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# CFIRM: AN INTEGRATED CODE PACKAGE FOR THE LOW-TEMPERATURE PLASMA SIMULATION ON STRUCTURED GRIDS

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**Abstract.** This paper presents a recently developed full kinetic particle simulation code package, which is a two-dimensional highly integrated and universal framework for low-temperature plasma simulation on both Cartesian and axisymmetric coordinate systems. This code package is named CFIRM, since it is designed based on the continuous Galerkin immersed-finite-element (IFE) particle-in-cell (PIC) model with the polynomial-preserving-recovery (PPR) technique and the Monte-Carlo-collision (MCC) method. Both the traditional and implicit PIC methods were implemented in the package. Incorporating the advantages of all these methods together, the CFIRM code can adopt explicit or implicit PIC schemes to track the motion trajectory of charged particles and deal with the collisions between plasma and neutral gas. Additionally, it can conveniently handle complex interface problems on structured grids. The CFRIM code has excellent versatility in low-temperature plasma simulation and can easily extend to various particle processing modules, such as the variable weights and adaptive particle management algorithms which were incorporated into this code to reduce the memory utilization rate. The implementation for the main algorithms and the overall simulation framework of the CFIRM code package are rigorously described in details. Several simulations of the benchmark cases are carried out to validate the reliability and accuracy of the CFIRM code. Moreover, two typical low-temperature plasma engineering problems are simulated, including a hall thruster and a capacitively coupled plasma reactor, which demonstrates the applicability of this code package.

**Key words.** Low-temperature plasma, particle-in-cell, immersed-finite-element, polynomial-preserving-recovery, Monte-Carlo-collision.

## 1. Introduction

Low-temperature plasma is a state of matter characterized by the electron temperature being significantly higher than the ion temperature. It is commonly generated by gas discharge at low pressures with the help of direct current, radio frequency, or microwave sources. Nowadays, low-temperature plasma technology has been widely used in many industries [1, 2], such as etching [3], electric propulsion [4], accelerators [5], and material surface modification [6]. Numerical simulations have been demonstrated to be an economical and powerful method for the research of low-temperature plasma. They can be used to reveal the basic physical mechanisms of plasma, assist in optimizing structural design, and significantly reduce research and development costs.

The commonly used simulation methods of the low-temperature plasma include fluid [7, 8], direct kinetic (Boltzmann) [9, 10], and particle-in-cell (PIC) models [11]. The fluid models solve the conservation equations of mass, momentum, and energy to obtain the macroscopic quantities of each physical parameter, like velocity, density, temperature, and so on. It always assumes that the velocity distribution function satisfies Maxwell's distribution. Although fluid models have been fully developed and have enough advantages in computational efficiency, their results will become less accurate once the thermodynamic equilibrium assumption is broken down. The direct kinetic models can obtain the time evolution of the distribution

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function by solving the Boltzmann or Vlasov equation, which provides the probability of particles in the given state of physical space and velocity space. However, the direct kinetic models have much higher computational cost, especially in the simulation of three-dimensional problems. On the other hand, the PIC method is a compromise between the fluid and direct kinetic models, which regards the plasma as a large number of particles and can capture the non-equilibrium phenomena of plasma by tracking the motion of particles. Hence the PIC models have become the most popular kinetic methods for low-temperature plasma simulations.

The classical PIC method was proposed by Birdsall et al [12]. It constantly updates the velocities and positions of particles through the 'leap-frog' scheme and updates the electric field by solving Poisson's equation. In order to simulate the collisions between the particles, the Monte Carlo collision (MCC) method was introduced in the PIC model [11], and then the PIC-MCC framework was widely used in low-temperature plasma simulation [13, 14, 15, 16]. Nevertheless, the traditional PIC method necessitates the use of sufficiently small spatial and temporal step sizes to precisely track the behaviors of the electrons. The step sizes of the PIC method should satisfy the following conditions, namely $\Delta x \leq \lambda_D$, $\Delta t \leq 2/\omega_{pe}$ and $\Delta x/\Delta t < v_{te}$, where $\Delta x$ is the spatial step size, $\Delta t$ is the temporal step size, $\lambda_D$ is the Debye length, $\omega_{pe}$ is the electron plasma frequency, and $v_{te}$ is the electron thermal velocity. This leads to a huge computational cost in the simulations with high plasma density and a large simulation domain. Therefore, the implicit PIC method [17, 18, 19, 20, 21, 22] was developed to reduce the cost of the traditional PIC algorithm. It can eliminate the limitations of step sizes by damping the high-frequency modes of the plasma. Although the high-frequency characteristic of the electron is lost when the step sizes are enlarged, most of the kinetic behaviors of the plasma are maintained. Thus, the implicit PIC model is an important method for large-scale plasma simulation. No matter which PIC scheme is adopted, the structured grids are the optimal option to improve the efficiency of particle localization, especially Cartesian meshes. However, the structured grids with traditional field solvers cannot accurately handle the problems that involve complex physical interfaces in the domain.

The immersed-finite-element (IFE) method [23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39] is a special finite element method, which was developed to solve the complex interface problems on structured grids. The meshes of the IFE method are independent of the interface, thus it has great advantages in dealing with complex and moving interfaces. The IFE method has been utilized as a field solver of the PIC model in recent years, which leads to the so called IFE-PIC method [40, 41, 42, 43, 44, 45, 46]. The IFE-PIC method has been applied to the simulations of low-temperature plasma problems, such as electric thrusters [47, 48, 49, 50, 51, 52, 53, 54, 55, 56] and lunar surface charging [57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67].

The polynomial-preserving-recovery (PPR) technique was proposed by Naga and Zhang [68]. This method uses the fitted numerical solutions to recover the gradient. Due to its superconvergence property, the PPR has received widespread attention and development [69, 70, 71, 72]. Thus, we utilized the PPR technology to recover the electric field for the IFE-PIC method.

The purpose of this paper is to develop a two-dimensional highly integrated continuous Galerkin immersed-finite-element particle-in-cell code package, named as CFIRM. In CFIRM, the electric field is obtained by the PPR method, and the collisions between plasma and neutral gas are simulated by the MCC method. The CFIRM code is designed for simulating low-temperature plasma in both Cartesian and axisymmetric coordinate systems. To enhance the code's versatility and computational efficiency, we have incorporated both traditional and implicit PIC models into the code. Additionally, we have introduced various numerical schemes into