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ABSTRACT

This paper presents a novel coupling of a kinetic description of neutrals with a fluid description of a fusion plasma. The code, plasma interacting super-atoms and molecules (PISAM), employs a grid-free Cartesian geometry and a direct simulation Monte Carlo approach to solve the kinetic equations of deuterium atoms and molecules. The grid-free geometry and the parallel nature of the neutral dynamics, in the absence of neutral-neutral interactions, allow for an unlimited and work-efficient parallelization of PISAM that always ensures a balanced workload. The highly optimized Python implementation obtains good performance while securing easy accessibility to new users. The coupling of PISAM with the edge turbulence model HESEL is outlined with emphasis on the technical aspects of coupling Message Passing Interface-parallelized Python and C++ codes. Furthermore, the paper presents and analyzes simulation results from running the coupled HESEL-PISAM model. These results demonstrate the impact of radial neutral transport and plasma–neutral dynamics perpendicular to the magnetic field. Specifically, they illustrate how the inward flow of neutral kinetic energy and the inhibition of radial electric shear, resulting from poloidal momentum transfer between atoms and ions, can affect the energy containment time. By comparing the results of the HESEL-PISAM model with those obtained from coupling HESEL with a diffusion models in predicting neutral transport in the plasma edge and scrape-off layer are elucidated.

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I. INTRODUCTION

On the boundary of toroidal fusion plasmas, the magnetic field curvature and strong pressure gradients give rise to turbulent motion making the SOL (scrape-off layer) inherently fluctuating of nature.¹ The interchange dynamics^{2,3} responsible for the macro-scale turbulence are unstable on the low field side of the plasma due to its unfavorable curvature. The resulting turbulent transport advects plasma across the LCFS (last closed flux surface) that forms elongated filaments expanding along the open field lines in the SOL. Viewed in the field-perpendicular plane, these filaments occur as radially propagating blobs.^{4–9} The ratio of the energy loss from this anomalous transport to the classical conduction loss is observed to be of order unity,^{10–12} making the understanding of turbulence at the plasma edge paramount in the design and operation of future reactors such as ITER and DEMO. The plasma dynamics in the vicinity of the LCFS are characterized by

non-linear and scale-free behavior, severely complicating their quantitative treatment. At present, the most commonly utilized codes for simulating plasma edge dynamics are based on drift-reduced Branginskii equations.^{13,14} These fluid approaches include GRILLIX,¹⁵ GDB,¹⁶ GBS,^{17–19} TOKAM3X,²⁰ and HESEL,^{21,22} the latter of which is the plasma model applied in this work. The difficulty of simulation is further increased due to the complex magnetic geometry around the separatrix and the presence of neutral particles. A range of processes, such as recycling, fueling,²³ and gas puff imaging,²⁴ contribute to the existence of multiple neutral species at the bulk plasma boundary of a Tokamak. Each neutral species interacts with the plasma through an array of reactions,^{25,26} which directly influence the particle and energy transport of the plasma. In various applications, such as heat exhaust simulations to assess the power load on wall and divertor plates, determining the lifespan of these crucial components,²⁷ simulations of gas puff imaging.^{28,29} and investigations into the effectiveness of different fueling techniques,^{30,31} it is essential to accurately predict the neutral transport and the impact of neutrals on the plasma. Moreover, momentum transfer from ion-neutral friction and an effective increase in ion viscosity caused by charge-exchange reactions influence the shear of the radial electric field,^{32–34} which is experimentally known to affect the accessibility of H-mode on which ITER and DEMO are highly dependent.^{35–37}

The field-perpendicular part of the plasma-particle orbits is constrained by the gyration motion around the field lines. In consequence, the field-perpendicular part of the effective mean free path is short in comparison to the characteristic length scale in fusion devices.¹³ The perpendicular dynamics of fusion plasma can, thus, be treated as collisional, allowing for the use of an asymptotic fluid closure. The flow of neutrals on the edge of fusion plasmas is, on the other hand, usually characterized by a high Knudsen number,³⁸ thus demanding the use of kinetic approaches, not dependent on a short mean path, to obtain accurate results. Most kinetic neutral codes apply a Markov-chain-Monte Carlo method as in EIRENE^{39,40} and DEGAS2.⁴¹ To avoid the associated Monte Carlo noise, deterministic solutions of the neutral kinetic equations have been sought as in the neutral part of the GBS code.⁴² In high-recycling and detached divertor operating regimes, the neutral mean free path may become short enough for fluid approaches to be valid in the divertor region. Under such conditions, recent research has shown a good agreement between EIRENE and neutralfluid models.^{43–45} HESEL, however, targets the plasma dynamics at the outboard mid-plane where the Knudsen number is generally too high to allow for an asymptotic fluid closure and, thus, should be coupled with a kinetic-neutral model to ensure its validity. Despite the long mean free path usually characterizing neutral flow, several fluid models for the description of neutrals at the plasma boundary have been developed.^{46–48} Among these, the fluid model nHESEL⁴⁸ is of special interest to the current work as it is rooted in the same plasma model as PISAM, i.e., HESEL. Thus, it serves as a direct comparison for the kinetic neutral model presented in this paper.

Transport codes consisting of coupled mean-field plasma models and neutral models, such as SOLPS-ITER,49 EDGE2D-EIRENE,51 UEDGE,⁵¹ Soledge2D-EIRENE,⁵² EMC3-EIRENE,⁵³ have been used extensively in fusion research for decades. At present, however, only a few codes self-consistently coupling an edge turbulence model with a kinetic neutral model have been reported. These achievements include the GBS code^{17-19,42} and the coupling of EIRENE with the TOKAM3X code.^{54,55} The present study adds to this collection of tools by introducing PISAM (plasma interacting super-atoms and molecules), a fully kinetic neutral model, and its coupling with HESEL. The combined model is denoted as HESEL-PISAM. The novel approach implemented by PISAM for the self-consistent inclusion of plasma-neutral interactions in plasma turbulence models is inspired by DSMC (direct simulation Monte Carlo) methods, traditionally used in the modeling of transition fluids.^{56–58} DSMC methods employ deterministic transport and probabilistic treatment of collisions to simulate superparticles, resulting in intuitive models that can be easily adjusted and expanded. When neglecting self-interactions of neutrals, the DSMC-based approach of PISAM allows for the implementation of a grid-free 3D geometry, making it possible to couple PISAM to any plasma model given that a mapping from the Cartesian coordinates of PISAM to the grid of the relevant plasma model is provided and that the boundary

conditions of PISAM are properly adjusted. Furthermore, the grid-free geometry and the embarrassingly parallel nature of the simulation problem are leveraged to implement PISAM with unlimited parallelism and a balanced workload among its parallel processes. To couple PISAM, implemented in Message Passing Interface-parallel Python, with the C++ implementation of HESEL, an MPI-intercommunicator is established between the two programs. While this approach was specifically developed for the current task, it can be employed to couple any two programs that support MPI compilation. As a result, this method offers broad applicability in enhancing the flexibility of the numerous MPIparallelized numerical tools applied in various fields of Physics.

Sections II-IX of this article are organized as follows. Following the "Introduction" section, Sec. II presents the HESEL equations augmented with source terms arising from plasma-neutral interactions. The fundamental principles of PISAM are described in Sec. III, encompassing the characteristics of plasma-neutral interactions, the kinematics of individual particles, the imposed boundary conditions on neutral particles, as well as the implementation of neutral transport and the sampling of reactions. In Sec. IV, the kinematics of the included plasma-neutral interactions are covered in detail and the assumptions utilized in calculating electron energy losses and the kinetic energy of resulting neutral fragments are presented. Section V provides the technical specifics of PISAM's parallelization, its coupling with HESEL, and the general workflow of HESEL-PISAM simulations. Additionally, Sec. VI outlines the neutral transport of nHESEL.48 The results obtained from the initial HESEL-PISAM simulations and their comparison with the outcomes of running nHESEL are presented in Sec. VII. Section VIII compares PISAM with similar codes representing the current state-of-the-art neutral modeling in turbulent plasma. Finally, Sec. IX concludes the article.

II. PLASMA MODEL

This section presents the HESEL equations augmented by source terms from inelastic collisions. HESEL,²² a successor of the ESEL model,⁵⁹ is a 2D, two-fluid, drift-reduced, Braginskii model developed to describe plasma edge turbulence. Assuming an electrostatic field with potential ϕ , the species-specific perpendicular drift, $u_{\perp,s}$, of a quasi-neutral plasma affected by plasma–neutral interactions can be written as

$$\boldsymbol{u}_{\perp} = -\frac{\boldsymbol{\nabla}\phi \times \hat{\boldsymbol{b}}}{B} + \frac{\hat{\boldsymbol{b}} \times \boldsymbol{\nabla}p}{qnB} + \frac{1}{\Omega_c}\hat{\boldsymbol{b}} \times \frac{d\boldsymbol{u}_{\perp}}{dt} + \frac{\hat{\boldsymbol{b}} \times \boldsymbol{\nabla} \cdot \bar{\pi}}{qnB} - \frac{\hat{\boldsymbol{b}} \times \boldsymbol{E}^{(mv)}}{qnB} - \frac{\hat{\boldsymbol{b}} \times \boldsymbol{I}^{(mv)}}{qnB} + \frac{\hat{\boldsymbol{b}} \times m\boldsymbol{u}_{\perp}\boldsymbol{I}^{(1)}}{qnB} = \boldsymbol{u}_E + \boldsymbol{u}_D + \boldsymbol{u}_p + \boldsymbol{u}_{\pi} + \boldsymbol{u}_R + \boldsymbol{u}_{IR} + \boldsymbol{u}_{In}, \qquad (1)$$

where the advective derivative $\frac{d_s}{dt} = \left(\frac{\partial}{\partial t} + \boldsymbol{u}_s \cdot \boldsymbol{\nabla}\right)$ has been used and the species subscript has been omitted to ease the notation. $\hat{\boldsymbol{b}}$ is the

the species subscript has been omitted to ease the notation. **b** is the unit vector parallel to a magnetic field of spatially varying strength *B*. *n* is the spatially varying plasma density assumed to be species-independent by quasi-neutrality. *q* and *m* are the charge and mass of the relevant species, respectively. *p*, Ω_c , and $\bar{\pi}$ are the pressure, cyclotron frequency, and viscous-stress tensor of the relevant species, respectively, all spatially varying. *v* denotes the velocity of a single particle. For later reference, when considering an ensemble of particle *v* can be divided into a mean velocity, *u*, and a random velocity, *w*, i.e.,

v = u + w. $E^{(\Phi)}$ and $I^{(\Phi)}$ denote moments over the elastic, \mathscr{E} , and inelastic, \mathscr{I} , part of the kinetic collision operator as given, for example, by Braginskii and Leontovich.¹³ The moments of the physical quantity Φ are defined as

$$E_s^{(\Phi)} = \int \Phi \mathscr{E}_s \mathrm{d} \boldsymbol{v}_s \quad \text{and} \quad I_s^{(\Phi)} = \int \Phi \mathscr{I}_s \mathrm{d} \boldsymbol{v}_s,$$
(2)

where a species subscript is included for clarity. In the remainder of the article, any subscripted i's and e's refer to ions and electrons, respectively. The last line of (1) names the drifts for later reference.

In the drift-reduced regime, the electric and diamagnetic drifts are of lowest order^{14,60} and we introduce the notation $u_{\perp,1} = u_E + u_D$ for the first-order perpendicular drift. Any appearance of u_{\perp} in the higher-order drifts of (1) is now substituted by $u_{\perp,1}$. The resulting approximation of $u_{\perp,s}$ is now substituted into the continuity and energy fluid equations of each species as given by Braginskii and Leontovich.¹³ Any terms that depend on the electron-to-ion mass ratio, m_e/m_i , are neglected.

Section II A provides a summary of the approximations leading from the drift-reduced Braginskii equations to the HESEL equations. For a detailed description, the reader should refer to Ref. 22.

A. HESEL

Slab geometry is utilized in formulating the equations of HESEL, the domain of which is limited to the outboard mid-plane. With x = 0at the last closed flux surface, the assumed vacuum magnetic field is

$$B(x) = \frac{RB_t}{R+a+x}, \quad B(0) = B_0 = \frac{RB_t}{R+a},$$
 (3)

where B_t is the toroidal magnetic field at the magnetic axis and R and a are the major and minor torus radii, respectively. Generally, subscript 0 indicates reference values at the LCFS in the following.

HESEL applies the thin-layer (Boussinesq) approximation and several similar linearizations, see Ref. 22. The thin-layer approximation is debatable when applied to edge-plasma simulations, due to the large density gradient in the vicinity of the LCFS. It is, however, widely used due to its numerical efficiency. Research targeting the effect of the thin-layer approximation in edge plasma simulations is sparse, but a recent study suggests that gyro-fluid models give rise to a lower blob growth rate than comparable models that apply the Boussinesq approximation.⁶¹

The diffusion and conduction coefficients are evaluated at the reference quantities of the LCFS and assumed to be constant across the domain, i.e., $D_{s0} \approx \nu_{ss'0} \rho_{s0}^2$, with $\nu_{ss'}$ and ρ_s being the collision frequency of species *s* with *s'* and the gyro radius of species *s*, respectively. The diffusion coefficients of collisional diffusion, $D_{e,i}$ are further modified to account for neoclassical effects by applying Pfirsch–Schlüter transport^{62,63}

$$D_s = \left(1 + \frac{R}{a}q^2\right) D_{s0},\tag{4}$$

where *q* is the safety factor.

The parallel dynamics are truncated by parameterization making HESEL effectively 2D. No parallel dynamics are considered within the LCFS, whereas outside the LCFS it is assumed that all parameterized parallel terms act as sinks since plasma is escaping along open field lines to the divertor plates and reactor wall. As blobs move into the SOL, they expand along the open field lines at velocities comparable to the ion sound speed $c_s = \sqrt{(T_e + T_i)/m_i}$, where T_s is the temperature of species *s*. This gives rise to a particle density damping rate approximated by $\frac{1}{\tau_a} = \frac{2v_b}{L_b}$, where v_b is the expansion velocity of each end of the blob, and L_b is the typical field-parallel blob length. Setting $v_b = Mc_s$, with $M = u_{\parallel i}/c_s$, and $L_b = qR_s^{22}$

$$\frac{1}{\tau_n} = \frac{2Mc_s}{qR}.$$
(5)

As vorticity is mainly transported by blobs in the SOL region, the damping rate of vorticity is assumed to be equal to that of density,

$$\frac{1}{\tau_w} = \frac{1}{\tau_n}.$$
(6)

The divergence of the parallel current present in the vorticity equation is approximated by sheath damping,^{22,64}

$$\nabla \cdot \left(\hat{\boldsymbol{b}} J_{\parallel} / \boldsymbol{e}\right) \approx \frac{e n_0 c_s}{L_c} \left[1 - \exp\left(\log \sqrt{\frac{m_i}{2\pi m_e}} - \frac{\boldsymbol{e} \phi}{T_e}\right) \right] = \mathscr{S}, \quad (7)$$

where J_{\parallel} is the field parallel current, n_0 is the reference density at the LCFS, and L_c is the outer divertor connection length.

The heat conduction of species *s* is mathematically represented as the divergence of the temperature-gradient-dependent part of the heat-flux vector, i.e., $\nabla q_{s,T}$. The parallel electron heat conduction, $\nabla_{\parallel} \cdot q_{e,T\parallel}$, is assumed to be given solely by Spitzer–Härm conduction,⁶⁵ which shall be approximated by

$$\nabla_{\parallel} \cdot \boldsymbol{q}_{e,T\parallel} \approx -\frac{T_e^{7/2}}{\tau_{SH}}, \quad \text{with} \quad \frac{1}{\tau_{SH}} = 3.16 \frac{n_0}{m_e \nu_{ei0} T_{e0}^{3/2} L_c^2}, \quad (8)$$

where ν_{ei0} is the electron–ion collision frequency, $\nabla_{\parallel} = \hat{b}(\hat{b} \cdot \nabla)$ and the 0 subscript indicates reference values at the LCFS. Parallel heat conduction is neglected for ions as advection is dominant in the SOL.²² Finally, the parallel damping rate of ion and electron pressure is parameterized through

$$\frac{1}{\tau_{pe}} = \frac{1}{\tau_{pi}} = \frac{9}{2} \frac{1}{\tau_n}.$$
 (9)

Damping is only applied in the unconfined region, i.e., outside the LCFS. A double step-function $\sigma(x)$ determines the extent to which the damping terms are applied in the various parts of the domain as illustrated by the shaded regions of Fig. 1, where the wall shadow region is exposed to damping eight times stronger than that of the scrape-off-layer. The plasma is fed by classical transport from the inner edge where the density and pressure fields are forced to preset profiles. To highlight characteristic quantities, the transport equations are gyro-Bohm normalized, i.e., temporally and spatially scaled by the scale of the ion gyration motion.⁶⁶ Specifically, the scaling procedure consists of the transformations

$$\Omega_{i0}t \to t, \quad \frac{x}{\rho_0} \to x, \quad \frac{T_{e,i}}{T_{e0}} \to T_{e,i},$$
(10)

$$\frac{e\phi}{T_{e0}} \to \phi, \quad \frac{n}{n_0} \to n, \quad \frac{u}{\rho_0 \Omega_{i0}} \to u,$$
 (11)

where $\Omega_{i0} = eB_0/m_i$ is the ion gyro frequency and $\rho_0 = \sqrt{\frac{T_{c0}}{m_i \Omega_{i0}^2}}$ is the hybrid ion thermal gyro radius evaluated at the reference values of the



FIG. 1. Simulation domain of the HESEL-PISAM model, with boundary conditions for plasma and neutrals. In the present slab coordinate system, the x-axis corresponds to the radial axis, and the y-axis corresponds to the poloidal axis. The dashed line indicates the last closed flux surface.

LCFS. In slab coordinates, it is practical to introduce the curvature operator

$$\mathscr{K}(f) = -\frac{\rho_0}{R+a}\frac{\partial}{\partial y}f.$$
 (12)

By inclusion of source terms from inelastic collisions and application of the simplifications listed above, the drift-reduced Braginskii equations reduce to the HESEL equations

$$\frac{d}{dt}n + n\mathscr{K}(\phi) - \mathscr{K}(p_e) = \Lambda_n + \Sigma_n,$$
(13)

$$\nabla \cdot \left(\frac{d^0}{dt} \nabla_{\perp} \phi^*\right) - \mathscr{K}(p_e + p_i) = \Lambda_w + \Sigma_w, \tag{14}$$

$$\frac{3}{2}\frac{d}{dt}p_e + \frac{5}{2}p_e\mathscr{K}(\phi) - \frac{5}{2}\mathscr{K}\left(\frac{p_e^2}{n}\right) = \Lambda_{p_e} + \Sigma_{pe}, \qquad (15)$$

$$\frac{3}{2}\frac{d}{dt}p_i + \frac{5}{2}p_i\mathscr{K}(\phi) + \frac{5}{2}\mathscr{K}\left(\frac{p_i^2}{n}\right) - p_i\mathscr{K}(p_e + p_i) = \Lambda_{p_i} + \Sigma_{p_i},$$
(16)

where the advective derivatives are defined solely through $E \times B$ -advection

$$\frac{d}{dt} = \frac{\partial}{\partial t} + B^{-1}\{\phi, \cdot\}, \quad \frac{d^0}{dt} = \frac{\partial}{\partial t} + \{\phi, \cdot\}$$

with

$$\{f,g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial y} - \frac{\partial f}{\partial y}\frac{\partial g}{\partial x}.$$
 (17)

Furthermore, the effective potential ϕ^* has been defined through

$$\phi^* = \phi + p_i. \tag{18}$$

Terms related to diffusion and parallel damping are denoted Λ_{i} , $i \in \{n, w, pe, pi\}$, and are given by

$$\Lambda_n = D_e(1+\tau)\nabla_{\perp}^2 n - \sigma(x)\frac{n}{\tau_n},\tag{19}$$

$$\Lambda_w = \frac{3}{10} D_i \nabla_\perp^2 \nabla_\perp^2 \phi^* - \sigma(x) \frac{\nabla_\perp^2 \phi^*}{\tau_n} + \sigma(x) \mathscr{S}, \qquad (20)$$

$$\begin{split} \Lambda_{p_e} &= D_e (1+\tau) \nabla \cdot (T_e \nabla_\perp n) + D_e \frac{11}{12} \nabla \cdot (n \nabla_\perp T_e) \\ &+ D_e (1+\tau) \nabla_\perp \ln n \cdot \nabla_\perp p_i - \frac{3m_e}{m_i} \nu_{ei0} (p_e - p_i) \\ &- \sigma(x) \left[\frac{9}{2} \frac{p_e}{\tau_n} + \frac{T_e^{7/2}}{\tau_{\rm SH}} \right], \end{split}$$
(21)

$$\begin{split} \Lambda_{p_i} &= \frac{5}{2} D_e (1+\tau) \nabla \cdot (T_i \nabla_\perp n) - D_e (1+\tau) \nabla_\perp \ln n \cdot \nabla_\perp p_i \\ &+ 2 D_i \nabla \cdot (n \nabla_\perp T_i) \frac{3}{10} D_i \bigg[\left(\partial_{xx}^2 \phi^* - \partial_{yy}^2 \phi^* \right)^2 + 4 \left(\partial_{xy}^2 \phi^* \right)^2 \bigg] \\ &+ \frac{3 m_e}{m_i} \nu_{ei0} (p_e - p_i) + \sigma(x) \bigg(p_i \mathscr{S} - \frac{9}{2} \frac{p_i}{\tau_n} \bigg), \end{split}$$
(22)

where $\tau = T_i/T_e$, $\sigma(x)$ is the step-function determining the strength of the parallel damping terms as a function of the radial coordinate, \mathscr{S} is the sheath-damping as defined by (7), $\mathbf{V}_{\perp} = \mathbf{\nabla} - \hat{\mathbf{b}}(\hat{\mathbf{b}} \cdot \mathbf{\nabla})$, and ∂_i^k is the *k*th derivative with respect to the *i*th coordinate where $k \in \mathbb{N}$ and $i \in \{x, y, z\}$. The terms entering the equations due to plasmaneutral interactions are given by

$$\Sigma_{n} = I^{(1)}, \quad \Sigma_{w} = \nabla \cdot (n u_{I,i}), \quad \Sigma_{pe} = I_{e}^{\left(\frac{1}{2}mv^{2}\right)}, \quad (23)$$
$$\Sigma_{pi} = I_{i}^{\left(\frac{1}{2}mv^{2}\right)} - u_{i\perp,1} \cdot I_{i}^{(mv)} + \frac{1}{2}u_{i\perp,1}^{2}I^{(1)}$$

$$+ p_i \nabla \cdot (n \boldsymbol{u}_{I,i}) - p_i \nabla \cdot (\boldsymbol{u}_{I,i}) - \frac{3}{2} \nabla \cdot (p_i \boldsymbol{u}_{I,i}), \qquad (24)$$

where $u_{I,i} = u_{IR,i} + u_{In,i}$ are defined in (1), and the moments, $I^{(\Phi)}$, are defined in (2). A neutral model is required to calculate the source

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terms, $I_i^{(1)}$, $I_i^{(mv)}$, $I_i^{(\frac{1}{2}mv^2)}$, and $I_e^{(\frac{1}{2}mv^2)}$, arising from inelastic plasmaneutral collisions and, thus, provide the final closure of the model equations (13)–(16). In Secs. III and VI, we present both a kinetic and fluid approach to performing this closure.

III. KINETIC NEUTRAL MODEL

PISAM can be considered a discrete Monte Carlo model as it monitors a large number of distinct superparticles, each representing an ensemble of physical particles. The objective is to find an approximate solution to the neutral kinetic equations by tracking the behavior of each superparticle individually during its interactions with the plasma. This approach enables a fully kinetic treatment of both the neutral transport and the computation of source terms from inelastic collisions. Due to the high Knudsen number characterizing the flow of neutrals at the outboard midplane, the kinetic approach of PISAM is a more accurate alternative to the fluid model of Sec. VI that has earlier been coupled to HESEL.

Each superparticle is assigned a species *s*, location *r*, velocity *v*, and weight *w*, equal to the number of physical particles it represents. The model proceeds through successive neutral time steps, that are not, in general, equal to the discrete time steps used in solving the plasma equations (see Sec. V for details). During each such intrinsic time step, three essential steps are performed: (1) breeding new superparticles from external sources, (2) sampling and simulating plasmaneutral interactions, and (3) transporting the superparticles. Similar to DSMC approaches, ⁵⁶ the transport component of PISAM is deterministic, while the collisions are treated stochastically.

A. Breeding superparticles

The breeding process currently supports the injection of each represented species at a user-defined temperature, T_{s} , and flux of physical particles, F_s . Each time step is initiated by injecting $n_{s,new}$ superparticles of the relevant species at the outer radial boundary of the domain with velocities sampled from a Maxwellian with temperature T_s , such that $F_s L_{pol} L_{tor} \Delta t = n_{s,new} w_{s,init}$, where Δt is the duration of a time step of the neutral model (see Sec. III C for details), $w_{s,init}$ is the initial weight of the injected superparticles, and L_{pol} and L_{tor} are the poloidal and toroidal domain sizes, respectively. (When coupling to a 2D model like HESEL, L_{tor} only affects the injection rate of neutrals and the calculation of the source terms such that the contributions to the source terms cancel. L_{tor} is, thus, set to 1 m in the current simulations.)

B. Sampling collisions

Individually for each superparticle, the initial phase of the collision routine involves sampling the plasma-neutral collisions that transpire within the specific neutral time step. Consider a particle identified by index *i* of species *s* that can react with the plasma through *R* different reactions. Let these reactions be indexed by $j \in \{1, ..., R\}$, such that a certain kind of reaction, e.g., atomic ionization, is uniquely defined by s_j . The frequency of the particle *i* undergoing the plasmaneutral collision s_j is given by $\Gamma_{ij} = [n\langle \sigma_{sj}g \rangle]_i$, where *n* is the plasma density, σ_{sj} is the cross section of the reaction, and *g* is the relative speed of the reaction particles. $\langle \cdot \rangle$ denotes the expectation value from integration over a Maxwellian and $[\cdot]_i$ indicates the evaluation concerning the plasma fluid variables that correspond to the position r_i of the superparticle in question. Let the total collision frequency of a

superparticle indexed by *i* be denoted $\Gamma_i = \sum_j \Gamma_{ij}$. The probability that particle *i* will undergo the collision s_j during Δt is then

$$P_{ij} = \frac{\Gamma_{ij}}{\Gamma_i} (1 - e^{-\Gamma_i \Delta t}).$$
⁽²⁵⁾

The reactions alter the densities of plasma and neutral species and so alter the reaction probabilities, i.e., the source terms of inelastic collisions are non-linear. For accuracy, we, thus require $P_i = \sum_j P_{ij}$ to be small which is satisfied to an acceptable degree when Δt is constrained by the Courant condition presented in Sec. III C. Under this constraint, $P_i <$ 0.05 for SOL and edge-relevant conditions of medium-sized Tokamaks. The sampling is now conducted by the standard method of constructing the cumulative sum from P_{ij} and generating a uniform random number u. If $u > P_i$, the particle does not collide in the given time step. The execution of the sampled collisions implies an alteration of the neutral velocity or complete removal of the neutral along with the generation of any neutral fragments produced in the collision. Section IV provides comprehensive details regarding the specific characteristics of each collision considered, including the computation of the corresponding source terms.

C. Transport of superparticles

Assuming that no forces act on the neutrals between collisions, their displacements are $\Delta t v_i$ during a time step Δt and their positions are updated by

$$\mathbf{r}_{i}^{t+\Delta t} = \mathbf{r}_{i}^{t} + \Delta t \mathbf{v}_{i}. \tag{26}$$

By applying the Braginskii closure scheme,¹³ we have implicitly assumed that $\rho_i \ll L_{\perp}$, where ρ_i is the ion gyro frequency and L_{\perp} is the characteristic length scale in the field perpendicular plane. Δt can, thus, be restricted by the Courant condition $\Delta t v_i < \rho_i$. Relaxing this condition by replacing v_i by the neutral thermal speed $v_{i,t}$, the Courant condition becomes

$$v_{i,t}\Delta t \le \rho_i \Rightarrow \Delta t \le \sqrt{\frac{T_i}{2T_{neut}}} \frac{1}{\Omega_i},$$
(27)

where T_i is the ion temperature and T_{neut} is a temperature characterizing the speed distribution of neutrals. The hottest neutrals are chargeexchanged atoms with $T_{neut} \approx T_i$ and so we take $\Delta t = \frac{1}{\Omega_{io}}$, i.e., the inverse ion gyro frequency at LCFS reference values. If the path between r_i^t and $r_i^{t+\Delta t}$ intersects with a boundary, the appropriate boundary condition is applied, as specified in Sec. III D.

D. Domain and boundary conditions

The domain of the coupled HESEL-PISAM model is sketched in Fig. 1. Neutral particles are injected at the outer radial boundary according to the breeding process described in Sec. III A. By intersection with this boundary, neutrals are absorbed with probability γ and otherwise reflected. The poloidal boundaries have periodic boundary conditions whereas neutral particles crossing the inner edge are removed from the system. To prevent an artificial accumulation of molecules with small radial velocities near the outer radial boundary, an additional boundary condition is enforced. If a particle travels sufficiently far in the poloidal or toroidal direction to intersect with the first wall, it is reflected with probability γ and otherwise re-emitted at wall temperature. In this regard, the poloidal cross section of the device is assumed circular such that the condition for being inside the wall is

$$y < \sqrt{2x'a - x'^2}$$
 and $z < \sqrt{2x'R - x'^2}$, (28)





where $x' = x_{max} - x + \tilde{x}$ with x_{max} being the x-coordinate of the outer radial boundary and \tilde{x} defined as in Fig. 1. *a* and *R* are the minor and major torus radii, respectively.

IV. KINEMATICS OF THE INCLUDED INELASTIC COLLISIONS

An overview of the plasma-neutral interactions included in PISAM is shown in Figs. 2 and 3 for deuterium molecules (D_2) and

atoms (D), respectively. The corresponding reaction rates are plotted in Fig. 4. The reaction rates of electron–neutral collisions are calculated by assuming a spherically symmetric non-shifted Maxwellian velocity distribution of the electrons and neglecting the neutral velocity, consistent with the small electron mass and the imposed drift regime. In consistency with the resulting spherical symmetry of electron–neutral collisions, the net momentum transfer between electrons and neutrals is assumed to be zero. Furthermore, the large relative mass difference



FIG. 3. An overview of the reactions of deuterium atoms with plasma particles included in PISAM. The orbitals are merely added to illustrate the difference in electronic states and do not necessarily match the physical orbitals.



FIG. 4. (a) Reaction rates of the groups of plasma-molecule reactions included in PISAM. The ionization rate is provided as an analytical fit in AMJUEL.⁶⁷ The MD reaction rates are calculated by integration over cross sections provided by Ref. 68. (b) Reaction rates of the plasma-atom reactions included in PISAM. The effective ionization rate and 2*p* excitation rate are provided by AMJUEL.⁶⁷ The charge-exchange rate is given in HYDHEL.⁶⁹

between electrons and neutrals allows for the assumption that in the included electron-neutral collisions the kinetic energy lost by the electron is converted entirely to internal energy of the neutral by excitation to an electronic state with higher potential energy. The velocity distribution of fragments resulting from electron-neutral collisions is, thus, assumed to be spherically symmetric in the rest frame of the colliding neutral particle prior to the collision. The remainder of this section describes the individual reactions in detail. The electron energy loss and average fragment energy of the various electron-plasma interactions are summarized in Table I. Section IV D describes the implementation of charge-exchange reactions in PISAM, which due to the inapplicability of the large mass ratio assumption demands a more rigorous mathematical treatment to be accurate and numerically feasible.

A. Molecular ion dissociation (MID)

PISAM assumes that molecular ions created by electron impact on deuterium molecules instantaneously dissociate into a deuterium atom in the ground state and a deuterium ion. This assumption is deemed acceptable by calculations based on simulation data from running HESEL-PISAM suggesting that the average mean free path of

 TABLE I. Average electron energy loss and fragment energy used in the electronneutral collisional processes of PISAM.

Collisional process	Electron energy loss (eV)	Fragment temperature
MD through $b^3 \Sigma_{\mu}^+$	10.62	2.75 eV
MD through $a^3 \Sigma_{\alpha}^+$ and $c^3 \Pi_u$	12.64	0.75 eV
MD through $B'^1 \Sigma_u^+$ and $D^1 \Pi_u$	17.25	0.3 eV
MD through $B^1 \Sigma_u^+$ and $C^1 \Pi_u$	12.75	0.17 eV
MID	$2E_{frag} + 17.04$	Dist. at 15 eV of Ref. 75
Ionization of D	13.60	
$D(1s) \rightarrow D(2p)$	10.61	

deuterium molecular ions is 4 mm corresponding to 2-5 ion gyro radii, depending on the magnetic field. The effective rate of ionization by electron impact is provided by the database AMJUEL.⁶⁷ Each molecular ionization yields an electron energy loss of 15.48 eV, equal to the ionization energy of D2.70 The vibrational states of the created molecular deuterium ions are assumed to be distributed according to the Franck Condon factors of the reaction $e + D_2(X^1\Sigma^+_{\alpha}, v = 0) \rightarrow$ $2e + D_2^+(1s\sigma_{\sigma}, v')$ provided by Refs. 71 and 72. Here, and in the following, the content of the parenthesis following a chemical symbol of an atom or molecule specifies its state. When specifying bound molecular states the content of the parenthesis is separated by a comma. In that case, the part before the comma specifies the electronic state, and the part after the comma specifies the vibrational state of the nuclei. The molecular and atomic states of this article are named by standard convention when specifying the relevant quantum numbers and symmetries. The ability to decode these chemical symbols is not a necessary prerequisite for this article, but the interested reader may refer to Refs. 139 and 140, among others. The potentials of the relevant molecular states are available in Refs. 73 and 74.

The dissociation of molecular deuterium ions by electron impact can proceed through multiple channels.⁷² Due to its dominant reaction rate at typical edge plasma temperatures, PISAM only considers nonresonant-dissociative excitation

$$e + D_2^+(1s\sigma_g, v) \to e + D_2^{+*} \to e + D^+ + D(1s),$$
 (29)

where D_2^{+*} denotes any singly excited state (one excited electron) of the deuterium molecular ion. Any such state is dissociative for this particular ion. In the center-of-mass frame, energy conservation demands $\Delta E_e(\nu) = 2E_{frag}(\nu) + E_{diss}(\nu)$, where $\Delta E_e(\nu)$ is the electron energy loss, $E_{frag}(\nu)$ is the fragment energy, $E_{diss}(\nu)$ is the dissociation energy of the deuterium molecular ion, and the dependence of the vibrational state ν has been stated explicitly. The kinetic energy release cross section of non-resonant-dissociative excitation processes in H_2^+ at 15 eV electron impact was measured by Ref. 75. Measurements,⁷⁵ and theoretical analysis,⁷⁴ at higher energies suggest that the probability distribution of fragment energies is very similar for hydrogen and deuterium. Furthermore, simulation of HESEL-PISAM shows that 15 eV is a typical electron impact energy for non-resonant-dissociative excitation at the positions of molecular ionization, and so the distribution obtained at this energy in Ref. 75 is used for sampling the fragment energies in HESEL-PISAM. Let E_{diss} be defined as the weighted average of $E_{diss}(v)$ according to the Franck Condon factors of the reaction $e + D_2(X^1\Sigma_g^+, v = 0) \rightarrow 2e + D_2^+(1s\sigma_g, v')$ and the cross sections of the reaction $e + D_2^+(1s\sigma_g, v) \rightarrow e + D_2^+(2p\sigma_u)$ evaluated at 15 eV given by Ref. 68 has been calculated. This calculation results in an average dissociation energy of 1.61 eV.

B. Molecular dissociation (MD)

Dissociation of the deuterium molecule into neutral fragments by electron impact can proceed through two fundamental processes: (1) dissociative excitation (DE) where the molecule is excited directly into the vibrational continuum of an excited electronic state, and (2) excitation decay dissociation (EDD) where an excitation to a bound vibrational level of an excited electronic state leads to spontaneous decay to the continuum of a lower electronic state.⁷³ Both of these processes proceed through multiple channels, all with different kinematic properties, i.e., electron energy loss and fragment energies. To represent the kinematics properly while limiting complexity the included reactions of molecular dissociation are implemented as four groups of reactions, described individually in the following.

1. Direct excitation to $b^3 \Sigma_u^+$

Excitation into the repulsive $b^3 \Sigma_u^+$ state leads to immediate dissociation. The excitation energy from the ground state at its most probable inter-nuclear separation is 10.62 eV.⁷⁶ The average temperature of dissociation through the relevant channel found in the current simulations is \approx 13eV. According to the calculations presented in Ref. 77, the most probable value of the kinetic fragment energy at 13 eV is 2.75 eV.

2. Dissociation through $a^{3}\Sigma_{a}^{+}$ and $c^{3}\Pi_{u}$

The $a^3 \Sigma_g^+$ state is radiatively coupled to the $b^3 \Sigma_u^+$ state with a lifetime of ~ 10ns.²⁵ $c^3 \Pi_u$ is metastable but decays to $a^3 \Sigma_g^+$ by electron impact. An extension of the analysis provided by Ref. 25 applied with SOL relevant plasma fields gives an approximate lifetime of $c^3 \Pi_u$ of ≈ 40 ns. Both of these decays shall, thus, be assumed to be instantaneous. The average excitation energy of these two triplet states is 12.64eV,^{78,79} which is used as the electron loss for the combined channel due to the similar cross sections of excitation to $a^3 \Sigma_g^+$ and $c^3 \Pi_u$.⁶⁸ The kinetic energy distributions of the neutral fragments produced by dissociation through $(a^3 \Sigma_g^+, v)$ and $(c^3 \Pi_u, v)$, where v is the vibrational quantum number, are given by Ref. 80. Averaging these distributions with respect to the cross sections of excitation to the vibrational states of $a^3 \Sigma_g^+$ and $c^3 \Pi_u$ from the ground state results in a fragment energy of 0.75 eV.

3. Dissociation through $B^{I}\Sigma^{+}_{u}$ and $D^{I}\Pi_{u}$

Considering solely the vibrational ground state of the electronic ground state of D₂ the only relevant singlet channel for DE is through $B^{J}\Sigma_{u}^{+}$.^{25,81,82} The EDD channel initialized by excitation to $D^{1}\Pi_{u}$ dissociates by decay to the continuum of $B^{\prime 1}\Sigma_{u}^{+}$ and, thus, produces the same neutral fragments, i.e., D(1s) and D(2s). The D(2s) is metastable but decays to the short-lived D(2p) state by electron impact. At SOL relevant conditions the typical collision time for this decay is \approx 30 ns and

D(2s) is, thus, assumed to decay instantaneously to the ground state, when created from molecular dissociation. Experimental measurements of these metastable atoms are presented in Ref. 83 and report a fragment energy of approximately 0.3eV. The dissociation threshold of $B^{I}\Sigma_{u}^{+}$ is 16.65eV above the ground state energy⁸¹ and the electron loss is, thus, assumed to be 16.65 eV + 2 × 0.3 eV = 17.25 eV. Only a fraction of the excitations of molecules to $B^{I}\Sigma_{u}^{+}$ and $D^{1}\Pi_{u}$ result in dissociation. These fractions are given in Ref. 73 and must be included when calculating the reaction frequencies from the cross sections given in Ref. 68.

4. Dissociation by EDD through $B^{1}\Sigma_{\mu}^{+}$ and $C^{1}\Pi_{\mu}$

The states $B^1\Sigma_u^+$ and $C_1\Pi_u$ decay to the ground state $X^1\Sigma_{\sigma}^+$ by emission of radiation with short lifetimes of approximately 1ns.8435 fraction of these decays are into the vibrational continuum of the ground state and lead to dissociation into 2D(1s) atoms.²⁵ The energy of the neutral fragments resulting from these dissociation channels are estimated by the emission spectra, presented in Refs. 80 and 86, of decays to the vibrational continuum of $X^1 \Sigma_g^+$ from the singlet states $B^1 \Sigma_u^+$, $C^1 \Pi_u$, $D^1 \Pi_u$, and $B'^1 \Sigma_u^+$, where $B^1 \Sigma_u^+$ is stated as the main contributor. These spectra are peaked around a significant resonance at approximately 1580 Å corresponding to a photon energy of 7.85eV. The energies of the states $B^1 \Sigma_{,,i}^+$ and $C^{1}\Pi_{u}$, which are the channels included for this mechanism, lie close at 12.75 and 13.22eV, relative to the ground state at its most probable internuclear separation of $R_0 = 1.40a_0^{.87,88}$ As $B^1 \Sigma_u^+$ is dominant, we use 12.75eV for the electron energy loss. The dissociation energy of the deuterium molecule is 4.56eV.89 The most probable value of the continuum energy ϵ_k is, thus, estimated as 12.75 eV - 7.85 eV - 4.56 eV =0.34eV giving an average fragment energy of 0.17eV.

C. Atomic excitation to 2p

As a consequence of the significant excitation rate of the 2p state at plasma edge relevant temperatures as shown by Fig. 4(b), this electron–neutral reaction is included in PISAM. 2p is short-lived with a lifetime of 1.6 ns^{90} and is, thus, assumed instantly to decay back to the ground state by emission of radiation, such that the reaction solely acts as an electron energy sink. The electron energy loss associated with the reaction is 10.61eV equal to the excitation energy of the 2p state.⁹¹

D. Atomic charge-exchange

In charge-exchange reactions, the velocities of the interacting deuterium ion, $v_i = w_i + u_i$ and deuterium atom, v_n , are simply assumed to be switched. Due to the small electron mass, as compared to ions and neutrals, this typical assumption yields only a minor violation of energy and momentum conservation. To ensure an accurate estimation of the momentum transfer mediated by charge-exchange reactions, it is necessary to incorporate both the ion fluid velocity and the neutral velocity in the calculation of the reaction rate. This consideration arises from the similarity in velocities exhibited by the colliding particles involved in these reactions. Assuming a Maxwellian distribution of ion velocities, the reaction rate is

$$\langle \sigma g \rangle_{ni} = \left(\frac{m}{2\pi T_i}\right)^{3/2} \int \sigma(g) g \exp\left(-\frac{m_i w_i^2}{2T_i}\right) \mathrm{d}\boldsymbol{v}_i,$$
 (30)

where $\langle \cdot \rangle$ denotes the expectation value from integration over the relevant Maxwellian and $g = |w_i + u_i - v_n|$ is the relative speed. By





FIG. 5. The lab frame is shown as the unprimed coordinate axes, while the rotated d-frame is denoted by primes. The angle θ' is the polar angle of the random ion velocity, w_i , in the d-frame. The axial symmetry obtained in the d-frame ensures that all w_i that intercept the periphery of the two black circles *and* the origin, contribute equally to the charge-exchange-reaction rate of the relevant neutral.

shifting (30) to the rest frame of the ions and rotating the coordinate system of integration to align the vertical axis with the velocity $d = v_n - u_i$, g^2 can be expressed as

$$g(w_i, \theta')^2 = d^2 + w_i^2 - 2dw_i \cos{(\theta')},$$
(31)

where θ' is the angle between *d* and *w_i*. The geometry of the interaction is illustrated in Fig. 5, emphasizing the axial symmetry with respect to *d* that appears in (31) which depends on the polar angle, θ' , but not on the azimuthal angle. Under this transformation, the reaction rate takes the form

$$\langle \sigma_{cx}g \rangle = \frac{1}{\sqrt{2\pi}} \left(\frac{m_i}{T_i}\right)^{3/2} \int_{0}^{\pi\infty} \int_{0}^{\infty} \exp\left(-\frac{m_i w_i^2}{2T_i}\right) \\ \cdot \sigma_{cx}(g)gw_i^2 \sin\left(\theta'\right) dw_i d\theta',$$
(32)

where $\sigma_{cx}(g)$ is the velocity-dependent cross section of the chargeexchange reaction. That is, the reaction rate only depends on the ion temperature and the neutral speed in the rest frame of the ions. The distribution defined by the integrand of (32) is used to sample w_i and θ' in each charge-exchange reaction of PISAM. v_i is finally obtained by random sampling of an azimuthal angle ϕ' and transformation back to the lab frame.

E. Atomic ionization

PISAM incorporates the effective atomic ionization rate of AMJUEL⁶⁷ when calculating the ionization probability, $P_{i,ion}$ of a superparticle according to (25), i.e., the ionization rate depends on electron temperature *and* density. However, instead of including

atomic ionization in the reaction sampling procedure, it is implemented as part of the translation routine by reducing the weight of superatoms. In the notation of Sec. III B, the weight of superatoms is reduced according to

$$w_i^{t+\Delta t} = w_i^t (1 - P_{i,ion}).$$
(33)

If $w_i^{t+\Delta t} < w_{thres}$, where w_{thres} is some user-defined threshold, the superparticle is assumed to be completely ionized. This procedure enhances the source resolution inside the LCFS, where neutrals are sparse.

The opposite process to atomic ionization, i.e., volumetric recombination is insignificant at the plasma densities and temperatures relevant to the domain of HESEL, and is not currently supported in PISAM.

V. WORKFLOW AND IMPLEMENTATION OF HESEL-PISAM

This section outlines the implementation and workflow of HESEL-PISAM, with a specific focus on PISAM and the technical aspects involved in establishing effective communication between MPI-parallelized Python (PISAM) and C++ (HESEL) programs. The nomenclature and underlying principles of MPI-implementations are available through various sources.^{92,93}

A. Workflow

Figure 6 outlines the workflow of HESEL-PISAM. The first part of the simulation process is the parsing of input parameters to HESEL and PISAM. From the input parameters, the plasma fields of HESEL are initialized and communicated to PISAM, which then iterates until the domain is saturated with neutrals. Next, PISAM runs a time step of userdefined length, t_{thres} to calculate the initial neutral source terms, and the main iterative simulation procedure can begin. In this procedure, the right-hand sides of the HESEL equations are evaluated with the aid of a second-order finite difference scheme and the neutral sources supplied by PISAM. The fields are then evolved using the adaptive time step solver $PVODE^{94}$ until the time passed in HESEL, t_p is larger than the time passed in PISAM, t_n , by more than some user-defined threshold, t_{thresh} This threshold value is conservatively set to Ω_i^{-1} in current simulations. When $t_p - t_n > t_{thres}$, the HESEL time step is completed and the updated fields are communicated to PISAM. PISAM then iterates with a user-defined internal time step, dt_n until $t_n - t_p < 2dt_n$. The last internal time step is set to $t_p - t_n$ for exact synchronization.

Before being communicated to HESEL, the neutral sources calculated by PISAM are smoothed. The smoothing procedure applies a low-pass filter in the Fourier domain, i.e., the source grid is Fourier transformed, multiplied entry-wise by a Fourier transformed Gaussian with a user-defined standard deviation, σ_b , and finally inversely Fourier transformed to obtain a smoothed version of the original source grid. To avoid edge artifacts and obtain a conservative smoothing procedure, the source grid must be mirror padded. For details on the smoothing procedure, the interested reader should consult an image processing textbook.^{95,96} Smoothing is performed to obtain source terms that are sufficiently continuous for the fluid model to handle while limiting the simulated number of superparticles. An obvious drawback of smoothing is that it limits the spatial resolution of the dynamics of the simulation. After the smoothing procedure has been performed, the source terms are communicated to HESEL, which concludes a full iteration.

B. Memory

At all times, the position and velocity of each active particle must be stored in memory. During the transient phase of the simulation, the number of active particles grows rapidly. After the transient phase, however, the number of active particles of each species only varies by $\approx 10\%$, depending on the extent of edge turbulence in the relevant simulation. By reusing the memory storing the information of inactive particles, the memory usage can, thus, be kept fixed during the simulation phase, by increasing the allocated memory at the end of the transient phase by a small safety factor.

C. Parallelization of PISAM

PISAM is implemented in Python, in an object-oriented style, making it easy to alter the code with new particles, reactions, and monitoring tools. It has been parallelized with MPI such as to exploit the embarrassingly parallel nature that the dynamics of neutrals exhibit when self-collisions are not included. The data parallel implementation creates N_{PISAM} non-interacting neutral simulations with a flux of each species of F_s/N_{PISAM} , where N_{PISAM} is the number of ranks on which PISAM is called and F_s is defined according to the notation of Sec. III A. At any time, all N_{PISAM} instances of PISAM see the same plasma fields and run through time steps of the same duration. At the end of each time step, the sources from each instance are summed before they are passed to HESEL. The summation is carried out by collective communication using MPI.Reduce(), with the intracommunicator grouping the ranks in the N_{PISAM} running PISAM. The setup of the communicators is covered in Sec. V D. Apart from its simplicity, this method of parallelization has the advantages of supporting

unrestricted parallelism and effortlessly securing a balanced workload on all processors.

D. Communication between HESEL and PISAM

Setting up the communication between the two codes requires some ingenuity as PISAM is implemented in Python using mpi4py,⁹ and HESEL is implemented using the C++ framework BOUT++. This section describes the robust and swift method for solving this communication challenge that was developed for the specific problem of coupling PISAM and HESEL. Figure 7 illustrates how the communication within each part of the program, i.e., PISAM and HESEL, is achieved, and how PISAM and HESEL communicate with each other. The C++ and Python parts of HESEL-PISAM are called simultaneously on n1 and n2 processors, respectively, using a command of the form mpirun -n n1 cpp_program: -n n2 python python_program. This call initiates the World Communicator with n1 + n2 ranks. The ranks belonging to each program can be identified by using the application number provided by MPI. This feature is utilized in a call to MPI.Split(), splitting the World_Communicator into two subcommunicators responsible for the internal communication in PISAM and HESEL, respectively. The communicator of BOUT + + is set to be the subcommunicator of the C++ part instead of World_Communicator, which is the default. The subcommunicator of the Python part is used to distribute the plasma fields to each rank of the Python part, before performing each time step. Moreover, it reduces the sources of each rank to the total sources obtained during each time step. To establish the communication between PISAM and HESEL the subcommunicaobtained from the split are used in a call of tors MPI_Intercomm_create. This call creates an intercommunicator that allows for collective communication from the root node of each program to all the nodes in the subcommunicator of the other program. In HESEL-PISAM the intercommunicator performs the vital tasks of sending the plasma fields from HESEL to PISAM and sending the



FIG. 6. Workflow of HESEL-PISAM. PISAM is run until the domain with the initial plasma fields is saturated with neutrals after which the initial neutral source terms are obtained, before the main simulation procedure is started. The blue area highlights a time step of HESEL. The neutral sources are constant in each such plasma time step, subdivided into smaller steps of variable size determined by the PVODE solver. The red area highlights a time step of PISAM. The plasma fields are constant in each such time step.



FIG. 7. An illustration of the method for simultaneously launching parallel C++ and Python programs and setting up the communication between them using MPI. The top line shows the command used to execute the programs when these are named cpp_program and python_program, respectively.

sources calculated by PISAM to HESEL. HESEL is parallelized along the radial axis, necessitating consideration during communication between PISAM and HESEL. To handle this spatial division, HESEL's fields are sent to the Python subcommunicator's rank_0 using MPI_Gather() and subsequently broadcasted to other PISAM ranks through MPI_Broadcast() within the same subcommunicator. Likewise, the Python subcommunicator employs MPI_Reduce() with rank_0 as the root to aggregate all sources from the *n*2 PISAM instances. The accumulated sources are then scattered to HESEL's rankspecific spatial domains using MPI_Scatter().

This communication scheme has been implemented on the HPC cluster Marconi,⁹⁹ with the C++ and Python parts spanning multiple nodes. In the simulations presented in Sec. VII, a 512×512 -grid was simulated in a duration of $500\Omega_{10}^{-1}$. Three nodes of 48 CPUs each were applied with HESEL running on 64 ranks and PISAM on 80 ranks. After saturation, the total number of active superparticles was on the order of 10^8 . The total wall time of the simulation was ≈ 30 h with approximately equal wall times of HESEL and PISAM. The time spent on the MPI communication in these simulations is minuscule. The method presented here should be directly applicable to coupling any two programming languages that can be compiled with MPI.

VI. FLUID NEUTRAL MODEL

In the nHESEL model, the neutrals are described as distinct isothermal fluids at characteristic temperatures. The modeled neutrals result from external injection and the interactions reviewed in Sec. IV and include sub eV cold molecules, warm neutral atoms from dissociation at the temperature of a few eV, and hot neutral atoms from charge-exchange collisions with a temperature similar to that of the ions. The transport of the neutral fluids is assumed convective and is, together with boundary conditions, described in detail in Ref. 48.

In the current study, the radial flux of neutral species (cold, warm, or hot) *s* in nHESEL is estimated from

$$F_{s,rad} = n_s V_{s,adv} - D'_s \frac{\partial n_s}{\partial x}, \qquad (34)$$

where n_s is the density of species *s* and the radial advective velocity $V_{s,adv}$ and the diffusion coefficient D'_s are assumed to be constant across the domain. The prime is added to D_s to distinguish it from the diffusion coefficients of the plasma model defined in (4). The values of $V_{s,adv}$ and D'_s are determined by the proposed method of Ref. 100 using recordings of the radial flux in HESEL-PISAM simulations. For each spatial gridpoint, a set of transport coefficients are fitted, and from characteristic values for the transport coefficients in the SOL region, global spatially independent values of $V_{s,adv}$ and D'_s are estimated and provided in Eqs. (41)–(43).

VII. RESULTS

In Sec. VII A, simulation results obtained from running HESEL-PISAM are presented, focusing on observations of mechanisms governing perpendicular plasma-neutral dynamics. Sec. VII B offers a comparative analysis of the results obtained using the kinetic model (PISAM) and the fluid model (See Sec. VI) in conjunction with HESEL. The HESEL-specific parameters of the current simulations resemble those for a medium-sized tokamak and are

$$R = 0.88 \text{ m}, \quad a = 0.225 \text{ m}, \quad q = 4.2, \quad L_c = 20 \text{ m}, \quad M = 0.5,$$
(35)

$$m_0 = 1.85 \times 10^{19} \text{m}^{-3}, \quad T_{e,0} = T_{i,0} = 30 \text{ eV}, \quad B_t = 1.11 \text{T}, \quad (36)$$

where M is the Mach number defining the assumed parallel velocity of the plasma outside the LCFS, see Sec. II A. The time and length scales are, thus, set by

$$\Omega_{i0} = 4.23 \times 10^7 \text{s}^{-1}, \quad \rho_{s0} = 1.7 \times 10^{-3} \text{ m.}$$
 (37)

The parameters of the neutrals are

$$F = 1.5 \times 10^{21} \text{s}^{-1} \text{m}^{-2}, \quad T_{cold} = 0.3 \text{ eV}, \quad \gamma = 0.2,$$
 (38)

where *F* is the injection flux of deuterium molecules, T_{cold} is the temperature defining the Maxwellian velocity distribution of the injected deuterium molecules, and γ is the wall absorption coefficient. Specific to the kinetic neutrals

$$w_{init,D_2} = 4.3 \times 10^6, \quad \sigma_b = 2\rho_0,$$
 (39)

where w_{init,D_2} is the initial superparticle weight of the injected D_2 supermolecules, and σ_b is the magnitude of the blur applied to the source terms when smoothing (see Sec. V). Specific to the fluid neutrals

$$T^{warm} = 2 \,\mathrm{eV}, \quad T^{hot} = T_{i,0},$$
 (40)

$$V_{adv}^{cold} = -758 \frac{\rm m}{\rm s}, \quad D_n^{cold} = 20 \frac{\rm m^2}{\rm s},$$
 (41)

$$V_{adv}^{warm} = -2000 \frac{\text{m}}{\text{s}}, \quad D_n^{warm} = 53 \frac{\text{m}^2}{\text{s}},$$
 (42)

$$V_{adv}^{hot} = -2800 \frac{\rm m}{\rm s} \,, \quad D_n^{hot} = 412 \frac{\rm m^2}{\rm s} \,, \tag{43}$$

where the superscripts indicate the type of neutral in question in accordance with the definitions of Sec. VI. The simulation domain has $L_x = L_y = 140\rho_0$ and the plasma spatial grid is $N_x \times N_y = 512 \times 512$. Initially, poloidally invariant profiles are perturbed by a mixture of Fourier modes. The system is found to enter a quasi-steady state after a transient period of approximately $100 \Omega_{i0}^{-1}$.

A. Simulation results of HESEL-PISAM

Figure 8 shows a typical snapshot of the plasma fields and electric field in a HESEL-PISAM simulation when a blob of plasma escapes into the SOL, as directly visible in Fig. 8(a). In agreement with the experimental studies of Refs. 4 and 101, the radial electric field of Fig. 8(f) results in a sheared $E \times B$ -flow detaching plasma transported outwards due to turbulent eddies in the vicinity of the LCFS. The turbulent eddies result from interchange modes' characterized by the harmonic fluctuations in the poloidal electric field of Fig. 8(e). The snapshots of Fig. 8 exemplify the local and intermittent nature of SOL transport due to coherent plasma filaments well known from experimental observations.^{1,102-104} The lower six shots of Fig. 8 show the neutral densities and the sources arising from plasma-neutral interactions in response to the present plasma fields. As evident from Fig. 8(g), the largest atom density occurs at the outer radial edge of the escaping plasma blob, as it gives rise to a large rate of molecular dissociation in the SOL. A further consequence is evident from Fig. 8(i) showing high rates of atomic and molecular ionization at the location of the radially propagating blobs resulting in a significant plasma density source. The density of the escaping blobs is hereby maintained due to the presence of neutrals, thus extending their lifetime as found by simulation of seeded blobs in Ref. 105. Expectantly, the electron energy source of Fig. 8(k) is strongly correlated with the density source as the ionization reactions responsible for the density source also give rise to the largest electron energy losses, see Table I. Figure 8(j) shows the rate of poloidal momentum transfer between ions and neutrals per unit volume. Charge-exchange reactions are the primary contributor, but ionization reactions of charge-exchanged atoms can also provide notable contributions. The momentum transfer is largest outside the LCFS where the radial electric field [see Fig. 8(f)] creates an $E \times B$ -flow in the negative poloidal direction and vice versa inside the LCFS due to the shear of the radial electric field. According to (1) and Fig. 8(j) the poloidal momentum transfer creates a radial ion drift away from the shear-center located just inside the LCFS. The charge separation arising from the ion drift partially inhibits the sheared radial electric field and, thus, weakens the poloidal-shear flow. The ion drift is most significant on the low field side of the LCFS due to the large density of atoms in this region. In 3D, the influence on the radial electric field would encompass additional effects arising from toroidal momentum transfer, as the radial electric field is linked to the toroidal flow through the force balance equation.^{34,106} Due to the efficiency of momentum transfer parallel to the field lines, the toroidal ion-neutral momentum transfer is expected to have a more pronounced impact on the radial electric field compared to the poloidal ion-neutral momentum transfer. Consequently, the latter mechanism, which is the focus of this paper, has received limited attention in previous studies. However, understanding the potential influence of radial electric shear is crucial, as a reduction in poloidal-shear flow can affect the accessibility of Hmode,³⁵ ³⁷ ultimately influencing the energy balance of the reactor. It is apparent from Fig. 8(1) that the energy balance is also directly affected by an inwards energy flux mediated by charge-exchange reactions. Outside the LCFS, especially in the regions of high ion temperature [see Fig. 8(c)], the warm ions transfer energy to the colder atoms through charge-exchange reactions. When the hot atoms created in these reactions are ionized their energy is transferred back to the ions. Some of the ionizations of hot atoms happen inside the LCFS such that energy is transported from the SOL into the plasma edge, thus positively contributing to the energy containment time. This effect is magnified by the reflections of hot atoms on the outer radial boundary.

B. The effects of fluid and kinetic neutrals

This section presents temporally averaged radial profiles of three sets of simulations: HESEL without neutrals, HESEL-PISAM, and HESEL with fluid neutrals (nHESEL). Each conducted simulation has a duration of $500\Omega_{i0}^{-1}$, where the initial $100\Omega_{i0}^{-1}$ are considered a transient period. The results from HESEL without neutrals represent the mean of eight runs seeded with different perturbations on the initial plasma density profile. The shaded regions in the HESEL profiles of Fig. 9 represent two times the standard deviation of the values obtained from these eight runs. Similarly, the results of HESEL-PISAM show the mean of five runs with identical perturbations on the initial plasma density profile, but different random seeds used in PISAM. The shaded regions in the HESEL-PISAM profiles of Fig. 9 represent two times the standard deviation of the values obtained from the five individual runs. The initial weight of superparticles was adjusted to ensure that the impact of Monte Carlo noise on the profiles obtained in HESEL-PISAM simulations with identical initial plasma fields but different random seeds (blue shades), was comparable to the profile noise resulting from repeated HESEL simulations with various initial perturbations (orange shades). This criterion on the superparticle weight ensures that the statistical certainty of HESEL-PISAM simulations is limited by the intermittent nature of the plasma dynamics and the limited simulation time rather than the Monte Carlo noise of the neutral model and, thus, serves as a reasonable criterion of convergence. The profiles obtained by using the nHESEL code rely on a single simulation. The uncertainty of this deterministic model is assumed equal to that of HESEL and HESEL-PISAM as it is likewise limited by the intermittent motion of the edge plasma and the limited simulation time.

Figure 9 shows profiles of the neutral densities and the source terms of plasma-neutral interactions and, thus, provides a direct comparison of the two neutral models. The profiles in Figs. 9(a) and 9(b) of the atom and molecule densities, respectively, indicate that the transport model of (34) with constant advection and diffusion coefficients is incapable of reproducing the kinetic model's results. Generally, the fluid model overestimates the capability of the neutrals to penetrate the plasma. The collision frequencies calculated in the fluid model are proportional to the neutral densities. The difference in densities of Figs. 9(a) and 9(b), thus, results in discrepancy is reflected in Fig. 9(c) where the density source of the fluid model is shifted inwards due to the overestimated radial transport of neutrals. The



FIG. 8. Snapshots of density (a), electron temperature (b), ion temperature (c), electrostatic potential (d), poloidal electric field (e), radial electric field (f), atom density (g), molecule density (h), density source (i), poloidal momentum source for ions (j), electron pressure source (k), and ion pressure source (l) for the simulations described in Sec. VII. Figures (a)–(f) show the plasma fields calculated by HESEL while the neutral densities and inelastic sources of (g)–(l) are calculated by PISAM. The discretized form of the sources arising from inelastic plasma–neutral collisions, as defined by (2), in figures (i)–(l) are smoothed as described in Sec. V. The white line indicates the position of the last closed flux surface.



FIG. 9. Time averaged radial profiles of atom density (a), molecule density (b), density source (c), radial ion drift resulting from plasma-neutral interactions (d), electron pressure source (e), and ion pressure source (f) for the simulations described in Sec. VII.

effect on the plasma density is seen in Fig. 10(a) where the shoulder formation (an experimentally observed effect¹⁰⁷) of HESEL-PISAM is more significant than that produced in nHESEL. The larger shoulder formation in PISAM simulations and the advanced charge-exchange sampling scheme applied in PISAM (see Sec. IV D) make the ion drift just outside the LCFS calculated in HESEL-PISAM simulations significantly larger than that of nHESEL simulations as apparent in Fig. 9(d). The charge separation created by this drift results in a reduction of the radial electric field which in correspondence with Fig. 9(d) is found to be larger for HESEL-PISAM than nHESEL, see Fig. 10(f). The most significant difference between the three simulations is present in Fig. 10(e) showing profiles of the radial $E \times B$ -flux. The level of anomalous transport resulting from interchange instability is contingent upon the amplitude of poloidal fluctuations in density and electric potential, along with the phase difference between these harmonic variations. The influence on the average anomalous radial flux of neutrals is, however, easiest understood by considering the time-averaged continuity equation $\nabla(\bar{n}\bar{u}_E) = D_e(1+\tau)\nabla_{\perp}^2\bar{n} - \sigma(x)\frac{\bar{n}}{\tau_{\perp}} + \bar{I}^{(1)}$, where the anomalous transport is only included to lowest order, and explicit effects of field inhomogeneity are neglected. The bars indicate an average over a time span sufficiently long for the plasma fields to be considered static, i.e., time independent. $\sigma(x)$ is the step function determining the strength and spatial extent of the parallel damping terms. The demand to balance this equation given the density source of Fig. 9(c) and the derived alterations of the plasma density of Fig. 10(a) directly accounts for the differences between the three profiles of Fig. 10(e). The decrease in the anomalous flux on the high field side of the LCFS in the presence of neutrals stems from the decrease in the plasma density gradient observed when adding neutrals, see Fig. 10(a). The lower density gradient causes the density perturbations induced by interchange dynamics to decrease, thus lowering the flux.¹⁰⁸ In the presence of neutrals, blobs escaping into the SOL are fueled by the ionization of neutrals and, thus, maintain a higher density when they propagate outwards yielding an increase in the anomalous flux as in Fig. 10(e). The larger anomalous flux, in the vicinity of the LCFS, of nHESEL-simulations in comparison to HESEL-PISAM simulations entails a larger radial energy transport and so explains why nHESEL simulations yield a larger electron temperature than the HESEL-PISAM simulations, even though the more sophisticated atomic and molecular physics of PISAM results in a larger electron energy loss [see Fig. 9(e)].

VIII. COMPARISON OF HESEL-PISAM WITH EXISTING CODES

Simulations from sophisticated codes such as GBS^{17–19,42} and TOKAM3X-EIRENE^{54,55} that couple an edge-turbulence model with a kinetic neutral model is already found in the literature. The neutral parts of these codes, especially EIRENE, currently include a larger variety of neutral species and interactions than PISAM. This is partly because these codes are designed to include the divertor region where



FIG. 10. Time averaged radial profiles of density (a), electron temperature (b), ion temperature (c), electrostatic potential (d), particle flux due to E × B-advection (e), and radial electric field (f) for the simulations described in Sec. VII.

volumetric and surface recombination contribute significantly to the plasma source terms. Furthermore, EIRENE also supports the simulation of a large array of impurities.⁴⁰ The main reason for developing PISAM is to allow a time-dependent simulation of the neutral dynamics on timescales as short as the characteristic timescale of filaments resulting from the interchange instability at the outboard mid-plane. The radial velocity of filaments across different tokamaks, MAST, 109,110 NSTX 111,112 ASDEX-U, 113 C-Mod, $^{114-117}$ DIII-D, 118,119 JET, 101,120 TORPEX, 121,122 is of the order $\sim 10^2 - 10^3$ m/s, i.e., similar to the speed of neutrals injected at ~ 0.1 eV. To the best of our knowledge, no other code resolves neutral dynamics on this short timescale. In the so-called neutral adiabatic regime,¹⁹ which is applied in the GBS code, the typical neutral time of flight $\tau_{tof,n}$ is explicitly assumed smaller than the characteristic timescale of turbulence, $\tau_{tof,n} \ll \tau_{turb}$. This assumption, required for numerical feasibility,¹⁹ is violated when radial blob propagation speeds exceed or are similar to neutral speeds. This hinders codes where the neutral adiabatic regime from describing certain phenomena arising in the interplay between SOL filaments and neutrals, e.g., trails of molecule depletion behind escaping blobs and the latent increase in atomic density at the LCFS arising from molecular dissociation caused by blobs escaping into the far SOL. The EIRENE code is also capable of time-dependent neutral modeling, although this feature is often, to the knowledge of the authors, not used in TOKAM3X-EIRENE simulations^{54,55} for numerical efficiency reasons, and static plasma fields are applied. Dynamical simulations are accelerated by updating the plasma fields that the neutrals react to

at a lower frequency than the plasma model. This method, however, quenches certain features of the plasma–neutral interplay similar to when the neutral adiabatic regime is applied. It is demonstrated in Sec. VII that HESEL-PISAM succeeds in simulating neutrals in time steps of $\Delta t < 2\Omega_{i0}^{-1}$ (see Sec. V) while providing source terms that are sufficiently smooth for the plasma fluid code to handle.

IX. SUMMARY AND CONCLUSION

This work presents a novel approach to the kinetic modeling of neutrals in fusion devices, currently implemented for deuterium atoms and molecules and coupled to the fluid turbulence model HESEL.^{21,22} The developed model, PISAM, handles neutral transport and the evaluation of source terms from inelastic collisions in a fully kinetic fashion and is, unlike similar codes, able to resolve the neutral dynamics on a timescale as short as that of the turbulent plasma, i.e., $\sim 1 \,\mu s.^{123,124}$ As the flow of neutrals at the outboard mid-plane is characterized by a high Knudsen number, PISAM offers a more accurate alternative to the fluid-diffusion model that has been used to include neutrals in HESEL before this work. To ensure the accuracy of the cross sections of molecular transitions, PISAM applies the most recent quantum mechanical data resulting from molecular close coupling methods.⁶ To ensure simulation accuracy, special care is shown in the treatment of charge-exchange collisions by considering both the ion fluid velocity and the velocity of the deuterium atom when sampling ions involved in charge-exchange reactions. By leveraging the system's axial symmetry, the dimensionality of the sampling problem is reduced, enabling a

numerically feasible implementation. The achieved precision in calculating the plasma–neutral momentum transfer, coupled with the limited scope of HESEL in only solving perpendicular dynamics, enables the isolation of the impact of field-perpendicular momentum transfer in plasma–neutral interactions on the radial electric field. Due to the close relation between the shear of the radial electric field and H-mode accessibility,^{125–129} the understanding and quantification of effects on the radial electric field are important in future reactor design and operation.

With inspiration from DSMC⁵⁶ approaches, the Monte Carlo procedure applied in PISAM solves transport deterministically while treating collisions stochastically. By neglection of neutral–neutral collisions, the neutral dynamics can be formulated as embarrassingly parallel. PISAM utilizes this simplicity by incorporating a grid-free neutral domain, thus facilitating unlimited parallelization with a balanced workload between the parallel processes. Furthermore, the intuitive nature of the DCSM approach in conjunction with the object-oriented Python implementation permits other researchers to easily adjust and extend the code. By incorporating an appropriate mapping from the neutral position to the grid of the relevant plasma model and reformulating the boundary conditions accordingly PISAM can be coupled to any plasma model in 1D, 2D, or 3D.

In this work, PISAM is coupled to the fluid plasma edge turbulence code $\text{HESEL}^{21,22}$ The mathematical coupling is achieved by including source terms from plasma-neutral collisions in the HESEL model. The derivation is summarized in Sec. II, where the resulting equations have been updated with higher-order terms. The coupling of the PISAM and HESEL codes written in Python and C++, respectively, relies on a novel technique for setting up an MPIintercommunicator between programming languages that are not otherwise directly compatible. This method facilitates effective communication between any MPI-compilable programs while allowing for extensive parallelism across multiple nodes. A detailed description of the technical aspects of this coupling method is given in Sec. V.

Section VII presents snapshots that highlight an array of mechanisms at play in the interaction between turbulent edge plasma and deuterium atoms and molecules. We show how escaping blobs create bursts in the atom creation rate due to molecular dissociation in the SOL. The intermittency of turbulent transport, thus, entails a corresponding intermittency in neutral transport phenomena. These phenomena include the radial transport of neutral atoms decisive for gas puff fueling efficiency. Additionally, the monitorization of the ionneutral energy exchange illustrates the inwards radial flux of energy arising from charge-exchange reactions and atomic ionization, and its close relation to the ion temperature field. Charge-exchange reactions also mediate a significant poloidal momentum transfer in the presence of a radial electric field. The flux divergence of the resulting ion drift directly inhibits the radial electric shear, which is apparent in the reported time-averaged radial profiles of the radial electric field.

To compare the kinetic and fluid neutral models coupled to HESEL, we report time-averaged radial profiles of the resulting neutral densities and the source terms produced from plasma-neutral interactions when running each of the models, i.e., HESEL-PISAM and nHESEL. Coupling the individual models to a common plasma turbulence model permits a direct comparison between the two fundamentally different approaches, i.e., a diffusive-fluid approach and a kinetic approach. Even though benchmark studies of fluid-neutral and kinetic-neutral codes coupled to transport codes have been published,¹³⁰⁻¹³² this paper reports the first direct comparison of fluidneutral and kinetic-neutral models coupled to an edge-turbulence code. This comparison enables an assessment of the capability of a neutral fluid model to reproduce the results of a more accurate kinetic model in the context of edge-turbulence modeling. Understanding the capabilities and weaknesses of nHESEL and similar fluid models can help in guiding future research in the appropriate application and development of fluid models for neutral modeling.

The reported results reveal the limitation of the diffusion fluid model to accurately assess the neutral transport and, thus, calculate the density of the neutral species. As the inelastic collision frequency of a certain plasma-neutral interaction is proportional to the density of the relevant neutral species, the inaccuracy in determining the neutral transport carries directly over to the source terms arising from inelastic collisions. The derived discrepancy of the plasma fields is exposed in the reported time-averaged radial profiles that also include the average fields without the presence of neutrals, thus emphasizing the general effects of neutral presence. We find that HESEL-PISAM simulations yield a more significant shoulder formation than nHESEL. Also, the inhibition of the radial electric field induced by the ion drift caused by plasma-neutral interactions is more prominent when applying kinetic neutrals. Furthermore, we find a reduction in radial plasma flux due to the presence of neutrals, again with the kinetic neutral model resulting in the largest deviation from the results of simulations conducted without neutrals.

The next natural investigation of this code is benchmarking it against well-established kinetic neutral codes. Future work is expected to shed light on the underlying neutral-dependent mechanism altering the correlation between fluctuations in the density and the poloidal electric field, which are ultimately responsible for the reduction in radial flux observed inside the LCFS in current simulations. Moreover, HESEL-PISAM should be applied to investigate the significance of the adiabatic neutral assumption, see Sec. VIII, to uncover whether efforts should be made to relax this assumption in the future development of coupled neutral and edge-turbulence models. PISAM is designed to ease the inclusion of new particles and reactions with the ambition that essential impurities should be included, making HESEL-PISAM a relevant tool in the exploration of impurity transport at the plasma edge. Furthermore, we hope to investigate the effect of Monte Carlo noise in the present model in detail. Only a small fraction of the superparticles of PISAM participate in reactions contributing to the source terms in each time step, and thus, the dependency of superparticle weight on the resulting Monte Carlo noise differs from that of Markow chain Monte Carlo solvers like EIRENE^{39,40} and DEGAS2⁴¹ that have been previously addressed in the literature.^{133,134} Moreover, the current numerical cost of noise reduction might be improved by splitting superparticles in each time step according to the probability of their individual reaction channels, rather than sampling reactions stochastically as described in Sec. III. To avoid an exponentially growing number of superparticles, this splitting approach requires the implementation of a merging scheme for like superparticles. Similar splitting-merging techniques have been applied to DSMC algorithms in related fields of physics.^{135–137} To improve the scaling of wall time when the neutral time step, one might tag the particles at creation in accordance with their speed, and collision frequency. The time step of the individual neutral particles should depend on this tag resulting in

slow molecules near the injection boundary with low collision frequency being rarely processed compared to charge-exchanged atoms inside the LCFS.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Kristoffer Kvist: Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). Alexander Simon Thrysøe: Conceptualization (supporting); Formal analysis (supporting); Software (supporting); Supervision (lead); Writing – review & editing (equal). Troels Haugboelle: Supervision (supporting); Writing – review & editing (equal). Anders H. Henry Nielsen: Conceptualization (supporting); Funding acquisition (lead); Project administration (lead); Supervision (lead).

DATA AVAILABILITY

The data that support the findings as well as the code used to conduct the simulations of this study have been published at https://doi. org/10.5281/zenodo.10512834, Ref. 138. For the latest stable update of HESEL-PISAM, refer to https://github.com/kristofferkvist/PISAM-HESEL, where a thesis clarifying the details of the relevant research is also available. By use of the full code or parts of it, this article should be cited.

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