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A fully-implicit Particle-In-Cell Monte Carlo Collision code for the simulation of inductively coupled plasmas

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A B S T R A C T

We present a fully-implicit electromagnetic Particle-In-Cell Monte Carlo collision code, called NINJA, written for the simulation of inductively coupled plasmas. NINJA employs a kinetic enslaved Jacobian-Free Newton Krylov method to solve self-consistently the interaction between the electromagnetic field generated by the radio-frequency coil and the plasma response. The simulated plasma includes a kinetic description of charged and neutral species as well as the collision processes between them. The algorithm allows simulations with cell sizes much larger than the Debye length and time steps in excess of the Courant–Friedrichs–Lewy condition whilst preserving the conservation of the total energy. The code is applied to the simulation of the plasma discharge of the Linac4 H^- ion source at CERN. Simulation results of plasma density, temperature and EEDF are discussed and compared with optical emission spectroscopy measurements. A systematic study of the energy conservation as a function of the numerical parameters is presented.

1. Introduction

In recent years there has been a strong interest in applications based on Inductively Coupled Plasmas (ICP): large-area integrated circuit manufacturing [1], medical devices [2], ion sources for accelerators [3] and fusion [4]. Key features of ICP driven discharges are the capability of obtaining high density plasmas (10^{17}–10^{18} m^{-3}) even at low gas pressures, and to operate without direct contact of the electrodes with the plasma. Modern applications set demanding specifications on the design and operation of ICP discharges, making it essential to develop detailed plasma models to gain insights into the underlying physics.

Theoretical and experimental studies have highlighted the importance of kinetic effects in ICPs [5–7] as well as local and non-local kinetics [8]. Modeling work of ICPs has mainly been performed using fluid [9,10] and hybrid codes [11,12], while only few papers can be found on kinetic modeling that are particularly targeted at the low-density regime [13–15]. This is partially because kinetic simulations of high density, low temperature plasmas require very large computational resources and remained intractable for many years. One of the techniques to simulate plasmas from a kinetic point of view is the Particle-In-Cell (PIC) algorithm [16]. In its classical implementation, the time dependent governing equations are solved with an explicit leap-frog integration scheme. While this technique is simple and second order accurate, its limitations arise from the stringent time step Δt and cell size Δx required for its stability. In fact Δt must be kept sufficiently small

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to resolve the fastest wave propagations, typically electromagnetic radiation or plasma oscillations (Langmuir waves), in order to satisfy the Courant–Friedrichs–Lewy condition [16]. Δx on the other hand must resolve the finest electron scales happening at the Debye length λ_{De} to avoid a numerical plasma heating known in the literature as finite-grid instability [17]. This is a strong limitation for the simulation of ICPs, as λ_{De} can be in the order of tens of μm, while the typical plasma chamber size is several centimeters large, leading to a considerable number of cells to be simulated.

To overcome these limitations, alternative PIC implementations using implicit integration schemes have been considered since the 80's, starting with the pioneering work of Mason [18] and Denavit [19]. Implicit PICs require the concurrent solution of the non-linear coupling of the field equations with the particles' equations of motion and originally, due to the complexity of the problem, a number of semi-implicit codes were first developed (implicit moment [18,19] and direct implicit [20]). Recently, thanks to advances in computing and numerical techniques, the fully-implicit solutions to the non-linear field-particles problem has been successfully addressed [21,22]. These algorithms are shown to be unconditionally stable for any choice of Δt and replace the constraint on Δx to resolve λ_{De} by a much more relaxed condition that particles should not cross more that one cell in one time step. This is a significant improvement over explicit codes because the choices of Δt and Δx are no longer bound to strict stability requirements, but can be chosen to resolve only the scales of interest in the plasma under investigation.

Based on these considerations, we have developed a fully-implicit electromagnetic PIC code, called NINJA, for the kinetic simulation of ICPs. Our motivation originated from the investigation of the Linac4 H^- ion source at CERN [3], whose plasma is created in an ICP in cylindrical configuration. NINJA is a 2.5D PIC in cylindrical coordinates, where the electromagnetic (EM) fields are solved in 2D assuming azimuthal symmetry ($\partial/\partial\theta = 0$), while the particles' motion is solved in 3D3V. The model is supplemented with a Monte Carlo Collision (MCC) algorithm to describe the plasma chemistry as well as a neutral transport module including atomic and molecular (vibrationally resolved) particle tracking for hydrogen. This study represents, in our best knowledge, the first application of a fully-implicit algorithm for the simulation of bounded, collisional plasmas, including the coupling with a Monte Carlo Collision module. This extends the previous work on the fully-implicit algorithm for unbounded, collision-less plasmas described in [21,22]. We present a description of the algorithms, their implementation, a performance analysis, a comparison to analytic solutions and the application of the code to the investigation of the hydrogen discharge in the Linac4 H^- ion source.

2. Method

2.1. Governing equations

The goal of our simulations is to describe the plasma dynamics in an ICP. This requires modeling the interaction between the EM field generated by the Radio-Frequency (RF) coil and the corresponding plasma response, composed of the particles' motion and the collision processes between them. We are interested in describing the high density regime of an ICP, in which the coupling between the coil and the plasma is of the inductive type (H-mode) [23]. The electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ are given by Maxwell's equations in which the current density $\mathbf{J}$ is the sum of the plasma $\mathbf{J}_{pl}$ and the RF coil $\mathbf{J}_{RF}$ contributions:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \tag{1}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{2}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \tag{3}$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\epsilon_0 \mu_0} \nabla \times \mathbf{B} - \frac{1}{\epsilon_0} \mathbf{J} \qquad \mathbf{J} = \mathbf{J}_{RF} + \mathbf{J}_{pl} \tag{4}$$

with t representing time, ρ the charge density and ϵ_0, μ_0 the permittivity and permeability of free space respectively.

While $\mathbf{J}_{RF}$ is externally imposed, the plasma contribution $\mathbf{J}_{pl}$ results from the motion of the charged particles in the plasma. Kinetically this is represented by the first moment of the distribution function f_s (normalized to the plasma density n_s) of each plasma species s (e.g. electron, ion), resulting in:

$$\mathbf{J}_{pl} = \sum_s q_s \int_V \mathbf{v} f_s(\mathbf{x}, \mathbf{v}, t) dv \tag{5}$$

with $\mathbf{x}$ the position, $\mathbf{v}$ the velocity and q_s the electric charge of the species s. The particles' position $\mathbf{x}_p$ and velocity $\mathbf{v}_p$ define the distribution function f_s, and are mathematically described by Newton's equations of motion:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \tag{6}$$

$$m_s \frac{d\mathbf{v}_p}{dt} = q_s(\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p) + \mathbf{F}_c \tag{7}$$