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Discontinuous Galerkin algorithms for fully kinetic plasmas

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ABSTRACT

We present a new algorithm for the discretization of the non-relativistic Vlasov–Maxwell system of equations for the study of plasmas in the kinetic regime. Using the discontinuous Galerkin finite element method for the spatial discretization, we obtain a high order accurate solution for the plasma's distribution function. Time stepping for the distribution function is done explicitly with a third order strong-stability preserving Runge–Kutta method. Since the Vlasov equation in the Vlasov–Maxwell system is a high dimensional transport equation, up to six dimensions plus time, we take special care to note various features we have implemented to reduce the cost while maintaining the integrity of the solution, including the use of a reduced high-order basis set. A series of benchmarks, from simple wave and shock calculations, to a five dimensional turbulence simulation, are presented to verify the efficacy of our set of numerical methods, as well as demonstrate the power of the implemented features.

1. Introduction

Plasmas are ubiquitous in nature, and the study of plasmas has application to a wide variety of problems, from the development of nuclear fusion, to understanding the dynamic interaction between the solar wind and the Earth's magnetosphere, to elucidating the mysteries of large scale astrophysical phenomena such as binary star collisions or the accretion disks of black holes. Unfortunately, many plasmas of interest are only weakly collisional and far from equilibrium, making the system best described by kinetic theory, in this case, the Vlasov equation. The use of kinetic theory significantly complicates the theoretical analysis and simulation of the plasma's dynamics due to the increased dimensionality of the corresponding equations, which are solved in a combined position and velocity phase space, along with the large collection of waves and instabilities that the kinetic system supports. This complication is usually mitigated in one of two ways: either a reduction of the system via asymptotic expansions of the corresponding equations in appropriate limits for the problem of interest or direct numerical simulation of the plasma by approximating it as a collection of "macroparticles," and employing the particle-in-cell (PIC) algorithm [1]. At scales much larger than the ion gyroradius, fluid models for the plasma are excellent tools for analyzing the macroscopic evolution of the plasma. Likewise, reductions of the system which retain kinetic effects, such as the gyrokinetic expansion of the Vlasov equation [2,3], which averages over the fast cyclotron motion of the particles in the plasma to eliminate one velocity space dimension, have been quite lucrative in both fusion and astrophysical contexts. The PIC algorithm has a long history of success in revealing many novel kinetic features of the plasma's dynamics because,

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outside of the approximation of integrating along “macroparticle” trajectories as opposed to individual particle trajectories, the algorithm makes no approximations of the plasma’s dynamics and retains the vast array of kinetic phenomena intrinsic to the system.

However, these two approaches are not without their disadvantages. Fluid models derived from asymptotic expansions of the Vlasov equation often require sub-grid models for the microphysics being approximated, and, while physically motivated, these closures are not always well-suited for the plasma being modeled. Even kinetic reductions which are closed, sometimes rigorously so, such as the aforementioned gyrokinetics, are almost certainly not valid in all contexts; for example, large amplitude fluctuations and waves above the cyclotron frequency observed in the solar wind and solar corona are beyond the scope of traditional gyrokinetic formulations. Thus, a tool like the PIC algorithm is ideal for studying physics in regimes where no tractable and physically reasonable asymptotic reduction exists. Even so, the approximation of the plasma as a collection of macroparticles introduces counting noise into the resulting solutions, which can pollute the results quite severely, or at the very least complicate the analysis. One can always mollify this concern by increasing the number of particles in the simulation, but the counting noise decreases like $1/\sqrt{N}$, where N is the number of particles per grid cell. This scaling can make the study of physics where the signal-to-noise ratio is low especially challenging. For example, Camporeale et al. [4] have demonstrated that a large number of particles-per-cell is required to correctly identify wave–particle resonances and to compare well with linear theory. One could employ the delta-f PIC method [5], but noise mitigation techniques such as the delta-f PIC method can break down if the distribution function deviates significantly from its initial value.

Therefore, if the problem of interest requires a full Vlasov–Maxwell description and is characterized by a low signal-to-noise ratio, an alternative approach which directly solves the Vlasov equation and gives access to a noise-free solution is desired. While computationally infeasible in the past due to the need to solve a six-dimensional system (three position and three velocity), plus time, to accurately capture the dynamics of the plasma, in recent years, directly solving the Vlasov equation has become a more popular alternative approach to illuminating the microphysics of the plasma’s evolution. Previous Vlasov work has focused almost exclusively on the so-called hybrid framework, treating the electrons as a fluid, usually massless and isothermal, to save significantly on computational cost [6–14], with some exceptions [15,16]. In this paper, we present the addition of a multi-species Vlasov–Maxwell solver to `Gkeyll`, a modular framework in which a variety of plasma physics and fluid dynamics solvers are currently being built [17–24]. Within `Gkeyll`, the Vlasov–Maxwell system is discretized in space with a discontinuous Galerkin finite element method, and discretized in time with a strong stability preserving Runge–Kutta method to form a fully explicit update. The discontinuous Galerkin method combines the power of finite element methods, including high order accuracy and the ability to handle complicated geometries, with the advantages of finite volume methods, including the introduction of limiters to enforce stability and physicality of the solution, and locality of data, for efficient parallelization [25–27]. The high order accuracy and locality of data in particular make our approach especially advantageous; higher order polynomials provide a level of accuracy equivalent to refining the grid at a fraction of the cost, and the locality of data significantly reduces the amount of communication required in the update, enabling the algorithm to scale well on both standard computing architecture and many-core devices. In fact, the discontinuous Galerkin algorithm has been gaining increased attention as a means of discretizing high dimensional transport equations and various flavors of the Vlasov equation, including Vlasov–Poisson, Vlasov–Ampere, and the aforementioned Vlasov–Maxwell [28–30].

The paper is organized as follows: Section 2 provides an overview of the relevant plasma kinetic equation, with discussion of pertinent conservation properties in the continuous system. Section 3 describes the Runge–Kutta discontinuous Galerkin discretization and proves relevant conservation properties of the discrete system in the continuous time limit. Section 4 covers the details of the implementation of the numerical algorithm, including the choice of basis functions to mitigate the computational cost in higher dimensions. Section 5 demonstrates the functionality of the algorithm, including scaling studies and performance analysis of the code on high dimensional benchmarks. Finally, Section 6 summarizes our findings and provides future directions for further numerical improvements while discussing current problems in plasma physics which are now within grasp with this new numerical tool.

2. The Vlasov–Maxwell system

2.1. Basic equations

The time evolution for the distribution function $f_s(t, \mathbf{x}, \mathbf{v})$ for species s in a plasma is given by the Vlasov equation,

$$\frac{\partial f_s}{\partial t} + \nabla \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = 0, \tag{1}$$

where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ is the Lorentz force. In the Lorentz force, q_s and m_s are the charge and mass of species s respectively, and $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields. The operators ∇ and $\nabla_{\mathbf{v}}$ are the gradient operators in configuration and velocity space respectively. Here we are considering two simultaneous limits: the non-relativistic[1] and the collisionless[2] limits.

Since the motion of charged particles creates currents and electromagnetic fields, the electric and magnetic fields in the Vlasov equation evolve self-consistently by the coupling of the Vlasov equation to Maxwell's equations,

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \tag{9}$$

$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}, \tag{10}$$

$$\nabla \cdot \mathbf{E} = \frac{\varrho_c}{\epsilon_0}, \tag{11}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{12}$$

where ϱ_c and $\mathbf{J}$ are the charge and current densities of the plasma. Charge and current densities are determined by moments of the distribution function

$$\varrho_c = \sum_s q_s \langle 1 \rangle_s, \tag{13}$$

and

$$\mathbf{J} = \sum_s q_s \langle \mathbf{v} \rangle_s, \tag{14}$$

where the moment operator for any function $\varphi(\mathbf{v})$ is defined as

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1 The special relativistic limit of the Vlasov equation can be obtained by substitution of the Lorentz boost factors where appropriate and a change of variables from velocity to momentum,

$$\frac{\partial f_s}{\partial t} + \nabla \cdot \left(\frac{\mathbf{p}}{m_s \gamma} f_s \right) + \nabla_{\mathbf{p}} \cdot \left(q_s \left(\mathbf{E} + \frac{\mathbf{p}}{m_s \gamma} \times \mathbf{B} \right) f_s \right) = 0, \tag{2}$$

where γ is the Lorentz boost factor,

$$\gamma = \frac{1}{\sqrt{1 - \frac{|\mathbf{p}|^2}{m_s^2 c^2}}}. \tag{3}$$

This definition of gamma is incorrect. It should be:
gamma = sqrt[1+p^2/(m^2c^2)]
See Wikipedia page https://en.wikipedia.org/wiki/Lorentz_factor

2 The weakly collisional or collisional limits can be obtained by the addition of the Landau–Fokker–Planck [31] collision operator to the right hand side of Eq. (1),

$$\left(\frac{\partial f_s}{\partial t} \right)_{\text{collisions}} = \sum_{s'} \nu_{s,s'} \nabla_{\mathbf{v}} \cdot \int d\mathbf{v}' \overleftrightarrow{\mathbf{U}}(\mathbf{v}, \mathbf{v}') \cdot \left(f_{s'}(\mathbf{v}') \nabla_{\mathbf{v}} f_s(\mathbf{v}) - \frac{m_s}{m_{s'}} f_s(\mathbf{v}) \nabla_{\mathbf{v}'} f_{s'}(\mathbf{v}') \right), \tag{4}$$

where

$$\nu_{s,s'} = \frac{q_s^2 q_{s'}^2 \ln(n_s \lambda_{Ds}^3)}{8\pi m_s \epsilon_0} \tag{5}$$

is the collision frequency of species s colliding with species s', and $\overleftrightarrow{\mathbf{U}}(\mathbf{v}, \mathbf{v}')$ is the Landau tensor,

$$\overleftrightarrow{\mathbf{U}}(\mathbf{v}, \mathbf{v}') = \frac{1}{|\mathbf{v} - \mathbf{v}'|} \left(\mathbf{I} - \frac{(\mathbf{v} - \mathbf{v}')(\mathbf{v} - \mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|^2} \right). \tag{6}$$

Here, $\mathbf{I}$ is the identity tensor. In the definition of the collision frequency, $\lambda_{Ds} = \sqrt{\frac{\epsilon_0 T_s}{n_s q_s^2}}$ is the Debye length. Often, the term in the logarithm, $n_s \lambda_{Ds}^3$, is abbreviated as Λ and called the plasma parameter. Reductions of the collision operator, such as the Bhatnagar–Gross–Krook (BGK) [32] collision operator,

$$\left(\frac{\partial f_s}{\partial t} \right)_{\text{collisions}} = \nu (f_{eq} - f_s), \tag{7}$$

where f_{eq} is some equilibrium distribution function to which the distribution function should relax, are also sometimes considered the weakly collisional or collisional limit. However, given the form of the Landau–Fokker–Planck collision operator, reduced collision operators which maintain a Fokker–Planck structure, i.e., a drag and diffusion term, such as the Lenard–Bernstein [33–35] collision operator,

$$\left(\frac{\partial f_s}{\partial t} \right)_{\text{collisions}} = \nu \nabla_{\mathbf{v}} \cdot ((\mathbf{v} - \mathbf{u}_s) f_s + v_{th_s}^2 \nabla_{\mathbf{v}} f_s), \tag{8}$$

where $\mathbf{u}_s$ and $v_{th_s}^2$ are related to the first and second moments of the distribution function respectively, are often preferred. Note that, while the Landau–Fokker–Planck operator naturally generalizes to a multi-species plasma, as well as the relativistic Vlasov equation, reduced collision operators such as the BGK and Lenard-Bernstein collision operators may require significant modification to include the effects of cross-species collisions and relativistic effects.

$$\langle \varphi(\mathbf{v}) \rangle_s \equiv \int_{-\infty}^{\infty} \varphi(\mathbf{v}) f_s(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v}. \tag{15}$$

If there are external fields, $\mathbf{B}_0$ and $\mathbf{E}_0$, e.g., created by coils or electrodes, we can replace $\mathbf{B} \rightarrow \mathbf{B} + \mathbf{B}_0$ and $\mathbf{E} \rightarrow \mathbf{E} + \mathbf{E}_0$ in the Lorentz force term. External fields do not appear in Maxwell's equations.

2.2. Conservation properties of the Vlasov–Maxwell system

As we mentioned previously, we are interested in deriving a discretization of the non-relativistic, collisionless, Vlasov–Maxwell system. Henceforth, when referring to the Vlasov equation, or the Vlasov–Maxwell system of equations, we emphasize that we are referring to the form of the Vlasov equation given in Eq. (1). Before proceeding to the derivation of the discretization, there are several key conservation properties of the continuous Vlasov–Maxwell system which we review here for the purposes of exploring these same conservation relations in the discrete system. To prove various properties of the Vlasov–Maxwell system we need to assume that $f(t, \mathbf{x}, \mathbf{v} \rightarrow \pm\infty) \rightarrow 0$ faster than $\mathbf{v}^n$ for finite n. Also, we will assume that either the configuration space is periodic, or that the distribution function vanishes on the boundaries.

Proposition 1. *The Vlasov–Maxwell system conserves particles.*

Proof. Upon integration of Eq. (1) over all of phase-space and summation over all species, we obtain

$$\frac{d}{dt} \int_{\Omega} \sum_s \langle 1 \rangle_s \, d\mathbf{x} = 0. \tag{16}$$

This relation is a straightforward consequence of the fact that the Vlasov–Maxwell system is written as a conservation law in phase-space. We further note that this relation holds independently for each species because in the absence of recombination and ionization, there is no mechanism for conversion of one particle species to another. □

Proposition 2. *The collisionless Vlasov–Maxwell system conserves the L_2 norm of the distribution function, i.e.,*

$$\frac{d}{dt} \int_K \frac{1}{2} f_s^2 \, d\mathbf{z} = 0, \tag{17}$$

where the integration is taken over the complete phase-space, K.

Proof. The Vlasov–Maxwell system can be written as a non-linear advection equation in phase-space. To do this, we introduce the phase-space velocity vector $\boldsymbol{\alpha}_s \equiv (\mathbf{v}, \mathbf{F}_s)$ and the phase-space gradient operator $\nabla_{\mathbf{z}} \equiv (\nabla, \nabla_{\mathbf{v}})$. The flow in phase-space is incompressible, i.e, $\nabla_{\mathbf{z}} \cdot \boldsymbol{\alpha}_s = 0$, because $\mathbf{v}$ is the velocity coordinate and thus has no configuration space dependence, and likewise, the Lorentz force $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ has no velocity space divergence. The latter point is slightly subtle because while the electric field $\mathbf{E}$ has no velocity space dependence, the $\mathbf{v} \times \mathbf{B}$ force has no velocity space divergence by properties of the cross product. Eq. (1) can then be written as

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha}_{\mathbf{s}} f_s) = 0, \tag{18}$$

where $f_s(t, \mathbf{z})$ is the distribution function. If we multiply Eq. (18) by f_s and integrate over all of phase-space we obtain

$$\frac{d}{dt} \int_K \frac{1}{2} f_s^2 \, d\mathbf{z} - \int_K \nabla_{\mathbf{z}} f_s \cdot \boldsymbol{\alpha}_{\mathbf{s}} f_s \, d\mathbf{z} = 0. \tag{19}$$

We have integrated by parts and used boundary conditions to eliminate the surface term. Now, using incompressibility of phase-space, we can write $\nabla_{\mathbf{z}} f_s \cdot \boldsymbol{\alpha}_{\mathbf{s}} f_s = \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha}_{\mathbf{s}} f_s^2)/2$. Using this relation in the above expression and converting the volume integral into a surface integral, combined with the use of boundary conditions, gives the desired conservation law. □

Proposition 3. *The collisionless Vlasov–Maxwell system conserves the entropy $S = -f \ln(f)$ of the system,*[3]

$$\frac{d}{dt} \int_K -f_s \ln(f_s) \, d\mathbf{z} = 0. \tag{20}$$

[3] The inclusion of the minus sign in the definition of the entropy is in concordance with the traditional physics definition of the entropy. It is common in the theory of hyperbolic conservation laws to drop the minus sign. This definition has the effect that the physicist's entropy is a non-decreasing quantity, while the mathematician's entropy is a non-increasing quantity.

Proof. We multiply Eq. (18) by $-\ln(f_s)$, integrate over all of phase space, and after a bit of algebra, we obtain,

$$\frac{d}{dt}\int_K -f\ln(f)\,d\mathbf{z} + \int_K \frac{\partial f_s}{\partial t} + \nabla_{\mathbf{z}}\ln(f_s)\cdot\boldsymbol{\alpha}_{\mathbf{s}} f_s\,d\mathbf{z} = 0. \tag{21}$$

In the first two terms, we have used the fact that $-\ln(f)\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} - \frac{\partial f\ln(f)}{\partial t}$ by the product rule, and in the last term, we have used integration by parts and eliminated the surface term. Now, since $\nabla_{\mathbf{z}}\ln(f_s) = \frac{\nabla_{\mathbf{z}} f_s}{f_s}$, we can see that the latter two terms just become the Vlasov equation written in the form of Eq. (18). Since in the collisionless limit the Vlasov equation equals 0, the latter two terms vanish and we are left with our desired conservation relation. □

Proposition 4. *The Vlasov–Maxwell system conserves total (particles plus field) momentum.*

Proof. We multiply Eq. (1) by $m_s\mathbf{v}$, integrate over all of phase-space, and sum over all species to obtain,

$$\frac{\partial}{\partial t}\int_\Omega \sum_s \langle m_s\mathbf{v}\rangle_s\,d\mathbf{x} + \underbrace{\int_\Omega \nabla\cdot\sum_s\langle m_s\mathbf{v}\mathbf{v}\rangle_s\,d\mathbf{x}}_{=0\text{ on integration by parts and use of BCs}} - \int_\Omega (\varrho_c\mathbf{E} + \mathbf{J}\times\mathbf{B})\,d\mathbf{x} = 0. \tag{22}$$

In the last term, we have used integration by parts and $\nabla_{\mathbf{v}}\mathbf{v} = \mathbf{I}$. To make further progress, we consider Maxwell's equations. Taking the cross-product of Eq. (9) with $\epsilon_0\mathbf{E}$, and the cross-product of Eq. (10) with $\mathbf{B}/\mu_0$ and subtracting the resulting equations we obtain

$$\epsilon_0\frac{\partial}{\partial t}(\mathbf{E}\times\mathbf{B}) + \epsilon_0\underbrace{\mathbf{E}\times(\nabla\times\mathbf{E})}_{(\nabla\mathbf{E})\cdot\mathbf{E}-(\mathbf{E}\cdot\nabla)\mathbf{E}} + \frac{1}{\mu_0}\underbrace{\mathbf{B}\times(\nabla\times\mathbf{B})}_{(\nabla\mathbf{B})\cdot\mathbf{B}-(\mathbf{B}\cdot\nabla)\mathbf{B}} = -\mathbf{J}\times\mathbf{B}. \tag{23}$$

Now, for any vector field $\mathbf{A}$ we have $(\nabla\mathbf{A})\cdot\mathbf{A} = \nabla|\mathbf{A}|^2/2$ and $(\mathbf{A}\cdot\nabla)\mathbf{A} = \nabla\cdot(\mathbf{A}\mathbf{A}) - \mathbf{A}\nabla\cdot\mathbf{A}$. Using these vector identities and the divergence Eqns. (11) and (12) gives

$$\epsilon_0\frac{\partial}{\partial t}(\mathbf{E}\times\mathbf{B}) + \nabla\left(\frac{\epsilon_0}{2}|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2\right) - \nabla\cdot\left(\epsilon_0\mathbf{E}\mathbf{E} + \frac{1}{\mu_0}\mathbf{B}\mathbf{B}\right) + \varrho_c\mathbf{E} = -\mathbf{J}\times\mathbf{B}. \tag{24}$$

Finally, inserting Eq. (24) into Eq. (22), integrating by parts, and using configuration space boundary conditions gives

$$\frac{d}{dt}\int_\Omega\left(\sum_s\langle m_s\mathbf{v}\rangle_s + \epsilon_0\mathbf{E}\times\mathbf{B}\right)d\mathbf{x} = 0. \tag{25}$$

The first term is the particle momentum, and the second term is the field momentum. □

Proposition 5. *The Vlasov–Maxwell system conserves total (particles plus field) energy.*

Proof. We multiply Eq. (1) by $m_s|\mathbf{v}|^2/2$, integrate over all phase-space, and sum over all species to obtain,

$$\frac{\partial}{\partial t}\int_\Omega\sum_s\langle\frac{1}{2}m_s|\mathbf{v}|^2\rangle_s\,d\mathbf{x} + \underbrace{\int_\Omega\nabla\cdot\sum_s\langle\frac{1}{2}m_s|\mathbf{v}|^2\mathbf{v}\rangle_s\,d\mathbf{x}}_{=0\text{ on integration by parts and use of BCs}} - \int_\Omega \mathbf{E}\cdot\mathbf{J}\,d\mathbf{x} = 0, \tag{26}$$

where we have used integration by parts and $\nabla_{\mathbf{v}}(m_s|\mathbf{v}|^2/2)\cdot\mathbf{F}_s = q_s\mathbf{v}\cdot\mathbf{E}$ to evaluate the third term on the left hand side. To make further progress, we again examine Maxwell's equations. Taking the dot product of Eq. (10) with $\mathbf{E}/\mu_0$ and the dot product of Eq. (9) with $\mathbf{B}/\mu_0$ and adding the resulting equations gives us

$$\frac{\partial}{\partial t}\left(\frac{\epsilon_0}{2}|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2\right) + \frac{1}{\mu_0}\underbrace{(\mathbf{B}\cdot(\nabla\times\mathbf{E}) - \mathbf{E}\cdot(\nabla\times\mathbf{B}))}_{=\nabla\cdot(\mathbf{E}\times\mathbf{B})} = -\mathbf{E}\cdot\mathbf{J}. \tag{27}$$

Using this result in Eq. (26), integrating by parts, and using configuration space boundary conditions gives the total energy conservation law

$$\frac{d}{dt}\int_\Omega\left(\sum_s\langle\frac{1}{2}m_s|\mathbf{v}|^2\rangle_s + \frac{\epsilon_0}{2}|\mathbf{E}|^2 + \frac{1}{2\mu_0}|\mathbf{B}|^2\right)d\mathbf{x} = 0. \tag{28}$$

The first term in this expression is the total particle energy, and the second two terms make up the electromagnetic field energy. □