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Hyperbolic divergence cleaning, the electrostatic limit, and potential boundary conditions for particle-in-cell codes

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ABSTRACT

In a numerical solution of the Maxwell–Vlasov system, the consistency with the charge conservation and divergence conditions has to be kept solving the hyperbolic evolution equations of the Maxwell system, since the vector identity $\nabla \cdot (\nabla \times \vec{u}) = 0$ and/or the charge conservation of moving particles may be not satisfied completely due to discretization errors. One possible method to force the consistency is the hyperbolic divergence cleaning. This hyperbolic constraint formulation of Maxwell's equations has been proposed previously, coupling the divergence conditions to the hyperbolic evolution equations, which can then be treated with the same numerical method. We pick up this method again and show that electrostatic limit may be obtained by accentuating the divergence cleaning sub-system and converging to steady state. Hence, the electrostatic case can be treated by the electrodynamic code with reduced computational effort. In addition, potential boundary conditions as often given in practical applications can be coupled in a similar way to get appropriate boundary conditions for the field equations. Numerical results are shown for an electric dipole, a parallel-plate capacitor, and a Langmuir wave. The use of potential boundary conditions is demonstrated in an Einzel lens simulation.

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1. Introduction

Particle-in-cell (PIC) codes are used to find an approximate solution of the collision-free Boltzmann equation [1,2], the so-called Vlasov equation:

$$\frac{\partial f_\alpha}{\partial t} + \vec{v}_\alpha \frac{\partial f_\alpha}{\partial \vec{x}_\alpha} + \frac{\vec{F}}{m_\alpha} \frac{\partial f_\alpha}{\partial \vec{v}_\alpha} = 0. \quad (1)$$

Here, $f_\alpha = f_\alpha(\vec{x}, \vec{v}, t)$ is the particle distribution function of species α depending on the position $\vec{x}$, the velocity $\vec{v}$ and the time t. In addition, m is the particle mass, and $\vec{F}$ is the Lorentz force, given by

$$\vec{F} = q_\alpha \left(\vec{E} + \vec{v}_\alpha \times \vec{B} \right) \quad (2)$$

with the particle charge q, the electric field $\vec{E}$ and the magnetic field $\vec{B}$.

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The electromagnetic fields $\vec{E}$ and $\vec{B}$ are solutions of the Maxwell's equations

$$\frac{\partial \vec{E}}{\partial t} - c^2 \nabla \times \vec{B} = -\frac{\vec{j}}{\epsilon_0}, \tag{3}$$

$$\frac{\partial \vec{B}}{\partial t} + \nabla \times \vec{E} = 0, \tag{4}$$

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}, \tag{5}$$

$$\nabla \cdot \vec{B} = 0. \tag{6}$$

Here, the source terms are the charge density ρ and the current density $\vec{j}$, defined as moments of the distribution function by

$$\rho(\vec{x}, t) = q \int_{\mathbb{R}^3} f(\vec{x}, \vec{v}, t) \mathrm{d}^3 v,$$

$$\vec{j}(\vec{x}, t) = q \int_{\mathbb{R}^3} \vec{v} f(\vec{x}, \vec{v}, t) \mathrm{d}^3 v. \tag{7}$$

In addition, the charge conservation equation reads as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0. \tag{8}$$

This coupled system is usually called the Maxwell–Vlasov system and is well-defined in the following sense. If the initial values satisfy the divergence constraints (5) and (6), the boundary values are consistent with these constraints, and the charge conservation (8) holds for all times, then the solution $f_\alpha, \vec{E}, \vec{B}$ of the hyperbolic evolution equations (1), (3), and (4) satisfies the whole set of the Maxwell–Vlasov equations for all times. The reason is that the divergence applied to the curl of a vector is zero. Hence, the divergence of Eq. (4) directly shows that Eq. (6) is satisfied at all times if satisfied initially. The same is true for Eq. (5) if the charge is conserved according to (8).

Due to the approximations used, this does not necessarily apply to a PIC code. Here, the particle distribution function is approximated as the linear combination of N δ-functions with a weighting factor w_k, i.e.,

$$f\left(\vec{x}, \vec{v}, t\right) \approx \sum_{k=1}^{N} w_k \delta\left(\vec{x} - \vec{x}_k(t)\right) \delta\left(\vec{v} - \vec{v}_k(t)\right). \tag{9}$$

This approximation is interpreted as N particles with the positions $\vec{x}_k$, the velocities $\vec{v}_k$ and the particle weights w_k. The distribution function of the Vlasov equation, which depends on three space and three velocity coordinates and the time, is then approximated by the time evolution of the particles in phase space. The path of every particle is determined by a system of ordinary differential equations for velocity and spatial location, called Lorentz equations.

These approximations of the Vlasov equation as well as Maxwell's equations changes the situation. Due to numerical errors the charge may not be conserved exactly and the divergence of a curl may vanish only up to some discretization errors. All these approximation errors will then affect the consistency within the Maxwell–Vlasov system. Hence, the approximate solution $f_\alpha, \vec{E}, \vec{B}$ of the approximated hyperbolic evolution equations (1), (3), and (4) does not guarantee the validity of discrete versions of (5) and (6) anymore. Moreover, errors of the divergence constraints may increase during a calculation and may produce instabilities or non-physical solutions [3,2,4].

Different approaches have been proposed to enhance the consistency also in the approximate case. Numerical methods that automatically preserve the algebraic conditions of $\nabla \cdot (\nabla \times \vec{u}) = 0$, which have been derived for Maxwell's or other equations, are not satisfying in this case, since they do not induce consistency regarding charge conservation. Hence, a constraint formulation of the Maxwell–Vlasov equations has to be introduced that couples the evolution equations with the divergence constraints. One of the basic concepts is to introduce Lagrange multipliers into the hyperbolic evolution equations that allows the coupling to the divergence constraints. Such an enlarged system was solved numerically within a finite difference framework by Boris [5], called the projection method, or within a finite element scheme via a penalization technique by Assous et al. [6]. An extension of the Lagrange multiplier approach has been proposed by Munz et al. [7,8] for Maxwell's equations and for the Maxwell–Vlasov equations [9]. It approximated the constrained system by approximating the infinite propagation speed by a finite one to obtain a set of hyperbolic evolution equations. The big advantage is that all equations remain essentially hyperbolic and can be numerically solved by any numerical approach for hyperbolic equations.

An alternative is the development of a numerical approximation that satisfies a discrete analogy of the necessary vector identities. In recent time, some novel methods have been developed that automatically handle the charge conservation in the full Maxwell system in the general case. In [10,11], this method is extended to unstructured grids and arbitrary order in time and space. To establish a discrete consistency seems to be the best approach, but it needs special numerical

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