Exact Charge Conservation in a High-Order Conforming Maxwell Solver coupled with Particles

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Abstract

We present a general mathematical framework for electromagnetic Particle-In-Cell (PIC) codes that can be used on structured as well as unstructured or hybrid grids using an exact sequence of conforming Finite Element spaces for the different components of the electromagnetic field. The structure of the Maxwell solver enables us to derive an exact discrete version of the continuity equation which generalized the charge conserving method of Villasenor and Buneman [2] on this kind of grids. The method has been implemented in 2D and 3D.

Introduction

Many important applications like nuclear fusion, microwave devices like klystrons, or particle accelerators rely on the numerical simulation of charged particles interacting non linearly with each other through the self-consistent electromagnetic field they generate. A mathematical model well suited for the description of these phenomena is the Vlasov-Maxwell model and the method, which has been the most often used for its discretization is the Particle-In-Cell method [1]. This method relies on the approximation of the Vlasov equation by a particle method coupled with the solution of Maxwell's equation on a grid often performed with the standard Yee algorithm. For charged particle applications it is essential that Gauss' law $\operatorname{div} E = \rho$ remains well approximated throughout the simulation. For this reason, one cannot merely rely on the solution of Maxwell's equation using Ampère's and Faraday's laws on their own. This can be done only if the scheme satisfies exactly an approximation charge conservation law. Such a method has been introduced for uniform cartesian grids and Yee's algorithm by Villasenor and Buneman [2]. Note that when this exact discrete charge conservation law is not available, one can still use a correction scheme in the Maxwell solver for most applications, but in some applications like laser-plasma interaction a local charge conservation is essential.

Developing new efficient and reliable Maxwell solvers has been an area of intense research in the last 40 years and a good understanding of the reasons why some solvers work well and other do not has only been achieved recently with the concept of discrete differential forms (see [3] for a review). The Yee scheme fits into this framework, but one can also define different classes of conforming Finite Element Spaces of arbitrary orders on structured and unstructured grids that fit in the same framework, which can also be used to derive an exact discrete charge conservation law. This is the aim of this presentation. For the sake of simplicity, all the constructions shall be presented in 2D, but they can be extended in a straightforward matter to 3D.

1 The 2D Time Domain Vlasov-Maxwell System

The charge conservation issue only depends in 2D on the (E_x, E_y, B_z) components of the electromagnetic field that satisfy

$$\partial_t \mathbf{E} - c^2 \,\mathbf{curl}\, B = -\frac{1}{\varepsilon_0}\mathbf{J} \tag{1}$$

$$\partial_t B + \operatorname{curl} \mathbf{E} = 0 \tag{2}$$

$$\operatorname{div} \mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{3}$$

where $\mathbf{E} = (E_x, E_y)^T$ and $B = B_z$ denote the relevant components of the electric and magnetic fields. These are the unknowns of the system, whereas $\mathbf{J} = (J_x, J_y)^T$ and ρ respectively denote given current and charge density, seen as sources. As usual, the vector and scalar curl operators are given in 2D by $\mathbf{curl}\,\varphi := (\partial_y\varphi, -\partial_x\varphi)^T$ and $\operatorname{curl}\boldsymbol{\varphi} := \partial_x\varphi_y - \partial_y\varphi_x$.

In the Vlasov model, the state of the plasma is represented by a time dependent *distribution function f* which, at any time t, is defined on the phase space $\hat{\Omega} := \{(\mathbf{x}, \mathbf{v}) \in \Omega \times \mathbb{R}^2\}$ consisting in all possible (physical) positions $\mathbf{x} = (x, y)$ and velocities $\mathbf{v} = (v_x, v_y)$ for the particles. For simplicity we shall only consider the evolution of one species of particles (namely, electrons) and assume the presence of a neutralizing uniform background ion distribution. The non relativistic Vlasov equation reads

$$\partial_t f + \mathbf{v} \cdot \boldsymbol{\nabla}_{\mathbf{x}} f + \frac{q}{m}\mathbf{F} \cdot \boldsymbol{\nabla}_{\mathbf{v}} f = 0, \tag{4}$$

where q, m denote the charge and mass of an electron, and where the force term is given by the Lorentz law, i.e., $\mathbf{F} := \mathbf{E} + \mathbf{v} \times B = (E_x + v_y B, E_y - v_x B)^T$, which yields a first coupling between the Maxwell and Vlasov equations.

The following equivalence, which is well known, is at the heart of our study. Given Ampere's law (1), the following properties are equivalent:

(i) Gauss' law (3) is satisfied at any time t,

(ii) Gauss' law (3) is satisfied at the initial time, and the sources ρ, $\mathbf{J}$ satisfy a charge conservation property (also called continuity equation)

$$\partial_t \rho + \operatorname{div} \mathbf{J} = 0. \tag{5}$$

2 The variational formulations

It reads: find $\mathbf{E}$ and B, such that $\mathbf{E}(0) = \mathbf{E}_0 \in \boldsymbol{H}_0(\mathrm{curl})$ and $B(0) = B_0 \in L^2$, with $\operatorname{div} \mathbf{E}_0 = \frac{\rho(0)}{\varepsilon_0}$ and such that for almost every t in $(0, T)$, we have

$$\int_\Omega \boldsymbol{\varphi}\, \partial_t \mathbf{E}(t) - c^2 \int_\Omega B(t) \operatorname{curl} \boldsymbol{\varphi} = -\varepsilon_0^{-1} \int_\Omega \boldsymbol{\varphi} \cdot \mathbf{J}(t) \qquad \forall \boldsymbol{\varphi} \in \boldsymbol{H}_0(\mathrm{curl}), \tag{6}$$

$$\int_\Omega \psi\, \partial_t B(t) + \int_\Omega \psi \operatorname{curl} \mathbf{E}(t) = 0 \quad \forall \psi \in L^2, \tag{7}$$

$$-\int_\Omega \mathbf{E}(t) \cdot \mathbf{grad}\, \phi = \varepsilon_0^{-1} \int_\Omega \phi\, \rho(t) \quad \forall \phi \in H_0^1. \tag{8}$$

Since the domain Ω is assumed polygonal and simply connected, we know that as long as the sources $\rho \in \mathcal{C}^1(0, T; L^2(\Omega))$, $\mathbf{J} \in \mathcal{C}^1(0, T; L^2(\Omega))$ satisfy the charge conservation property (5), there exists a unique solution to this variational formulation. Moreover the variational formulation of Gauss' law (8) needs only to be satisfied at $t = 0$ in order to be satisfied at all times.

This property is also verified by the discrete variational formulation provided the three discrete function spaces share the same property as their inifinite dimensional counterparts, namely the exact sequence property.

$$H_0^1 \overset{\mathbf{grad}}{\longrightarrow} \boldsymbol{H}_0(\mathrm{curl}) \overset{\mathrm{curl}}{\longrightarrow} L^2,$$

meaning that $\mathbf{grad}(H_0^1) \subset \boldsymbol{H}_0(\mathrm{curl})$, $\ker(\mathrm{curl}\,|_{\boldsymbol{H}_0(\mathrm{curl})}) = \mathbf{grad}(H_0^1)$ and $\mathrm{curl}(\boldsymbol{H}_0(\mathrm{curl})) \subset L^2$.

There are well known conforming approximations of these spaces of arbitrary order that satisfy this property as well on triangles as on quads, and they are naturally conforming on hybrid meshes of triangles and quads. These spaces have been defined by Nédélec [4]. Let us recall their form on quads: $\mathbb{Q}_k$ gives the conforming approximation of H_0^1, $\mathbb{Q}_{k-1,k} \times \mathbb{Q}_{k,k-1}$ gives the conforming approximation of $\boldsymbol{H}_0(\mathrm{curl})$ and $\mathbb{Q}_{k-1}$ gives the conforming approximation of L^2.

3 Discrete continuity equation

In order to have an exactly charge conserving discrete formulation there remains to find an exact discrete formulation of the continuity equation.

In a PIC method the distribution function and hence the charge and current densities ρ and $\mathbf{J}$ are approximated by a sum of Dirac masses. In the Finite Difference context these approximations need to be regularized in order to be able to define ρ and $\mathbf{J}$ at the points where they are needed. In the context of Finite Elements, these regularization is naturally performed by the variational formulations. Hence we define

$$\rho_h^n(\mathbf{x}) := \sum_{k=1}^{N_{\mathrm{part}}} w_k \delta(\mathbf{x} - \mathbf{x}_k^n),$$

$$\bar{\mathbf{J}}_h^{n+\frac{1}{2}}(\mathbf{x}) := \sum_{k=1}^{N_{\mathrm{part}}} w_k \mathbf{v}_k^{n+\frac{1}{2}} \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \delta(\mathbf{x} - \mathbf{x}_k(t))\, \mathrm{d}t,$$

with $\mathbf{x}_k(t)) = \mathbf{x}_k^n + (t - t_n)\mathbf{v}_k^{n+\frac{1}{2}}$, and w_k the weight of the particles.

Then putting these expressions in the discrete variational formulations, we can prove that the discrete Gauss law remains satisfied at all times if it is satisfied at time $t = 0$.

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