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A Spectral Algorithm for Solving
the Relativistic Vlasov-Maxwell Equations

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ABSTRACT

A spectral method algorithm is developed for the numerical solution of the full six-dimensional Vlasov-Maxwell system of equations. Here, the focus is on the electron distribution function, with positive ions providing a constant background. The algorithm consists of a Jacobi polynomial-spherical harmonic formulation in velocity space and a trigonometric formulation in position space. A transform procedure is used to evaluate nonlinear terms. The algorithm is suitable for performing moderate resolution simulations on currently available supercomputers for both scientific and engineering applications.

1. The Relativistic Vlasov-Maxwell Equations

The dynamics of a high-energy, collisionless plasma are described by the relativistic Vlasov-Maxwell equations [1]. These nonlinear equations include special relativistic effects [2] and couple the equations of the electromagnetic field (Maxwell's equations) with the evolution equations for single-particle distribution functions (Vlasov equations). In the simplest case, a plasma has two species, protons and electrons. Protons have charge $e>0$, mass m_p, and distribution function f_p, while electrons have charge $-e<0$, mass: m_e, and distribution function f_e. Although non-relativistic Vlasov-Poisson and Vlasov-Maxwell systems have received much attention in the distant [3-15] and more recent [16-23] past, relativistic systems appear to be somewhat less explored, although there have been linear treatments [24-27]. Here, an algorithm for a spectral method numerical solution of a fully relativistic, nonlinear Vlasov-Maxwell system is developed. The goal is to set up the basic framework necessary for numerical simulation in the full six-dimensional case. The purpose of this work is to provide a means to enable the study—and ultimately the prediction—of high-energy charged-particle distributions in space, both for intrinsic scientific interest and for optimizing human and robotic space exploration.

The *Vlasov* equations for the distribution functions $f_p(\mathbf{x},\mathbf{p},t)$ and $f_e(\mathbf{x},\mathbf{p},t)$ are

$$(1.1) \quad \frac{\partial f_p}{\partial t} + \mathbf{v} \cdot \frac{\partial f_p}{\partial \mathbf{x}} + e\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \cdot \frac{\partial f_p}{\partial \mathbf{p}} = 0$$

$$(1.2) \quad \frac{\partial f_e}{\partial t} + \mathbf{v} \cdot \frac{\partial f_e}{\partial \mathbf{x}} - e\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \cdot \frac{\partial f_e}{\partial \mathbf{p}} = 0 .$$

To determine the *self-consistent* fields $\mathbf{E}$ and $\mathbf{B}$, the Maxwell equations are needed:

$$(1.3) \quad \nabla \cdot \mathbf{B} = 0$$

$$(1.4) \quad \nabla \cdot \mathbf{E} = 4\pi \rho$$

$$(1.5) \quad \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$(1.6) \quad \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c}\mathbf{j} .$$

The sources present in (1.4) and (1.6) are the charge density ρ and the current density $\mathbf{j}$:

$$(1.7) \quad \rho = \rho_p + \rho_e = e \int \left(f_p - f_e \right) d\mathbf{p}$$

$$(1.8) \quad \mathbf{j} = \mathbf{j}_p + \mathbf{j}_e = e \int \left(f_p - f_e \right) \mathbf{v} \, d\mathbf{p} .$$

Additionally, **E** and **B** can have *external* components, as well as self-consistent ones, which can serve as external drivers of the coupled Vlasov-Maxwell system.

The solution of this set of integro-differential equations presents a great challenge, because of both the nonlinearity of the couplings and the six-dimensional nature of the solution space of the distribution function. Except in special cases, nonlinearity requires the use of computer simulation, while the presence of six dimensions has, in the past, pushed such simulations beyond the capabilities of then-available computer systems. However, we have now begun to move into an era of fast computers with large core memories, and these machines are providing the resources necessary to perform simulations of six-dimensional continua with a moderate amount of resolution. It is in this context that the following algorithm is presented and we hope that this will help further the development of computer simulations of the Vlasov-Maxwell system and will lead to a greater understanding of the evolution and distribution of high-energy charged particles in space (and other) plasmas.

2. Nondimensional Form of the Equations

First, let us nondimensionalize the equations of the previous section. To do this, we denote a characteristic length by L, and define

$$(2.1) \quad t' = \frac{ct}{L}, \quad \mathbf{x}' = \frac{\mathbf{x}}{L}, \quad \mathbf{v}' = \frac{\mathbf{v}}{c}, \quad \mathbf{p}' = \frac{\mathbf{p}}{mc}, \quad \nabla' = L\nabla .$$

In the previous section, Maxwell's equations were written in Gaussian form, in which the electric field **E** and magnetic induction **B** have the same units. To nondimensionalize Maxwell's equations, we choose B_0 as a characteristic electromagnetic field strength and n_0 as a characteristic number density, so that the fields and sources are transformed into

$$(2.2) \quad \mathbf{E}' = \frac{\mathbf{E}}{B_0}, \quad \mathbf{B}' = \frac{\mathbf{B}}{B_0}, \quad \rho_+ = \frac{\rho_p}{en_0}, \quad \rho_- = \frac{\rho_e}{en_0}, \quad \mathbf{j}_+ = \frac{\mathbf{j}_p}{en_0c}, \quad \mathbf{j}_- = \frac{\mathbf{j}_e}{en_0c} .$$

Here, the dimensional and dimensionless quantities are functions of $(\mathbf{x},\mathbf{p},t)$ and $(\mathbf{x}',\mathbf{p}',t')$, respectively. Also, using (1.4) and (1.6), a natural choice for B_0 is $B_0 = eLn_0$, so we will adopt this definition. The nondimensional Maxwell's equations are

(2.3) $\nabla' \cdot \mathbf{B}' = 0$

(2.4) $\nabla' \cdot \mathbf{E}' = 4\pi\left(\rho_+ + \rho_-\right)$

(2.5) $\dfrac{\partial \mathbf{B}'}{\partial t'} = -\nabla' \times \mathbf{E}'$

(2.6) $\dfrac{\partial \mathbf{E}'}{\partial t'} = \nabla' \times \mathbf{B}' - 4\pi\left(\mathbf{j}_+ + \mathbf{j}_-\right)$.

The distribution functions, in turn, take the form:

(2.7) $f_+(\mathbf{x}',\mathbf{p}',t') = \dfrac{(mc)^3}{n_0} f_p(\mathbf{x},\mathbf{p},t), \quad f_-(\mathbf{x}',\mathbf{p}',t') = \dfrac{(mc)^3}{n_0} f_e(\mathbf{x},\mathbf{p},t)$.

The nondimensional Vlasov equation is

(2.8) $\dfrac{\partial f_\pm}{\partial t'} + \mathbf{v}' \cdot \dfrac{\partial f_\pm}{\partial \mathbf{x}'} \pm \beta_\pm \left(\mathbf{E}' + \mathbf{v}' \times \mathbf{B}'\right) \cdot \dfrac{\partial f_\pm}{\partial \mathbf{p}'} = 0$.

The constants $\beta_\pm$ can be given in terms of L, n_0, and the classical radius of the electron r_e:

(2.9) $\beta_- = n_0 r_e L^2, \quad \beta_+ = \dfrac{m_e}{m_p}\beta_-, \quad r_e = \dfrac{e^2}{m_e c^2}$.

Unless a different characteristic length L is defined for protons and electrons, the relations in (2.9) indicate that the dynamic coupling of the electromagnetic field to the proton distribution function f_+ is less than that of the field to the electron distribution function f_- by a factor of m_p/m_e = 1830. Assuming that there is only one overall characteristic length L, then the dynamic evolution of f_- can be thought of as occurring on a static proton background, whose sole purpose is to provide overall charge neutrality, at least for times which are short compared to those required for an appreciable evolution of f_+. Here, it is the electron distribution function evolution that will be of primary concern and, to this end, we will simplify notation by choosing $\beta_- = 1$ and redefining $f_- = f$. Furthermore, we will henceforth drop all primes and accept that all variables

occurring in all equations are dimensionless. The nondimensional equations we will be concerned with are the following:

$$(2.10) \quad \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

$$(2.11) \quad \nabla \cdot \mathbf{B} = 0$$

$$(2.12) \quad \nabla \cdot \mathbf{E} = 4\pi \rho$$

$$(2.13) \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$(2.14) \quad \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - 4\pi \mathbf{j}$$

$$(2.15) \quad \rho = 1 - \int f \, d\mathbf{p}$$

$$(2.16) \quad \mathbf{j} = - \int f \, \mathbf{v} \, d\mathbf{p} .$$

3. Formulation in Velocity Space

The distribution function depends on $\mathbf{p}$ rather than $\mathbf{v}$ because the six-dimensional phase space volume element $d\mathbf{x}d\mathbf{p} = dxdydzdp_x dp_y dp_z$ and the distribution function $f(\mathbf{x},\mathbf{p})$ are invariant [2] under Lorentz transformations, while $d\mathbf{x}d\mathbf{v}$ and $f(\mathbf{x},\mathbf{v})$ are not. However, limits on the velocity components are $-1 \le v_k \le 1$, while the limits on momentum are $-\infty < p_k < \infty$. For computational purposes, we will work in velocity space, since the associated finite domain is more commensurate with the finite numerical structure of a digital computer.

The dimensionless relation between momentum and velocity is

$$(3.1) \quad \mathbf{p} = \frac{\mathbf{v}}{\sqrt{1 - v^2}} .$$

To transform from a momentum space formulation to one in velocity space, we need to calculate the Jacobian of the transformation, and to apply the chain rule of differential calculus to the equations of the previous section. These activities require the following partial derivatives, which can be derived from (3.1):

$$(3.2) \quad \frac{\partial p_i}{\partial v_k} = \frac{\left[\delta_{ik}\left(1-v^2\right)+v_iv_k\right]}{\left(1-v^2\right)^{3/2}}$$

$$(3.3) \quad \frac{\partial v_i}{\partial p_k} = \left(\delta_{ik}-v_iv_k\right)\left(1-v^2\right)^{1/2}.$$

Here, d is the dimension of the velocity space, and repeated indices, when used, will denote an implicit summation from 1 to d:

$$(3.4) \quad v^2 = v_iv_i \equiv \sum_{i=1}^{d} v_i^2.$$

The Jacobian for transforming the integrals in (2.15) and (2.16) is

$$(3.5) \quad \det\left|\frac{\partial p_i}{\partial v_k}\right| = \left(1-v^2\right)^{-d/2-1}.$$

Let us also transform the Vlasov equation (2.10) by using (3.2), along with

$$(3.6) \quad g(x,v) = f(x,p).$$

Then, equation (2.10) becomes

$$(3.7) \quad \frac{\partial g}{\partial t} + \mathbf{v}\cdot\frac{\partial g}{\partial \mathbf{x}} - (\mathbf{E}+\mathbf{u}\times\mathbf{B})_i\left(\delta_{ik}-v_iv_k\right)\left(1-v^2\right)^{1/2}\frac{\partial g}{\partial v_k} = 0.$$

(Again, repeated indices denote summation.)

Since no massive particles have a speed of c or greater, we must have $g = 0$ for $v^2 \geq 1$. The distribution function g can be written as

$$(3.8) \quad g(\mathbf{x},\mathbf{v}) = \begin{cases} \left(1-v^2\right)^n G(\mathbf{x},\mathbf{v}), & v^2 \leq 1, \quad n > 0 \\ 0, & v^2 > 1 \end{cases}.$$

We will assume that G can be represented by an analytic function in the v_k over the domain $v^2 \leq 1$. Also, using $n > 1$ in (3.8) will ensure that not only the distribution function, but also its first derivative, will be zero at $v^2 = 1$.

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Using (3.5) and (3.8), the density integral (2.15) becomes

$$(3.9) \quad \rho = 1 - \int_{-\infty}^{\infty} f \, d\mathbf{p} = 1 - \int_{-1}^{1} \left(1 - v^2\right)^{n - \frac{d}{2} - 1} G \, H\left(1 - v^2\right) d\mathbf{v}.$$

Here, $H(z)$ is the step function, which is equal to unity if $z \geq 0$, and equal to zero otherwise. The current integral (2.16) similarly becomes

$$(3.10) \quad \mathbf{j} = - \int_{-\infty}^{\infty} f \mathbf{v} \, d\mathbf{p} = - \int_{-1}^{1} \mathbf{v} \left(1 - v^2\right)^{n - \frac{d}{2} - 1} G \, H\left(1 - v^2\right) d\mathbf{v}$$

Using (3.9), equation (3.8) becomes

$$(3.11) \quad \frac{\partial G}{\partial t} + \mathbf{v} \cdot \frac{\partial G}{\partial \mathbf{x}} - (\mathbf{E} + \mathbf{u} \times \mathbf{B})_i \left(1 - v^2\right)^{\frac{1}{2}} \left[\left(\delta_{ik} - v_i v_k\right) \frac{\partial G}{\partial v_k} - 2n v_i G \right] = 0.$$

The choice of n in (3.9), (3.10) and (3.11) is determined so as to simplify the algorithm.

4. Spectral Method Formulation

Since we wish to consider a fully three-dimensional velocity space, we will set $d = 3$. When this three-dimensional velocity space ("v-space") is coupled with a three-dimensional position space, the result is the full six-dimensional phase space of the single particle distribution function. In a three-dimensional relativistic velocity space, the domain is the interior of the sphere $v^2 = 1$, so that a spherical polar coordinate system in velocity space is appropriate:

$$(4.1) \quad \mathbf{v} = v \left[\sin \theta \left(\cos\varphi \, \hat{\mathbf{x}} + \sin\varphi \, \hat{\mathbf{y}}\right) + \cos\theta \, \hat{\mathbf{z}}\right]$$

Here, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ are orthonormal Cartesian unit vectors. In the velocity-space spherical coordinate system (v, θ, φ), equation (3.11) takes the form:

$$(4.2) \quad \frac{\partial G}{\partial t} + \mathbf{v} \cdot \frac{\partial G}{\partial \mathbf{x}} - \left(1 - v^2\right)^{\frac{1}{2}} \left\{ (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial G}{\partial \mathbf{v}} - \mathbf{E} \cdot \mathbf{v} \left[v \frac{\partial G}{\partial v} + 2n\left(1 - v^2\right) G \right] \right\} = 0.$$

The density integral (3.10) and corresponding current integral become (here, the element of solid angle is $d\Omega = \sin\theta \, d\theta \, d\varphi$)

$$(4.3) \quad \rho = 1 - \int \left(1 - v^2\right)^{n - \frac{3}{2} - 1} G \, d\mathbf{v} = 1 - \int v^2 \left(1 - v^2\right)^{n - \frac{3}{2} - 1} G \, dv \, d\Omega$$

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$$(4.4) \quad \mathbf{j} = - \int \left(1 - v^2\right)^{n-\frac{3}{2}-1} \mathbf{v} \, G \, dv = - \int \mathbf{v} \, v^2 \left(1 - v^2\right)^{n-\frac{3}{2}-1} G \, dv \, d\Omega.$$

Our ultimate goal is to simulate numerically the evolution of the distribution function. To this end, a spectral method algorithm will be developed in which dependent variables are expanded in terms of known functions. Since the domain in v-space is a three-dimensional sphere, an appropriate choice of expansion functions for the angular dependence of the G is the well-known spherical harmonics $Y_{nm}(\theta,\varphi)$ [28] (the P_n^m are the associated Legendre functions):

$$(4.5) \quad Y_{nm}(\theta,\varphi) \equiv (-1)^m \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_n^m (\cos\theta) e^{im\varphi}.$$

A choice of radial expansion functions is complicated by the relativistic factor $(1-v^2)^{n-3/2-1}$ in the integrands of (4.3) and (4.4). This difficulty is eliminated by choosing $n = 5/2$, which removes the relativistic factor from (4.3) and (4.4), although not from (4.2). [If n = 2 is chosen, the integrands in (4.3) and (4.4) appear to gain a weight function appropriate to Chebyshev polynomials. However, the domain of v is $0 \le v \le 1$, while the Chebyshev polynomials $T_n(z)$ are orthogonal over the interval $-1 \le z \le 1$, and a transformation $z = 2v-1$ produces a weight function no longer in accord with the orthogonality properties of the $T_n(z)$.]

Using $n = 5/2$ reduces (4.3) and (4.4) to simpler forms:

$$(4.6) \quad \rho = 1 - \int_{v=0}^{1} dv \int_{\theta=0}^{\pi} d\theta \int_{\varphi=0}^{2\pi} d\varphi \, G \, v^2 \sin\theta$$

$$(4.7) \quad \mathbf{j} = - \int_{v=0}^{1} dv \int_{\theta=0}^{\pi} d\theta \int_{\varphi=0}^{2\pi} d\varphi \, G \, \mathbf{v} \, v^2 \sin\theta.$$

The choice of radial expansion function is now straightforward. We will use a set of polynomials that are orthogonal over the interval $0 \le v \le 1$, with a weighting function of v^2. These are the shifted Jacobi polynomials of index (0,2): $P_n^{0,2}(2v-1)$, which are described in detail elsewhere [29]. Here, the necessary results are

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$$P_0^{0,2}(s) = 1$$

$$P_1^{0,2}(s) = 2s - 1$$

$$(4.8) \quad P_2^{0,2}(s) = \frac{15}{4}s^2 - \frac{5}{2}s - \frac{1}{4}$$

$$\vdots$$

$$P_{n+1}^{0,2}(s) = \frac{2n+3}{n+3}\left[\frac{n+2}{n+1}s - \frac{1}{(n+1)^2}\right]P_n^{0,2}(s) - \frac{n}{n+3}\left(\frac{n+2}{n+1}\right)^2 P_{n-1}^{0,2}(s)$$

$$(4.9) \quad \int_{-1}^{1}(1+s)^2 P_n^{0,2}(s)P_m^{0,2}(s)\,ds = \frac{8}{2n+3}\delta_{nm}$$

$$(4.10) \quad P_{n+1}'^{0,2}(s) = \frac{(2n+3)(n+2)}{(n+1)(n+3)}\left[\frac{P_n^{0,2}(s)}{n+2} + \frac{nP_{n-1}^{0,2}(s)}{2n+3} + (n+1)P_n^{0,2}(s)\right].$$

The symbol $P_n' \equiv dP_n/ds$ denotes the first derivative of the nth order polynomial $P_n(s)$.

Using (4.9), let us define the normalized polynomial $R_n(v)$:

$$a) \quad R_n(v) \equiv \sqrt{2n+3}\, P_n^{0,2}(2v-1)$$

$$(4.11)$$

$$b) \quad \int_0^1 v^2 R_n(v)R_m(v)\,dv = \delta_{nm}.$$

The distribution function G then has the expansion:

$$(4.12) \quad G(v,\theta,\varphi) = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\gamma_{knm}R_k(v)Y_{nm}(\theta,\varphi).$$

Here, it should be noted that the $\gamma_{knm} = \gamma_{knm}(\mathbf{x},t)$ are functions of position $\mathbf{x}$ and time t.

The coefficients γ_{knm} can be determined by the inverse operation $\langle\cdots\rangle_{knm}$:

$$(4.13) \quad \gamma_{knm} = \langle G\rangle_{knm} \equiv \int G(v,\theta,\varphi)R_k(v)Y_{nm}^*(\theta,\varphi)\,v^2\,dv\,d\Omega.$$

If (4.12) is placed into (4.6) and (4.13) is used, the result is

$$(4.14) \quad \rho = 1 - \gamma_{000}.$$

To evaluate (4.7), (4.1) can be written as

$$(4.15) \quad \mathbf{v} = \sqrt{\frac{4\pi}{3}}\, v \left(Y_{11}^{*}\, \hat{\mathbf{e}}_{+} + Y_{1,-1}^{*}\, \hat{\mathbf{e}}_{-} + Y_{10}^{*}\, \hat{\mathbf{e}}_{0} \right).$$

Here, the complex unit vectors are

$$(4.16) \quad \hat{\mathbf{e}}_{+} = -\frac{\hat{\mathbf{x}}+i\hat{\mathbf{y}}}{\sqrt{2}}, \quad \hat{\mathbf{e}}_{-} = \frac{\hat{\mathbf{x}}-i\hat{\mathbf{y}}}{\sqrt{2}}, \quad \hat{\mathbf{e}}_{0} = \hat{\mathbf{z}}.$$

Similarly, using (4.1), (4.12) and (4.13), allows the integral (4.7) to be determined:

$$(4.17) \quad \mathbf{j} = \sqrt{\pi}\, \mathrm{Re}\left[\left(\frac{1}{\sqrt{15}} \gamma_{111} + \gamma_{011} \right) \hat{\mathbf{e}}_{+} \right] - \frac{\sqrt{\pi}}{2}\left(\frac{1}{\sqrt{15}} \gamma_{110} + \gamma_{010} \right) \hat{\mathbf{e}}_{0}$$

It is clear that the choice of expansion functions leads to an easy evaluation of the charge density and current, once the expansion functions of the distribution function are known. When ρ and $\mathbf{j}$ are determined, Maxwell's equations (2.11) to (2.14) can be used to find $\mathbf{E}$ and $\mathbf{B}$. These, in turn, affect the evolution of the γ_{knm} through (4.1). The spectral form of the evolution equations will be described next.

5. Spectral Form of the Vlasov Equation

The Vlasov equation (4.2) is, in a three-dimensional velocity space spherical polar coordinate system,

$$(5.1) \quad \frac{\partial G}{\partial t} + \mathbf{v} \cdot \frac{\partial G}{\partial \mathbf{x}} - \mathbf{E} \cdot \hat{\mathbf{v}}\left(1-v^2\right)^{3/2}\left(\frac{\partial G}{\partial v} - 5vG \right) - \left(1-v^2\right)^{1/2}\left(\mathbf{E} \cdot \frac{\mathbf{D}}{v} G - \mathbf{B} \cdot \hat{\mathbf{v}} \times DG \right) = 0.$$

Here $\mathbf{D}$ is the angular derivative part of the velocity space gradient operator:

$$(5.2) \quad \frac{\partial}{\partial \mathbf{v}} \equiv \hat{\mathbf{v}}\frac{\partial}{\partial v} + \frac{1}{v}\mathbf{D}, \qquad \mathbf{D} \equiv \hat{\boldsymbol{\theta}}\frac{\partial}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{\sin\theta}\frac{\partial}{\partial \phi}.$$

In the above, $\hat{\mathbf{v}}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}}$ are the unit vectors in the v, θ, ϕ directions, respectively.

Now, we subject equation (5.1) to the inverse operation $\langle \cdots \rangle_{knm}$ defined in (4.12):

$$(5.3) \quad \frac{\partial \gamma_{knm}}{\partial t} + \nabla \cdot \mathbf{N}_{knm}^{(0)} = \mathbf{E} \cdot \left[\mathbf{N}_{knm}^{(1)} + \mathbf{N}_{knm}^{(2)} \right] - \mathbf{B} \cdot \mathbf{N}_{knm}^{(3)}$$

where

$$(5.4) \quad \mathbf{N}^{(0)}_{knm} = \langle \mathbf{v}\, G \rangle_{knm}$$

$$(5.5) \quad \mathbf{N}^{(1)}_{knm} = \left\langle \hat{\mathbf{v}} \left(1 - v^2\right)^{3/2} \left(\frac{\partial G}{\partial v} - 5vG \right) \right\rangle_{knm}$$

$$(5.6) \quad \mathbf{N}^{(2)}_{knm} = \left\langle v^{-1} \left(1 - v^2\right)^{1/2} \mathbf{D}G \right\rangle_{knm}$$

$$(5.7) \quad \mathbf{N}^{(3)}_{knm} = \left\langle \left(1 - v^2\right)^{1/2} \hat{\mathbf{v}} \times \mathbf{D}G \right\rangle_{knm}.$$

At this point, we use the properties [28] of the angular momentum operator, **L**:

$$(5.8) \quad \mathbf{L} \equiv -i\,\hat{\mathbf{v}} \times \mathbf{D} = \frac{1}{\sqrt{2}}\left(L_+ \hat{\mathbf{e}}_- - L_- \hat{\mathbf{e}}_+ \right) + L_z \hat{\mathbf{e}}_0,$$

where

$$(5.9) \quad L_\pm = \pm e^{\pm i\varphi} \left(\frac{\partial}{\partial \theta} \pm i \cot\theta \frac{\partial}{\partial \varphi} \right), \quad L_z = -i \frac{\partial}{\partial \varphi}.$$

We will also need

$$(5.10) \quad \mathbf{D} \equiv -i\,\hat{\mathbf{v}} \times \mathbf{L} = \frac{1}{\sqrt{2}} \cos\theta \left(L_+ \hat{\mathbf{e}}_- + L_- \hat{\mathbf{e}}_+ \right) - \hat{\mathbf{e}}_0 \sin\theta \frac{\partial}{\partial \theta}$$

$$(5.11) \quad \hat{\mathbf{v}} = \frac{1}{\sqrt{2}} \sin\theta \left(e^{i\varphi} \hat{\mathbf{e}}_- - e^{-i\varphi} \hat{\mathbf{e}}_+ \right) + \cos\theta\, \hat{\mathbf{e}}_0.$$

The operators $\hat{\mathbf{v}}$, **D**, and **L** act on the spherical harmonics $Y_{nm}(\theta,\varphi)$ to produce linear combinations of other spherical harmonics with possibly raised and/or lowered indices n and/or m. The coefficients of these linear expansions can be made more succinct using

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$$C_n^m \equiv \sqrt{\frac{(n-m)(n+m)}{(2n-1)(2n+1)}}$$

$$(5.12) \quad S_n^m \equiv \sqrt{\frac{(n+m)(n+m-1)}{(2n-1)(2n+1)}} \ .$$

$$T_n^m \equiv \sqrt{(n-m)(n+m+1)}$$

Using the tabulated properties [28] of the $Y_{nm}(\theta,\varphi)$, along with the above definitions, produces, after a lengthy derivation, the following representations of (5.4), (5.5), (5.6) and (5.7):

$$
\begin{aligned}
\mathbf{N}_{knm}^{(\alpha)} &= \sum_j w_{k,j}^{(\alpha)} \left[\frac{\hat{\mathbf{e}}_-}{\sqrt{2}} \left(S_{n+1}^{-m+1} \gamma_{j,n+1,m-1} - S_n^m \gamma_{j,n-1,m-1} \right) \right. \\
&\quad + \frac{\hat{\mathbf{e}}_+}{\sqrt{2}} \left(S_{n+1}^{m+1} \gamma_{j,n+1,m+1} - S_n^{-m} \gamma_{j,n-1,m+1} \right) \\
&\quad \left. + \hat{\mathbf{e}}_0 \left(C_{n+1}^m \gamma_{j,n+1,m} + C_n^m \gamma_{j,n-1,m} \right) \right], \qquad \alpha = 0, \text{ or } 1
\end{aligned}
$$

(5.13)

$$
\begin{aligned}
\mathbf{N}_{knm}^{(2)} &= \sum_j w_{k,j}^{(2)} \left[\frac{\hat{\mathbf{e}}_-}{\sqrt{2}} \left(\{n+m+1\} S_{n+1}^{-m+1} \gamma_{j,n+1,m-1} + \{n-m\} S_n^m \gamma_{j,n-1,m-1} \right) \right. \\
&\quad + \frac{\hat{\mathbf{e}}_+}{\sqrt{2}} \left(\{n-m+1\} S_{n+1}^{m+1} \gamma_{j,n+1,m+1} + \{n+m\} S_n^{-m} \gamma_{j,n-1,m+1} \right) \\
&\quad \left. + \hat{\mathbf{e}}_0 \left(\{n+2\} C_{n+1}^m \gamma_{j,n+1,m} - \{n-1\} C_n^m \gamma_{j,n-1,m} \right) \right]
\end{aligned}
$$

(5.14)

$$
(5.15) \quad \mathbf{N}_{knm}^{(3)} = \sum_j w_{k,j}^{(3)} \ i \left[\frac{\hat{\mathbf{e}}_-}{\sqrt{2}} T_n^{m-1} \gamma_{j,n,m-1} - \frac{\hat{\mathbf{e}}_+}{\sqrt{2}} T_n^{-m-1} \gamma_{j,n,m+1} + \hat{\mathbf{e}}_0 m \gamma_{j,n,m} \right] .
$$

The terms $w_{k,j}^{(\alpha)}$ above are

$$(5.16) \quad w_{k,j}^{(0)} = \int_0^1 v^3 R_j R_k \, dv$$

$$(5.17) \quad w_{k,j}^{(1)} = \int_0^1 v^2 \left(1 - v^2\right)^{3/2} \left(R_j' - 5R_j\right) R_k \, dv$$

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$$(5.18) \quad w_{k,j}^{(2)} = \int_0^1 v \left(1 - v^2\right)^{1/2} R_j R_k \, dv$$

$$(5.19) \quad w_{k,j}^{(3)} = \int_0^1 v^2 \left(1 - v^2\right)^{1/2} R_j R_k \, dv \, .$$

Using (4.8) and (4.11), the integral in (5.16) is relatively simple to evaluate:

$$w_{k,j}^{(0)} = \tfrac{1}{2} \left[Q_k \, \delta_{j,k+1} + W_k \, \delta_{j,k} + Q_{k-1} \delta_{j,k-1} \right]$$

(5.20)

$$Q_k = \frac{(k+1)(k+3)}{(k+2)\sqrt{(2k+5)(2k+3)}}, \quad W_k = \frac{k^2 + 3k + 3}{(k+1)(k+2)}$$

The integrals in (5.17), (5.18) and (5.9) are more tedious to evaluate and will be deferred.

We now have a set of partial differential equations (5.3) in position space (x-space) that is nonlinearly coupled to the Maxwell equations. The velocity dependent part of the Vlasov equation has thus been transformed into a set of v-space spectral equations, i.e., equations for the spectra $\gamma_{knm}(\mathbf{x},t)$. This v-space spectral formulation is independent of the numerical method that is used in x-space. In x-space, we are free to choose whatever geometry, coordinate system and numerical method seems most appropriate and realizable. In fully ionized plasma problems, there are no distinct bounding surfaces since these generally preclude the existence of a fully ionized state. We must, of course, make some reasonable assumptions about the behavior of the plasma at the numerical boundary. We could assume that the number density falls to zero at such a boundary, for example, or we could assume that density is periodic at the boundary of the numerical grid that represents x-space. This choice then narrows the choices of numerical method to use in x-space. Here, for illustrative purposes and because it is applicable to so-called homogeneous plasmas, we will choose periodic boundary conditions. This leads to a straightforward spectral formulation in x-space. Thus, our next step is to consider solution of the Maxwell equations in the case of periodic boundary conditions.

6. Determination of the Electromagnetic Field

The full set of Maxwell's equations, (2.11) to (2.14), can be written in terms of the potential φ and the potential vectors $\mathbf{A}$ and $\mathbf{C}$ as follows [30]:

$$(6.1) \quad \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} = \mathbf{C}$$

$$(6.2) \quad \frac{1}{c}\frac{\partial \mathbf{C}}{\partial t} = \nabla^2 \mathbf{A} + 4\pi \mathbf{j}$$

$$(6.3) \quad \nabla^2 \varphi = -4\pi \rho - \nabla \cdot \mathbf{C}$$

$$(6.4) \quad \frac{1}{c^2}\frac{\partial \varphi}{\partial t} + \nabla \cdot \mathbf{A} = 0.$$

Equation (6.4) is the *Lorentz condition* [31]. The relations (6.1-4) are a set of coupled, first-order-in-time, partial differential equations for the electromagnetic potentials, in a form suitable for numerical integration. The associated electric and magnetic fields are

$$(6.5) \quad \mathbf{B} = \nabla \times \mathbf{A}$$

$$(6.6) \quad \mathbf{E} = -\nabla \varphi - \mathbf{C}.$$

In the case of periodic boundary conditions, we will expand electromagnetic fields and potentials, as well as the γ_{knm}, when necessary, using fast Fourier transforms:

$$\text{a)} \quad \mathbf{A}(\mathbf{x},t) = (2\pi)^{-3/2} \sum_{\mathbf{k}} \tilde{\mathbf{A}}(\mathbf{k},t) e^{i\mathbf{k}\cdot\mathbf{x}}$$

(6.7)

$$\text{b)} \quad \tilde{\mathbf{A}}(\mathbf{k},t) = (2\pi)^{-3/2} \sum_{\mathbf{x}} \mathbf{A}(\mathbf{x},t) e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

There is no time-frequency expansion here because the coupling between the electromagnetic field and matter is generally nonlinear, which generally precludes a simple dispersion relation between wave frequency ω and wave vector $\mathbf{k}$. In terms of Fourier coefficients (omitting t in the argument, for brevity), equations (6.1) to (6.6) take the form:

$$(6.8) \quad \frac{1}{c}\frac{d\tilde{\mathbf{A}}(\mathbf{k})}{dt} = \tilde{\mathbf{C}}(\mathbf{k})$$

$$(6.9) \quad \frac{1}{c}\frac{d\tilde{\mathbf{C}}(\mathbf{k})}{dt} = -k^2 \tilde{\mathbf{A}}(\mathbf{k}) + 4\pi \tilde{\mathbf{j}}(\mathbf{k})$$

(6.10) $\tilde{\varphi}(\mathbf{k}) = k^{-2}\left[4\pi\tilde{\rho}(\mathbf{k}) + i\mathbf{k}\cdot\tilde{\mathbf{C}}(\mathbf{k})\right]$

(6.11) $\dfrac{1}{c^2}\dfrac{d\tilde{\varphi}(\mathbf{k})}{dt} + i\mathbf{k}\cdot\tilde{\mathbf{A}}(\mathbf{k}) = 0$.

The sources in (6.9) and (6.11) are the Fourier transforms, using (6.7), of (4.14) and (4.17). (Also, note that the source coefficients corresponding to $\mathbf{k} = 0$ are zero.)

Using (6.7) and (6.10), equations (6.5) and (6.6) become

(6.12) $\tilde{\mathbf{B}}(\mathbf{k}) = i\mathbf{k}\times\tilde{\mathbf{A}}(\mathbf{k})$

(6.13) $\tilde{\mathbf{E}}(\mathbf{k}) = -4\pi\,i\dfrac{\mathbf{k}}{k^2}\tilde{\rho}(\mathbf{k}) - \left(\mathbf{I} - \dfrac{\mathbf{kk}}{k^2}\right)\cdot\tilde{\mathbf{C}}(\mathbf{k})$.

Here, $\mathbf{I}$ is the unit dyadic. Note that $\tilde{\varphi}(\mathbf{k})$ does not appear in these expression for $\tilde{\mathbf{B}}(\mathbf{k})$ and $\tilde{\mathbf{E}}(\mathbf{k})$. The scalar potential is thus only an auxiliary function, while $\tilde{\mathbf{A}}(\mathbf{k})$ and $\tilde{\mathbf{C}}(\mathbf{k})$ are seen to be more fundamental in classical electrodynamics. Furthermore, it is only those parts of $\tilde{\mathbf{A}}(\mathbf{k})$ and $\tilde{\mathbf{C}}(\mathbf{k})$ transverse to $\mathbf{k}$ that are essential to determining $\tilde{\mathbf{B}}(\mathbf{k})$ and $\tilde{\mathbf{E}}(\mathbf{k})$. (However, in numerical simulations of quantum electrodynamic processes, $\tilde{\varphi}(\mathbf{k})$ must also be calculated [32,33].)

7. The Complete Spectral Algorithm

A spectral method algorithm for the Vlasov-Maxwell system, as developed here, consists of a part in velocity space and a part in position space. The basic v-space spectral equation is (5.3) and its solution produces the coefficients γ_{knm}, which are time-dependent functions in x-space. We use a small subset of these coefficients to directly determine the electromagnetic sources, through (4.14) and (4.17). In x-space, Fourier transforms of these sources then allow the time-evolution of the electric and magnetic fields to be calculated through (6.8), (6.9), (6.12), and (6.13). These electromagnetic fields then enter the right-hand side of (5.3), completing the cycle. This is a coupled set of nonlinear equations, and a complete description of the algorithm developed here requires only a few additional details.

Equation (5.3) determines γ_{knm} and can be written as

(7.1) $\qquad \dfrac{\partial \gamma_{knm}}{\partial t} = \Gamma_{knm} + \Psi_{knm}$

where

(7.2) $\qquad \Gamma_{knm} = -\nabla \cdot \mathbf{N}^{(0)}_{knm}, \qquad \Psi_{knm} = \mathbf{E} \cdot \left[\mathbf{N}^{(1)}_{knm} + \mathbf{N}^{(2)}_{knm} \right] - \mathbf{B} \cdot \mathbf{N}^{(3)}_{knm}.$

To determine the Γ_{knm} we use the Fourier transform to **k**-space (6.20b), to find $\widetilde{\mathbf{N}}^{(0)}_{knm}$ and then form

(7.3) $\qquad \widetilde{\Gamma}_{knm} = -i\mathbf{k} \cdot \widetilde{\mathbf{N}}^{(0)}_{knm},$

after which we transform back to **x**-space with (6.20a) to get Γ_{knm}. Similarly, using (6.20a) to find $\mathbf{E}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$ from $\widetilde{\mathbf{E}}(\mathbf{k})$ and $\widetilde{\mathbf{B}}(\mathbf{k})$, allows us to form Ψ_{knm} point-wise on the numerical x-space grid. The transform method was pioneered many years ago [6] and has proven very useful in the solution of nonlinear problems involving many modes.

Equation (7.1) is now defined on all x-space grid points and can be used to advance the γ_{knm} forward in time with a suitable time-integration scheme (such as a Runge-Kutta [34] or an Adams-Bashforth [35] procedure). Since Γ_{knm} consists of only six coefficients γ_{knm}, it may be efficient and more accurate to treat this term implicitly when solving (7.1). Aliasing (i.e., higher-order coefficients affecting the determination of lower-order coefficients) can occur in determining the Ψ_{knm}, but this can be eliminated, if desired [36]. However, aliasing is often not critical, and run time can be reduced by neglecting aliasing effects (such methods are termed *pseudospectral* [37]). Lastly, one can introduce external parts to **E** and **B** in (7.2), in addition to those parts determined by (6.12) and (6.13), and these can serve as a source of external forcing, if appropriate to a given problem.

8. Discussion

The spectral method algorithm developed here provides a means for solving the coupled, nonlinear Vlasov-Maxwell system of equations in the full six-dimensional case. Numerical implementation requires the use of a discrete grid of points, and if we assume, for the purpose of illustration, that each dimension is given N points, then there are a total of N^6 grid points. If $N = 32$, then $N^6 \approx 10^9$, and if we assume 8 bytes per word in a computer, along with a factor of 25 to

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50 for all the arrays needed, then core memory requirements are in the range of 1 to 2 terabytes (10^{12} bytes), which is currently available on the largest existing supercomputers. The number of grid points allotted to each dimension in the six-dimensional x-v-space can also vary, to increase or decrease resolution, as appropriate.

However, remember that, in a spectral method, grid points are sampling points for an underlying continuous representation. The number of grid points is thus essentially equivalent to the number of coefficients (the 'spectra') kept after truncating a formally infinite function expansion. To prevent a 'pileup' at the higher-order coefficients and to ameliorate the effects of 'filamentation' [10,12,17], it may prove necessary to investigate the use of a collision term in the Vlasov equation, as done previously [3,16]. (These possibilities, and others unthought of, remain as potential challenges for future development.)

In spherical polar coordinates in v-space, the number of points in the radial, or v, direction sets the energy resolution of the code. This resolution may be defined by the relativistic factor $\gamma_n = (1-v_n^2)^{-\frac{1}{2}}$ corresponding to the largest positive zero v_n of $R_n(v)$ (all the zeros are used in the Gaussian quadrature formula [38] for integrals involving R_n, in which case the function to be evaluated is effectively known more or less precisely only at those zeros and interpolated in between [39]). Using known results [29], we can estimate $\gamma_n \approx 8n/3\pi$. For $n = 32$, this gives the resolution of electron energies an upper bound of around 14 MeV, a value which can be increased by making n larger (*e.g.*, by decreasing the number of grid points allotted to other coordinates). Thus, moderate resolution six-dimensional numerical simulations of relativistic electron distributions are possible on available computers.

9. Conclusion

The algorithm presented here provides a straightforward procedure with which to begin using supercomputer resources. The next steps are to evaluate certain integrals mentioned in this paper, to begin the numerical implementation of the algorithm, to gain access to the necessary computers, and to begin running numerical simulations. The probable outcome of proceeding is the creation of a numerical tool capable of studying the full six-dimensional dynamic evolution of charged-particle distributions, starting from various initial conditions and taking into account the influence of external fields. The benefits to be gained are a greater understanding of basic plasma processes and a new capability to predict radiation levels and effects in astrophysical, spaceflight, and engineering systems.

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A spectral method algorithm is developed for the numerical solution of the full six-dimensional Vlasov-Maxwell system of equations. Here, the focus is on the electron distribution function, with positive ions providing a constant background. The algorithm consists of a Jacobi polynomial-spherical harmonic formulation in velocity space and a trigonometric formulation in position space. A transform procedure is used to evaluate nonlinear terms. The algorithm is suitable for performing moderate resolution simulations on currently available supercomputers for both scientific and engineering applications.

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