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Development of PIFE-PIC-ESP: Parallel Immersed Finite Element Particle-In-Cell for ElectroSpray Propulsion

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As electrospray thrusters become more popular on small satellites, a multiscale, multiphysics modeling/simulation tool is needed to study the thruster performance and plume characteristics. This paper presents the preliminary work on the development of a multiscale (from single emitter to spacecraft plume) kinetic simulation framework specifically designed for electrospray propulsion, namely, Parallel Immersed Finite Element Particle-In-Cell for ElectroSpray Propulsion (PIFE-PIC-ESP). Legacy modules of the underlying framework PIFE-PIC are briefly described. New modules particularly related to electrospray thrusters are under development at different scales ranging from single emitter/extractor to thruster plume. Ongoing efforts are focused on carrying out benchmarking simulation cases across the scales to enable cross-scale capabilities.

I. Introduction

Electrospray thrusters refer to a category of electric propulsion (EP) devices that generate a stream of ions and/or charged droplets from a liquid reservoir through electrostatic acceleration. The liquid (propellant) from this reservoir is routed inside a capillary or around a needle (emitter). A large potential voltage difference is generated between this liquid and an electrode (extractor). The liquid forms what is known as a Taylor cone and is drawn through free space towards the electrode in a process referred to as emission [1]. This emission, depending on operating conditions, can be in the form of droplets, ions, or a mixture of both. There have been two main variations in realizing this concept for space propulsion: 1) field emission electric propulsion (FEEP) and 2) colloid thrusters. FEEP is denoted by the use of a liquid metal and emission of only ions (and neutralizing electrons) [2]. Colloid thrusters emit droplets/ions and use non-metallic liquids [3]. In addition to FEEP and colloid thrusters, a new type of electrospray source named ionic liquid ion sources (ILIS) has been firstly introduced by Lozano and Martinez-Sanchez [4]. ILIS are colloid thrusters capable of producing both positive and negative ions (cations and anions) as well as ion clusters from ionic liquids. Based on this concept, a new type of bimodal space propulsion, namely ion Electrospray Propulsion System (iEPS), has been developed [4, 5]. The iEPS utilizes ionic liquids exposed to strong electric fields in a microelectromechanical systems (MEMS) package to generate high energy beams of heavy molecular ions or charged droplets without gas-phase ionization, and has made significant advances in recent years [6–14].

In the past a few decades, electrospray propulsion research has gained significant momentum as a result of reduced spacecraft size and improved microscale manufacturing. Operational advantages of electrospray propulsion include high specific impulse (I_{sp}), thrust accuracy, efficiency, and volume/mass/scalability requirements [3, 15–17]. As electrospray thrusters become more popular on small satellites, which are of particular interest to the U.S. Air Force and Space Force [18], there is a gap between the current modeling capability and the knowledge needed for plume characteristics as well as spacecraft-plume interactions for electrospray propulsion. A multiscale (from emitter-extractor to spacecraft-plume), multiphysics (plume neutralization, spacecraft charging, contamination, etc.) modeling/simulation tool is needed for electrospray propulsion research.

This paper presents the preliminary work on the development of a multiscale (from single emitter to spacecraft plume) kinetic simulation framework specifically designed for electrospray propulsion, namely, Parallel Immersed Finite Element Particle-In-Cell for ElectroSpray Propulsion (PIFE-PIC-ESP). Section II reviews the current state of the art for electrospray modeling research. Section III describes the underlying framework, PIFE-PIC, for the development of PIFE-PIC-ESP. Section IV summarizes the legacy modules for electric propulsion applications, namely, ion optics and

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plume. Section V present related modules of PIFE-PIC-ESP at different scales ranging from single emitter/extrator to thruster plume. Lastly, Section VI summarizes the initial development and discuss the ongoing efforts.

II. Current State of the Art of Electrospray Modeling Research

The modeling approaches that have been applied to electrospray can be categorized based on the region / length scale. Near the cone-jet region, most of the modeling/simulation techniques are based on analytic models and molecular dynamics (MD) or fluid-continuum simulations, while near the emission/beam region, particle-kinetic methods have been mainly utilized. A number of modeling efforts have been made at Massachusetts Institute of Technology (MIT), University of Illinois at Urbana-Champaign (UIUC), University of California, Irvine (UCI), and University of California, Los Angeles (UCLA). Figure 1 illustrates a zoom-in view of a single emitter in an emitter array, labeled with typical state-of-the-art modeling approaches for different regions/processes.

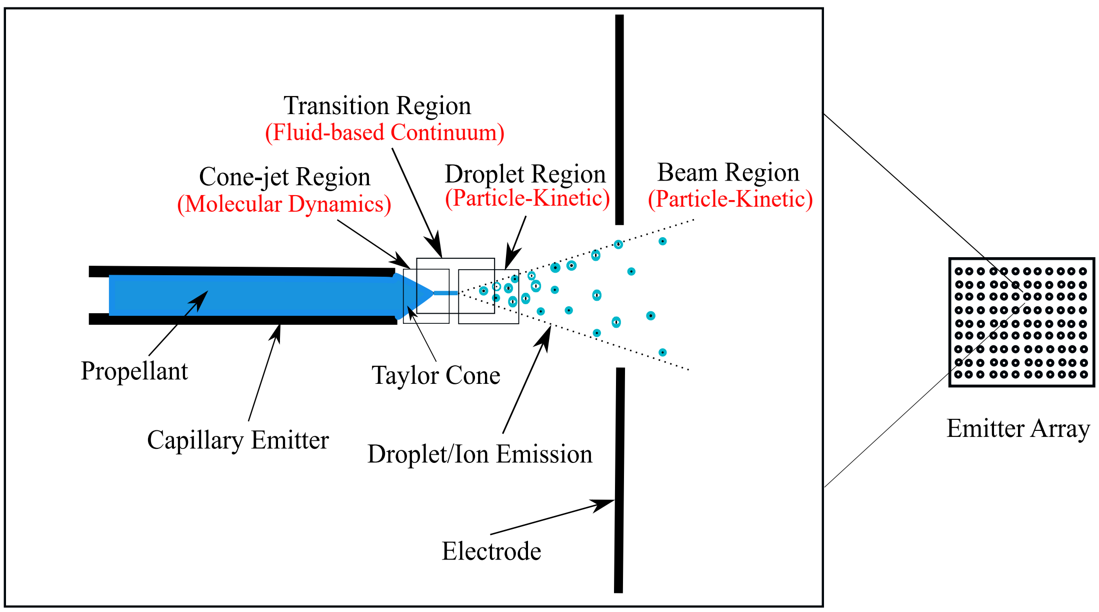

Fig. 1 A zoom-in view of a single emitter in an emitter array, labeled with typical state-of-the-art modeling approaches for different regions/processes.

Cone-Jet Region/Scale For the cone-jet region, the MIT group presented early numerical models [19, 20] and carried out MD simulations to study ion evaporation [21, 22], as well as the leaky-dielectric model accounting for charge evaporation [23]. The group at UIUC applied MD and kinetic techniques to model droplet evolution and fragmentation under electric field and long-range Coulomb interactions [24–33]. The UCI group introduced first-principle-based models of electrospraying in the cone-jet mode [34] [35], energy dissipation process [36, 37], and an electrohydrodynamic (EHD) model for coaxial electrosprays [38]. Recently, an EHD model integrated with OpenFOAM solver was developed by the group at UCLA [39, 40]. Other fluid-based methods have been used to study pressure feed systems [41], emitter flow [42], shape of the liquid cone jet [43], and ferrofluid propellant subject to electric and magnetic stresses [44].

Droplet/Ion Emission-Beam Region/Scale For the droplet/ion transition and emission-beam region, there are analytic formulations/models developed for the beam [45, 46], extractor design [47], spray deposition [48], and beam spreading caused by space charge and diffusion [49]. Computational efforts have utilized MD and particle-kinetic (i.e., PIC) approaches or coupling of the two [50–62], and discrete interaction models taking into account Coulomb interactions in plume expansion [39, 63]. It is noted here that recently a particle-particle (PP) method treating droplets as finite-sized particles and directly applying the Coulomb interactions among them has been introduced [64]. This PP method holds promise for significant computational speedup on shared-memory and/or GPU platforms.

Plume Region/Scale There have been a few attempts to model the electrospray up to the plume region/scale. Carretero et al. [65] used a quasi-1D EHD model and a 3D PIC code to study the cone-jet formation and charged particle spray dynamics in the droplet and the mixed ion-droplet regimes incorporating an electrically enhanced ion evaporation model. Results from the cone-jet model were extrapolated to the jet breakup region and then used as initial conditions for a PIC model to track individual droplets and ions. This model was used to estimate plume divergence angles and axial/radial energy distributions. Another multiscale study was carried out by Morris et al. [66], where molecular/particle/fluid modeling approaches were adopted to calculate the trajectories and characteristics of the droplets and ions.

III. The PIFE-PIC Framework

This section briefly describes the underlying framework, PIFE-PIC, for modeling plasma-material interactions with applications to problems of space plasma and electric propulsion. The fundamental phenomena of *plasma-material interactions* can be mathematically modeled as an interface problem including the electrostatic/electromagnetic field problem in self-consistent solution to the corresponding plasma dynamics problem, together with the appropriate boundary conditions at the interface between plasma region and material region. In EP applications, the shape of the interface is usually non-trivial (for example, the ion optics grids in ion thrusters and extractors in electrospray thrusters). Traditionally, when solving field problems involving complex-shaped objects, an unstructured body-fitting mesh is employed due to accuracy considerations. However, a Cartesian mesh is much-preferred in kinetic particle-in-cell modeling of plasma dynamics concerning computing speed and efficiency, although it has been limited to problems with relatively simple geometries due to accuracy considerations inherited with finite-difference-based Cartesian mesh. To solve this dilemma and to take into account both accuracy and efficiency, the immersed-finite-element particle-in-cell (IFE-PIC) method was developed to handle complex interface boundary conditions associated with irregular geometries while maintaining the computational speed of the Cartesian-mesh-based PIC. Over the past years, this method has matured to successfully model plasma dynamics problems arising from many space applications, such as ion thruster optics [67, 68], ion propulsion plume-induced contamination [69–71], charging of lunar and asteroidal surfaces [72–77], and dust transport dynamics around small asteroids [78].

The serial version of the IFE-PIC method has limited its applications to relatively small problem sizes with respect to practical interests. One of the objectives of the current research project is to develop/optimize a massively-scalable, first-principle-based, multiscale, multiphysics modeling capability for complex physics related to electrospray propulsion, such that practical and realistic simulations can be carried out routinely on supercomputers. Towards this goal, Han et al. have developed the Parallel IFE-PIC (PIFE-PIC) method using 3-D domain decomposition [79–81].

IV. Legacy Modules of PIFE-PIC-ESP for Electric Propulsion Modeling

A. Ion Optics Scale

The IFE-PIC method has been applied to simulations of plasma problems rising from ion propulsion [71]. At the ion optics scale, IFE-PIC method has been employed to resolve the geometry of the holes of the grids (Figure 2). It is noted here that the IFE scheme is also able to resolve the geometries of the emitter/extractor for electrospray thrusters.

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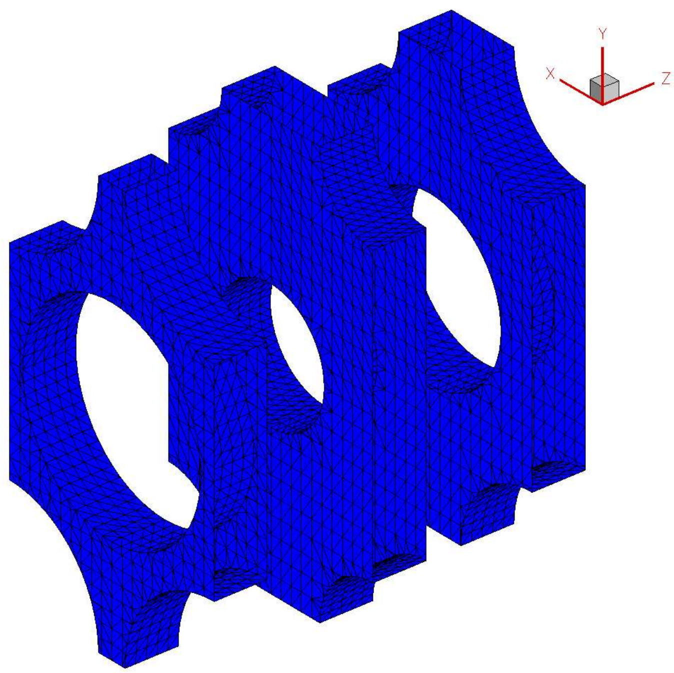

Fig. 2 Geometry resolution of IFE scheme applied to ion optics grids of an ion thruster. For PIFE-PIC-ESP, IFE scheme is used to resolve the geometries of extractor/accelerator for electrospray thrusters.

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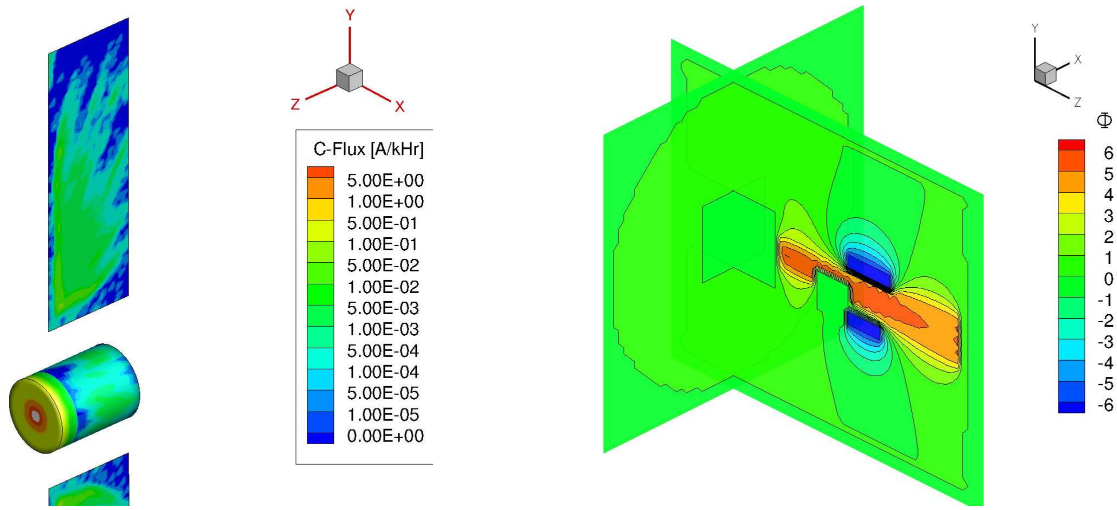
B. Spacecraft-Plume Scale

For the spacecraft-plume scale, the IFE-PIC method has been employed to perform contamination calculations [71] (Figure 3(a)) and plume expansion for in-chamber vs. in-space conditions [82, 83] (Figure 3(b)).



(a) Spacecraft contamination calculation using IFE-PIC [71].

(b) IFE-PIC simulation of a plume inside a cylinder chamber [83].

Fig. 3 Geometry resolution of IFE scheme applied to entire spacecraft (a) and full-scale ground chamber test of ion sources (b). In PIFE-PIC-ESP, IFE scheme will be used to resolve the geometries of spacecraft and vacuum chamber at the spacecraft-plume scale.

V. Modules of PIFE-PIC-ESP at Different Scales

Single Emitter/Extractor Scale The single-emitter/extractor module of PIFE-PIC-ESP starts with the domain including the emission site (Figure 4).

Extractor-Array Scale The extractor-array scale will extend the modules for single-emitter/extractor to extractor-array scale and take into account more array-scale interactions, as shown in Figure 5.

Spacecraft-Plume Scale The spacecraft-plume module will implement modules and models developed for smaller scales (i.e., single-emitter and emitter-array) into into existing plume modules inherited from the legacy IFE-PIC plume suite [69, 70], and develop the plume modules for PIFE-PIC-ESP. Additional modules will include fully-kinetic plume models, collision schemes including Direct Simulation Monte Carlo (DSMC) and Monte Carlo Collision (MCC), and surface-interaction models including secondary emission and sputtering, as illustrated in Figure 6.

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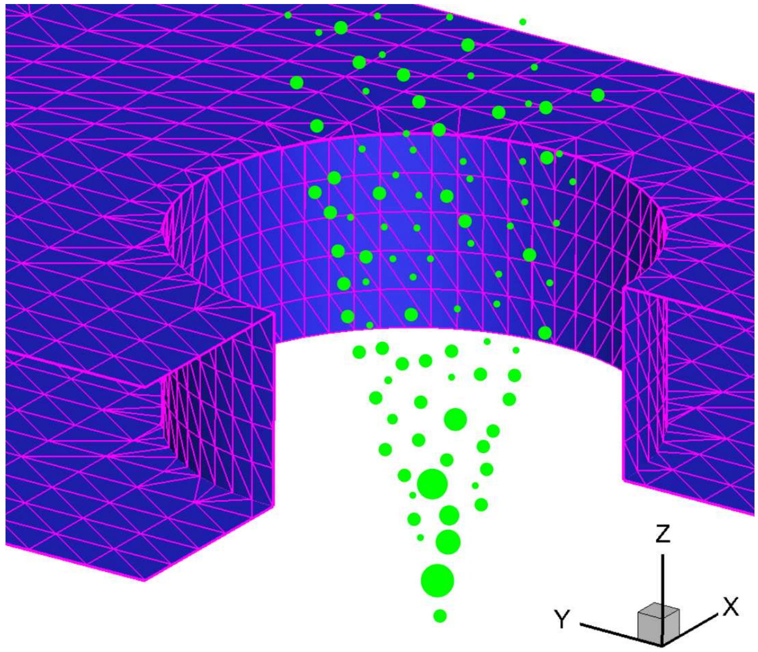

Fig. 4 Illustration of PIFE-PIC-ESP's single emitter/extractor module.

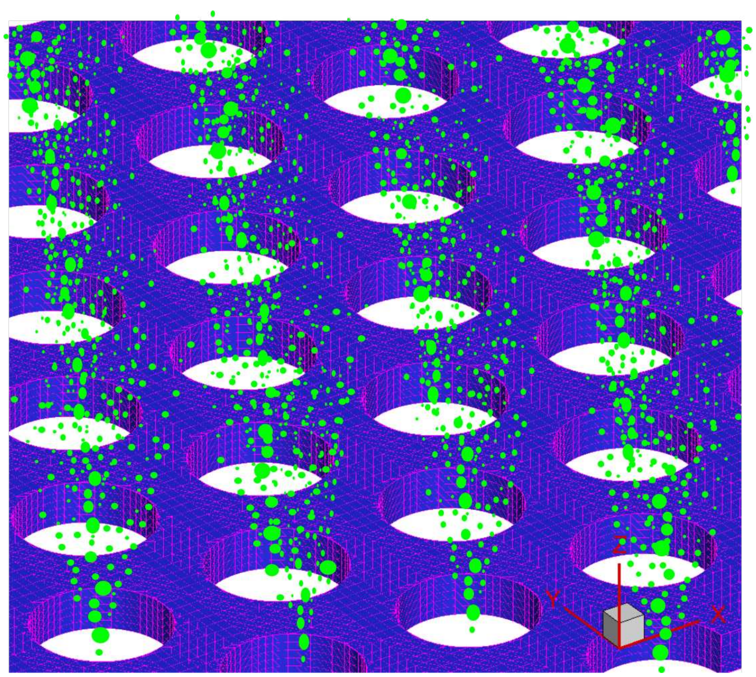

Fig. 5 Illustration of PIFE-PIC-ESP's extractor-array module.

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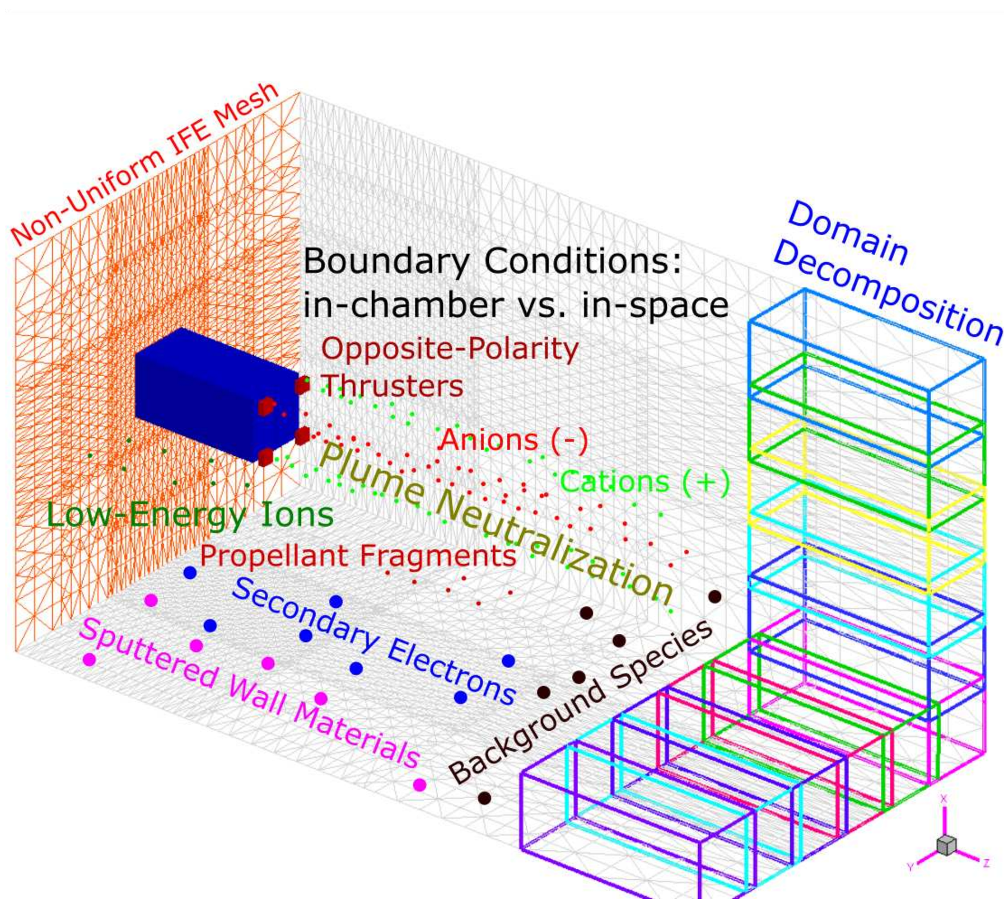

Fig. 6 Illustration of PIFE-PIC-ESP's spacecraft-plume module.

VI. Summary and Ongoing Work

Preliminary development status of a multiscale (from single emitter to spacecraft plume) kinetic simulation framework specifically designed for electrospray propulsion, namely, Parallel Immersed Finite Element Particle-In-Cell for ElectroSpray Propulsion (PIFE-PIC-ESP), is presented. Legacy modules of an existing framework PIFE-PIC are briefly described. New modules particularly related to electrospray thrusters are under development at different scales ranging from single emitter/extractor to thruster plume. Ongoing efforts are focused on carrying out benchmarking simulation cases across the scales to enable cross-scale capabilities.

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