C. R. Mecanique 342 (2014) 662–670

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

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Theoretical and numerical approaches for Vlasov–Maxwell equations

Coupled Particle-In-Cell and Direct Simulation Monte Carlo method for simulating reactive plasma flows

Claus-Dieter Munz [a,*], Monika Auweter-Kurtz [b], Stefanos Fasoulas [c], Asim Mirza [c], Philip Ortwein [a], Marcel Pfeiffer [c], Torsten Stindl [c]

[a] Institute of Aerodynamics and Gasdynamics (IAG), Universität Stuttgart, 70550 Stuttgart, Germany
[b] German Aerospace Academy (ASA), Forum 1 am Konrad-Zuse-Platz 1, 71034 Böblingen, Germany
[c] Institute of Space Systems (IRS), Universität Stuttgart, 70550 Stuttgart, Germany

ARTICLE INFO

Article history:
Received 22 March 2014
Accepted 28 June 2014
Available online 8 August 2014

Keywords:
Particle-In-Cell
Direct Simulation Monte Carlo
Discontinuous Galerkin
High-order
Plasma physics
Boltzmann equation

ABSTRACT

Plasma flows with high Knudsen numbers cannot be treated with classic continuum methods, as represented for example by the Navier–Stokes or the magnetohydrodynamic equations. Instead, the more fundamental Boltzmann equation has to be solved, which is done here approximately by particle based methods that also allow for thermal and chemical non-equilibrium. The Particle-In-Cell method is used to treat the collisionless Vlasov–Maxwell system, while neutral reactive flows are treated by the Direct Simulation Monte Carlo method. In this article, a combined approach is presented that allows the simulation of reactive, partially or fully ionized plasma flows. Both particle methods are briefly outlined and the coupling and parallelization strategies are described. As an example, the results of a streamer discharge simulation are presented and discussed in order to demonstrate the capabilities of the coupled method.

1. Introduction

Many plasma applications, including re-entry missions in high altitudes, electric space propulsion or streamer formation, are characterised by high Knudsen numbers and are dominated by strong deviations from thermal and/or chemical equilibrium conditions [1–4]. Therefore, it is physically not justified to apply classic continuum models like the Navier–Stokes or the magnetohydrodynamic equations for their description. Instead, the Boltzmann equation

$$\left(\frac{\partial}{\partial t}+\vec{v}\frac{\partial}{\partial \vec{x}}+\frac{\vec{F}}{m}\frac{\partial}{\partial \vec{v}}\right)f=\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \tag{1}$$

has to be solved, representing a more fundamental equation based on kinetic gas theory. Here, $f=f(\vec{v},\vec{x},t)$ is the particle distribution function at the six-dimensional phase space point $(\vec{x},\vec{v})$ at the time t. Furthermore, m is the particle mass, $\vec{F}$ an external force and $(\partial f/\partial t)_{\text{coll}}$ the so-called Boltzmann collision integral, which describes intermolecular collisions between the particles in the flow. A well-established way to find an approximate solution to the Boltzmann equation is the use of

* Corresponding author. Tel.: +49 711 685 63401; fax: +49 711 685 53402.
E-mail addresses: munz@iag.uni-stuttgart.de (C.-D. Munz), m.auweter-kurtz@german-asa.de (M. Auweter-Kurtz), fasoulas@irs.uni-stuttgart.de (S. Fasoulas), mirza@irs.uni-stuttgart.de (A. Mirza), ortwein@iag.uni-stuttgart.de (P. Ortwein), mpfeiffer@irs.uni-stuttgart.de (M. Pfeiffer), stindl@irs.uni-stuttgart.de (T. Stindl).

http://dx.doi.org/10.1016/j.crme.2014.07.005
1631-0721/

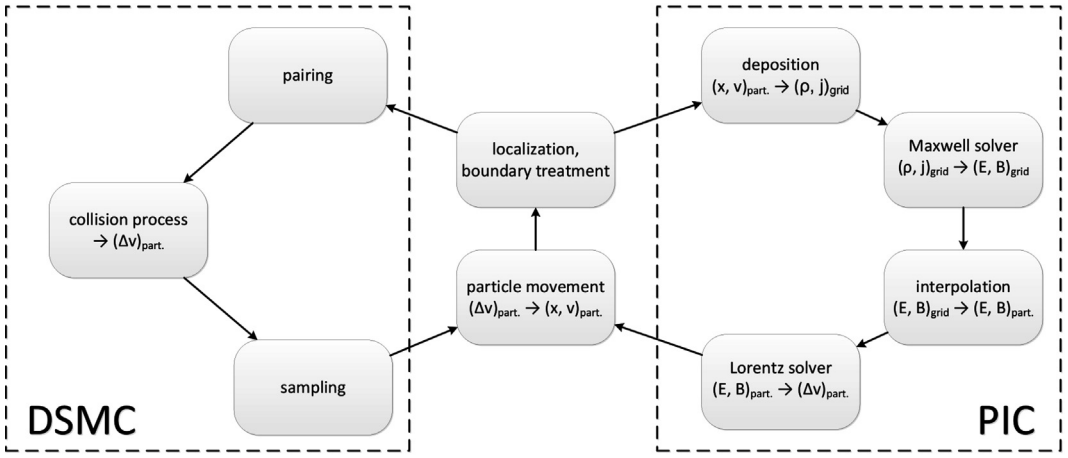

Fig. 1. Flow chart of PIC–DSMC simulation procedures performed during each time step.

numerical particle methods. Two of them, the Particle-In-Cell (PIC) and the Direct Simulation Monte Carlo (DSMC) method have continuously been advanced for decades and successfully applied to simulate a variety of plasma and gas applications and phenomena.

The basic idea of both methods is the approximation of the distribution function by a certain number of particles N at the position $\vec{x}_k$ and the velocity $\vec{v}_k$ at the corresponding time t, leading to

$$f(\vec{x},\vec{v},t)=\sum_{k=1}^{N} w_k \delta\big(\vec{x}-\vec{x}_k(t)\big)\delta\big(\vec{v}-\vec{v}_k(t)\big)$$

In addition, a particle weighting factor w_k is introduced, describing the number of real particles represented by one simulation particle k. This allows the handling of huge particle numbers with a lower number of simulation particles.

The PIC method describes the electromagnetic interaction between charged particles in a Vlasov plasma [5,6]. This means that the flow is collisionless, i.e. $(\partial f/\partial t)_{\text{coll}}=0$, and the only external force F considered in (1) is the Lorentz force, given by

$$\vec{F}_L = Q\,(\vec{E}+\vec{v}\times\vec{B}) \tag{2}$$

where Q, $\vec{E}$ and $\vec{B}$ are the particle charge, the electric and the magnetic field, respectively. The basic concept of the PIC method is the decoupling of the free-particle movement in the computational domain and the calculation of the electromagnetic fields on a fixed simulation grid. Therefore, the PIC method connects the Lagrangian particle handling and the electromagnetic fields that are handled in an Eulerian manner with different interpolation procedures that are described in Section 2. The first methods to calculate the electromagnetic fields were based on Yee's finite difference method [7] using structured grids. Later, finite volume (FV) [8] and finite element (FE) [9] methods were applied. Due to their excellent approximation of wave propagation and the flexible grid requirements, discontinuous Galerkin (DG) schemes have also been investigated in recent times. The successful application of the DG scheme as a field solver is demonstrated in [10], establishing a high-order explicit PIC method based on unstructured grids.

In contrast to the PIC method, the DSMC method includes the collision term $(\partial f/\partial t)_{\text{coll}}$, represented by binary collisions, and assumes that external forces are neglected, i.e. $\vec{F}=0$. As a consequence, the electromagnetic interaction of charged particles cannot be handled. The DSMC method, which was first introduced by Bird [1], performs collisions amongst freely moving particles and between particles and boundaries of the computational domain. Each collision includes an energy and momentum exchange and optionally a relaxation process of internal degrees of freedom as well as chemical reactions. The typical internal degrees of freedom handled in the DSMC method are the rotational and the vibrational energies of diatomic molecules, the latter being also introduced in a quantized model by Bergemann and Boyd [11]. In the last years, the inclusion of the electronic energy of atoms and molecules has become increasingly feasible [12,13]. The simulation of chemical reactions is mainly based on two models, the well-known macroscopic Arrhenius model [1,14] and a new microscopic quantum kinetic model by Bird [15]. The entire collision process, which includes relaxation processes and chemical reactions, is treated in a statistical manner using random numbers. Consequently, the results of the DSMC method, which have to be sampled from the microscopic particle value, contain a statistical noise.

In order to simulate collisional as well as electromagnetic interactions in a plasma flow, the coupled PIC–DSMC code "PICLas" has been developed in the last years and is described in this paper. The scheme uses unstructured, three-dimensional grids allowing one to be able to simulate complex geometries and flows. A schematic flow chart of the coupled code is depicted in Fig. 1. Both PIC and DSMC contribute to the particle movement, which represents the common module of the code together with localization and boundary treatment.