INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 14, Number 2, Pages 175–200



# AN IMMERSED-FINITE-ELEMENT PARTICLE-IN-CELL SIMULATION TOOL FOR PLASMA SURFACE INTERACTION

YUCHUAN CHU, DAORU HAN, YONG CAO, XIAOMING HE, AND JOSEPH WANG

**Abstract.** A novel Immersed-Finite-Element Particle-in-Cell (IFE-PIC) simulation tool is presented in this paper for plasma surface interaction where charged plasma particles are represented by a number of simulation particles. The Particle-in-Cell (PIC) method is one of the major particle models for plasma simulation, which utilizes a huge number of simulation particles and hence provides a first-principle-based kinetic description of particle trajectories and field quantities. The immersed finite element method provides an accurate approach with convenient implementations to solve interface problems based on structured interface-independent meshes on which the PIC method works most efficiently. In the presented IFE-PIC simulation tool, different geometries can be treated automatically for both PIC and IFE through the geometric information specified in an input file. The set of parameters for plasma properties is also assembled into a single input file which can be easily modified for a variety of plasma environments in different applications. Collisions between particles are also incorporated in this tool and can be switched on/off with one parameter in the input file. Efficient modules are adopted to integrate PIC and IFE together into the final simulation tool. Hence our IFE-PIC simulation package offers a convenient and efficient tool to study the microcosmic plasma features for a wide range of applications. Numerical experiments are provided to demonstrate the capability of this tool.

**Key words.** Particle-In-Cell, immersed finite elements, plasma surface interaction, electric propulsion.

## 1. Introduction

The problem of plasma interactions with a complex surface is typically very complicated to solve. Numerical simulations play an essential role in the study of plasma characteristics and have become an efficient tool to provide accurate performance predictions of the plasma devices. The standard tool to solve the interactions of a rarefied plasma with a complex surface is Particle-in-Cell (PIC) method, which has been widely used in many engineering and applied physics problems involving plasma-surface interaction, such as electric propulsion systems [41, 57, 73] and fusion reactors [20, 62]. Furthermore, the PIC method with Monte Carlo Collisions (MCC) [7, 36, 60, 64] and Direct Simulation Monte Carlo (DSMC) methods [3–5, 9, 33, 34, 58, 59] can simulate the interactions between different plasma species.

In the PIC method, a "gather" step is used to interpolate the electric field, which is solved by a numerical method, from mesh nodes to particle positions to push the particles. A "scatter" step is used to deposit particle charge to mesh nodes for the numerical method to solve for the electric field. In a typical PIC simulation, there are millions of simulation particles in the computation domain. Hence these two main steps cost a significant portion of computing time. Therefore, it is necessary to find an efficient way to perform these two steps for each particle. Since the particle locations can be easily identified via indexing in a Cartesian mesh, it is preferable to use a Cartesian mesh on which the PIC method works most efficiently. However, most PIC simulations in practical applications have

Received by the editors February 25, 2016 and, in revised form, October 8, 2016.
2010 Mathematics Subject Classification: 68N19, 65N30.

objects immersed in the plasma, which makes the problem an *interface* problem. For such problems, traditional numerical methods need to use body-fitting meshes, which are unstructured for non-trivial object geometry hence not very efficient for locating particles in the PIC method. Therefore, it is critical to develop a new numerical method to accurately solve the interface problem with complex interfaces on Cartesian meshes for PIC method.

The immersed finite element (IFE) method which adapts the finite element method for interface problems so that a structured mesh independent of the interface can be used to accurately solve interface problems [1,8,11–13,16,18,22,27,28, 31,32,35,43,44,46–50,52,53,56,63]. Based on the IFE method, the Immersed-Finite-Element Particle-In-Cell (IFE-PIC) method [37,39,40,54,55] has been developed to provide a promising approach for plasma simulations and applied to different applications [10,15,17,36,66,67,69,70]. The algebraic system arising from the IFE method is symmetric positive definite, which is a critical property for employing many fast solvers. While minimizing the extra efforts to modify the traditional finite element packages, IFE methods can also easily deal with complex interface with an optimal order of accuracy. These features make the IFE methods competitive for accurately solving the interface problems on structured meshes independent of the interface and providing the electric field to the PIC method.

In this paper we will present a featured simulation tool of the IFE-PIC method. The IFE and PIC methods will be briefly reviewed and the dynamic interactions between IFE and PIC modules are illustrated in details. Several critical features of the simulation tool will be discussed, such as the automatic treatment of the different geometries, the convenient input for different types of plasma, efficient modules for interactions between IFE and PIC methods, and optional modules for particle collisions. In order to illustrate the features of this simulation tool, two numerical experiments are carried out for the electric propulsion. Based on the automatic treatment of object surfaces and high-efficient particle simulation of our tool, various spacecraft/satellite parts of different geometries and high density plasma in electric propulsion can be modeled with our IFE-PIC package. Meanwhile, the physical mechanism of discharging process in electric propulsion and the erosion of key components, such as the grid erosion caused by charge-exchange ions, can be analyzed in detail with the particle collision module.

The rest of the paper is organized as follows. In Section 2 we will review the IFE method and discuss about the modules for obtaining the IFE solution. In Section 3 we will review the PIC method and introduce the modules and parameters for PIC. In Section 4 we will integrate PIC and IFE together under a dynamic framework with efficient modules for the interactions between PIC and IFE. In Section 5 numerical examples will be provided to illustrate the features of the simulation tool. Finally brief conclusions are given in Section 6.

## 2. Modules for immersed finite element method

In this section, we will introduce the modules of the immersed finite element method in the plasma environment simulation tool. First, we will briefly review the basic idea of IFE and the definition of the 3D linear IFE method. Then we will introduce the input file and the modules for dealing with the geometries which are needed to form the IFE basis functions and compute the integrals by Gauss quadratures. Moreover, we will introduce the modules to form the linear system arising from the immersed finite element method based on the charge density provided by