i(v) \mathbb{M}_{ij}^{-1} \sum_\alpha w_\alpha \varphi_j(v_\alpha^{n+1/2}). \tag{3.17}$$

With this, the implicit midpoint scheme for the system (3.6) can be written as follows:

$$v_\alpha^{n+1} = v_\alpha^n + ha\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right). \tag{3.18}$$

In order to verify conservation of the total momentum, let us consider the particle momentum at the $n+1$-th timestep:

$$\begin{aligned}
\sum_\alpha w_\alpha v_\alpha^{n+1} &= \sum_\alpha w_\alpha \left[v_\alpha^n + ha\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)\right], \\
&= \sum_\alpha w_\alpha v_\alpha^n + h \sum_\alpha w_\alpha a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right), \\
&= \sum_\alpha w_\alpha v_\alpha^n - h\nu \sum_\alpha w_\alpha \left[\frac{1}{f_s^{n+1/2}} \frac{\partial f_s^{n+1/2}}{\partial v}\left(v_\alpha^{n+1/2}\right) + A_1 + A_2 v_\alpha^{n+1/2}\right].
\end{aligned} \tag{3.19}$$

We observe that the sum in the second term of this equation is exactly given by the left-hand side of Equation (3.7), evaluated at $v_\alpha^{n+1/2}$, and so is equal to zero as (3.7) is satisfied for all times in the scheme by construction. Thus, the particle momentum is conserved exactly by the implicit midpoint scheme.

A similar result can be demonstrated for the total particle energy. At the $n+1$-th timestep, we have:

$$\begin{aligned}
\sum_\alpha w_\alpha \left(v_\alpha^{n+1}\right)^2 &= \sum_\alpha w_\alpha \left[v_\alpha^n + ha\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)\right]^2, \\
&= \sum_\alpha w_\alpha (v_\alpha^n)^2 + h^2 \sum_\alpha w_\alpha a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)^2 \\
&\quad + 2h \sum_\alpha w_\alpha v_\alpha^n a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right).
\end{aligned} \tag{3.20}$$

Now, we split the last term and replace one v_α^n by using the implicit midpoint rule,

i.e. $v_\alpha^n = v_\alpha^{n+1} - ha\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)$ to obtain the following:

$$\begin{aligned}
&2h\sum_\alpha w_\alpha v_\alpha^n a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) \\
&\quad = h\sum_\alpha w_\alpha v_\alpha^n a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) + h\sum_\alpha w_\alpha v_\alpha^n a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) \\
&\quad = h\sum_\alpha w_\alpha v_\alpha^n a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) \\
&\qquad + h\sum_\alpha w_\alpha \left[v_\alpha^{n+1} - ha\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)\right] a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) \\
&\quad = h\sum_\alpha w_\alpha \left(v_\alpha^n + v_\alpha^{n+1}\right) a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right) - h^2\sum_\alpha w_\alpha a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right)^2 . \quad (3.21)
\end{aligned}$$

The last term in this equation cancels the second term on the right-hand side of (3.20), and we are left with:

$$\sum_\alpha w_\alpha \left(v_\alpha^{n+1}\right)^2 = \sum_\alpha w_\alpha \left(v_\alpha^n\right)^2 + 2h\sum_\alpha w_\alpha v_\alpha^{n+1/2} a\left(v_\alpha^{n+1/2}, f_s^{n+1/2}\right). \quad (3.22)$$

The second term on the right-hand side of (3.22) equals the expression in (3.8) evaluated at the midpoint $v_\alpha^{n+1/2}$, and therefore is zero. Thus, the particle energy is preserved exactly in time.

3.3 Numerical results

In this chapter, we present numerical experiments for the one-dimensional conservative Lenard-Bernstein operator using B-spline basis functions of arbitrary order for projecting the particle distribution function. The implementation is based on the Julia programming language (Bezanson *et al.* 2017), and the package is available publicly (Kraus *et al.* 2023).

3.3.1 Convergence of the semi-discrete operator

We demonstrate convergence properties of the semi-discretisation under projection onto a B-spline basis and particle sampling. First, we verify that the semi-discretisation indeed preserves the Maxwellian as an equilibrium solution under projection. To this end, we compute the projection of an exact Maxwellian onto the spline basis as follows:

$$\int \sum_j f_j \varphi_j(v)\varphi_i(v)\mathrm{d}v = \int f_M(v)\varphi_i(v)\mathrm{d}v, \quad (3.23)$$

where f_j are the coefficients of the spline for which we are solving, and $f_M(v) = 1/\sqrt{2\pi}\exp(-v^2/2)$ is the Maxwellian of mean $\mu = 0$ and variance $\sigma^2 = 1$. Rearranging this expression, we obtain the following spline coefficients for the projected Maxwellian:

$$f_j = \mathbb{M}_{ij}^{-1} \int f_M(v)\varphi_i(v)\mathrm{d}v, \tag{3.24}$$

where $\mathbb{M}_{ij} = \int \varphi_i\varphi_j \mathrm{d}v$ are the elements of the mass matrix $\mathbb{M}$ as before. The spline-projected representation of the Maxwellian distribution $f_M(v)$ is then given by $f_{s,M}(v) = \sum_j f_j\varphi_j(v)$ with the coefficients f_j from (3.24). We use this projected Maxwellian to compute the right-hand side of Equation (3.6), as follows

$$\dot{v}_\alpha = -\nu\left(\frac{1}{f_{s,M}(v_\alpha)}\frac{\partial f_{s,M}}{\partial v}(v_\alpha) + A_1 + A_2 v_\alpha\right), \tag{3.25}$$

where the coefficients A_1 and A_2 are computed using the projected Maxwellian distribution $f_{s,M}$ in (3.11). The L^2 norm of the time derivative of the particle velocities, $\|\dot{v}_\alpha\|_2$, can then be used to check if the Maxwellian is an equilibrium solution under projection, as this norm should approach zero with increasing spline resolution in such case. We compute this quantity for a range of spline resolutions, using a sample of $N = 100,000$ particles from a normal distribution where the sample is strictly used for evaluation of Equation (3.25) and never for projection. Figure 3.1 shows the convergence of $\|\dot{v}_\alpha\|_2$ with an increasing number of splines, computed using cubic spline basis functions. As expected, the norm of the time derivative approaches zero with an increasing number of splines at a rate which corresponds to the order of the splines used (cubic splines have order $k = 4$).

Secondly, we demonstrate convergence of the semi-discretisation under particle sampling. Here, we instead compute the sample variance of the particle velocity time derivatives, i.e. $\sum \dot{v}_\alpha^2/N$, keeping the spline resolution fixed and varying the number of particles in the sample. We directly project the particles to compute the spline representation of f, as per Equations (3.2) and (3.6). The results of this are shown in Figure 3.2, and we observe that the sample variance converges at a rate slightly above $1/N$, which is the expected convergence rate for the sample variance generated by statistical sampling methods.

These two results demonstrate that the Maxwellian distribution remains an equilibrium solution under semi-discretisation, and the method demonstrates the expected convergence properties with both number of splines and particles.

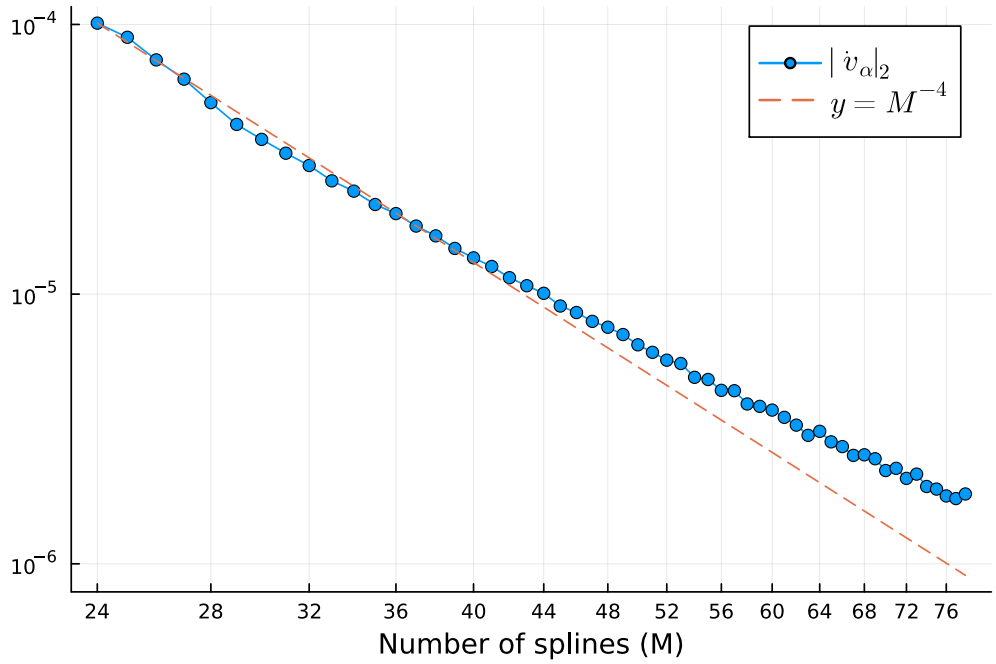

Figure 3.1: Convergence of the L^2 norm of the particle velocity gradient, $\|\dot{v}_\alpha\|_2$, when computed using a true Maxwellian f, against the number of splines. The dashed line shows the reference curve $y = x^{-4}$.

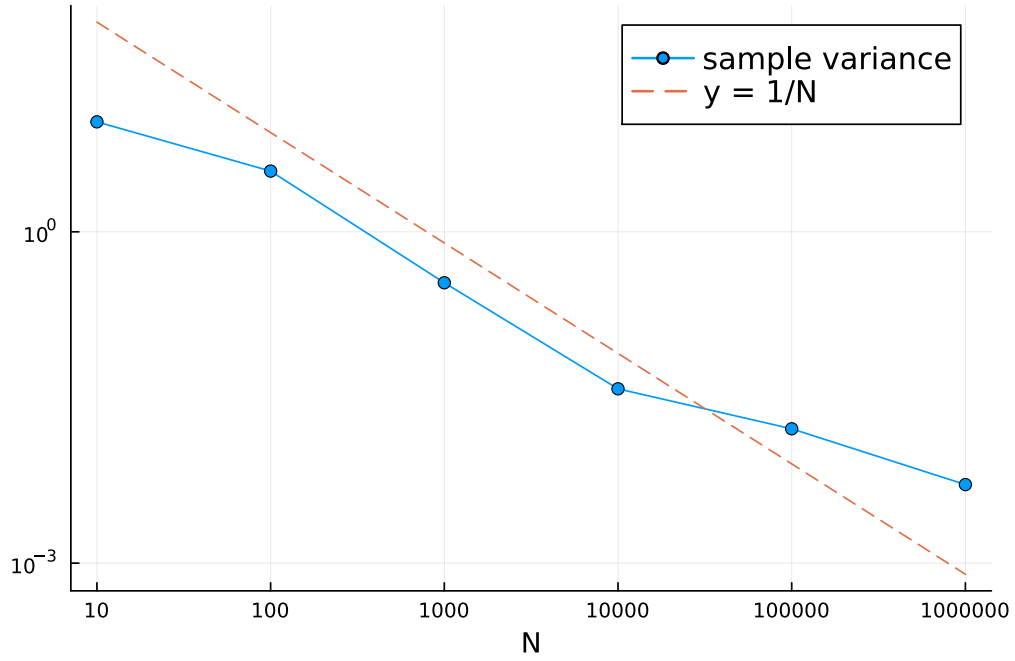

Figure 3.2: Convergence of the sample variance of the particle velocity time derivative, $\sum \dot{v}_\alpha^2/N$, with the number of particles, shown on a logarithmic scale. The dashed line represents the reference curve $y = 1/N$.

3.3.2 Relaxation of a shifted normal distribution

In the first example, we initialise the distribution function with a standard normal distribution shifted to the right by $\mu = 2$, obtaining a distribution with mean $\mu = 2$ and variance $\sigma^2 = 1$ as shown in the following equation:

$$f(v, t = 0) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(v-2)^2}. \tag{3.26}$$

The particles are then initialised by independently and identically (iid) sampling from this distribution, for $N = 1000$ particles. The spline distribution is initialised by L^2 projecting the initial particle distribution onto the spline basis, with the spline coefficients computed as per Equation (3.2). A cubic-spline basis of 41 elements is used, with equally spaced knots on the velocity domain $v \in [-10, 10]$. The time integration is performed using the implicit midpoint scheme, which is of second order. A time-step of $h = 8 \times 10^{-4}$ and a collision frequency of $\nu = 1$ is used. The simulation was run until a final normalised time of $t = 1$, corresponding to 1250 timesteps.

In the initial condition, shown on the left of Figure 3.3, we observe slight variations in the spline-projected distribution function due to the sampling error of the particles. In the final distribution, we observe the expected behaviour of the projected distribution approaching an exact normal with the initial variations smoothed out, and due to the momentum conservation, the mean of the distribution stays at the same value ($v = 2$). Here, the particle momentum and the energy are conserved up to machine precision. The evolution of the energy and momentum error are shown in Figure 3.4. The evolution of the entropy, $S = \int f_s \log f_s dv$, is shown in Figure 3.5 (normalised by the magnitude of its initial value), and we observe the monotonic dissipation of the entropy over the course of the simulation as expected.

We also observe that the method works well even for small numbers of particles. Results for the same simulation using a sample of $N = 200$ particles instead are shown in Figure 3.6. The particle energy and momentum are again conserved up to machine precision in relative error, with similar behaviour as shown in Figure 3.4.

3.3.3 Relaxation of a bi-Maxwellian distribution

Next, we consider a double Maxwellian distribution as the initial condition. Each peak is a standard normal distribution which has been shifted from the origin by

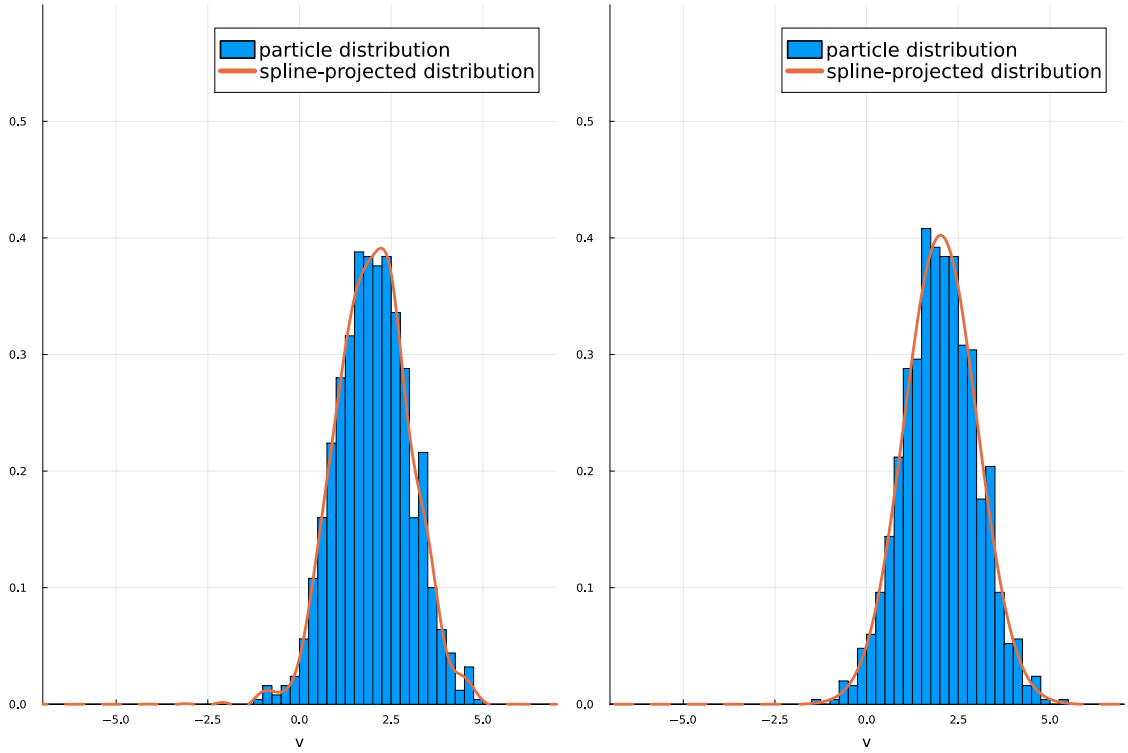

Figure 3.3: The initial and final distributions when the initial condition is chosen to be a normal distribution of mean $\mu = 2$ and variance $\sigma^2 = 1$, for a sample of $N = 1000$ particles.

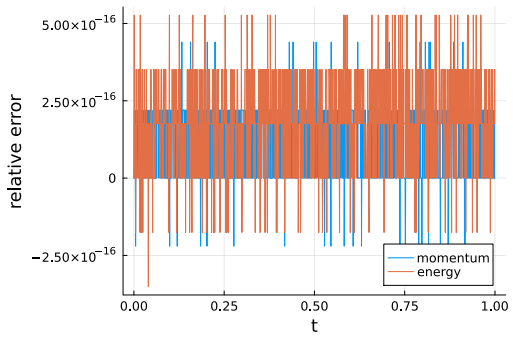

Figure 3.4: Energy and momentum conservation during the simulation, for the initial condition of a shifted normal distribution

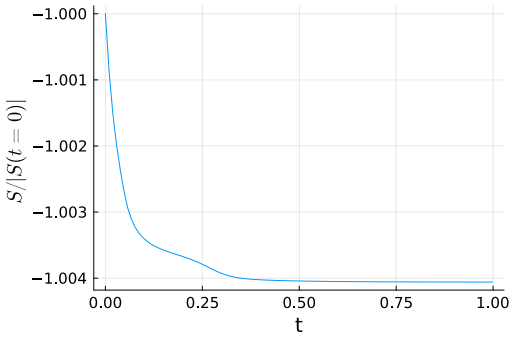

Figure 3.5: Evolution of the normalised entropy, i.e. $S/|S(t = 0)|$ where $S = \int f_s \log f_s dv$, during the simulation

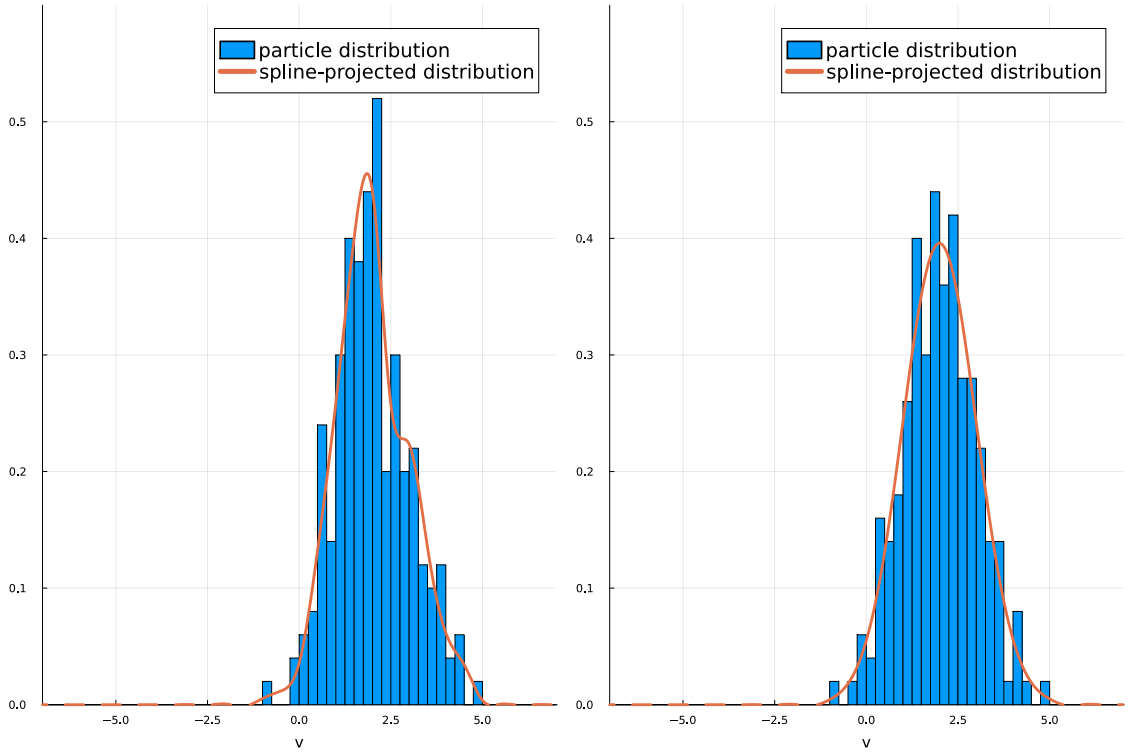

Figure 3.6: The initial and final distributions when the initial condition is chosen to be a normal distribution of mean $\mu = 2$ and variance $\sigma^2 = 1$, for a sample of $N = 200$ particles.

$v = \pm 2$ as per the following equation:

$$f(v, t = 0) = \frac{1}{\sqrt{2\pi}} \left(e^{-\frac{1}{2}(v-2)^2} + e^{-\frac{1}{2}(v+2)^2} \right), \tag{3.27}$$

and the sampled distribution is shown in Figure 3.7 on the left. The sample for the particle distribution function is again of size $N = 1000$ particles. We use the identical numerical setup as the previous example, in particular the same time-step of $h = 8 \times 10^{-4}$ and the same collision frequency of $\nu = 1$. The final distribution obtained after time integration until $t = 5$ is shown in Figure 3.7 on the right. Again, the equilibrated distribution is a Gaussian with equal mean and variance to the initial condition. The particle energy is conserved up to machine precision in relative error. The particle momentum is conserved up to a relative error on the order of 10^{-14}. The behaviour of the two quantities over time is oscillatory and similar to Figure 3.4. The normalised entropy also decreases monotonically in time, and this is illustrated in Figure 3.8.

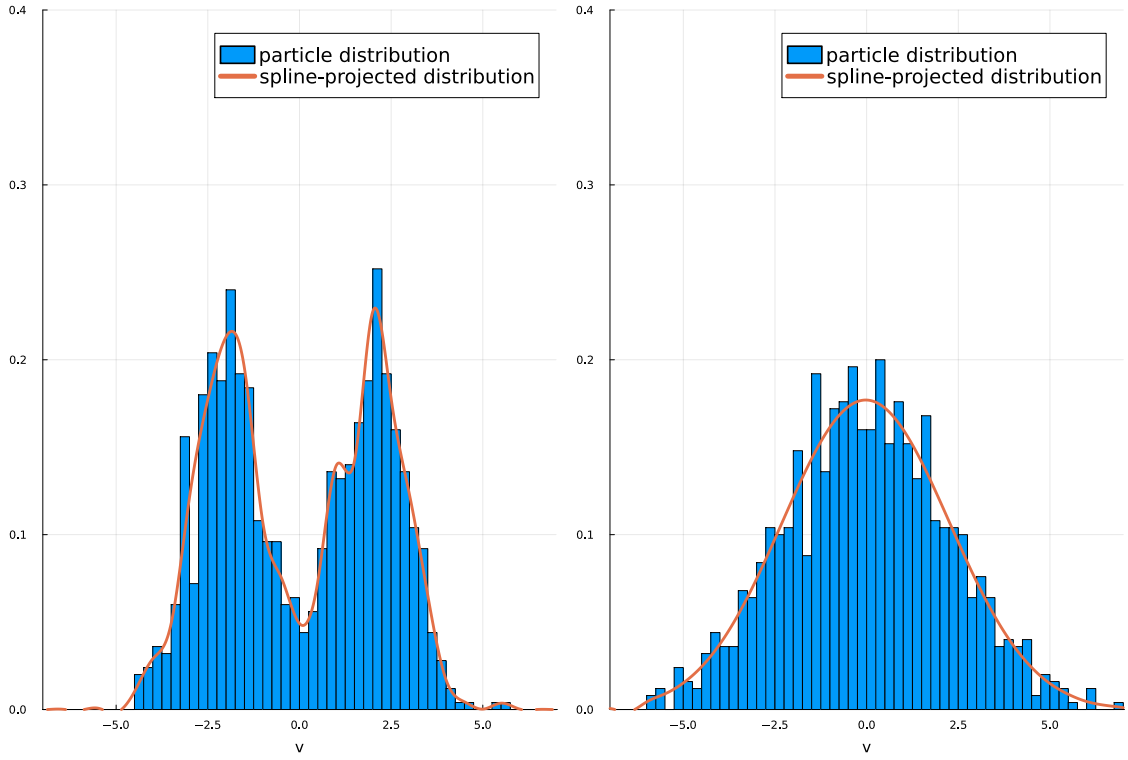

Figure 3.7: The initial and final distribution functions when the initial condition is chosen to be a bi-Maxwellian, in both particle and spline bases, for $N = 1000$ particles.

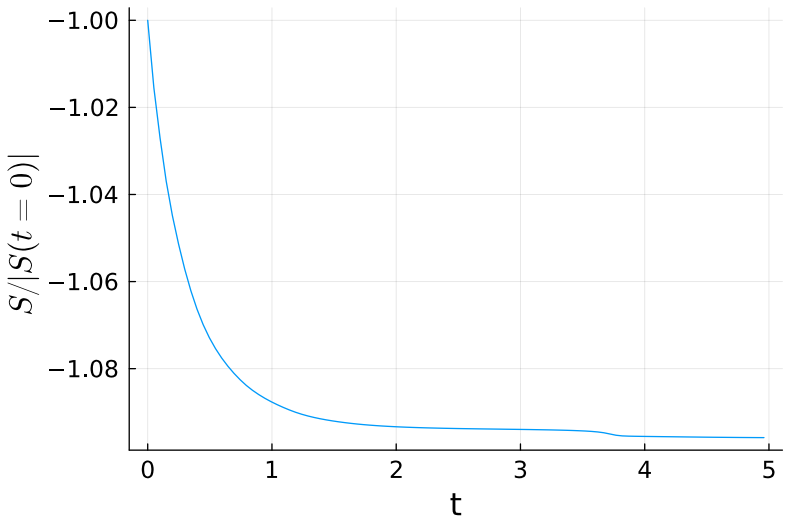

Figure 3.8: Evolution of the normalised entropy over the simulation, where the initial condition is a bi-Maxwellian.

3.3.4 Relaxation of a uniform distribution

In the last example, we initialise the distribution function with a uniform distribution shifted and scaled to the interval $v \in [-2, 2]$, i.e.:

$$f(v, t = 0) = \begin{cases} \frac{1}{4}, \text{ if } v \in [-2, 2], \\ 0, \text{ else.} \end{cases} \tag{3.28}$$

A sample of $N = 200$ particles is taken from this distribution. A timestep of $h = 1 \times 10^{-4}$ is used and the final integration time is $t = 1$. All other parameters are kept the same. Figure 3.9 shows the initial and final distributions obtained in the simulation, demonstrating again the expected result that the initial distribution relaxes to a normal distribution. The resultant particle distribution function retains the same mean up to a relative error on the order of 10^{-14} (which is equivalent to momentum being preserved at this level). The energy is preserved to a relative error on the order of 10^{-15}. The entropy decreases monotonically as expected and is illustrated in Figure 3.10. We note that the method performs as well here as it does in the other examples despite this being a more challenging case, as the uniform distribution is discontinuous and therefore not amenable to being represented using B-spline basis functions.

3.3.5 Remarks

It is important to ensure that the chosen velocity domain for a simulation is sufficiently large such that no particle leaves this domain at any time. There is no sensible method for returning a particle to the simulation domain, as the true velocity space domain for this problem is infinite. Practically, a particle leaving the domain will return zero when the spline projected distribution is evaluated on the particle's velocity, which leads to the evaluation of (3.6) becoming undefined due to division by zero.

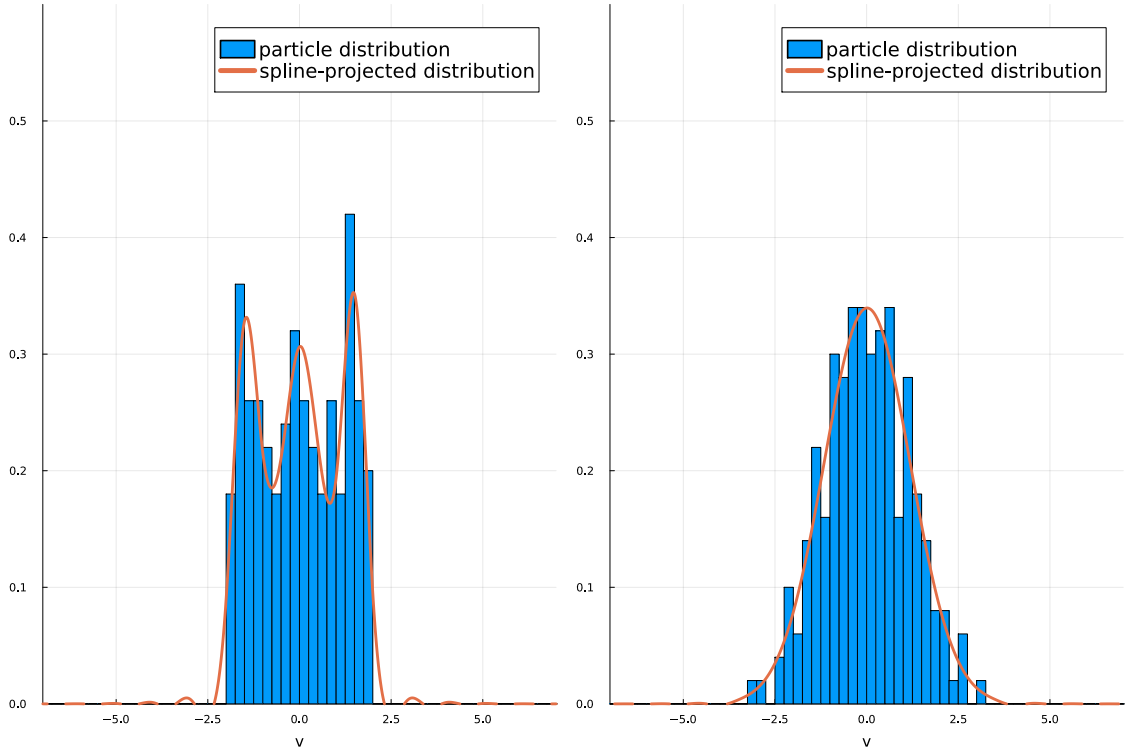

Figure 3.9: The initial and final distribution functions for the case of a uniform initial condition, with the initial condition shown on the left and the final result shown on the right. A sample of $N = 200$ particles is used.

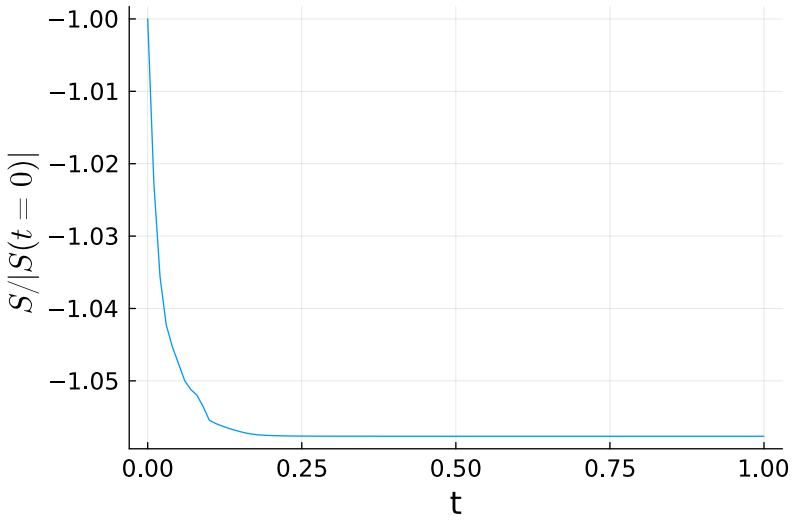

Figure 3.10: Evolution of the normalised entropy over the simulation, where the initial condition is a uniform distribution.

Chapter 4

Discretisation of the Landau operator

In this chapter, we present several different approaches for discretising the Landau collision operator (1.68) in a structure-preserving manner. That is, we are interested in solving the equation:

$$\partial_t f = C[f], \tag{4.1}$$

where

$$C[f] = \nu \frac{\partial}{\partial v} \cdot \int U(v, v') \left(f(v') \frac{\partial f}{\partial v} - f(v) \frac{\partial f}{\partial v'} \right) \mathrm{d}v', \tag{4.2}$$

$$U_{ij}(v, v') = \frac{1}{|v - v'|} \left(\delta_{ij} - \frac{(v_i - v_i')(v_j - v_j')}{|v - v'|^2} \right), \tag{4.3}$$

for the time-evolution of the single-particle distribution function, f, while preserving mass, momentum, and energy.

First, we present a direct discretisation of the equation using a deterministic particle method, following a similar approach to that used for the Lenard-Bernstein operator, as shown in Chapter 3. Then, we present two approaches for discretisation following the metriplectic approach.

Part of this chapter is based on our manuscript on the arXiv, "Structure-preserving particle methods for the Landau collision operator using the metriplectic framework" (Jeyakumar *et al.* 2024*b*).

4.1 Discretising using a deterministic particle method

Following the work of Chertock (2017), we begin by rewriting the equations in divergence form as follows:

$$\partial_t f - C[f] = \partial_t f + \frac{\partial}{\partial v} \cdot (a(v, f) f) = 0, \tag{4.4}$$

where

$$a(v, f) = -\int U(v, v') \left(\frac{f(v')}{f(v)} \frac{\partial f}{\partial v} - \frac{\partial f}{\partial v'} \right) \mathrm{d}v' \tag{4.5}$$

for $U(v, v')$ as defined in Equation (4.3).

Thus, we have that solutions to Equation (4.4) are given by:

$$f_p(v, t) = \sum_{\alpha} \delta(v - v_\alpha(t)), \tag{4.6}$$

where the particle velocities, $\{v_\alpha\}$, satisfy the following ODEs

$$\dot{v}_\alpha = a(v_\alpha, f). \tag{4.7}$$

For the right-hand side, $a(v_\alpha, f)$, to be well-defined, we require a representation of f such that $\partial f / \partial v$ is well-defined. Thus, we follow the same approach as shown in Chapter 3 to define a projected distribution function:

$$f_s(v, t) = \sum_j f_j(t) \varphi_j(v) = \sum_{i,j} \mathbb{M}^{-1}_{ij} \sum_{\alpha} w_\alpha \varphi_i(v_\alpha(t)) \varphi_j(v), \tag{4.8}$$

which is obtained via L^2 projection of f_p onto the basis $\{\varphi_j(v)\}$. The basis itself can be chosen to provide sufficient differentiability for the problem.

Using the projected distribution, f_s, we can now compute the equations of motion for the particle velocities as follows:

$$\dot{v}_\alpha = a(v_\alpha, f_s), \tag{4.9}$$

$$= -\int U(v_\alpha, v') \left[\frac{f_s(v')}{f(v_\alpha)} \frac{\partial f_s}{\partial v}(v_\alpha) - \frac{\partial f_s}{\partial v'}(v') \right] \mathrm{d}v'. \tag{4.10}$$

There is, however, one major issue with this discretisation and that is the fact that the integration in v' in the above equation must be performed for *each* particle individually, due to the coupling of v_α and v' by the tensor U. This is extremely

expensive, and thus not a viable approach to solving the problem.

As such, we turn to discretisations of the Landau operator via the metriplectic approach, and this is discussed in the following two sections.

4.2 Discretising the metric bracket directly

We discretise the Landau collision operator by discretising its metriplectic formulation using particles. This is to say that we do not discretise the dynamical equations as shown in the previous section, but instead we discretise the entropy and metric bracket and obtain discrete equations via the metriplectic approach detailed in Section 1.2. This approach consists of the following main steps: (a) discretising the distribution function, (b) discretising functionals, and (c) discretising functional derivatives, all of which will be detailed in the following.

4.2.1 Approximating the distribution function

The distribution function is represented by a collection of N macro-particles (Klimontovich representation):

$$f_p(v,t) = \sum_{\alpha=1}^{N} w_\alpha \delta(v - v_\alpha(t)), \tag{4.11}$$

where $v_\alpha(t) \in \mathbb{R}^d$ is the velocity of the α-th particle, w_α is its weight, and $d \in \{2,3\}$ is the number of velocity dimensions being considered.

This representation of the distribution function, however, does not allow for an immediate discretisation of the entropy functional (1.73) as the expression resulting from evaluating entropy $\mathcal{S}$ on the particle distribution f_p is not well-defined. To overcome this, we use a projection method as in Chapter 3 and adopt a projected distribution function as follows:

$$f_s(v,t) = \sum_i \varphi_i(v) f_i, \tag{4.12}$$

where $\{\varphi_i(v)\}_{i=1}^M$ are a set of differentiable basis functions with local/compact support in $\mathbb{R}^d$ and $\{f_i(v_1(t),\ldots,v_N(t))\}_{i=1}^M$ are the coefficients of the projected distribution function in this basis.

While it is not possible to evaluate the entropy (1.73) on the particle distribution function f_p, evaluation on the projected distribution function f_s poses no issues. This second representation of the distribution function can thus be seen as a method of

regularisation in a similar vein as previous works that used radial basis functions and similar methods to this end (Carrillo *et al.* 2020; Hirvijoki 2021).

4.2.2 Discrete functional derivatives

Following the metriplectic formulation, we will discretise the entropy functional and bracket separately, and then apply the discrete bracket to the discrete entropy to obtain the semi-discrete equations of motion. Discretising the metric bracket for the Landau operator (1.74) requires the discretisation of the functional derivatives appearing therein. This is facilitated by the observation that functionals of the distribution function, $\mathcal{A}[f]$, can be considered as functions of the particle velocities $V = \{v_\alpha\}_{\alpha=1}^{N}$, upon evaluation on the particle distribution f_p:

$$\mathcal{A}[f_p] = A(V). \tag{4.13}$$

By considering variations of both sides of this expression, we obtain an approximation of the functional derivatives of $\mathcal{A}[f_p]$ in terms of the function A as follows[1]. Starting with the left-hand side, variation and integration by parts gives,

$$\begin{aligned}
\delta\mathcal{A}[f_p] &= \int \frac{\delta\mathcal{A}}{\delta f}\,\delta f_p\,dv \\
&= -\sum_{a=1}^{N_p} w_a \int \frac{\delta\mathcal{A}}{\delta f}\,\nabla_v\delta\big(v - v_a(t)\big)\cdot\delta v_a\,dv \\
&= \sum_{a=1}^{N_p} w_a\,\nabla_v \frac{\delta\mathcal{A}}{\delta f}\bigg|_{v=v_a}\cdot\delta v_a.
\end{aligned} \tag{4.14}$$

Upon equating this expression with the variation of the right-hand side of (4.13), namely

$$\delta A(V) = \sum_{a=1}^{N_p} \frac{\partial A}{\partial v_a}\,\delta v_a, \tag{4.15}$$

[1]We note that, generally speaking, this approach to discretising the functional derivatives requires the functional being differentiated to be linear in the distribution function f. While, in theory, this may seem very restrictive, in practise, this choice has no impact on the type of "discrete functionals" on which the resulting bracket may be evaluated. Regardless of this ansatz, the discrete bracket will be applicable to any function of the discrete degrees of freedom, no matter if it depends linearly or nonlinearly on the degrees of freedom, and independently from how it is constructed, e.g. by evaluating a continuous functional on the particle distribution, f_p, or in some other way.

we obtain:

$$\frac{\partial A}{\partial v_\alpha} = w_\alpha \frac{\partial}{\partial v} \left.\frac{\delta \mathcal{A}}{\delta f}\right|_{v=v_\alpha}. \tag{4.16}$$

Evaluating the bracket of Equation (1.74) on the particle distribution from Equation (4.11), we obtain the following bracket on functionals:

$$(\mathcal{A}, \mathcal{B}) = \frac{1}{2} \sum_{\alpha,\beta} w_\alpha w_\beta \int \left(\frac{\partial \mathcal{A}_f}{\partial v} - \frac{\partial \mathcal{A}_{f'}}{\partial v'} \right) \delta(v - v_\alpha) U(v, v') \delta(v' - v_\beta) \left(\frac{\partial \mathcal{B}_f}{\partial v} - \frac{\partial \mathcal{B}_{f'}}{\partial v'} \right) dv dv', \tag{4.17}$$

for some functionals $\mathcal{A}, \mathcal{B}$. Using relation (4.16) to replace the functional derivatives $\mathcal{A}_f$, etc., we obtain the discrete bracket on *functions*:

$$(A, B)_h = \frac{1}{2} \sum_{\alpha,\beta} w_\alpha w_\beta \left(\frac{1}{w_\alpha} \frac{\partial A}{\partial v_\alpha} - \frac{1}{w_\beta} \frac{\partial A}{\partial v_\beta} \right) U(v_\alpha, v_\beta) \left(\frac{1}{w_\alpha} \frac{\partial B}{\partial v_\alpha} - \frac{1}{w_\beta} \frac{\partial B}{\partial v_\beta} \right), \tag{4.18}$$

where A, B are functions of the particle velocities $V = \{v_\alpha\}_{\alpha=1}^N$.

4.2.3 Discrete entropy

The remaining ingredient required for constructing the discrete collision operator is the entropy. The entropy functional (1.73) is not amenable to plain evaluation on the particle distribution f_p as the resulting expression is not well-defined. Thus, we evaluate the entropy functional (1.73) on the projected distribution function f_s instead, such that the discrete entropy becomes:

$$S_h = -\int f_s \log f_s \, dv = -\int \left(\sum_i \varphi_i(v) f_i \right) \log \left(\sum_j \varphi_j(v) f_j \right) \mathrm{d}xv. \tag{4.19}$$

Using this expression for entropy, we now compute its derivative with respect to the degrees of freedom (this will be required to apply the metric bracket to the entropy):

$$\frac{\partial S_h}{\partial v_\alpha} = -\int \left[\sum_i \frac{\partial f_i}{\partial v_\alpha} \varphi_i(v) \log \left(\sum_j \varphi_j(v) f_j \right) + \frac{\sum_i \varphi_i(v) f_i}{\sum_j \varphi_j(v) f_j} \sum_j \frac{\partial f_j}{\partial v_\alpha} \varphi_j(v) \right] \mathrm{d}xv, \tag{4.20}$$

where the derivative $\partial f_i / \partial v_\alpha$ is given by Equation (2.30). Simplifying the second

term and using Equation (2.30) to compute $\partial f_i/\partial v_\alpha$ gives us the following:

$$\begin{aligned}\frac{\partial S_h}{\partial v_\alpha} &= -\int \left[\sum_i \frac{\partial f_i}{\partial v_\alpha}\varphi_i(v)\log\left(\sum_j \varphi_j(v) f_j\right) + \sum_j \frac{\partial f_j}{\partial v_\alpha}\varphi_j(v)\right] \mathrm{d}xv, \\ &= -\int \left[\sum_{i,k} \mathbb{M}^{-1}_{ik} w_\alpha \nabla\varphi_k(v_\alpha)\varphi_i(v)\log\left(\sum_{j,l}\varphi_j(v)\mathbb{M}^{-1}_{jl}\sum_\beta w_\beta\varphi_l(v_\beta)\right)\right. \\ &\qquad \left. + \sum_{j,l}\mathbb{M}^{-1}_{jl} w_\alpha \nabla\varphi_l(v_\alpha)\varphi_j(v)\right] \mathrm{d}v. \end{aligned} \tag{4.21}$$

We define the following for convenience:

$$\mathbb{L}_k = \sum_i \mathbb{M}^{-1}_{ik}\int \varphi_i(v)\left[1+\log\left(\sum_j f_j\varphi_j(v)\right)\right]\mathrm{d}v. \tag{4.22}$$

Relabelling indices in (4.21) and using (4.22), we obtain our final expression for the derivative of the discrete entropy with respect to the degrees of freedom:

$$\frac{\partial S_h}{\partial v_\alpha} = -\sum_k w_\alpha \mathbb{L}_k \nabla\varphi_k(v_\alpha). \tag{4.23}$$

With this, we can now compute the collision contribution for a given particle, $\dot{v}_\gamma$, through the metric bracket.

4.2.4 Discrete collision operator

The discrete collisional dynamics are given by

$$\dot{v}_\gamma = -(v_\gamma, S_h)_h. \tag{4.24}$$

Upon inserting the expression of the discrete bracket (4.18) and the derivative of the entropy (4.23), we obtain:

$$\dot{v}_\gamma = \frac{1}{2}\sum_{\alpha,\beta} w_\alpha w_\beta \left(\frac{1}{w_\alpha}\delta_{\alpha\gamma} - \frac{1}{w_\beta}\delta_{\beta\gamma}\right) U(v_\alpha, v_\beta) \sum_k \mathbb{L}_k(\nabla\varphi_k(v_\alpha) - \nabla\varphi_k(v_\beta)), \quad (4.25)$$

$$= \frac{1}{2}\left[\sum_\beta w_\beta U(v_\gamma, v_\beta) \sum_k \mathbb{L}_k(\nabla\varphi_k(v_\gamma) - \nabla\varphi_k(v_\beta)) \right.$$

$$\left. - \sum_\alpha w_\alpha U(v_\alpha, v_\gamma) \sum_k \mathbb{L}_k(\nabla\varphi_k(v_\alpha) - \nabla\varphi_k(v_\gamma))\right], \quad (4.26)$$

$$= \sum_\alpha w_\alpha U(v_\gamma, v_\alpha) \sum_k \mathbb{L}_k(\nabla\varphi_k(v_\gamma) - \nabla\varphi_k(v_\alpha)). \quad (4.27)$$

Here, we obtain Equation (4.26) through separating the two Kronecker delta terms in (4.25) and contracting the appropriate indices. Equation (4.27) then comes from relabelling indices and recognising that the two sums in (4.26) are in fact identical by symmetry of the kernel $U(\cdot,\cdot)$. Equation (4.27) is the final semi-discretised system of equations.

For the purpose of discretising the system in time, it will be useful to rewrite the semi-discretised system of equations as a gradient system. To obtain this form, we rearrange Equation (4.25) as follows with the use of (4.23):

$$\dot{v}_\gamma = \mathbb{G}_{\gamma\sigma}\frac{\partial S_h}{\partial v_\sigma} = -\sum_\beta \left(\frac{w_\beta}{w_\gamma}\delta_{\gamma\sigma} - \delta_{\beta\sigma}\right) U(v_\gamma, v_\beta)\frac{\partial S_h}{\partial v_\sigma}. \quad (4.28)$$

Here, the operator $\mathbb{G}$ can be expressed as:

$$\mathbb{G}(v_1,\ldots,v_n) = \begin{bmatrix} -\sum\limits_{\beta\neq 1} U(v_1,v_\beta)\frac{w_\beta}{w_1} & U(v_1,v_2) & U(v_1,v_3) & \ldots \\ U(v_2,v_1) & -\sum\limits_{\beta\neq 2} U(v_2,v_\beta)\frac{w_\beta}{w_2} & U(v_2,v_3) & \ldots \\ \vdots & & \ddots & \end{bmatrix}. \quad (4.29)$$

The matrix $\mathbb{G}$ is a $Nd \times Nd$ block matrix, where d is the number of velocity-space dimensions and N the number of particles, and each $d \times d$ block is given by

$$\mathbb{G}_{\gamma\sigma} = \begin{cases} -\sum\limits_{\beta\neq\gamma} U(v_\gamma, v_\beta)\frac{w_\beta}{w_\gamma} & \text{if } \gamma = \sigma, \\ U(v_\gamma, v_\sigma) & \text{else.} \end{cases} \quad (4.30)$$

We observe by the symmetry of the kernel $U(\cdot,\cdot)$ that the operator $\mathbb{G}$ is also symmetric. It is also negative semi-definite. To see this, take a vector $p \in \mathbb{R}^{dN}$ and

interpret it as structured into N blocks p_γ of size d, in analogy to the structure of $\mathbb{G}$, so that each block $p_\gamma \in \mathbb{R}^d$. Multiplying the operator $\mathbb{G}$ from both sides with p, we have:

$$\begin{aligned} p_\gamma^T \mathbb{G}_{\gamma\sigma} p_\sigma &= -\sum_{\gamma,\sigma=1}^{N}\sum_{\beta=1}^{N} p_\gamma^T \left(\frac{w_\beta}{w_\gamma}\delta_{\gamma\sigma} - \delta_{\beta\sigma}\right) U(v_\gamma, v_\beta) p_\sigma, \\ &= -\sum_{\sigma=1}^{N}\sum_{\beta=1}^{N} \frac{w_\beta}{w_\sigma} p_\sigma^T U(v_\sigma, v_\beta) p_\sigma + \sum_{\gamma=1}^{N}\sum_{\beta=1}^{N} p_\gamma^T U(v_\gamma, v_\beta) p_\beta, \\ &= -\sum_{\sigma=1}^{N}\sum_{\beta=1}^{N} \left(\frac{w_\beta}{w_\sigma} p_\sigma^T U(v_\sigma, v_\beta) p_\sigma - p_\sigma^T U(v_\sigma, v_\beta) p_\beta\right). \end{aligned} \tag{4.31}$$

Here, we have expanded out the two terms, contracted the appropriate indices with the delta functions, and relabelled the resulting indices in the second sum. Factoring out the left-multiplying terms, we obtain:

$$p_\gamma^T \mathbb{G}_{\gamma\sigma} p_\sigma = -\sum_{\sigma=1}^{N}\sum_{\beta=1}^{N} \frac{p_\sigma^T}{w_\sigma} U(v_\sigma, v_\beta) \left(w_\beta p_\sigma - w_\sigma p_\beta\right), \tag{4.32}$$

$$= -\frac{1}{2}\sum_{\sigma=1}^{N}\sum_{\beta=1}^{N} \left(w_\beta p_\sigma - w_\sigma p_\beta\right)^T \frac{U(v_\sigma, v_\beta)}{w_\sigma w_\beta} \left(w_\beta p_\sigma - w_\sigma p_\beta\right) \leq 0. \tag{4.33}$$

The final equation is obtained by realising that swapping indices in Equation (4.32) results in the same term up to a minus sign, and further re-arranging results in the form shown above. As the matrix U is a projector and therefore positive semi-definite, and is being multiplied from the left and right by the same vector, we have that every term in the sum is non-positive. Thus the entire sum is non-positive and the operator $\mathbb{G}$ is negative semi-definite.

4.2.5 Conservation of momentum and energy

We now demonstrate that the semi-discrete equations of motion preserve total momentum and energy. We note that mass is trivially preserved by this scheme, due to the particle weights being held constant. We start by looking at the evolution of the total particle momentum, $P = \sum_\gamma w_\gamma v_\gamma$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_\gamma w_\gamma v_\gamma = \sum_\gamma w_\gamma \dot{v}_\gamma = \sum_\gamma w_\gamma \mathbb{G}_{\gamma\sigma} \frac{\partial S_h}{\partial v_\sigma}, \tag{4.34}$$

which gives us that $dP/dt = 0$, as the product $w_\gamma \mathbb{G}_{\gamma\sigma}$ is equal to a vector which is zero element-wise. Thus, the semi-discretisation preserves total particle momentum

over time.

To demonstrate energy conservation, it will be useful to consider the action of the operator $U(\cdot,\cdot)$. We note that $U(v,v')$ is an orthogonal projector onto the subspace orthogonal to the vector $v-v'$. It follows that $U(v,v')(v-v') = U(v',v)(v-v') = \vec{0}$. We now follow the same process as before to check conservation, where the energy density is given by $E = \sum_\gamma w_\gamma v_\gamma^2/2$:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_\gamma w_\gamma v_\gamma \dot{v}_\gamma = \sum_\gamma w_\gamma v_\gamma \mathbb{G}_{\gamma\sigma} \frac{\partial S_h}{\partial v_\sigma}. \tag{4.35}$$

Without loss of generality, we choose $\sigma = 1$. If we consider the contraction $\sum_\gamma w_\gamma v_\gamma \mathbb{G}_{\gamma 1}$, we obtain:

$$\begin{aligned}\sum_\gamma w_\gamma v_\gamma \mathbb{G}_{\gamma 1} &= -\sum_{\beta\neq 1} U(v_1,v_\beta) w_\beta v_1 + U(v_1,v_2) w_2 v_2 \\ &\qquad + U(v_1,v_3) w_3 v_3 + \cdots + U(v_1,v_n) w_n v_n \\ &= \sum_{\beta\neq 1} w_\beta U(v_1,v_\beta)(v_\beta - v_1) \\ &= 0,\end{aligned} \tag{4.36}$$

where the last line follows by the property of $U(\cdot,\cdot)$ being an orthogonal projector. As this argument holds for all σ, it follows that $dE/dt = 0$ and the semi-discretisation preserves energy.

4.2.6 H-Theorem

The semi-discrete collisional dynamics (4.24) satisfies a H-theorem, such that entropy is monotonically dissipated. This can be seen by considering the time evolution of the discretised entropy:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} S_h &= -(S_h, S_h)_h \\ &= -\frac{1}{2}\sum_{\alpha,\beta} w_\alpha w_\beta \left(\frac{1}{w_\alpha}\frac{\partial S_h}{\partial v_\alpha} - \frac{1}{w_\beta}\frac{\partial S_h}{\partial v_\beta}\right)^T U(v_\alpha, v_\beta) \left(\frac{1}{w_\alpha}\frac{\partial S_h}{\partial v_\alpha} - \frac{1}{w_\beta}\frac{\partial S_h}{\partial v_\beta}\right),\end{aligned} \tag{4.37}$$

where $(\cdot,\cdot)_h$ is the semi-discrete metric bracket given in Equation (4.18).

As the matrix U is positive semi-definite, and the terms multiplying it in the above equation are identical for a given α and β, and $w_\alpha, w_\beta \geq 0$, each term in the sum is

non-negative. As such, we have that $dS_h/dt \leq 0$ and so the discretised entropy is monotonically dissipated.

We can also compute the discrete equilibrium state by using the energy-Casimir principle, as before. The energy-Casimir principle for the discrete system reads:

$$\delta S_h(f_{s,eq}) + \delta \sum_i \lambda_i C_i(f_{s,eq}) = 0, \tag{4.38}$$

where $S_h(f_{s,eq})$ is the discrete entropy (4.19), evaluated at the discrete equilibrium distribution $f_{s,eq}$, that is the spline representation of the particles with equilibrated velocities $v_{\alpha,eq}$. The C_i's are the discrete Casimir invariants, i.e. the discrete mass, momentum, and energy. Thus, the above equation becomes:

$$\left[\delta S_h + \lambda_{M_h}\delta\left(\sum_\alpha w_\alpha\right) + \lambda_{P_h}\delta\left(\sum_\alpha w_\alpha v_\alpha\right) + \lambda_{E_h}\delta\left(\sum_\alpha w_\alpha v_\alpha^2\right)\right]_{v_\alpha = v_{\alpha,eq}} = 0, \tag{4.39}$$

where λ_{M_h}, λ_{P_h}, and λ_{E_h} are the corresponding Lagrange multipliers for the discrete quantities. Computing the variations in this equation, we have:

$$\sum_\alpha \left[\frac{\partial S_h}{\partial v_\alpha} + \lambda_{P_h} w_\alpha + \lambda_{E_h} w_\alpha v_\alpha\right] \delta v_\alpha \Bigg|_{v_\alpha = v_{\alpha,eq}} = 0, \tag{4.40}$$

where the quantity $\partial S_h/\partial v_\alpha$ is given by Equation (4.23), and the term corresponding to the mass does not appear as it does not depend on the particle velocities, thus having zero variation. Thus, we find that an equilibrium distribution's degrees of freedom, i.e. the particle velocities $\{v_{\alpha,eq}\}$ must satisfy:

$$\left[\frac{\partial S_h}{\partial v_\alpha} + \lambda_{P_h} w_\alpha + \lambda_{E_h} w_\alpha v_\alpha\right]_{v_\alpha = v_{\alpha,eq}} = 0, \tag{4.41}$$

for the appropriate Lagrange multipliers based on the chosen initial conditions.

4.2.7 Time discretisation

In the case of the Landau operator, Equation (4.28) is the gradient form of the semi-discrete system of ODE's. Applying the discrete gradient approximation of Equation (2.37), we have:

$$\frac{v_\gamma^{n+1} - v_\gamma^n}{h} = \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}), \tag{4.42}$$

where $\bar{\nabla}_\sigma S_h(v_n, v_{n+1})$ represents the discrete gradient of $\partial S_h/\partial v_\sigma$, satisfying the properties in (2.38), and v_n represents a vector of all particle velocities at time n. Here, we take the midpoint approximation for the matrix $\tilde{\mathbb{G}}_{\gamma\sigma}$, i.e.:

$$\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1}) = \mathbb{G}_{\gamma\sigma}\left(\frac{v_n + v_{n+1}}{2}\right). \tag{4.43}$$

In the treatment of the full Vlasov–Maxwell-Landau system, this approach for time discretisation of the dissipative part can immediately be adopted for the conservative part as well, possibly in conjunction with some kind of operator splitting.

Conservation of momentum and energy

Under this scheme, we can show that momentum and energy are conserved in time as well. We first consider the total particle momentum:

$$\begin{aligned}\sum_\gamma w_\gamma v_\gamma^{n+1} - \sum_\gamma w_\gamma v_\gamma^n &= h\sum_\gamma w_\gamma \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\ &= h\sum_\gamma w_\gamma \mathbb{G}_{\gamma\sigma}\left(\frac{v_n + v_{n+1}}{2}\right)\bar{\nabla}_\sigma S_h(v_n, v_{n+1}),\end{aligned} \tag{4.44}$$

where we have used Equation (4.43) to obtain the second line. By the structure of the matrix $\mathbb{G}_{\gamma\sigma}$ as shown in Equation (4.29), we have that the sum $\sum_\gamma w_\gamma \mathbb{G}_{\gamma\sigma}(\cdot) = 0$, and so:

$$\Delta P = \sum_\gamma w_\gamma v_\gamma^{n+1} - \sum_\gamma w_\gamma v_\gamma^n = 0. \tag{4.45}$$

Thus, total particle momentum is conserved exactly in time.

Now, we consider the total particle energy. We have:

$$\begin{aligned}\frac{1}{2}\sum_\gamma w_\gamma \left(v_\gamma^{n+1}\right)^2 &= \frac{1}{2}\sum_\gamma w_\gamma \left[v_\gamma^n + h\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\right]^2, \\ &= \frac{1}{2}\sum_\gamma w_\gamma \left(v_\gamma^n\right)^2 + h\sum_\gamma w_\gamma v_\gamma^n \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\ &\quad + \frac{1}{2}h^2\sum_\gamma w_\gamma \left(\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\right)^2.\end{aligned} \tag{4.46}$$

Rewriting the second term of the above equation using the discrete gradient update rule rearranged as $v_\gamma^n = v_\gamma^{n+1} - h\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})$, we have the following

useful expression

$$
\begin{aligned}
h\sum_{\gamma} w_\gamma v_\gamma^n \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\
&= h\sum_{\gamma} w_\gamma \left(v_\gamma^{n+1} - h\tilde{\mathbb{G}}_{\gamma\beta}(v_n, v_{n+1})\bar{\nabla}_\beta S_h(v_n, v_{n+1})\right) \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}), \\
&= h\sum_{\gamma} w_\gamma v_\gamma^{n+1} \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\
&\quad - h^2\sum_{\gamma} w_\gamma \left(\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\right)^2. \qquad (4.47)
\end{aligned}
$$

Now, we rewrite Equation (4.46) by splitting up the second term into two halves. Using Equation (4.47) to replace one of those terms, we have:

$$
\begin{aligned}
\Delta E &= \frac{1}{2}\sum_{\gamma} w_\gamma \left(v_\gamma^{n+1}\right)^2 - \frac{1}{2}\sum_{\gamma} w_\gamma \left(v_\gamma^{n}\right)^2 \\
&= \frac{1}{2}h\sum_{\gamma} w_\gamma v_\gamma^n \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\
&\quad + \frac{1}{2}h\sum_{\gamma} w_\gamma v_\gamma^{n+1} \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}) \\
&\quad - \frac{1}{2}h^2\sum_{\gamma} w_\gamma \left(\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\right)^2 \\
&\quad + \frac{1}{2}h^2\sum_{\gamma} w_\gamma \left(\tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\right)^2, \qquad (4.48)
\end{aligned}
$$

where the last two terms in the above equation cancel exactly. Factorising the first two terms and then using the definition of $\tilde{\mathbb{G}}_{\gamma\sigma}(\cdot,\cdot)$, we have:

$$
\begin{aligned}
\Delta E &= h\sum_{\gamma} w_\gamma \left(\frac{v_\gamma^n + v_\gamma^{n+1}}{2}\right) \tilde{\mathbb{G}}_{\gamma\sigma}(v_n, v_{n+1})\bar{\nabla}_\sigma S_h(v_n, v_{n+1}), \\
&= h\sum_{\gamma} w_\gamma \left(\frac{v_\gamma^n + v_\gamma^{n+1}}{2}\right) \mathbb{G}_{\gamma\sigma}\left(\frac{v_n + v_{n+1}}{2}\right) \bar{\nabla}_\sigma S_h(v_n, v_{n+1}). \qquad (4.49)
\end{aligned}
$$

By the arguments given in the semi-discrete energy conservation proof, we have that $\sum_\gamma w_\gamma v_\gamma \mathbb{G}_{\gamma\sigma} = 0$, where v_γ and $\mathbb{G}_{\gamma\sigma}$ are evaluated at the same point in time. As such, we have that $\sum_\gamma w_\gamma[(v_\gamma^n + v_\gamma^{n+1})/2]\mathbb{G}_{\gamma\sigma}[(v_\gamma^n + v_\gamma^{n+1})/2] = 0$, and so:

$$
\Delta E = \frac{1}{2}\sum_{\gamma} w_\gamma \left(v_\gamma^{n+1}\right)^2 - \frac{1}{2}\sum_{\gamma} w_\gamma \left(v_\gamma^{n}\right)^2 = 0. \qquad (4.50)
$$

Thus, the total particle energy is also conserved exactly in time.

H-theorem

We can demonstrate that entropy is also monotonically dissipated in time, from the properties of the discrete gradient method. From Equation (2.38), we have that:

$$S(v_{n+1}) - S(v_n) = (v_\gamma^{n+1} - v_\gamma^n) \cdot \bar{\nabla}_\gamma S_h(v_n, v_{n+1}). \tag{4.51}$$

Using the discrete gradient update rule (4.42), this becomes:

$$S(v_{n+1}) - S(v_n) = h\bar{\nabla}_\sigma S_h(v_n, v_{n+1})\tilde{\mathbb{G}}_{\sigma\gamma}\bar{\nabla}_\gamma S_h(v_n, v_{n+1}). \tag{4.52}$$

As the matrix $\tilde{\mathbb{G}}$ is simply $\mathbb{G}$ evaluated at the midpoint (c.f. Equation (4.43)), it is also negative semi-definite. Since the vectors multiplying $\tilde{\mathbb{G}}$ from the left and right are identical, we have:

$$S(v_{n+1}) - S(v_n) \leq 0, \tag{4.53}$$

and so entropy is monotonically dissipated in time. Thus, the H-theorem is maintained at the discrete level.

4.2.8 Final comments on the direct bracket discretisation

In this section, we have constructed a structure-preserving particle method for the Landau operator by directly discretising the metric bracket and entropy with particle-based distribution functions. The final equations of motion obtained via this method were as follows:

$$\dot{v}_\gamma = \sum_\alpha w_\alpha U(v_\gamma, v_\alpha) \sum_k \mathbb{L}_k(\nabla\varphi_k(v_\gamma) - \nabla\varphi_k(v_\alpha)). \tag{4.54}$$

While this discretisation preserves momentum and energy, as well as the H-theorem, it faces a downside from the perspective of computational efficiency. Specifically, the equation of motion for a given particle is coupled to the velocity of *every* other particle in the system via the tensor U in the above equation. Thus, for the whole system, this results in a complexity of $\mathcal{O}(N^2)$, where N is the number of particles.

In the following section, we approach the discretisation of the metric bracket via a different approach in order to resolve this problem. Namely, we try to leverage the smaller number of degrees of freedom of the projected distribution function f_s to reduce the computational complexity of the resulting discretised bracket.

4.3 Discretising the metric bracket via a two-stage approach

In this section, we describe a second approach to discretising the metric bracket, in order to produce a dicretisation of the Landau operator. We recall that in the previous section, there are three separate components that must be discretised: 1. functionals in the bracket, 2. functionals derivatives in the bracket, and 3. the entropy functional itself. The previous discretisation was produced by adopting the particle, or Klimontovich, representation for discretised functions for the first two, and the projected representation for the entropy. In this approach, we will consider discretising throughout by using the projected representation, i.e. using f_s (4.12) to discretise all three required components.

We will discretise the metric bracket via a two-step approach. First, we will restrict the bracket to act on discrete functions of the form

$$f_h = \sum_j f_j \varphi_j, \tag{4.55}$$

for some set of basis functions $\{\varphi_j\}$. This step will closely mirror the approach of Kraus & Hirvijoki (2017), who obtain a finite element discretisation of the Landau operator, also via the metriplectic approach. Then, we will further restrict the discrete bracket to such functions f that are obtained via projecting particles, such as the projected distribution function f_s:

$$f_s(v,t) = \sum_j f_j(t)\varphi_j(v) = \sum_{i,j} \mathbb{M}^{-1}_{ij} \sum_\alpha w_\alpha \varphi_i(v_\alpha(t))\varphi_j(v). \tag{4.56}$$

4.3.1 First step in discretisation

We begin by restating the metric bracket on functionals of Morrison (1986) in its general form:

$$(\mathcal{A},\mathcal{B}) = \frac{1}{2}\int\int \left(\frac{\partial \mathcal{A}_f}{\partial v} - \frac{\partial \mathcal{A}_{f'}}{\partial v'}\right) M(f(v))U(v,v')M(f(v')) \left(\frac{\partial \mathcal{B}_f}{\partial v} - \frac{\partial \mathcal{B}_{f'}}{\partial v'}\right) dv dv'. \tag{4.57}$$

Here, $M(f)$ is a function that defines the statistics that are modelled by the bracket, with the Landau operator being produced by $M(f) = f$ when paired with entropy as $S = -\int f \log f \mathrm{d}v$.

The aim, as stated above, is to obtain a discretisation of this bracket on functions of the form of Equation (4.55). We first consider the discretisation of functionals.

A functional $\mathcal{A}$ can be discretised by being restricted to functions of the form (4.55) as follows:

$$A_h(\hat{f}) = \mathcal{A}[f_h], \qquad \text{with} \qquad \hat{f}(t) = (f_1(t), ..., f_M(t))^T. \tag{4.58}$$

Here, the function $A_h(\hat{f})$, resulting from the evaluation of the functional $\mathcal{A}$ on f_h, is a function of the degrees of freedom $\hat{f}$.

With this, we can now consider the discretisation of the functional derivatives appearing in (4.57). We will construct this by requiring equality of the following pairings:

$$\left\langle \frac{\delta \mathcal{A}[f_h]}{\delta f}, g_h \right\rangle_{L^2} = \left\langle \frac{\partial A_h}{\partial \hat{f}}, \hat{g} \right\rangle_{\mathbb{R}^M} = \sum_{i=1}^{M} \frac{\partial A_h}{\partial f_i}\, g_i, \tag{4.59}$$

where $\hat{g}(t) = (g_1(t), ..., g_M(t))^T$ denotes the degrees of freedom of a test function g_h, so that

$$g_h(v,t) = \sum_{i=1}^{M} g_i(t)\, \varphi_i(v). \tag{4.60}$$

In order to compute the term on the left-hand side of (4.59), we will require the dual basis in L^2 to $\{\varphi_j\}_{j=1}^M$. Let us denote this dual basis by $\{\psi_i\}_{i=1}^M$, such that it satisfies

$$\int_\Omega \psi_i(v)\, \varphi_j(v) \mathrm{d}v = \delta_{ij} \quad \text{for} \quad 1 \leq i, j \leq M. \tag{4.61}$$

Thus, the functional derivative on the left-hand side of (4.59) can be represented in the dual basis as follows

$$\frac{\delta \mathcal{A}[f_h]}{\delta f} = \sum_{i=1}^{M} a_i\, \psi_i(v), \tag{4.62}$$

where $\{a_i\}$ are the degrees of freedom in this dual basis, which are to be determined.

In order to determine the coefficients $\{a_i\}$, let us choose the test function g_h such that $\hat{g} = (0, \ldots, 0, 1, 0, \ldots, 0)^\top$ with 1 at the i-th position and 0 everywhere else, i.e. $g_h = \varphi_i$. By using Equations (4.59) and (4.62), we obtain the result for the i-th coefficient:

$$a_i = \frac{\partial A_h}{\partial f_i}. \tag{4.63}$$

Thus, the functional derivative in (4.59) can be represented in the dual basis as

follows

$$\frac{\delta \mathcal{A}[f_h]}{\delta f} = \sum_{i=1}^{M} \frac{\partial A_h}{\partial f_i}\, \psi_i(v). \tag{4.64}$$

We can re-express this in terms of our original, or primal, basis $\{\varphi_j\}$:

$$\frac{\delta \mathcal{A}[f_h]}{\delta f} = \sum_{i,j=1}^{M} \frac{\partial A_h}{\partial f_i}\, \mathbb{A}_{ij}\, \varphi_j(v), \tag{4.65}$$

where $\mathbb{A}_{ij}$ relates the two bases as follows

$$\psi_i(v) = \sum_{j=1}^{M} \mathbb{A}_{ij}\, \varphi_j(v). \tag{4.66}$$

We can compute the coefficients $\mathbb{A}_{ij}$ by computing the inner product of (4.66) with a given basis function φ_k

$$\begin{aligned} \int_{\Omega} \psi_i(v)\, \varphi_k(v) dv &= \int_{\Omega} \sum_{j=1}^{M} \mathbb{A}_{ij}\, \varphi_j(v)\, \varphi_k(v) \mathrm{d}v, \\ &= \sum_{j=1}^{M} \mathbb{A}_{ij} \int_{\Omega} \varphi_j(v)\, \varphi_k(v) \mathrm{d}v, \\ &= \sum_{j=1}^{M} \mathbb{A}_{ij} \mathbb{M}_{jk}, \end{aligned} \tag{4.67}$$

where $\mathbb{M}$ is the mass matrix for the basis $\{\varphi_j\}$. Using (4.61), we have the result that $\mathbb{I} = \mathbb{A}\mathbb{M}$, where $\mathbb{I}$ is the identity matrix of size $M \times M$. Thus we have that $\mathbb{A} = \mathbb{M}^{-1}$, and so the functional derivative expression in (4.65) becomes

$$\frac{\delta \mathcal{A}[f_h]}{\delta f} = \sum_{i,j=1}^{M} \frac{\partial A_h}{\partial f_i}\, (\mathbb{M}^{-1})_{ij}\, \varphi_j(v). \tag{4.68}$$

We can now use this expression for the discrete functional derivative to obtain the discrete version of the metric bracket in (4.57):

$$(A_h, B_h)_h = \sum_{i,j,k,l=1}^{M} \frac{\partial A_h}{\partial f_i}\, (\mathbb{M}^{-1})_{ij}\, \mathbb{L}_{jk}(\hat{f})\, (\mathbb{M}^{-1})_{kl} \frac{\partial B_h}{\partial f_l}, \tag{4.69}$$

where A_h, B_h are functions of the form (4.55), and the elements of the symmetric

matrix $\mathbb{L}(\hat{f})$ are as follows:

$$\mathbb{L}_{ij}(\hat{f}) = \frac{1}{2}\int_\Omega\int_\Omega \left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right) \cdot M(f_h(v))\,U(v,v')\,M(f_h(v'))\cdot\left(\frac{\partial\varphi_j(v)}{\partial v} - \frac{\partial\varphi_j(v')}{\partial v'}\right)\mathrm{d}v\mathrm{d}v'. \quad (4.70)$$

It should be noted that this discrete bracket is still positive semi-definite, which will be an important property to prove that the operator produced by the bracket satisfies an H-theorem. A sufficient condition for this is provided by the non-negativity of the function $M(f_h)$.

4.3.2 Step 2: Particle discretisation

Now that we have a discrete bracket on functions of the form of (4.55), we consider further restricting the bracket to functions of this form that are obtained *specifically* from a projection of particles, i.e. those of the form (4.56). Thus, we are moving to functions with particle velocities, $\{v_\alpha\}$, as their degrees of freedom, rather than rather than basis coefficients $\{f_i\}$.

There are two components of the discrete bracket (4.69) to consider for this. The first is that the partial derivatives with respect to f_i's must be converted to derivatives with respect to the particle degrees of freedom, i.e. $\{v_\alpha\}$. Secondly, the matrix $\mathbb{L}$ should also depend on the particle velocities.

As in the first part, we will obtain the relationship between the derivatives by requiring the following

$$\delta A_h[\hat{f}] = \delta A_s[\hat{v}], \quad (4.71)$$

where A_h is our finite-element type function as in (4.55), with degrees of freedom $\hat{f}$, and A_s is the projected function which has degrees of freedom $\hat{v} = (v_1, \ldots, v_N)$.

Computing these variations, we have:

$$\delta A_h[\hat{f}] = \sum_{\alpha=1}^{N}\sum_{i=1}^{M}\frac{\partial A_h}{\partial f_i}\frac{\partial f_i}{\partial v_\alpha}\,\delta v_\alpha, \quad (4.72)$$

$$= \sum_{i,j=1}^{M}\frac{\partial A_h}{\partial f_i}\mathbb{M}^{-1}_{ij}\sum_{\alpha=1}^{N} w_\alpha\nabla\varphi_j(v_\alpha)\,\delta v_\alpha, \quad (4.73)$$

where the expression for $\partial f_i/\partial v_\alpha$ comes from (2.30), and

$$\delta A_s[\hat{v}] = \sum_{\alpha=1}^{N} \frac{\partial A_s}{\partial v_\alpha}\, \delta v_\alpha. \tag{4.74}$$

Equating the two variations, we obtain

$$\sum_{i,j=1}^{M} \frac{\partial A_h}{\partial f_i} \mathbb{M}^{-1}_{ij} \sum_{\alpha=1}^{N} w_\alpha \nabla\varphi_j(v_\alpha)\, \delta v_\alpha = \sum_{\alpha=1}^{N} \frac{\partial A_s}{\partial v_\alpha}\, \delta v_\alpha. \tag{4.75}$$

We introduce the matrix $\mathbb{K} \in \mathbb{R}^{M\times N}$, such that

$$\mathbb{K}_{j,\alpha} = w_\alpha \nabla\varphi_j(v_\alpha). \tag{4.76}$$

As this matrix is generally not square, it is also not invertible. However, we can define a pseudo-inverse, $\mathbb{K}^+$, such that $\mathbb{K}\mathbb{K}^+ = \mathbb{I}_{M\times M}$. [2] We can then rewrite (4.75) as follows:

$$\sum_{i=1}^{M} \frac{\partial A_h}{\partial f_i}\, \mathbb{M}^{-1}_{ij} = \sum_{\alpha=1}^{N} \frac{\partial A_s}{\partial v_\alpha}\, \mathbb{K}^+_{\alpha,i}. \tag{4.77}$$

Thus, the discrete bracket on particles becomes:

$$(A_s, B_s)_s = \sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \frac{\partial A_s}{\partial v_\alpha}\, \mathbb{K}^+_{\alpha,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial B_s}{\partial v_\beta}, \tag{4.78}$$

where the matrix $\mathbb{L}$ is now evaluated on the particle velocities $\hat{v}$.

4.3.3 Semi-discrete equations of motion

The equation of motion for a given particle can then be obtained by taking the bracket on particles from (4.78) and evaluating it on the particle velocity and discrete entropy (4.19) as follows:

$$\dot{v}_\gamma = -(v_\gamma, S_h)_p \tag{4.79}$$

$$= -\sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \frac{\partial v_\gamma}{\partial v_\alpha}\, \mathbb{K}^+_{\alpha,i(\hat{v})}\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial S_h}{\partial v_\beta}. \tag{4.80}$$

Using the fact that $\partial v_\gamma/\partial v_\alpha = \delta_{\gamma\alpha}$, and the expression for $\partial S_h/\partial v_\alpha$ from Equa-

[2] It should be noted that $\mathbb{K}^+\mathbb{K} \neq \mathbb{I}_{N\times N}$

tion (4.23), we have:

$$\dot{v}_\gamma = -\sum_{\alpha,\beta=1}^{N}\sum_{i,j=1}^{M} \delta_{\gamma\alpha}\,\mathbb{K}^{+}_{\alpha,i}(\hat{v})\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{K}^{+}_{\beta,j}\left(-\sum_k w_\beta \mathbb{J}_k \nabla\varphi_k(v_\beta)\right), \tag{4.81}$$

where we have renamed the vector $\mathbb{L}_k$ to $\mathbb{J}_k$ to avoid confusion with the matrix $\mathbb{L}_{ij}$, i.e.:

$$\mathbb{J}_k(\hat{f}(\hat{v})) = \sum_i \mathbb{M}^{-1}_{ik}\int \varphi_i(v)\left[1+\log\left(f_s(\hat{v})\right)\right]\mathrm{d}v. \tag{4.82}$$

Simplifying Equation (4.81), we have:

$$\dot{v}_\gamma = \sum_{\beta=1}^{N}\sum_{i,j=1}^{M} \mathbb{K}^{+}_{\gamma,i(\hat{v})}\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{K}^{+}_{\beta,j}(\hat{v})\sum_k w_\beta \nabla\varphi_k(v_\beta)\mathbb{J}_k(\hat{f}(\hat{v})) \tag{4.83}$$

which using the definition of $\mathbb{K}_{k,\beta} = w_\beta\nabla\varphi_k(v_\beta)$ can be rewritten as:

$$\dot{v}_\gamma = \sum_{\beta=1}^{N}\sum_{i,j,k=1}^{M} \mathbb{K}^{+}_{\gamma,i}(\hat{v})\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{K}^{+}_{\beta,j}(\hat{v})\,\mathbb{K}_{k,\beta}(\hat{v})\,\mathbb{J}_k(\hat{f}(\hat{v})).$$

As we have that $\sum_\beta \mathbb{K}^{+}_{\beta,j}\,\mathbb{K}_{k,\beta} = \mathbb{K}\mathbb{K}^{+} = \mathbb{I}_{M\times M}$, this equation can be simplified to obtain the following:

$$\dot{v}_\gamma = \sum_{i,j=1}^{M} \mathbb{K}^{+}_{\gamma,i}(\hat{v})\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{J}_j(\hat{f}(\hat{v})), \tag{4.84}$$

and this is now the final set of equations of motion for the particle velocities.

4.3.4 Conservation of invariants

Now, we demonstrate that the obtained semi-discrete equations preserves the required invariants, namely mass, total momentum and energy. Interestingly, the discrete quantities that are preserved intrinsically by this discretisation are different to those that are preserved by the direct bracket discretisation shown in Section 4.2.

We recall that at a continuous level, the conserved quantities of the Landau operator (when purely considering collisions) are as follows:

$$\mathcal{M} = \int f\mathrm{d}v, \qquad \mathcal{P} = \int vf\mathrm{d}v, \qquad \mathcal{E} = \int v^2 f\mathrm{d}v. \tag{4.85}$$

The discrete invariants in the direct metric bracket discretisation of Section 4.2 are

the following *particle* invariants:

$$M_p = \int f_p \, \mathrm{d}v = \sum_\alpha w_\alpha, \tag{4.86}$$

$$P_p = \int v f_p \, \mathrm{d}v = \sum_\alpha w_\alpha v_\alpha, \tag{4.87}$$

$$E_p = \int v^2 f_p \, \mathrm{d}v = \sum_\alpha w_\alpha v_\alpha^2. \tag{4.88}$$

In the case of the two-step discretisation presented in this section, however, the discrete invariants which are preserved are the *projected* invariants:

$$M_s = \int f_s \, \mathrm{d}v = \hat{\mathbb{1}}^T \mathbb{M} \hat{f}, \tag{4.89}$$

$$P_s = \int v f_s \, \mathrm{d}v = \hat{v}^T \mathbb{M} \hat{f}, \tag{4.90}$$

$$E_s = \int v^2 f_s \, \mathrm{d}v = \hat{\varepsilon}^T \mathbb{M} \hat{f}, \tag{4.91}$$

where $\mathbb{M}$ is the mass matrix for the basis $\{\varphi_j\}$ as before, $\hat{f} \in \mathbb{R}^M$ are the coefficients of the projected distribution function f_s in this basis, and the vectors $\hat{\mathbb{1}}, \hat{v}, \hat{\varepsilon} \in \mathbb{R}^M$ satisfy:

$$\sum_{j=1}^M \hat{\mathbb{1}}_j \varphi_j = 1, \qquad \sum_{j=1}^M \hat{v}_j \varphi_j = v, \qquad \sum_{j=1}^M \hat{\varepsilon}_j \varphi_j = v^2. \tag{4.92}$$

It should be noted that to obtain (4.92), there is a requirement that the chosen basis is able to represent the functions $\{1, v, v^2\}$.

To show the conservation properties of this discretisation, we will require the following property to be satisfied by the vectors $\hat{\mathbb{1}}, \hat{v}, \hat{\varepsilon}$:

$$\hat{\mathbb{1}}^T \mathbb{L}(\hat{f}) = 0, \tag{4.93}$$

$$\hat{v}^T \mathbb{L}(\hat{f}) = 0, \tag{4.94}$$

$$\hat{\varepsilon}^T \mathbb{L}(\hat{f}) = 0, \tag{4.95}$$

for any vector $\hat{f} \in \mathbb{R}^M$.

To show that these properties hold, let us first restate the expression for the elements

of the matrix $\mathbb{L}(\hat{f})$:

$$\mathbb{L}_{ij}(\hat{f}) = \frac{1}{2}\int_\Omega\int_\Omega \Bigg(\overbrace{\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}}^{\text{depends on } i}\Bigg) \cdot M(f_h(v))\,U(v,v')\,M(f_h(v'))\cdot\left(\frac{\partial\varphi_j(v)}{\partial v} - \frac{\partial\varphi_j(v')}{\partial v'}\right)\mathrm{d}v\mathrm{d}v'. \quad (4.96)$$

As the dependence of $\mathbb{L}_{ij}$ on the index i is purely in the first term, let us consider the contraction of just this term with the vector $\hat{\mathbb{1}}$:

$$\begin{aligned}\sum_i \hat{\mathbb{1}}_i\left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right) &= \sum_i \hat{\mathbb{1}}_i\frac{\partial\varphi_i(v)}{\partial v} - \sum_i \hat{\mathbb{1}}_i\frac{\partial\varphi_i(v')}{\partial v'}\\ &= \frac{\partial}{\partial v}(1) - \frac{\partial}{\partial v'}(1) = 0, \end{aligned} \quad (4.97)$$

where we have used (4.92) and the fact that $\hat{\mathbb{1}}_i$ does not depend on v to obtain the second line. Thus, we have that

$$\hat{\mathbb{1}}^T\mathbb{L}(\hat{f}) = \frac{1}{2}\int_\Omega\int_\Omega \sum_i \hat{\mathbb{1}}_i\left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right) \cdot M(f_h(v))\,U(v,v')\,M(f_h(v'))\cdot\left(\frac{\partial\varphi_j(v)}{\partial v} - \frac{\partial\varphi_j(v')}{\partial v'}\right)\mathrm{d}v\mathrm{d}v' = 0, \quad (4.98)$$

which holds for any vector $\hat{f} \in \mathbb{R}^M$. We note that here, we are free to carry the sum inside the integral in (4.96) as the vector $\hat{\mathbb{1}}$ does not depend on v or v'.

Following the same procedure for $\hat{v}$, we have

$$\begin{aligned}\sum_i \hat{v}_i\left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right) &= \sum_i \hat{v}_i\frac{\partial\varphi_i(v)}{\partial v} - \sum_i \hat{v}_i\frac{\partial\varphi_i(v')}{\partial v'}\\ &= \frac{\partial}{\partial v}v - \frac{\partial}{\partial v'}v' = 1 - 1 = 0, \end{aligned} \quad (4.99)$$

where we have again used (4.92). Thus, by the same logic as in (4.98), we have that $\hat{v}^T\mathbb{L}(\hat{f}) = 0$ for any vector $\hat{f} \in \mathbb{R}^M$.

Finally, let us consider $\hat{\varepsilon}$:

$$\begin{aligned}\sum_i \hat{\varepsilon}_i\left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right) &= \sum_i \hat{\varepsilon}_i\frac{\partial\varphi_i(v)}{\partial v} - \sum_i \hat{\varepsilon}_i\frac{\partial\varphi_i(v')}{\partial v'}\\ &= \frac{\partial}{\partial v}v^2 - \frac{\partial}{\partial v'}v'^2 = v - v'. \end{aligned} \quad (4.100)$$

In this case, we obtain

$$\hat{\varepsilon}^T \mathbb{L}(\hat{f}) = \frac{1}{2} \int_\Omega \int_\Omega (v - v') \cdot M(f_h(v))\, U(v, v')\, M(f_h(v')) \cdot \left(\frac{\partial \varphi_j(v)}{\partial v} - \frac{\partial \varphi_j(v')}{\partial v'} \right) \mathrm{d}v \mathrm{d}v'. \tag{4.101}$$

Here, we must use the fact that the tensor $U(v, v')$ is the orthogonal projector onto the subspace orthogonal to the vector $v - v'$, and so $U(v, v')(v - v') = 0$. Thus, we have that $\hat{\varepsilon}^T \mathbb{L}(\hat{f}) = 0$ for any $\hat{f} \in \mathbb{R}^M$, as required.

In order to show the conservation laws, we will also need the derivatives of a given projected quantity, $A_s = \hat{a}^T \mathbb{M} \hat{f}$, with respect to the particle degrees of freedom, v_α. Computing this derivative, we have:

$$\begin{aligned} \frac{\partial A_s}{\partial v_\alpha} &= \hat{a}^T \mathbb{M} \frac{\partial \hat{f}}{\partial v_\alpha}, \\ &= \sum_{i,j,k} \hat{a}_i \mathbb{M}_{ij}\, \mathbb{M}^{-1}_{jk} \mathbb{K}_{k,\alpha}, \\ &= \sum_k \hat{a}_k\, \mathbb{K}_{k,\alpha}, \end{aligned} \tag{4.102}$$

where we have expanded $\partial \hat{f} / \partial v_\alpha$ using (2.30) and the definition of the matrix $\mathbb{K}$ (4.76).

Now, we have the required components to demonstrate the conservation of the discrete projected invariants. As the procedure is the same for mass, momentum, and energy, let us consider a general invariant, $A_s = \hat{a}^T \mathbb{M} \hat{f}$, which satisfies the property $\hat{a}^T \mathbb{L} = 0$.

The time evolution of the invariant A_s is as follows

$$\frac{d}{dt} A_s = -(A_s, S_h)_s, \tag{4.103}$$

$$= - \sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \frac{\partial A_s}{\partial v_\alpha}\, \mathbb{K}^+_{\alpha,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial S_h}{\partial v_\beta}. \tag{4.104}$$

We use (4.102) to expand $\partial A_s / \partial v_\alpha$ and so the above equation becomes:

$$\frac{d}{dt} A_s = - \sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \sum_{k=1}^{M} \hat{a}_k\, \mathbb{K}_{k,\alpha}\, \mathbb{K}^+_{\alpha,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial S_h}{\partial v_\beta}, \tag{4.105}$$

$$= - \sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \hat{a}_i\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial S_h}{\partial v_\beta}. \tag{4.106}$$

Since A_s is an invariant such that it satisfies $\hat{a}\mathbb{L} = 0$, the above equation becomes $dA_s/dt = 0$, and so A_s is conserved under this semi-discretisation. As we have that the projected mass, momentum, and energy (4.89)-(4.91) take the form of A_s, and satisfy (4.93)-(4.95), we thus have:

$$\frac{d}{dt}M_s = 0, \tag{4.107}$$

$$\frac{d}{dt}P_s = 0, \tag{4.108}$$

$$\frac{d}{dt}E_s = 0, \tag{4.109}$$

i.e. the projected mass, momentum, and energy are conserved by the semi-discretisation.

4.3.5 H-Theorem

We also demonstrate that this semi-discretisation satisfies a H-theorem. First, we consider the dissipation of entropy, $S_h = -\int f_s \log f_s \mathrm{d}v$:

$$\begin{aligned}\frac{d}{dt}S_h &= -(S_s, S_h)_s, \\ &= -\sum_{\alpha,\beta=1}^{N}\sum_{i,j=1}^{M} \frac{\partial S_h}{\partial v_\alpha}\, \mathbb{K}^+_{\alpha,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}\, \frac{\partial S_h}{\partial v_\beta},\end{aligned} \tag{4.110}$$

where we have used (4.78) to expand the bracket. Since the matrix $\mathbb{L}$ is positive semi-definite, and we are multiplying it from the left and right by the same terms, we thus have that:

$$\frac{d}{dt}S_h \leq 0. \tag{4.111}$$

Thus, entropy is monotonically dissipated by this semi-discretisation.

We can also determine the equilibrium state through the energy-Casimir principle. Recalling that the energy-Casimir principle in the discrete case is as follows:

$$\delta S_h(f_{s,eq}) + \delta \sum_i \lambda_i C_i(f_{s,eq}) = 0, \tag{4.112}$$

where $S_h(f_{s,eq})$ is the discrete entropy (4.19), $f_{s,eq}$ is the discrete equilibrium distribution with equilibrium particle velocities $\{v_{\alpha,eq}\}$, and C_i are the Casimir invariants of the bracket, given in this case by Equations (4.89)-(4.91).

Expanding on these quantities, we obtain the following equation:

$$\left[\delta S_h + \lambda_{M_s}\delta\left(\hat{\mathbb{1}}^T\mathbb{M}\hat{f}\right) + \lambda_{P_s}\delta\left(\hat{v}^T\mathbb{M}\hat{f}\right) + \lambda_{E_s}\delta\left(\hat{\varepsilon}^T\mathbb{M}\hat{f}\right)\right]_{v_\alpha = v_{\alpha,eq}} = 0, \tag{4.113}$$

where $\lambda_{M_s}, \lambda_{P_s}, \lambda_{E_s}$ are the corresponding Lagrange multipliers for mass, momentum, and energy, respectively. Computing the variations in this equation and using (4.102) to obtain the derivative of each invariant with respect to the particle velocities, we have the following:

$$\sum_{\alpha=1}^{N}\left[\frac{\partial S_h}{\partial v_\alpha} + \sum_{j=1}^{M}\left(\lambda_{M_s}\hat{\mathbb{1}}_j\mathbb{K}_{j,\alpha} + \lambda_{P_s}\hat{v}_j\mathbb{K}_{j,\alpha} + \lambda_{E_s}\hat{\varepsilon}_j\mathbb{K}_{j,\alpha}\right)\right]\Bigg|_{v_\alpha = v_{\alpha,eq}} \delta v_\alpha = 0, \tag{4.114}$$

where the derivative $\partial S_h/\partial v_\alpha$ is given by Equation (4.23) as before, and the matrix $\mathbb{K}$ is defined as in (4.76).

Thus, we have that the discrete equilibrium state must satisfy the following equations:

$$\left[\frac{\partial S_h}{\partial v_\alpha} + \sum_{j=1}^{M}\left(\lambda_{M_s}\hat{\mathbb{1}}_j\mathbb{K}_{j,\alpha} + \lambda_{P_s}\hat{v}_j\mathbb{K}_{j,\alpha} + \lambda_{E_s}\hat{\varepsilon}_j\mathbb{K}_{j,\alpha}\right)\right] = 0, \tag{4.115}$$

where the Lagrange multipliers $\lambda_{M_s}, \lambda_{P_s}, \lambda_{E_s}$ can be obtained by matching the mass, momentum, and energy of the equilibrium state to that of the initial conditions.

4.3.6 Final comments on the two-step discretisation and challenges in implementation

The semidiscrete equations of motion we obtained by following the two-step discretisation approach are the following:

$$\dot{v}_\gamma = \sum_{i,j=1}^{M}\mathbb{K}^{+}_{\gamma,i}(\hat{v})\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{J}_j(\hat{f}(\hat{v})), \tag{4.116}$$

where solving this ODE in time gives us the evolution of the velocity of the γ-th particle, and the quantities on the right-hand side of the ODE are as follows:

$$\mathbb{K}_{j,\alpha} = w_\alpha \nabla \varphi_j(v_\alpha), \tag{4.117}$$

$$\mathbb{K}\mathbb{K}^+ = \mathbb{I}_{M\times M}, \tag{4.118}$$

$$\begin{aligned}\mathbb{L}_{ij}(\hat{f}) = \frac{1}{2}\int_\Omega\int_\Omega &\left(\frac{\partial\varphi_i(v)}{\partial v} - \frac{\partial\varphi_i(v')}{\partial v'}\right)\\ &\cdot f_s(v)\,U(v,v')\,f_s(v')\cdot\left(\frac{\partial\varphi_j(v)}{\partial v} - \frac{\partial\varphi_j(v')}{\partial v'}\right)\mathrm{d}v\mathrm{d}v',\end{aligned} \tag{4.119}$$

$$\mathbb{J}_j(\hat{f}(\hat{v})) = \sum_i \mathbb{M}^{-1}_{ij}\int \varphi_i(v)\left[1+\log\left(f_s(\hat{v})\right)\right]\mathrm{d}v. \tag{4.120}$$

where $\{\varphi_j\}_{j=1}^M$ are the basis functions of the chosen basis for projection, and $f_s(v)$ is the projected distribution function. As we have seen in the previous section, this semi-discretisation preserves mass, momentum and energy exactly by construction. It also preserves the H-theorem, meaning that the discrete entropy is monotonically dissipated. Thus, this discretisation preserves all the required properties for the Landau operator.

There are significant computational advantages of this scheme as opposed to the one obtained in Section 4.2 via the direct discretisation of the bracket. The primary advantage is that the cost of this scheme is $\mathcal{O}(NM^2)$, where N is the number of particles. This is the cost associated with computing the pseudo-inverse matrix $\mathbb{K}^+$, as that is the most expensive step to compute. This is a significant improvement over the scheme in Section 4.2 which had a cost of $\mathcal{O}(N^2)$, as cases of interest typically have $M \ll N$, i.e. the number of basis functions required to represent the projected distribution function are much less than the number of particles in the simulation.

There are, however, some challenges in implementation that apply to this discretisation. This issue effectively arises from the computation of the vector $\mathbb{J}$, as in (4.120). Following our discussion of projections in Chapter 2, we can recognise that the vector $\mathbb{J}$ is the result of a projection. In fact, $\mathbb{J}$ is the vector of coefficients in the basis $\{\varphi_j\}$ as a result of projecting the function $1+\log f_s$ onto this basis. This can be considered as a projection of the gradient of the discrete entropy, $S_h = -\int f_s \log f_s \mathrm{d}v$.

While this in itself is not an issue, the problem becomes more clear when we consider that the basis $\{\varphi_j\}$ is chosen for projecting the distribution function, which satisfies very different boundary conditions to the function $1+\log f_s$. At a continuous level, the distribution function f is a probability density function, and so we can assume

that $f \to 0$ as $v \to \pm\infty$. In the computational domain, as we did in the Lenard-Bernstein discretisation of Chapter 3, we can choose the velocity-space domain to be sufficiently large, and then set homogeneous Dirichlet boundary conditions for the basis on this domain so that the projected f_s approximately satisfies the required boundary conditions.

The function $1 + \log f$, however, does not satisfy these boundary conditions. If f is a Maxwellian, for example, then we have that $1 + \log f \to -\infty$ as $v \to \pm\infty$, which is directly incompatible with the boundary conditions for f. In general, we have that $1 + \log f \to -\infty$ as the distribution function $f \to 0$, and so we can see that representing these two functions in the same basis poses an issue.

When using B-splines as our basis functions, as in the implementation in Chapter 3, it is possible to alleviate this issue by considering boundary conditions other than Dirichlet. For example, under natural boundary conditions (i.e. where no boundary conditions are enforced), it is possible to represent both functions in the same basis. When using a linear splines basis, it is also possible to represent both functions using periodic boundary conditions (as we only need to match the values of the function on either boundary to enforce periodicity in the linear case; this would fail for higher orders). However, this causes another issue, namely in the computation of the pseudo-inverse matrix $\mathbb{K}^+$. For either of these boundary conditions, the matrix $\mathbb{K}$ becomes rank-deficient, and so the computed pseudo-inverse no longer satisfies $\mathbb{K}\mathbb{K}^+ = \mathbb{I}_{M\times M}$. This is an issue as the derivation of the semi-discretisation depends on this property, and it not being respected results in the right-hand side of (4.116) no longer being computed accurately.

One possible way to resolve this would be to return to the discrete bracket in (4.78):

$$(A_s, B_s)_s = \sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \frac{\partial A_s}{\partial v_\alpha} \mathbb{K}^+_{\alpha,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j} \frac{\partial B_s}{\partial v_\beta}. \tag{4.121}$$

Recall that the equations of motion are computed by evaluating the bracket on a particle velocity, v_γ, and the discrete entropy $S_h = -\int f_s \log f_s \mathrm{d}v$:

$$\begin{aligned}
\dot{v}_\gamma &= -(v_\gamma, S_h)_p, \\
&= -\sum_{\alpha,\beta=1}^{N} \sum_{i,j=1}^{M} \frac{\partial v_\gamma}{\partial v_\alpha} \mathbb{K}^+_{\alpha,i(\hat{v})}\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j} \frac{\partial S_h}{\partial v_\beta}, \\
&= \sum_{\beta=1}^{N} \sum_{i,j,k=1}^{M} \mathbb{K}^+_{\gamma,i}(\hat{v})\, \mathbb{L}_{ij}(\hat{f}(\hat{v}))\, \mathbb{K}^+_{\beta,j}(\hat{v}) \underbrace{\mathbb{K}_{k,\beta}(\hat{v})\, \mathbb{J}_k(\hat{f}(\hat{v}))}_{\partial S_h/\partial v_\beta},
\end{aligned} \tag{4.122}$$

where the final line is obtained by the fact that $\partial S_h/\partial v_\beta = \mathbb{K}_{k,\beta}(\hat{v})\,\mathbb{J}_k(\hat{f}(\hat{v}))$ (4.23). From here, we used the pseudo-inverse property, which in index form is $\sum_\beta \mathbb{K}_{j,\beta}\mathbb{K}^+_{\beta,k} = \delta_{jk}$, to simplify (4.122) and obtain the equations of motion in (4.116).

From here, an alternative approach can be to use a different basis $\{\psi_j\}_{j=1}^K$ to compute $\partial S_h/\partial v_\beta$ to the rest of the right-hand side of (4.122). This effectively means that a suitable basis can be used for the computation of $\mathbb{J}$, and a different basis can be used for the computation of the pseudo-inverses $\mathbb{K}^+$ which will not result in the same rank-deficiency as if the same basis was used for both. However, there is a cost trade-off to this approach. Using a different basis to compute $\partial S_h/\partial v_\beta$ in (4.122) implies that we can no longer use the pseudo-inverse property, as the $\mathbb{K}$ in the entropy derivative is now a different matrix:

$$\dot{v}_\gamma = \sum_{\beta=1}^{N}\sum_{i,j,k=1}^{M} \mathbb{K}^{+,\varphi}_{\gamma,i}(\hat{v})\,\mathbb{L}_{ij}(\hat{f}(\hat{v}))\,\mathbb{K}^{+,\varphi}_{\beta,j}(\hat{v})\,\mathbb{K}^{\psi}_{k,\beta}(\hat{v})\,\mathbb{J}_k(\hat{f}(\hat{v})), \tag{4.123}$$

where the superscripts denote which basis a particular matrix is computed with respect to. To compute this equation, we now need to compute the product $\mathbb{K}^{\psi}\mathbb{K}^{+,\varphi}$, which is an operation with cost $\mathcal{O}(N^2)$. This is the same cost as that of the direct bracket discretisation in Section 4.2, and is extremely expensive for realistic particle numbers N. Thus, this approach is also not viable.

Chapter 5

Conclusions

In this work, we have presented two families of approaches for the construction of structure-preserving particle discretisations for collision operators. The first is a deterministic particle approach, which is applied to a modified conservative version of the Lenard-Bernstein operator. The second is based on the metriplectic framework, and is demonstrated through two different discretisations of the Landau collision operator. Both methods use L^2 projections to regularise the particle solutions.

In Chapter 3, we have demonstrated how a deterministic particle method can be used to construct a discretisation of a conservative Lenard-Bernstein operator (the derivation of which is given in Chapter 1). A second representation of the distribution function is introduced (based on a finite element approach) which is computed by projecting the particle solution onto the chosen basis. The obtained semi-discretisation is shown to preserve mass, momentum, and energy exactly. Time integration is performed using the implicit midpoint scheme, which is shown to conserve the invariants exactly as well. The method was implemented in a one-dimensional case, with a cubic spline basis for the projected representation. Several examples are given to demonstrate the method's validity, and the conservation properties are verified up to machine precision. Though it was not possible to produce a proof of a semi-discrete H-theorem, the monotonic dissipation of entropy is verified numerically, and the obtained equilibrium states are shown to be Maxwellians with the expected properties.

In Chapter 4, we have constructed three separate discretisations of the Landau collision operator. The first is again through a deterministic particle method, though the discretisation is shown to be computationally too expensive. Two discretisations based on the metriplectic approach of Morrison (1986) are then presented, and both use the same projection method as in the Lenard-Bernstein case to regularise the particle solution. The first method is constructed by directly discretising the Landau metric bracket using the particle distribution function, and the projected representation is only used to compute the entropy. This leads to a semi-discretisation with all

the required conservation properties, which are shown to be preserved in time when the method of discrete gradients is used for time integration. However, the method is shown to have a cost of $\mathcal{O}(N^2)$, where N is the number of particles. The second method follows a two-step approach to discretising the metric bracket. The first step is to restrict the bracket to act on finite-element type functions, and then the bracket is further restricted to those finite-element functions which are obtained by projecting a particle solution. Thus, we obtain a discrete metric bracket that acts on functions of the particle velocities. The method is shown to have a cost of $\mathcal{O}(NM^2)$, where M is the number of basis functions for the computing the projection. This is a marked improvement on the first metriplectic discretisation. However, there are some implementation challenges for this method, and these are discussed in detail in the chapter.

5.1 Future outlook

There are several pathways for the work in this thesis to be extended. The first is to solve the implementation challenges for the Landau operator discretisation, so that the method can be numerically verified. It is necessary to investigate different bases for the projection, so that the required terms can be computed without issue in the semi-discretisation. Another extension of this work is to also consider how best to enforce positivity preservation, as this is not something that can be achieved using splines with the current discretisation. Finally, the time discretisation must still be verified analytically for the two-step bracket discretisation (i.e. whether or not the method of discrete gradients preserves all the required properties in time, or if it is necessary to use a different method).

There are several options to choose from there. One is to consider the coupling of either collision operator to an ideal solver, i.e. one which solves the Vlasov–Poisson or the Vlasov–Maxwell equations. The effect that the collisions have on a particle-in-cell method is of particular interest, especially in terms of how they affect the statistical noise that is inherent to PIC. This can then be used to investigate classical examples such as Landau damping, or the two-stream instability, which are useful benchmarks for such methods. Another topic of interest is how the methods constructed in this thesis compare to other existing structure-preserving methods for collision operators. There are several such methods in the literature (including grid-based, particle-based, and stochastic approaches), as we have discussed in the introduction, and it is of interest to quantify this comparison both in terms of cost and accuracy of the methods.

Bibliography

Bailo, Rafael, Carrillo, José A. & Hu, Jingwei 2024 The Collisional Particle-In-Cell Method for the Vlasov-Maxwell-Landau Equations , arXiv: 2401.01689.

Bezanson, Jeff, Edelman, Alan, Karpinski, Stefan & Shah, Viral B 2017 Julia: A fresh approach to numerical computing. *SIAM Review* **59** (1), 65–98.

Boozer, Allen H. & Kuo-Petravic, Gioietta 1981 Monte Carlo evaluation of transport coefficients. *The Physics of Fluids* **24** (5), 851–859.

Burby, J W 2017 Finite-dimensional collisionless kinetic theory. *Physics of Plasmas* **24** (3), 32101.

Campos Pinto, Martin, Kormann, Katharina & Sonnendrücker, Eric 2022 Variational Framework for Structure-Preserving Electromagnetic Particle-in-Cell Methods. *Journal of Scientific Computing* **91** (2), 46.

Carrillo, Jose A., Hu, Jingwei, Wang, Li & Wu, Jeremy 2020 A particle method for the homogeneous Landau equation. *Journal of Computational Physics: X* **7**, 100066.

Chen, G., Chacón, L. & Barnes, D.C. 2011 An energy- and charge-conserving, implicit, electrostatic particle-in-cell algorithm. *Journal of Computational Physics* **230** (18), 7018–7036.

Chertock, A. 2017 A Practical Guide to Deterministic Particle Methods. *Handbook of Numerical Analysis* **18**, 177–202.

Degond, Pierre & Mustieles, Francisco-Jose 1990 A deterministic approximation of diffusion equations using particles. *SIAM Journal on Scientific and Statistical Computing* **11** (2), 293–310.

Evstatiev, Evstati G. & Shadwick, Bradley A. 2013 Variational formulation of particle algorithms for kinetic plasma simulations. *Journal of Computational Physics* **245**, 376–398.

Filbet, F. & Sonnendrücker, E. 2003 Comparison of Eulerian Vlasov solvers. *Computer Physics Communications* **150** (3), 247–266.

Gonzalez, O. 1996 Time Integration and Discrete Hamiltonian Systems. *Journal of Nonlinear Science* **6** (5), 449–467.

Grmela, Miroslav 1984*a* Bracket formulation of dissipative fluid mechanics equations. *Physics Letters A* **102** (8), 355–358.

Grmela, Miroslav 1984*b* Particle and bracket formulations of kinetic equations. In *Fluids and Plasmas: Geometry and Dynamics*, pp. 125–132. American Mathematical Society.

Grmela, Miroslav 1985 Bracket formulation of dissipative time evolution equations. *Physics Letters A* **111** (1-2), 36–40.

Hairer, E. & Wanner, G. 2006 *Geometric numerical integration algorithms for ordinary differential equations*.

Hakim, Ammar, Francisquez, Manaure, Juno, James & Hammett, Gregory W. 2020 Conservative discontinuous Galerkin schemes for nonlinear Dougherty-Fokker-Planck collision operators. *Journal of Plasma Physics* , arXiv: 1903.08062.

Hirvijoki, Eero 2021 Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes. *Plasma Physics and Controlled Fusion* **63** (4), 44003.

Hirvijoki, E. & Adams, M. F. 2017 Conservative discretization of the Landau collision integral. *Physics of Plasmas* **24** (3).

Hirvijoki, Eero, Kraus, Michael & Burby, Joshua W. 2018 Metriplectic particle-in-cell integrators for the landau collision operator, arXiv: 1802.05263.

Jeyakumar, S., Kraus, M., Hole, M. J. & Pfefferlé, D. 2024*a* A structure-preserving particle discretisation for the Lenard–Bernstein collision operator. *Journal of Plasma Physics* **90** (3).

Jeyakumar, Sandra, Kraus, Michael, Hole, Matthew J. & Pfefferlé, David 2024*b* Structure-preserving particle methods for the Landau collision operator using the metriplectic framework , arXiv: 2404.18432.

Kaufman, Allan N. 1984 Dissipative hamiltonian systems: A unifying principle. *Physics Letters A* **100** (8), 419–422.

Kaufman, Allan N. & Morrison, Philip J. 1982 Algebraic structure of the plasma quasilinear equations. *Physics Letters A* **88** (8), 405–406.

Kraus, Michael 2013 Variational Integrators in Plasma Physics. PhD thesis, Technische Universität München.

Kraus, Michael, Blickhan, Tobias M. & Jeyakumar, Sandra 2023 VlasovMethods.jl. DOI: 10.5281/zenodo.8123648.

Kraus, Michael & Hirvijoki, Eero 2017 Metriplectic integrators for the Landau collision operator. *Physics of Plasmas* **24** (10), arXiv: 1707.01801.

Kraus, Michael, Kormann, Katharina, Morrison, Philip J. & Sonnendrücker, Eric 2017 GEMPIC: Geometric electromagnetic particle-in-cell methods. *Journal of Plasma Physics* **83** (4).

Laidin, Tino & Pareschi, Lorenzo 2024 Conservative polynomial approximations and applications to Fokker-Planck equations , arXiv: 2402.06473.

Lenard, A. & Bernstein, Ira B. 1958 Plasma oscillations with diffusion in velocity space. *Physical Review* **112** (5), 1456–1459.

Markidis, Stefano & Lapenta, Giovanni 2011 The energy conserving particle-in-cell method. *Journal of Computational Physics* **230** (18), 7037–7052.

Marsden, Jerrold E. & Weinstein, Alan 1982 The Hamiltonian structure of the Maxwell-Vlasov equations. *Physica D: Nonlinear Phenomena* **4** (3), 394–406.

McLachlan, Robert I., Quispel, G. R.W. & Robidoux, Nicolas 1999 Geometric integration using discrete gradients. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* **357** (1754), 1021–1045.

Morrison, Philip J 1980 The Maxwell-Vlasov equations as a continuous Hamiltonian system. *Physics Letters* **80**.

Morrison, Philip J. 1984*a* Bracket formulation for irreversible classical fields. *Physics Letters A* **100** (8), 423–427.

Morrison, Philip J. 1984*b* Some observations regarding brackets and dissipation. *Tech. Rep.*. Center for Pure and Applied Mathematics Report PAM–228, University of California, Berkeley.

Morrison, Philip J. 1986 A paradigm for joined Hamiltonian and dissipative systems. *Physica D: Nonlinear Phenomena* **18** (1-3), 410–419.

Morrison, P. J. 1998 Hamiltonian description of the ideal fluid. *Reviews of Modern Physics* **70** (2), 467–521.

Morrison, P. J. 2017 Structure and structure-preserving algorithms for plasma physics. *Physics of Plasmas* **24** (5), arXiv: 1612.06734.

Morrison, Philip J. & Updike, Michael H. 2023 An inclusive curvature-like framework for describing dissipation: metriplectic 4-bracket dynamics, arXiv: 2306.06787.

Qin, Hong, Liu, Jian, Xiao, Jianyuan, Zhang, Ruili, He, Yang, Wang, Yulei, Sun, Yajuan, Burby, Joshua W., Ellison, Leland & Zhou, Yao 2016 Canonical symplectic particle-in-cell method for long-term large-scale simulations of the Vlasov-Maxwell equations. *Nuclear Fusion* **56** (1).

Quispel, G R W & Turner, G S 1996 Discrete gradient methods for solving odes numerically while preserving a first integral. *Journal of Physics A: Mathematical and General* **29** (13), L341.

Schnake, Stefan, Kendrick, Coleman, Endeve, Eirik, Stoyanov, Miroslav, Hahn, Steven, Hauck, Cory D, Green, David L, Snyder, Phil & Canik, John 2024 Sparse-grid Discontinuous Galerkin Methods for the Vlasov-Poisson-Lenard-Bernstein Model , arXiv: 2402.06493.

Shiroto, Takashi & Sentoku, Yasuhiko 2019 Structure-preserving strategy for conservative simulation of the relativistic nonlinear Landau-Fokker-Planck equation. *Physical Review E* **99** (5), 1–7.

Squire, J, Qin, H & Tang, W M 2012 Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme. *Physics of Plasmas* **19** (8), 84501.

Taitano, W. T., Chacón, L., Simakov, A. N. & Molvig, K. 2015 A mass, momentum, and energy conserving, fully implicit, scalable algorithm for the multi-dimensional, multi-species Rosenbluth-Fokker-Planck equation. *Journal of Computational Physics* **297**, 357–380.

Tyranowski, Tomasz M. 2021*a* Stochastic variational principles for the collisional Vlasov-Maxwell and Vlasov-Poisson equations. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **477** (2252), arXiv: 2102.09611.

Tyranowski, Tomasz M. 2021*b* Stochastic variational principles for the collisional Vlasov-Maxwell and Vlasov-Poisson equations. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **477** (2252).

Yoon, E. S. & Chang, C. S. 2014 A Fokker-Planck-Landau collision equation solver on two-dimensional velocity grid and its application to particle-in-cell simulation. *Physics of Plasmas* **21** (3).

Zhang, Chenglong & Gamba, Irene M. 2017 A conservative scheme for Vlasov Poisson Landau modeling collisional plasmas. *Journal of Computational Physics* **340**, 470–497.

Appendix A

Derivation of the Vlasov Equation

A.1 The BBGKY hierarchy

The Vlasov equation possesses deep roots in the theories of statistical mechanics, as it fundamentally attempts to capture the microscopic behaviour of a plasma through a more simplified, or macroscopic, lens. The Bogoliubov-Born-Green-Kirkwood-Yvon (or BBGKY) hierarchy stands for a series of approximations in statistical mechanics by which the Vlasov equation is derived from the general Liouville equation.

First, we begin by stating the Liouville equation. Let us suppose we have a system of N bodies that are identical with mass m, and whose position and momentum coordinates are denoted $x_i = (q_i, p_i)$, for $i = 1 \dots N$. The Hamiltonian for such a system is given by:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{1 \le i < j \le N} V\left(|q_i - q_j|\right) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{1 \le i < j \le N} V_{ij}, \tag{A.1}$$

where $V(\cdot)$ is a two-body interaction potential function. In the case of plasmas, this interaction potential is given by Coulomb interactions between particles. Hamilton's equations of motion are then:

$$\dot{q}_i = \frac{p_i}{m}, \qquad \dot{p}_i = -\sum_{j \neq i}^{N} (\nabla_i V_{ij}), \tag{A.2}$$

where $\nabla_i = \partial / \partial q_i$.

The N-body distribution function is denoted by $f_N(x_1, \dots, x_N, t)$. Rather than a probability density function for particles, as appears in the Vlasov equation, f_N is a probability density function for *systems*, such that the following quantity

$$f_N(x_1, x_2, \dots, x_N) \mathrm{d}x_1 \mathrm{d}x_2 \dots \mathrm{d}x_N \tag{A.3}$$

represents the probability of finding a *system* of N particles in a state such that $X_1 \in (x_1, x_1 + \mathrm{d}x_1)$, $X_2 \in (x_2, x_2 + \mathrm{d}x_2)$, up to $X_N \in (x_N, x_N + \mathrm{d}x_N)$. Integrating over the whole $6N$-dimensional space, we have that

$$\int f_N(x_1, x_2, \ldots, x_N)\mathrm{d}x_1\mathrm{d}x_2 \ldots \mathrm{d}x_N = 1, \tag{A.4}$$

implying that a system of N particles will be found almost surely in this space.

Its time evolution is obtained via the continuity equation for this function:

$$\frac{\partial}{\partial t} f_N + \sum_{i=1}^{N} \frac{\partial}{\partial q_i}(\dot{q}_i f_N) + \sum_{i=1}^{N} \frac{\partial}{\partial p_i}(\dot{p}_i f_N), \tag{A.5}$$

which through the use of Hamilton's equations (A.2) gives us the Liouville equation:

$$\frac{\partial}{\partial t} f_N + \sum_{i=1}^{N} \frac{p_i}{m} \cdot \nabla_i f_N - \sum_{i=1}^{N} \sum_{j \neq i}^{N} (\nabla_i V_{ij}) \cdot \frac{\partial f_N}{\partial p_i} = 0. \tag{A.6}$$

One of the notable characteristics of this equation is that it can be expressed as:

$$\frac{\mathrm{d}f_N}{\mathrm{d}t} = 0, \tag{A.7}$$

implying that the N-particle distribution function is constant along the phase-space trajectories of the system, and this is referred to as *Liouville's theorem*.

While the statement and implications of Liouville's equation are quite notable, practically speaking, it is an intractable problem to solve for a meaningful number of particles in a plasma ($N \sim 10^{23}$). As such, it is imperative to simplify this equation in a way that makes it more tractable.

First, we begin by noting that the N-body distribution function contains much more information than is desired. For instance, there are many configurations where particle positions in phase-space may be interchanged, resulting in new configurations that are effectively equal to the original. Additionally, many quantities of interest in a plasma are averaged (i.e. they are integrated against the distribution function) and so the microscopic granularity of the full N-body distribution function may not be required.

Thus, we can define a reduced s-particle distribution function, where the dependency on $N - s$ particles has been integrated over:

$$f_s(x_1, \ldots, x_s, t) = \frac{N!}{(N-s)!} \int \mathrm{d}x_{s+1} \ldots \mathrm{d}x_N f_N(x_1, \ldots, x_N, t), \tag{A.8}$$

for $s \in \{1, \ldots, N-1\}$. Thus, $f_1(x_t, t)$ is the probability density function for a single *particle*, whereas f_2 up to f_s are *joint* probability density functions for systems of two particles up to s particles respectively.

By following the same reduction process in the Liouville equation (A.6), we obtain the following:

$$\frac{\partial}{\partial t} f_s + \sum_{i=1}^{s} \frac{p_i}{m} \cdot \nabla_i f_s - \sum_{i=1}^{s} \sum_{j \neq i}^{s} (\nabla_i V_{ij}) \cdot \frac{\partial f_s}{\partial p_i} = \sum_{i=1}^{s} \int \left(\nabla_i V_{i,s+1} \cdot \frac{\partial f_{s+1}}{\partial p_i} \right) \mathrm{d}x_{s+1}, \quad \text{(A.9)}$$

where $s \in \{1, \ldots, N-1\}$, and $V_{i,s+1}$ denotes the interaction potential between the i-th and $s+1$-th particles. This is a system of $N-1$ coupled integro-differential equations, where the evolution equation of the reduced s-particle distribution function f_s depends on f_{s+1}, as seen in the terms on the right-hand side. These $N-1$ coupled equations, together with the Liouville equation, are referred to as the *BBGKY hierarchy*. It should be noted that no approximation has been made in obtaining this set of equations. Solving the $N-1$ equations of the hierarchy is equivalent to solving the Liouville equation itself, and so we must further approximate the system to obtain something that is solvable.

As a result of the coupling between these equations, it is not possible to truncate the hierarchy at any $s < N$ and obtain a closed system of equations simply by doing so. However, we can truncate the system at some s and *approximate* the dependence on f_{s+1} by some function of f_s, resulting in a closed, albeit possibly non-linear, equation. Examples of equations obtained in this manner are the Boltzmann equation, the Landau equation, and of course, the Vlasov equation.

A.2 The Vlasov Equation

We now detail the main steps involved in the derivation of the Vlasov equation.

We are interested in obtaining a closed equation for the case of $s = 1$, i.e. for the single-particle distribution function, f_1. If we consider the $s = 1$ equation in the BBGKY hierarchy,

$$\frac{\partial}{\partial t} f_1 + \frac{p_1}{m} \cdot \nabla_1 f_1 = \int \left(\nabla_1 V_{12} \cdot \frac{\partial f_2}{\partial p_1} \right) \mathrm{d}x_2, \quad \text{(A.10)}$$

we observe that the dependence on the second particle (and therefore the entire system via the hierarchy) arises in two terms: the interaction potential V_{12}, and the two-body distribution function f_2.

First, we consider the treatment of f_2. Treating this as a joint probability distribution function for two particles, we can define it as follows:

$$f_2(x_1, x_2, t) = f_1(x_1, t) f_2(x_2, t) + g(x_1, x_2, t), \tag{A.11}$$

where g is the two-body correlation function. Assuming these correlations are negligible, we insert this approximation into Equation (A.10):

$$\frac{\partial}{\partial t} f_1 + \frac{p_1}{m} \cdot \nabla_1 f_1 = \int \left(\nabla_1 V_{12} \cdot \frac{\partial}{\partial p_1} \left[f_1(x_1, t) f_2(x_2, t) \right] \right) \mathrm{d}x_2. \tag{A.12}$$

Rearranging the right-hand side of the equation, we obtain:

$$\frac{\partial}{\partial t} f_1 + \frac{p_1}{m} \cdot \nabla_1 f_1 = \left(\int f_1(x_2, t) \nabla_1 V_{12} \mathrm{d}x_2 \right) \cdot \frac{\partial}{\partial p_1} f_1(x_1, t). \tag{A.13}$$

Recognising that $a_{12} = -\nabla_1 V_{12}$ is the acceleration experienced by particle 1 due to particle 2, we can consider the following term:

$$a(x_1, t) = -\left(\int f_1(x_2, t) \nabla_1 V_{12} \mathrm{d}x_2 \right) \tag{A.14}$$

as an *ensemble-averaged* acceleration experienced by the first particle. Thus, we obtain

$$\frac{\partial}{\partial t} f_1 + \frac{p_1}{m} \cdot \nabla_1 f_1 + a \frac{\partial}{\partial p_1} f_1(x_1, t) = 0, \tag{A.15}$$

which is referred to as the correlation-less kinetic equation or, in the case where a is generated by electromagnetic fields, as the Vlasov equation.