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A 3D immersed finite element method with non-homogeneous interface flux jump for applications in particle-in-cell simulations of plasma–lunar surface interactions ☆

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ABSTRACT

Motivated by the need to handle complex boundary conditions efficiently and accurately in particle-in-cell (PIC) simulations, this paper presents a three-dimensional (3D) linear immersed finite element (IFE) method with non-homogeneous flux jump conditions for solving electrostatic field involving complex boundary conditions using structured meshes independent of the interface. This method treats an object boundary as part of the simulation domain and solves the electric field at the boundary as an interface problem. In order to resolve charging on a dielectric surface, a new 3D linear IFE basis function is designed for each interface element to capture the electric field jump on the interface. Numerical experiments are provided to demonstrate the optimal convergence rates in L^2 and H^1 norms of the IFE solution. This new IFE method is integrated into a PIC method for simulations involving charging of a complex dielectric surface in a plasma. A numerical study of plasma–surface interactions at the lunar terminator is presented to demonstrate the applicability of the new method.

1. Introduction

The Particle-in-Cell (PIC) method is a standard tool to model the interactions of a rarefied plasma with complex surfaces of different types of objects. In PIC simulations of plasma–object interaction, the objects' surfaces divide the domain into two or more sub-domains. In order to take into account the electrical interactions between the objects and plasma, the following three-dimensional interface elliptic equation involving the electric field ($\mathbf{E}$) discontinuity across the interface needs to be considered for the electric potential $\phi(X)$ [12,30,68]:

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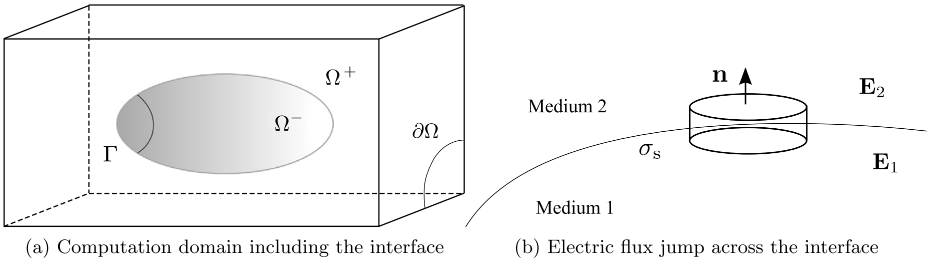

Fig. 1. A sketch of the interface problem.

$$-\nabla\cdot\big(\varepsilon\nabla\phi(X)\big)=\rho(X),\quad X=(x,y,z)\in\Omega^-\cup\Omega^+, \tag{1.1}$$

$$\phi(X)|_{\Gamma_D}=g(X), \tag{1.2}$$

$$\frac{\partial\phi(X)}{\partial\mathbf{n}_{\Gamma_N}}|_{\Gamma_N}=p(X), \tag{1.3}$$

together with the jump conditions across the interface Γ:

$$[\phi(X)]|_\Gamma=0, \tag{1.4}$$

$$\left[\varepsilon\frac{\partial\phi(X)}{\partial\mathbf{n}_\Gamma}\right]\Big|_\Gamma=q(X)=-(\varepsilon_2\mathbf{E_2}-\varepsilon_1\mathbf{E_1})\cdot\mathbf{n}_\Gamma=-\sigma_s. \tag{1.5}$$

Here, see the sketch in Fig. 1, without loss of generality, we assume that $\Omega\subset\mathbb{R}^3$ is a box domain, the interface Γ is a curved surface separating Ω into two sub-domains (Ω^- and Ω^+) such that $\overline{\Omega}=\overline{\Omega^-}\cup\overline{\Omega^+}\cup\Gamma$, Γ_D and Γ_N are the Dirichlet and Neumann boundaries such that $\partial\Omega=\Gamma_D\cup\Gamma_N$, $\mathbf{n}_{\Gamma_N}$ is the unit outer normal vector of Γ_N, $\mathbf{n}_\Gamma$ is the unit normal vector of Γ pointing from Ω^- to Ω^+, E_i $(i=1,2)$ is the electric field in the medium i, and the material-dependent coefficient $\varepsilon(x,y)$ is a piecewise constant function defined by

$$\varepsilon(X)=\begin{cases}\varepsilon^-, & X\in\Omega^-,\\ \varepsilon^+, & X\in\Omega^+.\end{cases}$$

Because PIC simulations spend a significant amount of time on locating a huge number of simulation particles in the mesh at each iteration, it is preferable to utilize structured meshes that can deal with the complex interfaces. However, when conventional numerical methods [3,5,8,28,59] are used to solve the interface problem (1.1)–(1.5), body-fitting meshes, which are unstructured, need to be utilized in order to guarantee these methods' performance. Therefore, the immersed finite element (IFE) methods, which were developed for solving interface problems on meshes independent of interface [1,6,9,15,19,22,23,26,27,31,39–41,43–47,49,50,53,69], have been integrated into the PIC method as the electric field solver on structured meshes. This resulted in the IFE-PIC method [7,11,33,37,51,52,64,68], which has been employed in the modeling of plasma flow in ion thrusters and plume–spacecraft interactions. In these applications, the electric potentials of the objects are assumed to be fixed and known, which yields the homogeneous flux jump condition across the interface for the interface model. Therefore, the existing IFE-PIC method and 3D IFE method [34,58,63] consider only the homogeneous flux jump condition.

This study concerns application problems involving a dielectric object immersed in a plasma. The surface potential on a dielectric surface is determined by local charge deposition, which results in a non-homogeneous flux jump (i.e. electric field) conditions across the interface. In this paper, we develop a three-dimensional immersed finite element method for the second order interface elliptic problems with non-homogeneous flux jump condition, and integrate it to the PIC method. This new IFE-PIC method allows one to solve self-consistently the surface potential of a complex dielectric object and the plasma flow directly from local charge deposition on the surface.

The basic idea of the new IFE method is to locally enrich the 3D linear IFE space in [34] by adding new piecewise polynomials that can approximate the non-homogeneous flux jump conditions satisfactorily [24]. The major difficulty for proposing the new IFE-PIC method lies in the dynamic interaction between the IFE and PIC methods, especially the accumulation of the surface charging q expressed by surface charge density σ_s as shown in Fig. 1b. In addition to the traditional advantages of the IFE and PIC methods, another practical advantage of this new method is the convenience to implement it based on the existing 3D IFE-PIC package for homogeneous interface conditions since the new method keeps the basic framework of the existing IFE space and the method developed in [34].

This new IFE-PIC method is applied to study plasma–surface interactions at the lunar terminator. Without a global magnetic field, the lunar surface is directly exposed to the solar radiation and the space plasma environments. Substantial studies have been carried out to understand the near surface plasma environment on the Moon [14,16,55–57,66–68]. The lunar polar region is of particular interest to future lunar exploration missions due to the availability of solar power and the existence of cold-trapped lunar water/ice. Modeling plasma–surface interactions in the terminator region is a challenging numerical problem as it requires the model to calculate the charging of a complex shaped surface terrain self-consistently