The Particle in Diffuse Cell Method for Plasmas Simulations

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Abstract. *In this work we propose the Particle-In-Diffuse-Cell (PIDC) method for plasma simulation. The foundation of this method relies in the standard Particle-In-Cell (PIC) model and in the Element-Free Galerkin method (EFGM), which has been widely studied in electromagnetism and magneto-hydrodynamic fields. The absence of mesh in the EFGM formulation leads to a generalization of the geometric concept of cells in the PIC model. We aim investigate the advantages of this formulation in comparison with the mesh-based PIC models, as well as to introduce the formalism of meshfree approaches in the context of PIC models.*

Resumo. *Neste trabalho propomos o método Particle-In-Diffuse-Cell (PIDC) para simulação de plasmas, fundamentado no modelo Particle-In-Cell (PIC) e no método Element-Free Galerkin (EFG), o qual vem sendo amplamente estudado em eletromagnetismo e magneto-hidrodinâmica. A inexistência de malha na formulação do método EFG conduz à generalização do conceito geométrico das células no modelo PIC, e nosso objetivo é explorar suas vantagens em comparação às abordagens PIC baseadas em malha, formalizando a incorporação de abordagens meshfree em modelos PIC.*

1. INTRODUCTION

The study o plasmas is of high interest due the enormous number of scientific and industrial applications which can take advantage of improved knowledge about plasma phenomena. The applications of plasma-based technologies include a wide variety of research areas such as the development of plasma-based devices in medicine, material processing, plasma thrusters, controlled nuclear fusion, aerodynamic drag reduction, and many others (Hrach *et al,* 2003; Kafafy & Wang, 2006; Nam *et al*, 2005; Shang, 2001).

The Particle-In-Cell (PIC) model is a very versatile approach for plasmas simulation (Dawson, 1984; Birdsall, 1985) and allows the treatment of many physical and chemical phenomena in plasmas, like reactive and non-reactive collisional processes. In the PIC models the plasma is represented by many thousands of charged particles whose motion is governed by their self-consistent electric and/or magnetic field. In this work we are interested in the electrostatic plasma approximation. The force acting on each particle is computed by means of the self-consistent electric field. Thus there is two main solvers in a PIC code, one for the particle dynamic and other for the field computation. Due the enormous number of particles required for representing the plasma correctly, PIC codes require considerable amount of memory and high performance computers. Although the PIC model has been proposed in the end of fifties, its application always were dependent of high performance computer architectures like supercomputers which were a computational resource unavailable for the majority of the researchers. Nowadays, due the increasing availability of high performance computers at low cost experienced in the past decades, the PIC methodology has been widely investigated.

This scenario of increasing availability of memory and processing capability has allowed the improvement of the PIC models, as it enables the coupling with specific techniques and methods for treating physical or chemical

phenomena of interest, or even it allows the choice for more robust numerical methods for the field computation.

Plasma-based devices often present complex geometries, therefore, PIC codes that supports CAD (Computer Aided Design) tools are desired, and sometimes indispensable for design properly the geometrical model. In these cases, the coupling of the PIC and the Finite Element Method (FEM) proposed by Paes *et al* (2003) seems to be very adequate, since the finite elements of the mesh coincide to the cells of the PIC model, it allows that the device boundaries be properly represented by the computational model.

Another difficulty, commonly present in many plasmas applications is the occurrence of regions with charge accumulation and thin regions with strong field variation, *e.g.* plasmas sheaths. Two difficulties rises in this scenario. Firstly, the high number of charged particles accumulated in some regions require the subdivision of the cells in these regions, in other words, a mesh refinement process is required for preserving the plasma properties. The task of mesh refinement is time-consuming, and may lead to an inappropriate refined mesh depending on the complexity of the geometric model and specially in three dimensional problems. Secondly, the electric field may hardly change across a cell, in such a way that a linear finite element approximation (for the potential variable) would not be able to properly reproduce the physical variation of the field inside the cell. Taking into account that the motion of the charged particles are governed by the computed electric field components, inaccurate calculations for the field variable may lead to incorrect expectations about the behavior of the plasma-device.

The proposed formulation is stated on the PIC model and the Element-Free Galerkin Method (EFGM). The meshless feature of the EFGM enable us to avoid the mesh refinement processes however, there is no finite elements, or mesh elements in the EFGM formulation to make them coincide with the cells of the PIC model. We recall the concept of *diffuse elements* introduced by Nayroles *et al.* (1992) in the proposition of the Diffuse Element Method (DEM), which has been popularized as EFGM two years latter, with the work of Belytschko *et al* (1994). The concept of diffuse elements is the key for coupling the PIC model and the EFGM, pointing to the idea of diffuse cells, which lead us to a generalization of the geometric concept of cells in PIC models. Thus, we called the present formulation as the Particle-In-Diffuse-Cell (PIDC) method (Marques *et al.*, 2007.a). Additionally, the approximation provided by the EFGM has high order of continuity, therewith it is more able to reproduce strong field variation across thin regions, even inside a cell. In few words, this work introduces the meshfree formalism based on the EFGM in the PIC context.

2. THE PIC AND PIDC MODELS

Like a classic particle system, the motion of the charged particles are given by the forces that act on the particles. The resulting forces acting on the particles are given by the Lorentz force-relation,

$$\mathbf{F} = q\left(\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right), \tag{1}$$

thus, in the electrostatic approximation, the acceleration acting on the j^{th} particle can be written as:

$$\mathbf{a}_j = \frac{q_j}{m_j}\left(\mathbf{E}(\mathbf{x}_j)\right) . \tag{2}$$

The acceleration of the particles are calculated from the electrical field. In the absence of externally applied electric or magnetic fields, the resulting field is the self-consistent electric one, governed by the Maxwell equations. Using a scalar potential formulation, $\mathbf{E} = -\nabla u(x, y)$, for simplifying the Maxwell equations for the electric field variable, one can gets the Poisson's equation for the electric potential variable $u(x,y)$:

$$\nabla\cdot\left(\varepsilon\nabla u(x, y)\right) = -4\pi\rho(x, y), \tag{3}$$

where it was used the constitutive relation for the electric field vector $\mathbf{D} = \varepsilon\cdot\mathbf{E}$.

In the PIDC model, the EFGM is employed to solve equation (3), but first it is necessary to determine de charge density $\rho(x, y)$. The PIC cycle starts at this point. In the PIC model the domain is decomposed by a cell structure, a mesh over the entire domain. The charge of the particles of each cell are distributed among the cell vertexes, following an area or distance criteria. In the PIDC, based on theoretical considerations about how the local approximations are constructed in the FEM and the EFGM, we propose that the *diffuse elements* of the EFGM be properly adjusted to define the diffuse cells. These diffuse cells are not regular polygons, neither non-intersecting ones, however its regularity is ensured by the shape functions associated with the cell vertexes. This issue is well detailed in the work of Marques *et al* (2007.a). After distribute the charge of all particles, we have determined the total charge accumulated on each i^{th} cell vertex (x_i,y_i), that is, $\rho(x_i, y_i)$.

Once we have determined $\rho(x_i, y_i)$, we go to the second stage of PIC cycle: the field computation stage, where we solve the Poisson's equation (3). In the PIDC approach we used the EFGM as described in Marques *et al.* (2007.b). The third stage of the PIC cycle is the field interpolation stage, where from the electric potential computed at the cell vertexes we interpolate the field value at the particle locations. Thus, equation (2) can be computed, from which the new positions and velocities of the particles can be calculated by integrating the motion equations. As the particles move the charge net changes as well, and the PIC cycle restarts from the first stage.

3. FINAL REMARKS

We present a meshfree method for plasma simulation based on PIC model and the EFGM. The absence of mesh and the high order of continuity of the approximations provided by the EFGM makes the PIDC method an interesting and unexplored alternative for plasma simulation involving complex three-dimensional domains, charge accumulation and/or plasma sheaths. We have developed an object-oriented C^{++} code that implements the PIDC method similarly the one described in Passaro *et al* (2004), and now we are conducting some performance analysis on Beowulf PC clusters.

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