

Verification of the generalized reduced-order particle-in-cell scheme in a radial-azimuthal $E \times B$ plasma configuration

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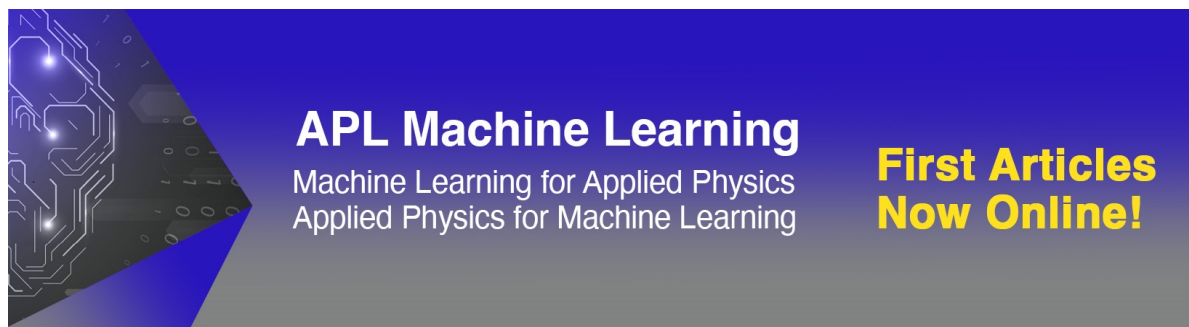
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Verification of the generalized reduced-order particle-in-cell scheme in a radial-azimuthal $E \times B$ plasma configuration

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ABSTRACT

In this article, we present an in-depth verification of the generalized electrostatic reduced-order particle-in-cell (PIC) scheme in a cross electric and magnetic field configuration representative of a radial-azimuthal section of a Hall thruster. The setup of the simulations follows a well-established benchmark case. The main purpose of this effort is to demonstrate that our novel PIC scheme can reliably resolve the complex two-dimensional dynamics and interactions of the plasma instabilities in the radial-azimuthal coordinates of a Hall thruster at a fraction of the computational cost compared to full-2D PIC codes. To this end, we first present the benchmarking of our newly developed full-2D PIC code. Next, we provide an overview of the reduced-order PIC scheme and the resulting “quasi-2D” code, specifying that the degree of order reduction in the quasi-2D PIC is defined in terms of the number of “regions” along the simulation’s directions used to divide the computational domain. We compare the predictions of the quasi-2D simulation in various approximation degrees of the 2D problem against our full-2D simulation results. We show that, with an increase in the number of regions in the Q2D simulations, the quasi-2D results converge to the 2D ones. Nonetheless, we also highlight that a quasi-2D simulation that provides a factor of 5 reduction in the computational cost resolves the underlying physical processes in an almost indistinguishable manner with respect to the full-2D simulation and incurs an L2-norm error of only about 2% in the ion number density and below 1% in the electron temperature.

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I. INTRODUCTION

Nowadays, the $E \times B$ plasma discharges, where the applied magnetic field is perpendicular to the discharge current, have several important applications, from magnetrons for material processing to Hall thrusters for spacecraft plasma propulsion. The operation of the $E \times B$ technologies mainly relies on effectively impeding the cross-magnetic-field electron current. Nonetheless, the plasma in an $E \times B$ configuration is subject to strong anisotropies and gradients that lead to the excitation of various instabilities and turbulence, spanning over a broad range of spatial and temporal scales.^{1,2} The instabilities and turbulent mechanisms are demonstrated through numerical^{3,4} and experimental^{5,6} efforts to induce notable cross-field transport of particles and energy. As a result, the global dynamics of the plasma discharge and, hence, the performance of the $E \times B$ devices are affected by these plasma processes. Therefore,

acquiring an all-round knowledge of the instabilities’ behavior and their effects on $E \times B$ plasmas in conjunction with having predictive modeling tools available will greatly enhance the development cycle of the technologies reliant on these plasmas, enabling methodical and cost-effective design, optimization, and testing of the devices.

Although many insights into the excitation and evolution of the instabilities in $E \times B$ plasmas have been gathered over the past decades, a comprehensive knowledge basis of these phenomena and their interplays is still lacking.⁷ The reason for this status quo is twofold: on the one hand, the dominant phenomena are three-dimensional and greatly multi-scale,⁷ they are kinetic in nature,⁸ and their evolution and interactions are characterized by highly nonlinear processes.^{4,9} On the other hand, a comprehensive study of the complex dynamics of the instabilities and their associated effects on the plasma discharge requires a high-fidelity and

computationally affordable 3D kinetic model capable of resolving the full-3D dynamics in real-size devices over real-world operational timeframes. Such a modeling tool is currently unachievable due to the significant computational burden of the existing kinetic simulation codes. Even lower dimension 2D kinetic simulations are prohibitively expensive for real-scale devices; for instance, a 2D PIC simulation of a Hall thruster for a representative period of 150 μ s simulated time, without any scaling of the physical or geometrical parameters, requires a run time of *about 1 year using 1500 CPUs*.¹⁰ In view of the unavailability of a cost-effective 3D kinetic code, the main unresolved questions in the physics of $E \times B$ plasmas revolve around the 3D effects and interactions⁷ as well as the mechanisms for energy transfer across instabilities spectrum over time that can lead to the formation of large-scale spatiotemporally coherent structures (i.e., inverse energy cascade and self-organization).¹¹ Consequently, the puzzle of the dynamics of the particles and energy transport due to the instabilities and turbulence in various phases of their evolution has still important missing pieces.

The reduced-order, or quasi-multi-dimensional, PIC scheme is an innovative approach based on a dimensionality-reduction technique that reduces the computational cost of electrostatic kinetic simulations by 1–3 orders of magnitude.^{12,13} As a result, it serves as a potential solution to the long-persisting challenge of the unavailability of a self-consistent, high-fidelity 3D kinetic code to reveal the full picture of the underlying plasma phenomena in $E \times B$ configurations. In this respect, it is important to also acknowledge the other efforts initiated in the past years within the community to tackle the computational cost issue of kinetic plasma simulations through alternative approaches such as applying the sparse grid methods to the PIC scheme.¹⁴

So far, the reduced-order PIC has been verified in detail in an axial–azimuthal Hall thruster configuration, demonstrating that it is able to approximate the full-2D results from conventional PIC codes with high accuracy and remarkable computational efficiency.^{13,15} Moreover, the formulation underlying the reduced-order PIC scheme, which enables the decomposition of the multi-dimensional Poisson's equation into a system of coupled 1D ODEs, is proven to be mathematically consistent and applicable to solve general Poisson problems with arbitrary boundary conditions.¹³

Based on the already observed promises in the axial–azimuthal configuration, and ahead of extending the reduced-order PIC to 3D, we evaluate, in this effort, the applicability and predictions' accuracy of the reduced-order PIC in another 2D $E \times B$ configuration, which is representative of a radial–azimuthal section of a Hall thruster. Prior research into the physics of plasma in the radial–azimuthal Hall thruster configuration has revealed the development of microscopic instabilities^{16,17} and intricate interactions between the plasma sheath and the bulk plasma processes that affect the evolution of the excited kinetic instabilities.¹⁸ Thus, verifying the “quasi-2D” PIC in the radial–azimuthal configuration allows us to ascertain further the abilities of the scheme in resolving closely coupled, highly two-dimensional phenomena, hence gaining additional confidence that the generalized implementation of the reduced-order scheme serves as the required strong foundation upon which we can build to enable reliable and computationally efficient 3D simulations of the $E \times B$ plasmas.

Toward the above aim, we provide in Sec. II a brief review of the reduced-order quasi-2D PIC scheme and the corresponding kinetic code, IPPL-Q2D, developed at Imperial Plasma Propulsion Laboratory (IPPL). We also introduce our laboratory's recently developed full-2D conventional PIC code, IPPL-2D. Since the full-2D and the quasi-2D PIC codes share several similarities, the comparison of the quasi-2D results against our own 2D ones, rather than the reference benchmark results,¹⁹ allows us to unequivocally link the potential discrepancies to the reduced-order description of the problem inherent to the quasi-2D scheme. In Sec. III, we provide an overview of the radial–azimuthal simulation setup and conditions. Moreover, we present the verification results of the IPPL-2D code against the benchmark in this section, which is the first benchmarking of this newly developed code. We compare the predictions of the IPPL-Q2D code in various number-of-region approximations and those from the IPPL-2D in Sec. IV, discussing the results in terms of the radial distribution of the time-averaged plasma properties, ion number density and electron temperature, the time evolution of these plasma properties, the wavenumber content of the resolved azimuthal electric field fluctuations, and the 2D radial–azimuthal snapshots of several plasma parameters at two instances of the discharge evolution. In Sec. V, we further evaluate the flexibility of the reduced-order PIC by investigating the effect that adopting non-uniform regions' extent in the quasi-2D simulations has on the results. Section VI is dedicated to the analysis of the sensitivity of the quasi-2D results to the initial number of macroparticles per cell. Finally, in Sec. VII, we highlight the main outcomes of this study and outline the planned follow-up activities.

II. IPPL-2D AND IPPL-Q2D PARTICLE-IN-CELL CODES

Here, we first introduce the IPPL-2D code and then provide an overview of our reduced-order PIC scheme and the IPPL-Q2D code. The difference between these two electrostatic particle-in-cell codes is limited to two aspects: first, the formulation underlying the Poisson solver and, second, the computation grid that we use to deposit the particle-based information, such as the charge density, and from which we gather the grid-based information, such as the electric field, on particles' location. All other module implementations, such as the random number generator, particles' push, and the diagnostics, are the same between the two codes. Both full-2D and quasi-2D PIC codes are parallelized with the Message Passing Interface (MPI) protocol. The parallelization is based on the domain decomposition, which is carried out along a single simulation direction.

A. Introducing the IPPL-2D particle-in-cell code

IPPL-2D is an explicit, conventional fully kinetic particle-in-cell code whose overall structure and function implementations follow the standard particle-in-cell method, as explained in Refs. 20 and 21.

The code is written in Julia language.²² The main reasons for choosing Julia have been its special focus on scientific computing and its built-in capabilities to simplify CPU parallelization. Julia is a just-in-time compiled language, and as such, a code in Julia can, in principle, run as fast as an equivalent version written in legacy languages such as C++. However, to achieve the highest computational performance possible, the code needs to be compatible with Julia's

compiler optimizations, which implies that the “Julian” way of writing the code can sometimes be different from the common practices used for code development in other programming languages, such as C++ or Fortran.

The code uses Julia’s built-in Random Number Generator (RNG) function, which follows the Xoshiro256++ algorithm²³ by default. The sampling of the distribution function for macroparticles’ load is done using the Box–Muller algorithm.²⁴ Bilinear weighting is used to deposit particle-based information onto the 2D grid nodes and to gather the grid-based information on particles’ position. Particle’s push function is based on the classic leapfrog scheme²⁰ with the position of the magnetized electrons being updated following the Boris method.²⁵ The electric potential is resolved by numerically solving the 2D Poisson equation using Julia’s built-in direct matrix solve algorithm based on the LU decomposition.

B. Overview of the generalized reduced-order PIC scheme and the IPPL-Q2D PIC code

As mentioned in Sec. I, the reduced-order PIC scheme, described in detail in Refs. 13 and 26, is a novel kinetic plasma modeling approach to significantly lower the computational resource requirement of the traditional multi-dimensional PIC codes. In this PIC scheme, the computational domain is decomposed into multiple rectangular (in 2D) or cubic (in 3D) “regions,” which can be thought of as the discretization of the domain using a “coarse” grid (Fig. 1, left). Within any specific region, denoted as Ω on the left-hand side of Fig. 1, we discretize each simulation dimension separately using 1D “elongated” cells (orange-shaded elements in Fig. 1, right). The criterion for the cell size along the x and y directions, Δx and Δy , is the same as that in a conventional 1D PIC, i.e., smaller than the Debye length. This fine-discretization step yields a decoupling between the different coordinates in each region, allowing us to reduce the number of cells and, hence, the required total number of macroparticles from $O(N^2)$ to $O(2N)$ in a “quasi-2D” (or from $O(N^3)$ to $O(3N)$ in a “quasi-3D”) simulation, with N being the number of cells along each simulation direction. The vertical and horizontal cells in each region (Fig. 1, right) capture separately the variations of the plasma properties along the x and y directions, respectively.

The dimensionality-reduction formulation underpinning the generalized reduced-order PIC scheme¹³ is formulated in a flexible way that allows the user to determine the desired level of accuracy of predictions and, hence, to define the order of approximation or, equivalently, the number of regions to use. This, in turn, changes the required computational resources.¹³ In other words, the accuracy and the computational cost of a reduced-order simulation depend on the fineness of the coarse grid (Fig. 1, left). Therefore, our quasi-multi-dimensional PIC scheme offers a unique flexibility to have a trade-off between fidelity and the computational gain of the simulation depending on its specific purpose.

The IPPL-Q2D code, which is based on the reduced-order PIC scheme, features an electric potential field solver, which we have termed “Reduced-Dimension” Poisson Solver, or RDPS.¹³ The RDPS numerically solves a system of 1D Poisson’s equations along the simulation coordinates obtained from our dimensionality-reduction formulation, Eqs. (1) and (2), using the same Julia’s built-in direct matrix solve algorithm as that of IPPL-2D. The detailed derivation of Eqs. (1) and (2) and the verification results of RDPS for generic 2D Poisson’s problems are reported in Ref. 13.

In Eqs. (1) and (2), ϕ^x and ϕ^y are 1D potential functions along the x and y directions, respectively, that are used to approximate the 2D potential $\phi(x, y)$ in each region Ω as $\phi(x, y) = \phi^x + \phi^y$; l_x and l_y are the horizontal and vertical extents of each region; x_i is the x coordinate of each computational node i along a horizontal computation grid; and y_j is the y coordinate of each node j along a vertical computation grid. In addition, x_g and y_g are the locations of the y and x computation grids, respectively, with respect to the origin, ϵ_0 is the permittivity of free space, and $\rho(x, y)$ is the 2D charge density distribution in region Ω ,

$$\begin{aligned} & \left(\frac{d^2 \phi^x}{dx^2} \Big|_{x=x_i} \right) l_y + \frac{\partial \phi^x}{\partial y} \Big|_{y=y_g + \frac{l_y}{2}} - \frac{\partial \phi^x}{\partial y} \Big|_{y=y_g - \frac{l_y}{2}} \\ &= -\frac{1}{\epsilon_0} \int_{y_g - \frac{l_y}{2}}^{y_g + \frac{l_y}{2}} \rho(x, y) dy - \frac{\partial \phi^y}{\partial y} \Big|_{y=y_g + \frac{l_y}{2}} + \frac{\partial \phi^y}{\partial y} \Big|_{y=y_g - \frac{l_y}{2}} \\ & - \left(\int_{y_g - \frac{l_y}{2}}^{y_g + \frac{l_y}{2}} \left(\frac{\partial \phi^y}{\partial x} \Big|_{x=x_i + \frac{\Delta x}{2}} \right) dy - \int_{y_g - \frac{l_y}{2}}^{y_g + \frac{l_y}{2}} \left(\frac{\partial \phi^y}{\partial x} \Big|_{x=x_i - \frac{\Delta x}{2}} \right) dy \right) \frac{1}{\Delta x}, \end{aligned} \quad (1)$$

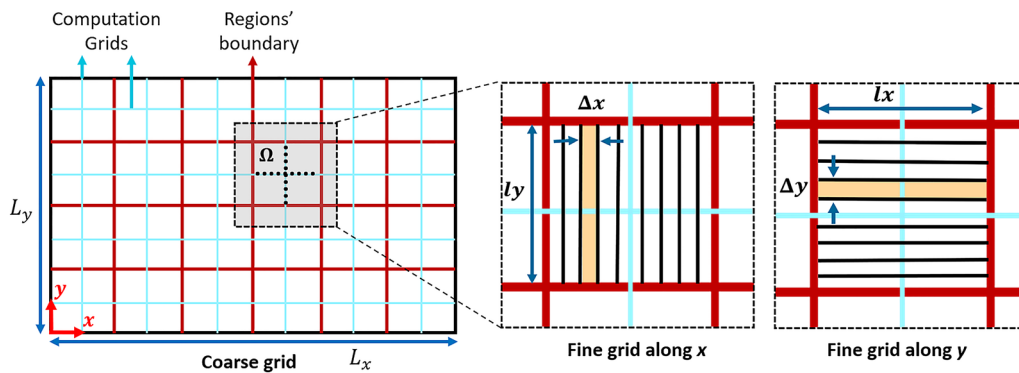


FIG. 1. Schematic of the domain decomposition corresponding to the reduced-order PIC scheme: (left) decomposition into multiple “regions” using a coarse grid; (right) 1D computational cells for discretization of each region along the x and y directions.

$$\begin{aligned}
& \left(\frac{d^2 \phi^y}{dy^2} \Big|_{y=y_j} \right) l_x + \frac{\partial \phi^y}{\partial x} \Big|_{x=x_g+\frac{l_x}{2}} - \frac{\partial \phi^y}{\partial x} \Big|_{x=x_g-\frac{l_x}{2}} \\
&= -\frac{1}{\epsilon_0} \int_{x_g-\frac{l_x}{2}}^{x_g+\frac{l_x}{2}} \rho(x, y) dx - \frac{\partial \phi^x}{\partial x} \Big|_{x=x_g+\frac{l_x}{2}} + \frac{\partial \phi^x}{\partial x} \Big|_{x=x_g-\frac{l_x}{2}} \\
&\quad - \left(\int_{x_g-\frac{l_x}{2}}^{x_g+\frac{l_x}{2}} \left(\frac{\partial \phi^x}{\partial y} \Big|_{y=y_j+\frac{\Delta y}{2}} \right) dx - \int_{x_g-\frac{l_x}{2}}^{x_g+\frac{l_x}{2}} \left(\frac{\partial \phi^x}{\partial y} \Big|_{y=y_j-\frac{\Delta y}{2}} \right) dx \right) \frac{1}{\Delta y}.
\end{aligned} \quad (2)$$

It is worth pointing out that, at each simulation time step, the derivative terms on the right-hand side of Eqs. (1) and (2) are obtained from the solutions of ϕ^x and ϕ^y from the previous time step.¹³

RDPS is one of the differences between IPPL-Q2D and IPPL-2D codes. It provides the solution of the electric potential and, hence, the electric field, on the reduced-dimension computation grids illustrated using blue lines in Fig. 1. As a result, in the IPPL-Q2D code, these are the grids that we use for the deposition of the particles' charge density and for gathering the electric field components using a 1D linear interpolation. This is the second and last difference between our quasi-2D and full-2D codes.

III. DESCRIPTION OF THE RADIAL-AZIMUTHAL SIMULATION SETUP AND IPPL-2D BENCHMARKING

The setup of the full-2D and quasi-2D simulations presented in this work exactly follows that of the well-established radial-azimuthal benchmark case by Villafana *et al.*¹⁹ We provide an overview of the simulation setup and conditions in Sec. III A. Next, in Sec. III B, we present and compare the results from our full-2D code against the reference benchmark results.

A. Simulation domain and conditions

Figure 2 illustrates the domain for the 2D and quasi-2D simulations, which is a Cartesian (x - z) plane with x along the radial direction and z along the azimuthal coordinate. The y direction represents the axial coordinate. A constant radial magnetic field (B_x) with an intensity of 20 mT and a constant axial electric field (E_y) with a magnitude of 1×10^4 Vm⁻¹ are applied. A summary of the initial plasma properties and the computational parameters used for the simulations is provided in Table I.

Initially, the electrons and ions are sampled from a Maxwellian distribution at 10 and 0.5 eV, respectively, and are loaded uniformly as electron-ion pairs over the (x - z) simulation plane. In all simulations, the macroparticle weight of the plasma species is equal and constant. In order to mimic the downstream convection of the azimuthal waves and to limit the growth of the particles' energy in the simulations,²⁷ the approach of Ref. 19 is adopted and a virtual axial extent with a length of $L_y = 1$ cm is considered. Along this axial extent, we do not solve the Poisson equation. Rather, the particles crossing a domain's boundary along the y direction are resampled from a Maxwellian at their initial load temperature, i.e., 10 eV for electrons and 0.5 eV for ions. These particles are re-injected on the simulation plane, maintaining their azimuthal and radial positions.

Referring to Fig. 2, the two radial extremes of the domain, which represent the channel walls of a Hall thruster, are grounded

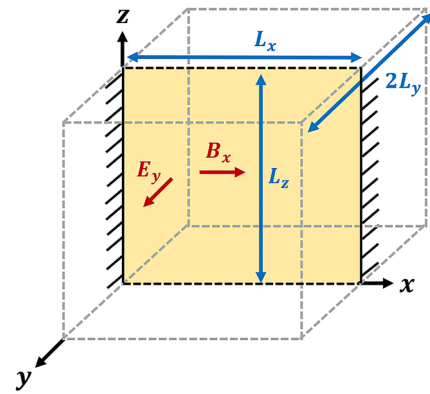


FIG. 2. Schematics of the simulation's coordinate system, the computational plane, and the applied constant electric and magnetic fields.

and the secondary electron emission from the walls is neglected. As a result, a Dirichlet boundary condition is applied for the electric potential at $x = 0$ and $x = L_x$ and any particle hitting a wall is removed from the simulation. The domain along the azimuthal direction is periodic. Hence, a periodic potential boundary condition is implemented and the particles exiting the azimuthal extent at one end of the domain are re-introduced into the domain from the opposite end.

The simulation case is completely collisionless. However, to compensate for the flux of particles lost to the walls, following the benchmark approach,¹⁹ a cosine-shaped ionization source, covering 86% of the radial extent of the domain, from $x = 0.09$ cm to $x = 1.19$ cm, is imposed. The source is uniform along the azimuthal direction. The peak of the ionization source is $S_0 = 8.9 \times 10^{22}$ m⁻³s⁻¹,

TABLE I. Summary of the computational and physical parameters used for the radial-azimuthal 2D and quasi-2D simulations.

Parameter	Value (unit)
Computational parameters	
Domain length ($L_x = L_z$)	1.28 (cm)
Virtual axial length (L_y)	1 (cm)
Cell size ($\Delta x = \Delta z$)	50 (μ m)
Number of cells in each direction ($N_i = N_j$)	256
Time step (t_s)	1.5×10^{-11} (s)
Total simulated duration (t_{sim})	30 (μ s)
Initial number of macroparticles per cell (N_{ppc})	100
Physical parameters	
Initial plasma density ($n_{i,0}$)	5×10^{16} (m ⁻³)
Initial electron temperature ($T_{e,0}$)	10 (eV)
Initial ion temperature ($T_{i,0}$)	0.5 (eV)
Axial electric field (E_y)	10 000 (Vm ⁻¹)
Radial magnetic field (B_x)	0.02 (T)
Potential at walls (ϕ_w)	0 (V)

which corresponds to an axial ion current density of 100 Am^{-2} . The electron-ion pairs injected at each time step due to the ionization source are sampled from a Maxwellian at the respective initial temperature of each species.

B. Verification of the IPPL-2D against the radial-azimuthal benchmark results

Figure 3 shows the comparison between the radial distributions of the time-averaged plasma properties, ion number density and electron temperature, from IPPL-2D and from the benchmark's 2D code, CERFACS.¹⁹ Referring to Ref. 19, the participating codes in the radial-azimuthal benchmarking activity had a maximum prediction error of $\pm 2.5\%$ in ion number density and electron temperature with respect to the CERFACS code. Thus, we also took the results from CERFACS as the reference to verify our 2D results. Figure 3 shows that the time-averaged radial distributions from IPPL-2D are almost identical to those from CERFACS, with only a negligible difference of about 0.5% observable in the zoomed-in view on the ion number density profile [Fig. 3(a)].

The time evolution of the spatially averaged ion number density and the radial component of the electron temperature from IPPL-2D is shown in Fig. 4. The radial electron temperature (T_{ex}) is obtained from Eq. (3), whereas the azimuthal electron temperature (T_{ez}), to be used for the discussions in Sec. V, is given by Eq. (4). In Eqs. (3) and (4), m_e is the electron mass; e is the unit charge; n is the number density; $V_{de,x}$ and $V_{de,z}$ are, respectively, the electrons' radial and azimuthal drift velocities; and $f_e(\mathbf{v})$ is the electrons' velocity distribution function,

$$T_{ex}(x, z) = \frac{m_e}{en} \left(\int_{-\infty}^{+\infty} v_x^2 f_e(\mathbf{v}) d^3 v - n V_{de,x}^2 \right), \quad (3)$$

$$T_{ez}(x, z) = \frac{m_e}{en} \left(\int_{-\infty}^{+\infty} v_z^2 f_e(\mathbf{v}) d^3 v - n V_{de,z}^2 \right). \quad (4)$$

Comparing the evolution plots of the plasma properties in Fig. 4 with those shown in Fig. 7 of the benchmarking code,¹⁹ we found that the resolved trends from IPPL-2D are very similar to those from the 2D codes that participated in the benchmarking, both over the first $3 \mu\text{s}$ of the simulation [Fig. 4(a)] and over the entire simulation duration [Fig. 4(b)].

According to the above results and discussions, we verified that our full-2D PIC code provides predictions in the radial-azimuthal

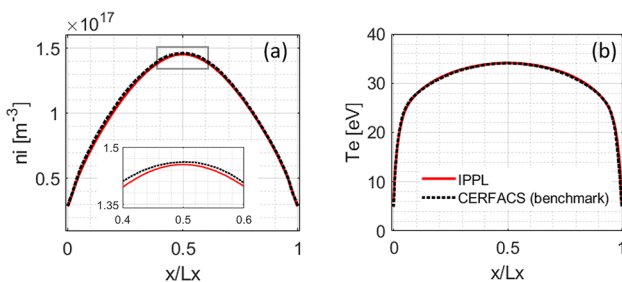


FIG. 3. Comparison between the time-averaged radial profiles of (a) ion number density (n_i) and (b) electron temperature (T_e), obtained from IPPL-2D and the CERFACS code.¹⁹ The profiles are averaged over 25–30 μs .

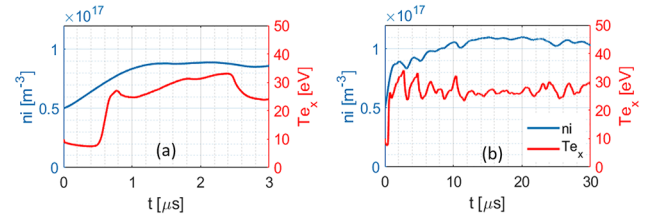


FIG. 4. Time evolution of the ion number density (n_i) and the radial component of the electron temperature (T_{ex}) over (a) the first $3 \mu\text{s}$ of the simulation time and (b) the entire simulation duration. The left y axis in both plots corresponds to the ion number density, whereas the right y axis represents the radial electron temperature.

configuration that are highly consistent with the other benchmarked conventional full-2D codes in the $E \times B$ plasma community. Consequently, the comparison of the results of the quasi-2D simulations against the full-2D results, as presented in Sec. IV, is justified.

IV. COMPARISON BETWEEN IPPL-Q2D PREDICTIONS IN VARIOUS NUMBER-OF-REGION APPROXIMATIONS AND IPPL-2D RESULTS

We performed a series of quasi-2D radial-azimuthal simulations using different orders of approximation of the 2D problem, which, as mentioned in Sec. II B, amounts to using various number-of-region approximations. In all of the quasi-2D simulations discussed in this section, the number of regions used is equal along the radial and azimuthal directions. For reference, we also report, in this section, the results from a 1D radial and a 1D azimuthal PIC simulation that we carried out using the same conditions and setup of the 2D and quasi-2D simulations (Sec. III A) but adapted accordingly for the 1D simulations. In the 1D radial case, the same ionization source as that described in Sec. III A was used. However, for the 1D azimuthal simulation, noting that the plasma density remains constant throughout the simulation, the initial plasma density ($n_{i,0}$) was increased to $1 \times 10^{17} \text{ m}^{-3}$, which approximately corresponds to the radially averaged density value from the 2D simulation (Sec. III B) after reaching the quasi-steady state.

Figure 5 presents the time-averaged radial distributions of the ion number density (n_i) and the electron temperature (T_e) from the 1D radial simulation, from the quasi-2D simulations at “low” and “high” approximation orders, and from our 2D simulation. The “low-order” quasi-2D simulations correspond to the number of regions of 1, 3, and 5, whereas for the “high-order” simulations, we used 10, 25, 50, and 100 regions.

Looking at the radial profiles of the plasma properties from the high-order quasi-2D simulations [Figs. 5(c) and 5(f)], it is evident that, by increasing order of approximation, the quasi-2D results converge to the full-2D ones at the 100 number-of-regions limit. Indeed, the 100-region quasi-2D simulation results show an error of about 2.5% in peak ion number density and peak electron temperature with respect to the 2D results. This is deemed a reasonably low error considering that it is consistent with the error observed among various 2D codes that participated in the radial-azimuthal benchmark activity.¹⁹

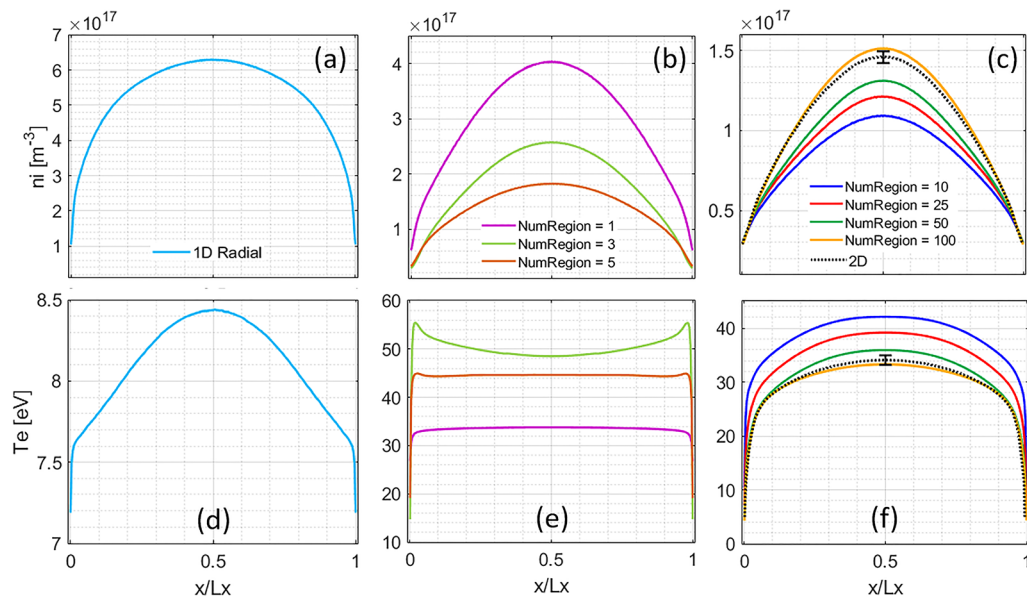


FIG. 5. Radial profiles of the ion number density (first row) and the electron temperature (second row) averaged over 25–30 μ s. Plots (a) and (d) are from the 1D radial simulation, plots (b) and (e) are from low-order quasi-2D simulations, and plots (c) and (f) are from high-order quasi-2D simulations. The reference 2D profiles are shown in plots (c) and (f) with a $\pm 2.5\%$ error band superimposed at the peak values. Note the difference in the y axis scale between plots (a)–(c) and (d)–(f); the scales are chosen in this manner to allow distinguishing more clearly the time-averaged profiles from various simulations.

Referring now to plots (b) and (e) in Fig. 5, it is observed that, by increasing the number of regions from 1 to 5, the ion number density profile becomes consistently more similar to the 2D one, whereas the electron temperature profile first shows an increase in values and a deviation in distribution compared to the 2D results from 1 region to 3 regions before starting to approach the 2D profile at 5 regions.

An interesting point to highlight is that the “single-region” quasi-2D simulation, which resolves an average effect of the radial and azimuthal processes,¹⁵ predicts a value of the electron temperature at the mid-radial location ($x/L_x = 0.5$) that is very close to the corresponding value from the 2D simulation. However, the radial T_e distribution from the single-region simulation is rather different from the 2D one. In addition, the predicted ion number density profile is also quite different in terms of values compared to the 2D result. Regardless of these discrepancies, comparing the single-region profiles against those from the 1D radial simulation [Figs. 5(a) and 5(d)], it is seen that the single-region simulation provides a good improvement to the 1D radial results. In particular, the average mutual effects of the physical mechanisms along the azimuthal and radial directions are captured by the single-region simulation. This can be noticed by comparing the 1D radial and the single-region profiles, where an increase in the electron temperature due to particles’ heating by azimuthal waves and a corresponding decrease in the ion number density are observed.

Figure 6 shows the time evolution of the ion number density and the radial electron temperature, averaged over the entire domain, from the 1D radial, quasi-2D, and full-2D simulations. First, comparing the 1D radial and the single-region quasi-2D simulations, we notice that resolving an average mutual effect of the

azimuthal and radial processes by the single-region simulation also affects the temporal variations of the plasma properties. In fact, in the 1D radial simulation, the ion number density [Fig. 6(a)] approaches an asymptotic value near the end of the simulation duration and the radial electron temperature [Fig. 6(d)] drops to a value of about 3 eV very early into the simulation. In contrast, in the single-region simulation, the ion number density [Fig. 6(b)] becomes asymptotic within the last 10 μ s of the simulation at a value 0.6 times that in the 1D radial case. In addition, the radial electron temperature shows a relatively small decrease from the initial load temperature of 10 eV and then oscillates around a mean value of 7.5 eV.

The reason for the above observations is the specific coupling that exists between the electron temperature and the number density in the adopted radial–azimuthal simulation case. In this regard, when T_{ex} increases, an increased flux of particles is lost to the walls. Now, since the simulation setup features a constant ionization source that does not receive feedback from the system’s energy and injects electron–ion pairs at a constant rate, the plasma density will consequently decrease. Accordingly, in the 1D radial case, after the initial transient where the tail of the electrons’ radial energy distribution function (EDF) is depleted due to being lost to the wall and, hence, the radial electron temperature decreases, the absence of any mechanism to thermalize the electron population and, thus, to replenish the EDF tail implies that the flux of particles with enough energy to overcome the sheath potential drop decreases. As a result, the ion number density evolution shows the increasing behavior seen in plot (a) of Fig. 6. In the single-region simulation, the excitation of azimuthal waves limits the decrease in the radial electron

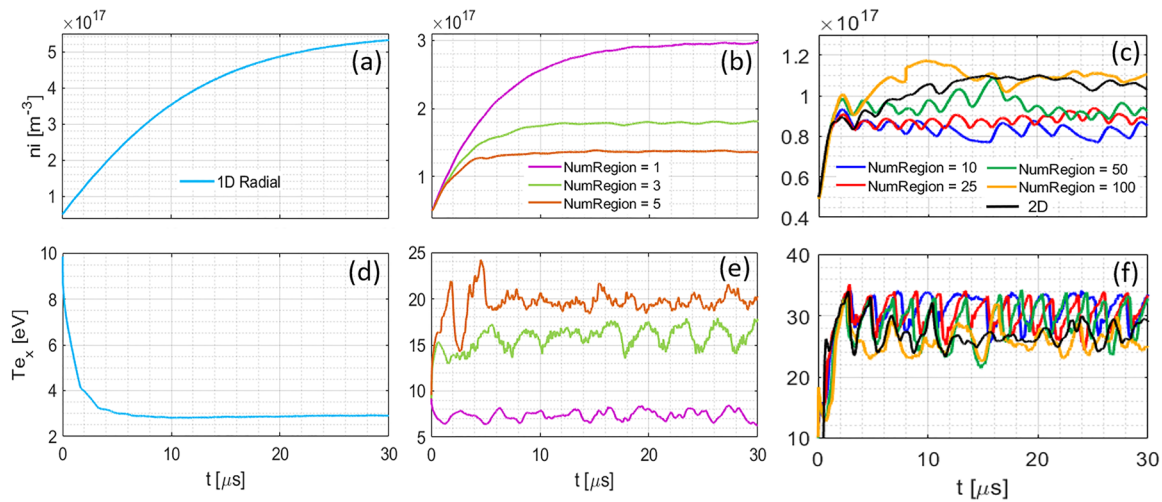


FIG. 6. Time evolution of the ion number density (first row) and the radial electron temperature (second row) obtained from the performed simulations: (a) and (d) 1D radial, (b) and (e) quasi-2D in low number-of-region limit, and (c) and (f) quasi-2D in high number-of-region approximation limit. The 2D simulation results are shown in plots (c) and (f). Note the difference in the y axis scale between plots (a)–(c) and (d)–(f); the scales are chosen in this manner to allow distinguishing more clearly the time evolutions from various simulations.

temperature, which, as explained above, limits the increase in the ion number density.

As the second point concerning the plots in Fig. 6, the high-order quasi-2D simulations [Figs. 6(c) and 6(f)] have resolved the time evolution of the radial electron temperature in a consistent manner compared to the 2D simulation. The temporal variations in T_{ex} from all quasi-2D simulations feature a characteristic oscillation similar to that visible in the 2D result, which is associated with the periodic growth and damping of the Modified Two-Stream Instability (MTSI).¹⁹ Due to the coupling between the plasma density and the electron temperature in the present simulation case, which was explained in the preceding paragraph, the ion number density trends also show an oscillatory behavior over time [Fig. 6(c)]. In this regard, as the number of regions is increased from 10 to 100, the ion density time evolutions become increasingly more similar to that of the 2D simulation, with 50- and 100-region simulations showing the highest degree of similarity overall.

Looking now at plots (b) and (e) in Fig. 6, we notice that as the approximation order in the low number-of-region quasi-2D simulations is increased from 1 to 5, the time to reach steady state for the ion number density decreases. Moreover, the mean value of the radial electron temperature oscillations becomes more comparable with the high-order quasi-2D and the full-2D ones from the single-region to 5-region simulations.

In Fig. 7, we present the time evolution of the ion number density and the radial electron temperature from the high-order quasi-2D and the full-2D simulations over the first 3 μs of the simulation. It is observed that whereas the quasi-2D simulations have all resolved the initial transient in the ion number density rather consistently with the 2D simulation, the evolution trend of the radial electron temperature is quite different from the 2D one over approximately the first 1.5 μs of the simulation. This difference highlights that the reduced-order simulations did not properly resolve the very

initial evolution of the discharge most likely due to the highly small-scale physical interactions occurring over the first few microseconds of the simulation as explained in Ref. 19. Nevertheless, noting that the quasi-2D results are consistent with the 2D ones from about 2 μs onward, we believe that the observed discrepancy here does not undermine the applicability and/or reliability of the reduced-order scheme, which is primarily intended to enable self-consistent kinetic simulations over long durations, which is currently not feasible using conventional full-2D codes without any simulation speed-up technique.²⁸

The 1D Fast Fourier Transforms (FFTs) of the azimuthal electric field signal, averaged over three time intervals along the simulation duration, from the 1D azimuthal simulation, from the quasi-2D simulations in low- and high-order approximation limits, and from the 2D simulation are shown in Fig. 8. The approach adopted to obtain these spatiotemporally averaged FFT plots is similar to that explained in detail in Refs. 16 and 19.

The x axis in the plots of Fig. 8 represents the normalized azimuthal wavenumber (k_z/k_0), with the normalization factor (k_0)

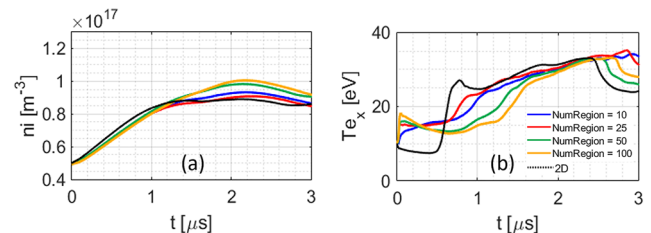


FIG. 7. Time evolution of (a) ion number density and (b) radial electron temperature from the high-order quasi-2D and 2D simulations over the first 3 μs of the simulation.

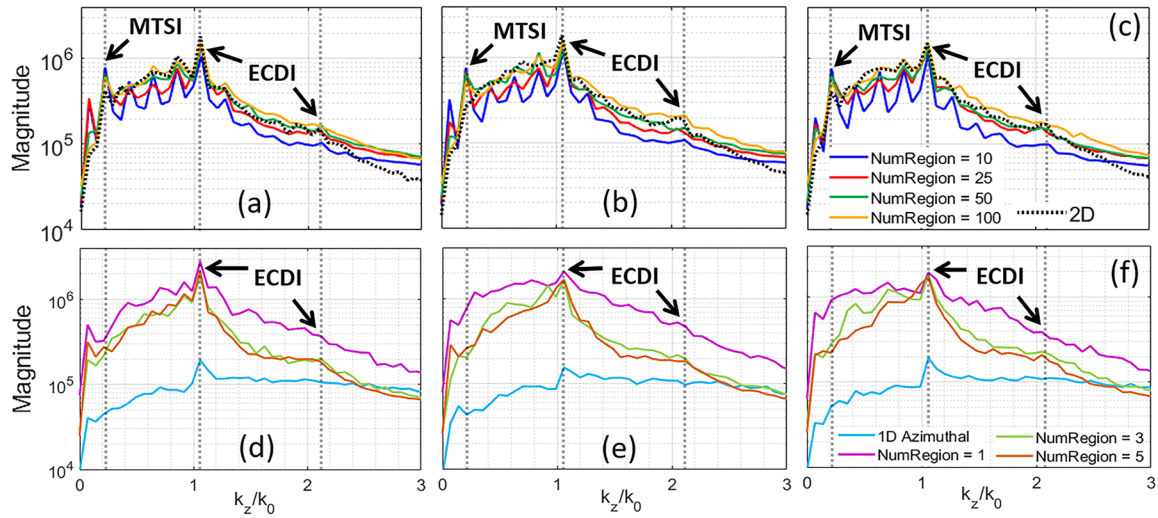


FIG. 8. 1D FFTs of the azimuthal electric field signal averaged over all radial positions and over three time intervals: (a) and (d) 5–10 μs , (b) and (e) 15–20 μs , and (c) and (f) 25–30 μs . The top row is related to the quasi-2D simulations with high number-of-region limits and the 2D simulation; the bottom row is related to the quasi-2D simulations with low number-of-region limits and the 1D azimuthal simulation.

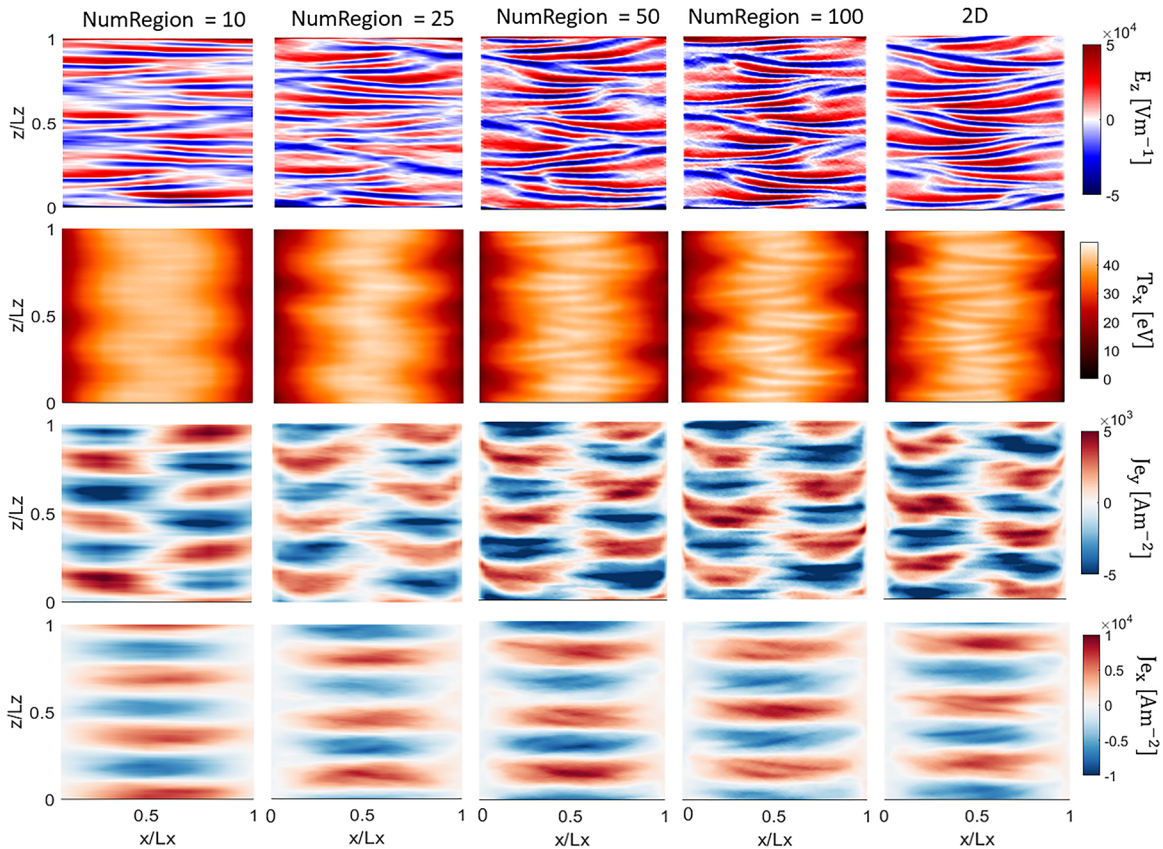


FIG. 9. 2D snapshots of the plasma properties at the time of local maximum of the radial electron temperature obtained from high-order quasi-2D simulations and the 2D simulation. The rows, from top to bottom, represent the azimuthal electric field (E_z), the radial electron temperature (T_{ex}), and the axial and radial electron current densities (J_{ey} and J_{ex}).

being the fundamental resonance wavenumber of the Electron Cyclotron Drift Instability (ECDI) defined as $k_0 = \frac{\Omega_{ce}}{v_{de}}$,¹⁹ where Ω_{ce} is the electron cyclotron frequency and v_{de} is the electrons' $\mathbf{E} \times \mathbf{B}$ drift velocity.

Referring to the top-row plots in Fig. 8, which illustrate the FFTs of the azimuthal electric field from the high-order quasi-2D simulations and the 2D simulation, we notice the presence of two distinct instabilities, similar to the observations reported in the benchmark study.¹⁹ The peak in the FFT plots at $\frac{k_z}{k_0} \sim 0.2$ is associated with the azimuthal component of the MTSI,¹⁹ whereas the peak at $\frac{k_z}{k_0} \sim 1$ corresponds to the fundamental ECDI mode.¹⁹ The second peak at $\frac{k_z}{k_0}$ slightly higher than 2 is related to the second harmonic of the ECDI. Comparing the FFTs from the high-order quasi-2D simulations with respect to those from the 2D simulation, it is observed that the above three peaks are captured in all reduced-order simulations. Moreover, the FFT plots from the 50- and 100-region simulations closely resemble the FFTs from the 2D simulation within each time interval.

Concerning the FFT plots from the low-order quasi-2D and the 1D azimuthal simulations (Fig. 8, bottom row), we see that the

fundamental ECDI mode is captured in all simulations. However, comparing the azimuthal FFT from the 1D azimuthal simulation against that from the single-region simulation, the magnitude of the ECDI mode and the overall FFT spectrum from the single-region simulation are observed to be more consistent with the high-order quasi-2D and 2D simulations' FFTs. The 3-region and 5-region simulations also resolve the second harmonic of the ECDI. The MTSI is noticed to be absent in the 1D azimuthal and low-order quasi-2D simulations most likely because, in these simulations, the radial wavenumber component of the MTSI is not properly captured so as to allow the formation of the corresponding wave modes.

The FFT analysis results presented above confirm that the azimuthal wave content from the quasi-2D simulations is quite similar to that from our full-2D simulation. It is discussed in Ref. 19 based on the results of full-2D simulations that the existing ECDI and MTSI modes exhibit a nonlinear coupling throughout the simulation, which is the reason behind the oscillatory evolution of the radial electron temperature (also the ion number density, albeit to a lesser extent) in the time interval of 2–10 μs and then from 20 μs onward. Accordingly, the discharge in the present radial–azimuthal simulation case is reported to overall oscillate between two distinct

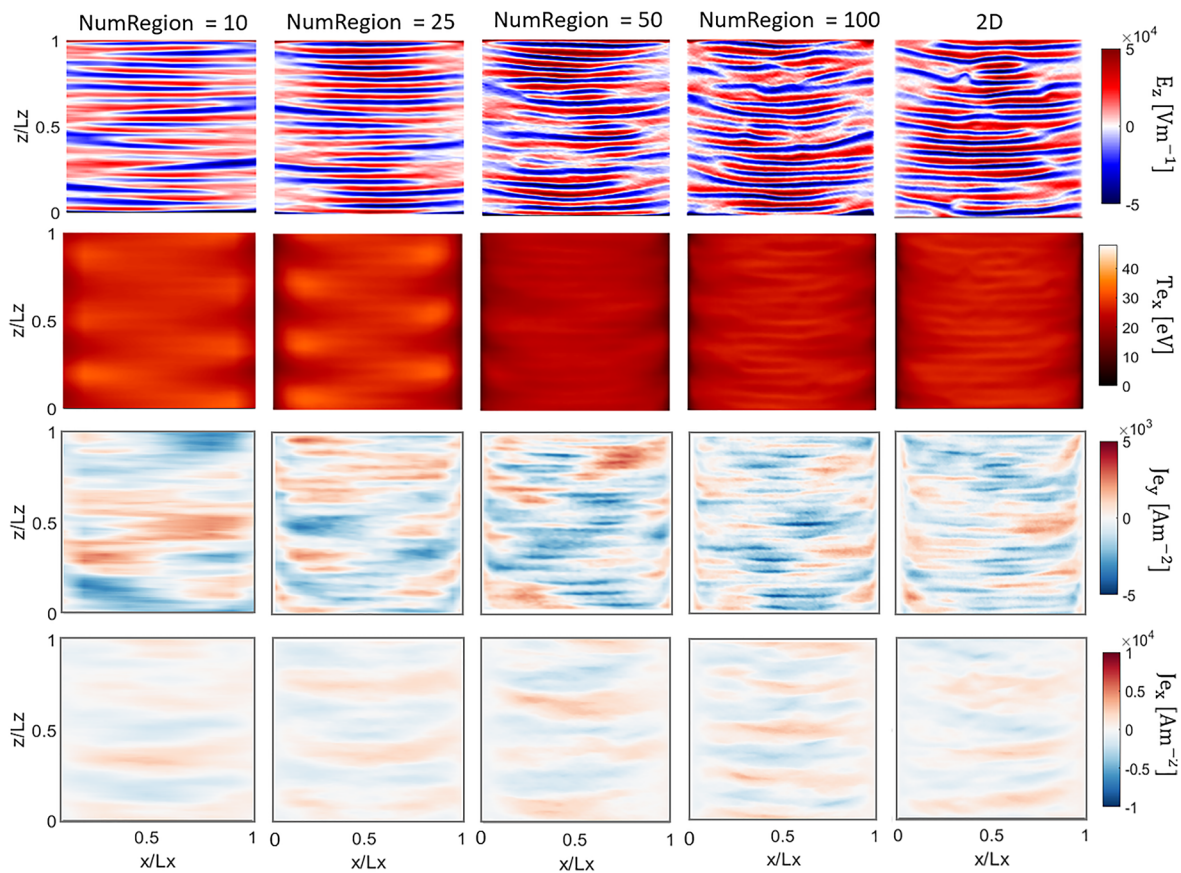


FIG. 10. 2D snapshots of the plasma properties at the time of local minimum of the radial electron temperature obtained from high-order quasi-2D simulations and the 2D simulation. The rows, from top to bottom, represent the azimuthal electric field (E_z), the radial electron temperature (T_{ex}), and the axial and radial electron current densities (J_{ey} and J_{ex}).

states corresponding to the local maxima and the local minima of the electron temperature evolution plot [Fig. 6(f)].¹⁹ When the radial electron temperature is at its local maximum, the MTSI is dominant, whereas the ECDE becomes more dominant when the radial electron temperature reaches a local minimum.¹⁹

These insights from conventional full-2D simulations are also recovered using the high-order quasi-2D simulations. Indeed, looking at Figs. 9 and 10, which show the 2D snapshots of several plasma properties at a time instance corresponding to a local maximum and a local minimum of the radial electron temperature, respectively, it is evident that with as few numbers of regions as 10, the resolved 2D distributions are in good agreement compared to the distributions from our full-2D simulation. Moreover, as it might be expected based on the results presented so far, the 50- and 100-region simulations provide predictions of 2D distributions of the plasma properties that are almost indistinguishable compared to the full-2D results. In this respect, it is particularly seen that both the azimuthal and radial wavenumber components of the MTSI are resolved, which is best visible from the 2D snapshots of the axial electron current density (J_{ey}) on the third row of Fig. 9.

Of course, moving to the lower end of the high-order quasi-2D simulations, i.e., the 10-region and 25-region simulations, some of the small-scale features observable from the other simulations are absent, for instance, the tilts in the plasma distributions near the walls. However, the overall patterns and the main characteristics are still faithfully captured by these relatively low-cost reduced-order kinetic simulations.

To conclude the discussions in this section, we first refer to Fig. 11(a), which shows the variation in the L2 error of the quasi-2D predictions in terms of the radial distribution of the time-averaged ion number density and electron temperature compared to the corresponding full-2D profiles. The L2-norm error is calculated using Eq. (5), in which ζ denotes either the ion number density or the electron temperature, i is the index of each node along the radius, and N_i is the number of cells along the radial direction,

$$err_{L2} = \sqrt{\frac{1}{N_i} \sum_{i=1}^{N_i} \left(\frac{\zeta_{Q2D}(i) - \zeta_{2D}(i)}{\zeta_{2D}(i)} \right)^2}. \quad (5)$$

Overall, it is noticed that, from the 3-region quasi-2D simulation, the error in both plasma parameters continuously decreases. In particular, the high-order quasi-2D simulations (25, 50, and 100 regions) all have an L2 error of below 5% in terms of both plasma properties.

We now look at Fig. 11(b), where we have plotted the ratio between the computational times of the quasi-2D simulations and

the 2D one vs the number of regions used for the quasi-2D simulations. This plot, together with the L2 error plot in Fig. 11(a), underlines the cost-effectiveness and fidelity of the reduced-order PIC scheme. Indeed, the highest order quasi-2D simulation carried out in this work, i.e., the 100-region simulation, has a computational time that is only 40% of the 2D one and provides results that are almost identical to the full-2D results. The 50-region simulation with an L2 error of about 2% in n_i and below 1% in T_e has a computational time ratio of 20% compared to the 2D simulation. The computational time ratio decreases monotonically to below 5% for the 10-region simulation for which the L2 error remains below 10% in terms of both n_i and T_e .

V. ANALYSIS OF THE EFFECT OF USING NON-UNIFORM REGIONS' EXTENT IN THE REDUCED-ORDER SIMULATIONS

The quasi-2D simulations, the results of which have been presented and discussed so far, all featured a uniform regions' extent along the radial and azimuthal directions. Here, we investigate the variation in the quasi-2D predictions in case of adopting a non-uniform regions' extent along the radial direction. This is to assess that, by using more refined regions near the walls, where the potential gradient is strong due to the plasma sheath, whether a reduced-order simulation with an overall number of regions quite lower than 100 can provide results that resemble those from the 100-region quasi-2D simulation. In the studies presented in this section, the regions along the azimuthal direction are always spaced uniformly. Furthermore, it is emphasized that the extent of the regions and the cells' size remain constant throughout the simulations with a non-uniform radial length of the regions.

In this regard, Fig. 12(a) shows the schematics of a 2D domain with a non-uniform domain decomposition along the x-direction. Figure 12(b) shows a comparison of the normalized radial extent of the regions (l_x/L_x) in the four cases investigated here against three reference quasi-2D simulations with a uniform regions' definition, namely, the 10-, 25-, and 100-region simulations. Cases 1 and 2 have a total number-of-region count along the radius (M) of 25, whereas in cases 3 and 4, M is equal to 30. It is observed from Fig. 12(b) that, in all cases, the smallest radial regions' extent near the walls is equivalent to that of the 100-region simulation. Moving toward the center of the domain along the radial direction, cases 1 and 2 have a middle region whose radial length is larger than that in the 10-region simulation. In cases 3 and 4, the middle regions have a radial length larger than that in the 25-region simulation but smaller than that in the 10-region simulation.

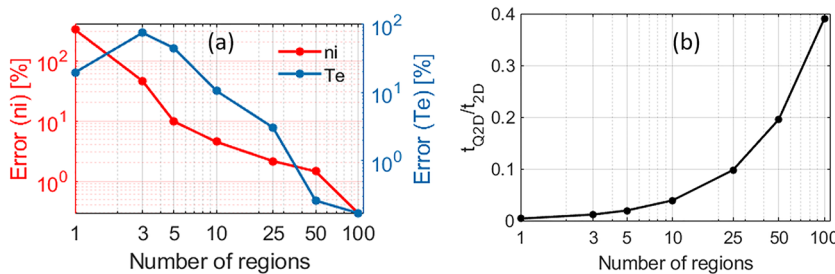


FIG. 11. (a) Variation in the L2 error of the quasi-2D predictions vs the number of regions used. The y axes in plot (a) are in logarithmic scale. (b) Variation in the computational time ratio between the quasi-2D and full-2D simulations vs the number of regions used in the quasi-2D simulations.

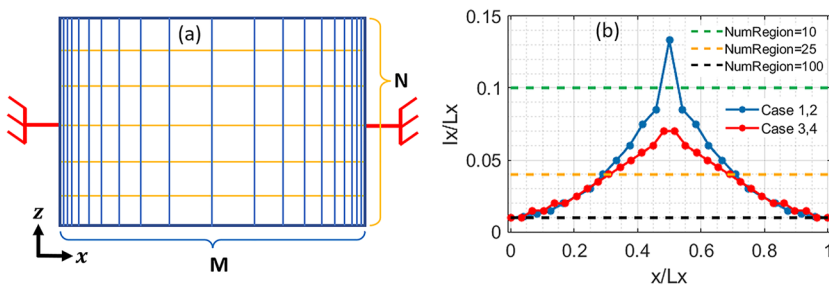


FIG. 12. (a) Illustration of non-uniform regions' extent along the radial direction. (b) Comparison of the variation in regions' extent along the radial direction in the different cases investigated. The values on the x axis of plot (b) show the normalized axial position of the centerline of each region.

TABLE II. Summary of the numerical parameters used for the quasi-2D simulations with a non-uniform radial regions' extent.

	M (non-uniform)	N (uniform)	$N_{p,init}$	N_{ppc} (in smallest cell)	N_{ppc} (in largest cell)
Case 1	25	10	$100 * \max(N * N_i, 100 * N_k)$	100	1330
Case 2	25	10	$100 * \max(N * N_i, M * N_k)$	25	332
Case 3	30	10	$100 * \max(N * N_i, M * N_k)$	33	231
Case 4	30	100	$100 * \max(N * N_i, M * N_k)$	100	700

Table II provides a summary of the number of radial (M) and azimuthal (N) regions used in the quasi-2D simulations of this section alongside the initial total number of macroparticles ($N_{p,init}$) and the initial number of macroparticles per cell (N_{ppc}) in each case. It is noticed from Table II that cases 1–3 all have 10 regions along the azimuth, whereas case 4 has 100 azimuthal regions. The difference between cases 1 and 2 is the initial total number of macroparticles and, consequently, N_{ppc} . It is recalled that, in the reduced-order PIC scheme, the number of cells to be used for the calculation of $N_{p,init}$ is obtained from the relation $\max(N * N_i, M * N_k)$, as described in Ref. 13. In this relation, N_k denotes the number of cells along the azimuthal direction. Accordingly, in case 1, we have exactly 100 macroparticles at the beginning of the simulation in the smallest cells adjacent to the walls. In case 2, however, there are 100 macroparticles per cell, on average, which implies an N_{ppc} of 25 in the smallest cells near the walls. The difference between cases 3 and 4 is in the number of azimuthal regions (N). The difference in terms of N_{ppc} is a consequence of this variation.

The results from the non-uniform quasi-2D simulations in terms of the time-averaged profiles of the ion number density (n_i), the total electron temperature (T_e), and the radial and azimuthal components of the electron temperature (T_{ex} and T_{ez}), given by Eqs. (3) and (4), are compared in Fig. 13 against the 10-region, 25-region, and 100-region quasi-2D simulations with a uniform radial domain decomposition. Overall, it is observed in the plots of Fig. 13 that, by refining the regions' extent near the walls, the ion number density [Fig. 13(a)] and the radial electron temperature [Fig. 13(c)] distributions closely follow the 100-region profiles shown as dashed black lines in Fig. 13. In particular, case 3 (solid green lines) with only 30 radial regions can reproduce with good accuracy the 100-region results in terms of n_i and T_{ex} profiles.

Nevertheless, the T_e and T_{ez} profiles shown in plots (b) and (d) of Fig. 13 approach the 100-region results only in case 4, where the number of azimuthal regions is increased to 100. Indeed, the T_{ez} profiles for cases 1–3 with 10 azimuthal regions are similar to

the T_{ez} profile from the 10-region quasi-2D simulation (dashed blue lines) and, hence, the T_e profiles for these cases are also representative of that in the 10-region simulation. Having a fine resolution of regions along the azimuth in case 4 yields improved predictions of T_e and T_{ez} , whereas the n_i and T_{ex} profiles are noticed to deviate, to some extent, from the 100-region profiles. A plausible reason for this observation concerning case 4 is the disparate resolution of the plasma potential gradient along the radial and the azimuthal coordinates due to quite a different domain decomposition performed in case 4 along the two directions of the simulation. In any case, it is emphasized that the main motive behind the simulations

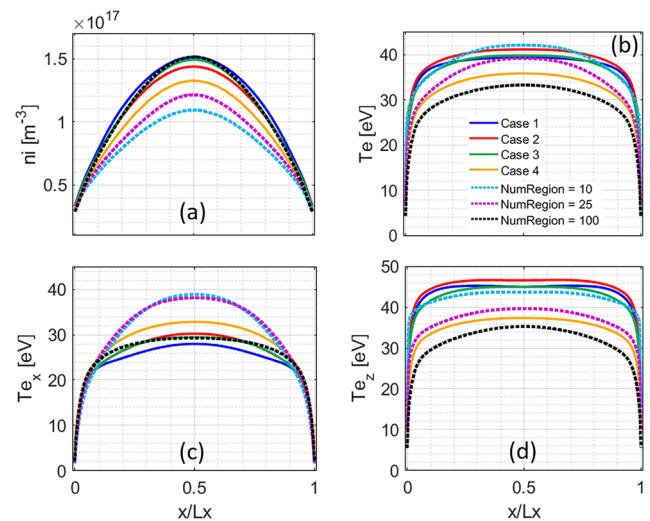


FIG. 13. Radial profiles of (a) ion number density, (b) total electron temperature, (c) radial electron temperature, and (d) azimuthal electron temperature from the non-uniform and uniform quasi-2D simulations, averaged over 25–30 μ s.

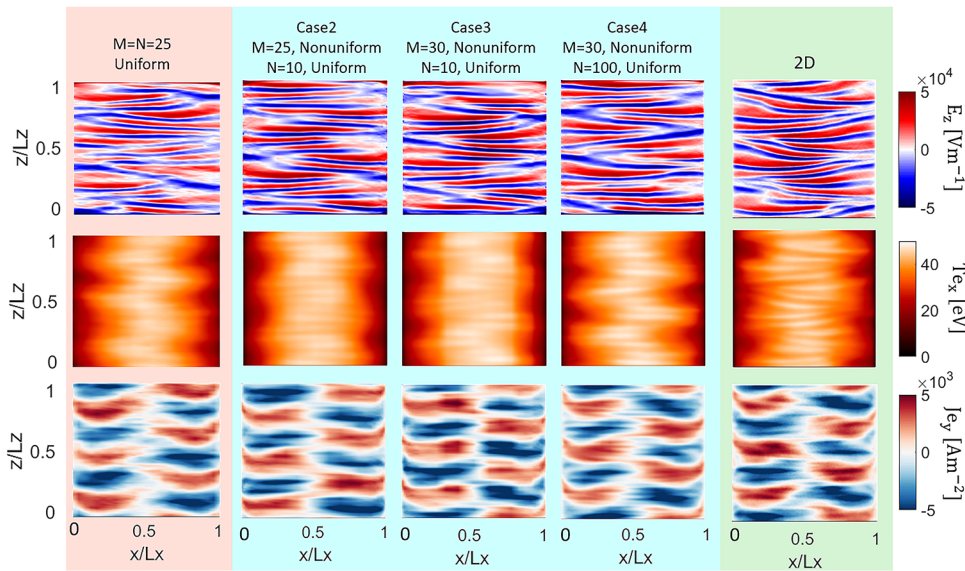


FIG. 14. 2D snapshots of the plasma properties at the time of local maximum of the radial electron temperature obtained from the non-uniform quasi-2D simulations (cases 2–4) as well as the uniform 25-region quasi-2D simulation and the full-2D simulation. The rows, from top to bottom, represent the azimuthal electric field (E_z), the radial electron temperature (T_{ex}), and the axial electron current density (J_y).

in this section has been to demonstrate the flexibility of the reduced-order PIC scheme to allow a non-uniform regions' extent. In a plasma configuration where the coupling between the involved simulation's directions would not occur over such small scales as in the case studied here, the non-uniform domain decomposition informed by the macroscopic gradients in the plasma properties, particularly the electric field, is expected to improve the predictions. In such a scenario, the overall number of regions can be more readily reduced without a notable impact on the fidelity of the results. The verification of this hypothesis is left for future work.

Comparing the profiles of the plasma properties from cases 1 and 2 in Fig. 13, it is noticed that the distributions are almost identical, particularly in terms of n_i and T_{ex} . Noting that the difference between these two cases was related to the initial number of macroparticles, specifically in the regions near the walls (Table II), we conclude that a lower N_{ppc} in the smallest regions does not have a noticeable influence on the results.

Finally, Fig. 14 shows the 2D snapshots of the plasma properties for cases 2–4 as well as the uniform 25-region simulation and the full-2D at a time instance corresponding to the local maximum of the radial electron temperature. In contrast to the conclusions drawn above from the time-averaged profiles, it is noticed from Fig. 14 that refining the regions near the walls had overall a minor effect on the 2D snapshots of various plasma properties from the non-uniform quasi-2D simulations compared to the uniform quasi-2D and the full-2D ones. Nevertheless, it is interesting to note that, in case 4, the small-scale features and patterns visible in the snapshots of the full-2D simulation are more closely captured.

VI. ANALYSIS OF THE EFFECT OF THE INITIAL NUMBER OF MACROPARTICLES PER CELL ON THE QUASI-2D RADIAL-AZIMUTHAL SIMULATION

To evaluate the influence of the initial number of macroparticles per cell on the quasi-2D results, we used the uniform 50-region

quasi-2D simulation, which was shown in Sec. IV to provide high-fidelity results at relatively low computational cost, to simulate the radial-azimuthal case with a range of N_{ppc} from 10 to 1024. The results in terms of the normalized, time-averaged radial distributions of the ion number density and total electron temperature are shown in Fig. 15. Referring to plot (a) in this figure, the ion number density profiles are seen to have converged at a peak density ratio of about 2.45 from 100 macroparticles per cell. Looking at plot (b) of Fig. 15, even though the convergence trend is not monotonic, the temperature profiles does not show any noticeable variation from an N_{ppc} of 200 and the simulation case with 100 N_{ppc} has a maximum discrepancy of less than 10% in normalized T_e compared to the simulations with higher N_{ppc} values.

As a result, it is possible to say that the quasi-2D simulations show a clear statistical convergence behavior with increasing N_{ppc} and an initial number of macroparticles per cell in the range of 100–200 can be sufficient to ensure statistically converged results. This conclusion is consistent with that from similar

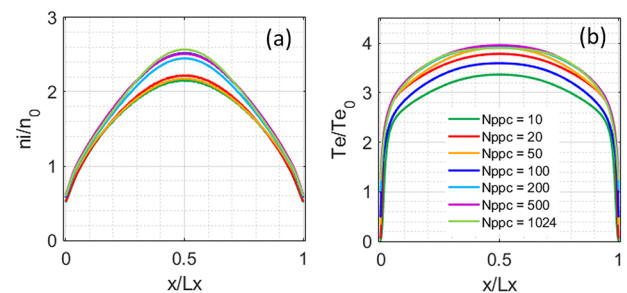


FIG. 15. Time-averaged radial profiles of (a) normalized ion number density and (b) normalized electron temperature obtained from the uniform 50-region quasi-2D simulation with various values of initial number of macroparticles per cell. n_0 and T_{e0} denote the initial ion number density and electron temperature used for initial particles' loading.

studies reported in the literature^{19,29} and also from our previous studies.^{13,15}

VII. CONCLUSIONS

In this article, we presented the verification results of two PIC codes: the conventional IPPL-2D and the reduced-order IPPL-Q2D, in a radial–azimuthal $E \times B$ configuration representative of a Hall thruster. The simulation setup and conditions were based on a well-defined benchmark case in the same configuration.¹⁹ We introduced the IPPL-2D code and presented its benchmarking against the 2D results from the literature. Accordingly, we confirmed that our full-2D results can be used as a trustworthy reference for the verification of the reduced-order PIC code. In this respect, we first provided an overview of the reduced-order PIC scheme and highlighted the two aspects with respect to which the resulting IPPL-Q2D code is different from IPPL-2D, namely, the formulation behind the Poisson solver, and the computation grids used for the information exchange between the particles and the grids.

Second, we presented an extensive comparison between the quasi-2D simulation results at various approximation orders (or, equivalently, different numbers of regions) and the full-2D results. We compared the quasi-2D and full-2D predictions in terms of the time-averaged radial profiles of the plasma properties, the time evolution of the plasma properties, 1D FFTs of the azimuthal electric field signals, and, finally, the 2D snapshots of the plasma properties at two instances of the discharge evolution at the quasi-steady state corresponding to a local minimum and a local maximum of the radial electron temperature. Considering the highly two-dimensional nature of the plasma phenomena in the radial–azimuthal coordinates of a Hall thruster, we observed that reduced-order simulations at the approximation orders that yield from about 2.5 to 25 times speed-up compared to the 2D simulation provide results that compare reasonably well with the full-2D ones. In particular, we demonstrated that a quasi-2D simulation with 50 regions along the radial and azimuthal directions has a speed-up factor of 5, while its predictions in terms of the time-averaged plasma profiles and the 2D distributions of the plasma properties are well consistent with the corresponding predictions from the 2D simulation.

On the highly low-cost end of the reduced-order approximations, the single-region simulation, which practically amounts to in-parallel 1D PIC simulations along each of the simulation coordinates, was shown to provide results that are notably improved with respect to the corresponding 1D radial and 1D azimuthal simulations. This improvement in predictions was underlined to be due to an average mutual effect of the radial and azimuthal physical processes that is resolved by the single-region simulation. In addition, in a general case, other low-order approximations, such as the 3- and 5-region simulations, whose results were demonstrated to be on the same order as the full-2D results but are still notably less computationally expensive, can be useful to tune the initial conditions or the configuration of the higher-order higher-fidelity simulations.

We also investigated the effect of using a non-uniform domain decomposition along the radius in the quasi-2D simulations as well

as the influence of the initial number of macroparticles per cell. Concerning the former, we confirmed the flexibility of the reduced-order formulation to allow for arbitrary selection of the regions' extent. In addition, we highlighted that refining the domain decomposition around the locations of large gradients in the plasma properties can enable a non-uniform quasi-2D simulation with relatively low number of regions to have a fidelity of the results on a par with the higher-order quasi-2D simulations with a uniform, refined regions' extent throughout the domain.

The results and in-depth analyses presented in this paper complement our previous detailed evaluations of the reduced-order scheme in the axial–azimuthal coordinates of a Hall thruster.^{12,13} As a result, we further progressed toward establishing the maturity, versatility, and reliability of the generalized reduced-order PIC scheme. Consequently, in the near term, our PIC scheme can be used for extensive physical parametric studies that are essential to better understand and untangle the roles played by various mechanisms in the overall picture of the multi-dimensional processes in Hall thrusters and similar cross-field plasma configurations. In any case, we acknowledge that in both the axial–azimuthal and radial–azimuthal verification cases, the domain decomposition associated with the reduced-order scheme was aligned with the direction of the dominant physical processes. Therefore, as the next verification step, we are performing reduced-order simulations of a Penning discharge in which the direction of the involved phenomena is constantly changing. This effort serves to further prove the broad applicability of the generalized reduced-order PIC scheme.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

F. Faraji: Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Writing – original draft (lead). **M. Reza:** Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Visualization (lead); Writing – review & editing (equal). **A. Knoll:** Conceptualization (equal); Project administration (lead); Supervision (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

- ¹J.-P. Boeuf, "Tutorial: Physics and modeling of Hall thrusters," *J. Appl. Phys.* **121**, 011101 (2017).
- ²E. Y. Choueiri, "Anomalous resistivity and heating in current-driven plasma thrusters," *Phys. Plasmas* **6**, 2290 (1999).
- ³T. Lafleur, S. D. Baalrud, and P. Chabert, "Characteristics and transport effects of the electron drift instability in Hall-effect thrusters," *Plasma Sources Sci. Technol.* **26**, 024008 (2017).
- ⁴S. Janhunen, A. Smolyakov, O. Chapurin, D. Sydorenko, I. Kaganovich, and Y. Raitses, "Nonlinear structures and anomalous transport in partially magnetized $E \times B$ plasmas," *Phys. Plasmas* **25**, 011608 (2018).
- ⁵M. S. McDonald and A. D. Gallimore, "Parametric investigation of the rotating spoke instability in Hall thrusters," IEPC-2011-242, in Proceedings of 32nd International Electric Propulsion Conference, Wiesbaden, Germany, 2011.
- ⁶C. L. Ellison, Y. Raitses, and N. J. Fisch, "Cross-field electron transport induced by a rotating spoke in a cylindrical Hall thruster," *Phys. Plasmas* **19**, 013503 (2012).
- ⁷I. D. Kaganovich, A. Smolyakov, Y. Raitses *et al.*, "Physics of $E \times B$ discharges relevant to plasma propulsion and similar technologies," *Phys. Plasmas* **27**, 120601 (2020).
- ⁸M. Reza, F. Faraji, T. Andreussi, and M. Andrenucci, "A model for turbulence-induced electron transport in Hall thrusters," IEPC-2017-367, in Proceedings of 35th International Electric Propulsion Conference, Atlanta, Georgia, 2017.
- ⁹O. Koshkarov, A. I. Smolyakov, A. Kapulkin, Y. Raitses, and I. Kaganovich, "Nonlinear structures of lower-hybrid waves driven by the ion beam," *Phys. Plasmas* **25**, 061209 (2018).
- ¹⁰T. Charoy, "Numerical study of electron transport in Hall thrusters," Plasma Physics [physics.plasm-ph], Institut Polytechnique de Paris. English., 2020 (NNT: 2020IPPAX046) (tel-02982367).
- ¹¹O. Koshkarov, A. Smolyakov, Y. Raitses, and I. Kaganovich, "Self-organization, structures, and anomalous transport in turbulent partially magnetized plasmas with crossed electric and magnetic fields," *Phys. Rev. Lett.* **122**, 185001 (2019).
- ¹²F. Faraji, M. Reza, and A. Knoll, "Enhancing one-dimensional particle-in-cell simulations to self-consistently resolve instability-induced electron transport in Hall thrusters," *J. Appl. Phys.* **131**, 193302 (2022).
- ¹³M. Reza, F. Faraji, and A. Knoll, "Generalized reduced-order particle-in-cell scheme for Hall thruster modeling: Concept and in-depth verification in the axial-azimuthal configuration," [arXiv:2208.13106](https://arxiv.org/abs/2208.13106) (2022).
- ¹⁴L. F. Ricketson and A. J. Cerfon, "Sparse grid techniques for particle-in-cell schemes," *Plasma Phys. Controlled Fusion* **59**, 024002 (2017).
- ¹⁵M. Reza, F. Faraji, and A. Knoll, "Resolving multi-dimensional plasma phenomena in Hall thrusters using the reduced-order particle-in-cell scheme," *J. Electr. Propul.* **1**, 19 (2022).
- ¹⁶S. Janhunen, A. Smolyakov, D. Sydorenko, M. Jimenez, I. Kaganovich, and Y. Raitses, "Evolution of the electron cyclotron drift instability in two dimensions," *Phys. Plasmas* **25**, 082308 (2018).
- ¹⁷V. Croes, T. Lafleur, Z. Bonaventura, A. Bourdon, and P. Chabert, "2d particle-in-cell simulations of the electron drift instability and associated anomalous electron transport in Hall-effect thrusters," *Plasma Sources Sci. Technol.* **26**, 034001 (2017).
- ¹⁸A. Heron and J. C. Adam, "Anomalous conductivity in Hall thrusters: Effects of the non-linear coupling of the electron-cyclotron drift instability with secondary electron emission of the walls," *Phys. Plasmas* **20**, 082313 (2013).
- ¹⁹W. Villafana, F. Petronio, A. C. Denig, M. J. Jimenez *et al.*, "2D radial-azimuthal particle-in-cell benchmark for $E \times B$ discharges," *Plasma Sources Sci. Technol.* **30**, 075002 (2021).
- ²⁰C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation* (CRC Press, 1991).
- ²¹L. Brieda, *Plasma Simulations by Example* (CRC Press, 2019).
- ²²J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah, "Julia: A fresh approach to numerical computing," *SIAM Rev.* **59**, 65–98 (2017).
- ²³D. Blackman and S. Vigna, "Scrambled linear pseudorandom number generators," *ACM Trans. Math. Softw.* **47**, 1–32 (2021).
- ²⁴G. E.P. Box and M. E. Muller, "A note on the generation of random normal deviates," *Ann. Math. Stat.* **29**(2), 610 (1958).
- ²⁵J. P. Boris, "The acceleration calculation from a scalar potential," Plasma Physics Laboratory, Princeton University, MATT-152 (1970).
- ²⁶M. Reza, F. Faraji, and A. Knoll, "Dimensionality reduction of Poisson's equation with application to particle-in-cell simulations of Hall thrusters," [arXiv:2206.13892](https://arxiv.org/abs/2206.13892) (2022).
- ²⁷T. Lafleur, S. D. Baalrud, and P. Chabert, "Theory for the anomalous electron transport in Hall effect thrusters. I. Insights from particle-in-cell simulations," *Phys. Plasmas* **23**, 053502 (2016).
- ²⁸J. J. Szabo, "Fully kinetic numerical modeling of a plasma thruster," PhD dissertation (Massachusetts Institute of Technology, 2001).
- ²⁹T. Charoy, J. P. Boeuf, A. Bourdon, J. A. Carlsson *et al.*, "2D axial-azimuthal particle-in-cell benchmark for low-temperature partially magnetized plasmas," *Plasma Sources Sci. Technol.* **28**, 105010 (2019).