On the kinetic modeling of fusion processes in IEC devices

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The spherical IEC concept as well as driving research objectives in the context of a potential application as an innovative plasma propulsion system in space are briefly introduced. The numerical approach currently under development is outlined. Focus is on the DSMC code development for the kinetic treatment of fusion reactions. Correspondingly, typical criteria like resolution necessities are derived. We find that for a fully kinetic all-scale particle simulation of a typical IEC device only one spatial scale needs to be considered. However, with the applied field solver (explicit, full Maxwell) three different time scales have to be accounted for, but the number of time scales might be reduced by one if e.g. a Poisson solver is used instead.

Numerical problems are expected from an inappropriate definition of the Debye length as well as from the divergence of the Coulomb cross section. Potential countermeasures as well as certain solution paths are sketched.

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Nomenclature

c	= index collision
cou	= index Coulomb collision
E	= energy
e	= index electron
ee, ei, en	= indices electron-electron, electron-ion, electron-neutral
$\vec{F}$	= force
f	= velocity distribution function
fus	= index fusion reaction
g	= relative velocity
i, j	= index interaction
ii, in	= indices ion-ion, ion-neutral
k	= index ion species
m	= particle mass
n	= particle density
nn	= index neutral-neutral
P	= interaction probability
Q	= number of possible particle pairs
R	= equally distributed random number $\in [0, 1]$
t	= time
T	= index total cross section
T_e, T_k	= electron and ion temperature
U	= electrostatic potential
V_{cell}	= cell volume
$\vec{v}$	= velocity coordinate
$\vec{x},\ x$	= spatial coordinate
$\alpha,\ \beta$	= indices species
λ_D	= Debye length
σ	= interaction cross section
$\sigma_{f,1}, \sigma_{f,2}$	= approximated fusion cross sections
τ	= characteristic time
Ω	= space angle
$\triangle t_{sim}$	= global simulation time step

I. Introduction

INERTIAL Electrostatic Confinement (IEC) devices were originally developed and used for fusion research purposes.[1] The exothermal nuclear fusion process is the energy releasing process with the second highest energy density right after the annihilation. Binding energy is released once two highly energetic light ions collide in a way that fusion is induced, resulting in the creation of fusion products with a total rest mass which is lower than the total rest mass of the educts. The released amount of energy E_{fus} can be calculated via the well known equation $E_{fus} = \triangle m_0 c_0^2$ where $\triangle m_0$ and c_0 are the difference in rest mass and the vacuum speed of light. Some of the most prominent fusion propellants and corresponding reaction equations are listed in Table 1.

Table 1. Some prominent fusion reactions and released energies per event. D - deuteron ion ($^2H^+$), T - triton ion ($^3H^+$), p - proton, n - neutron, α - α particle ($^4He^{2+}$), ν - gamma photon.

Educt 1	E2		Product 1	P2	E_{fus} / MeV
D	T	$\rightarrow$	n	α	17.6
D	^3He	$\rightarrow$	p	α	18.3
^{11}B	p	$\rightarrow$	ν	3α	8.7
^3He	^3He	$\rightarrow$	$2p$	α	12.9

The very high E_{fus} values motivate the utilization of fusion technology in space. From an engineering point of view, a reasonable starting point to study fusion technology is a simple set-up which can be build and controlled at low cost. Within the field of IEC technology, the simplest set-up contains a spherical electrode which is placed in a vacuum chamber, see Fig. 1. The sphere made of stainless steel wires is negatively charged while the vacuum chamber is grounded. The vacuum chamber contains a highly rarefied gas. Once the voltage difference between the inner electrode and chamber is high enough a glow discharge is induced. The produced ions are accelerated by radial electric fields towards the center of the sphere where they collide with other ions building a positively charged ion cloud. This ion cloud accelerates electrons towards the center of the sphere, correspondingly leading to the creation of a certain potential distribution. Detailed discussions of the resulting potential distributions in IEC device can be found in literature.[2–5]

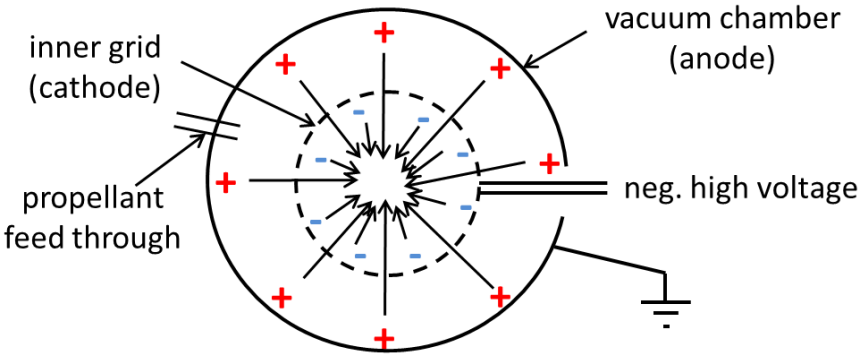

Figure 1. Schematic of a so-called Farnsworth-Hirsch Fusion Reactor.

A. IEC in fusion mode

It has been repeatedly demonstrated that such an IEC device can be operated in fusion mode[6] if the electrode's potential difference is increased up to at least 20 kV and if the background gas consists of fusion educts. Once the discharge is initiated the accelerated ions carry only radial momentum (which makes them constitute a radial ion beam) such that a head-on collision with another ion coming from the opposite

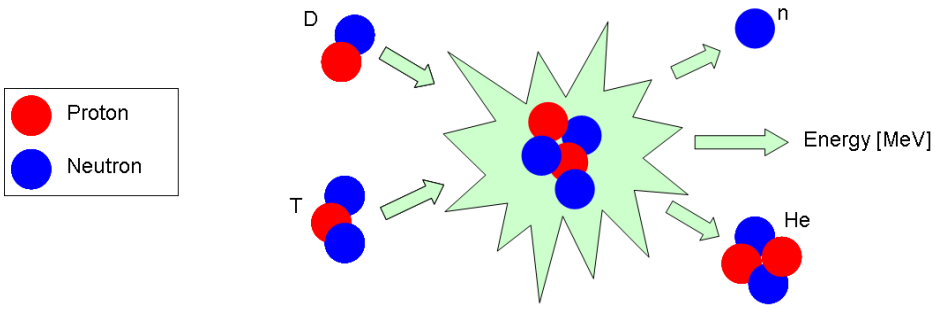

Figure 2. Basic scheme of a D-T fusion process.

direction might initiate a fusion process, accompanied by the creation of highly energetic ($\sim MeV$) fusion products, see Fig. 2.

The ionized products are supposed to transfer their energy to the educts such that the plasma core energy can be sustained at a level higher than without fusion. However, Coulomb scattering leads also to a decrease of radial momentum and to an increase of angular momentum of the ions. Additionally, the initially directed energy is converted into thermal energy with corresponding effects like radiation, especially Bremsstrahlung radiation. This process cannot be damped significantly because the ion-electron coupling is very strong.[2] In fact, one can show that Bremsstrahlung radiation coming from the hot electrons is one of the reasons why such an IEC device will not be able to reach energetic break-even. This has led to a loss of interest in such configurations for power production.

B. IEC in jet mode

One can construct the confinement grid in a way that at one side the electrostatic potential barrier is lower than at all other sides. This is usually achieved by designing the inner grid with one grid opening larger than the other grid openings. Under such conditions and as depicted in Fig. 3 it is possible to extract a plasma jet from the plasma core. In order to keep the operation steady neutrals are added according to the extracted plasma mass flow. IEC in jet mode would thus be, in principle, usable for propulsion purposes.

However, the microscopic physical mechanisms leading to the jet extraction are not well understood so far. The acceleration process is described as electrostatic[7] but it differs significantly from the acceleration method in gridded ion thrusters. In IEC set-ups some electrons are able to overcome the locally decreased potential barrier such that they attract ions to follow them out. However, a detailed theoretical description of the acceleration mechanism is still lacking. Another difference with respect to gridded ion thrusters worth

Figure 3. IEC driven in jet mode.[7]

mentioning affects the grid transparency: The geometric transparency of the inner IEC grid (cathode) is much higher (in the order of 90% in case of a single grid IEC[8] leading to an effective grid transparency of 98-99%) which provides better conditions with respect to grid losses. This has also a huge impact on erosion processes and, correspondingly, on grid lifetime.

C. IEC in jet *and* fusion mode

As mentioned before, simple IEC configurations will never reach energetic break-even as the loss mechanisms are dominant with respect to the energy gain mechanisms.[2] Hence, potential IEC based propulsion systems are not considered as fusion propulsion systems but as EP systems with basically unknown thrust and thruster properties.

As nuclear fusion leads to a release of highly energetic ions the plasma core energy density is increased due to thermalization of the fusion products. This consequently favors power loss due to Bremsstrahlung radiation. However, since the fusion rate is low and the generation of highly energetic fusion educts is non-thermal, fusion processes might improve IEC thruster performance. Identification of respective configurations and operational modes (if existing) needs deep understanding and intense modeling of the underlying physical processes.

This paper is part of an attempt to address the jet extraction mechanisms in general and particularly the impact of fusion processes on these mechanisms. The methodology of choice is to develop and apply a fully kinetic approach which is able to resolve the relevant microscopic processes and the unknown energy distribution functions of interest. The second section gives a brief introduction to the numerical scheme we intend to utilize for the kinetic modeling of IEC devices. In section three we discuss basic elements of the collision solver like resolution necessities and probability models. The shortcomings arising from the definition of the so-called Debye length motivated us the propose a numerical experiment for the definition of a more accurate expression of the Coulomb collision cross section which is explained in section four. Major conclusions are drawn in section five.

II. Numerical Scheme

This section contains basic information on the fully kinetic modeling of an IEC device. The numerical scheme is purely kinetic as several aspects limit the applicability of a continuum approach. Just to mention two of them:

1. Direct Coulomb collisions might play a central role in the jet extraction process which implies a significant (but local) violation of the quasi-neutrality assumption.

2. The fusion products can be regarded as mono-energetic. Such an energy distribution (essentially a peak) is far away from the equilibrium (or near-equilibrium) distribution function implemented in continuum approaches.

Having in mind the thermalization process of the products which is supposed to affect the thrust efficiency, it appears to be sensible to apply an approach which does not imply the assumption of a certain energy or velocity distribution function inherent to continuum methods. Such approaches are called fully kinetic as, apart from initial and boundary conditions, any distribution function is an outcome of the simulation.

Kinetic approaches are mostly particle approaches, the relevant interactions in a flow are modeled on a microscopic level. Those approaches solve the Boltzmann equation

$$\frac{\partial f_\alpha}{\partial t} + \vec{v_\alpha}\frac{\partial f_\alpha}{\partial \vec{x}} + \frac{\vec{F}_\alpha}{m_\alpha}\frac{\partial f_\alpha}{\partial \vec{v}_\alpha} = \int_{-\infty}^{\infty}\int_0^{4\pi}\left[f'_\alpha f'_\beta - f_\alpha f_\beta\right] g\sigma_T \mathrm{d}\Omega \mathrm{d}\vec{v} \tag{1}$$

which is the governing equation for rarefied gas and plasma flows. In Eq. (1) f, t, $\vec{v}$, $\vec{x}$, $\vec{F}$, g, σ_T, and $\mathrm{d}\Omega$ are the unknown velocity distribution function, the time coordinate, the velocity coordinate, the space coordinate, the force acting on a test particle of species α with mass m_α, the relative velocity $g = |\vec{v}_\alpha - \vec{v}_\beta|$ between a test particle and a field particle of species β, the total (integral) collision cross section for a given pair of particles, and the space angle over which it is integrated. Primed quantities denote the post-collisional

state. One can see that f is influenced by several phenomena: spatial gradients (second left-hand term)), external forces (third left-hand term), and collisions (right-hand side).

All these different phenomena act on different space and time scales such that different kinetic methodologies have been established: Neglecting the elastic collisions between charged particles (Coulomb collisions) but considering forces originating from applied and/or self-induced electric and magnetic fields one gets the non-collisional Boltzmann equation in combination with the Maxwell equations. The resulting Maxwell-Vlasov equations[9] are solved kinetically by use of Particle-In-Cell (PIC) codes.[10] Instead, if the mentioned fields are neglected and one aims for the direct Coulomb collisions, the collision term in the Boltzmann equation can be reformulated, yielding the Fokker-Planck equation.[11] But, considering only short range collisions in gases and partially ionized plasmas allows to use e.g. Monte Carlo based approaches of which the most successful one is the DSMC method.[12] DSMC stands for Direct Simulation Monte Carlo and is a probabilistic particle approach. It allows a treatment of large particle systems as the computational needs scale only linearly with the number of simulated particles.

The respective code we utilize for the kinetic IEC simulation contains a PIC solver developed by the Institute of Aerodynamics and Gas Dynamics of the Universität Stuttgart,[13] a DSMC solver developed by the Institute of Space Systems of the Universität Stuttgart,[14] and a FP solver developed by Institute of Pulsed Power and Microwave Technology of the Karlsruhe Institute of Technolgy.[11] However, for faster computations a Monte Carlo based FP solver[15] was implemented in the DSMC module and will be used for upcoming IEC simulations.

The PIC module provides not only self-consistent solutions of the full set of Maxwell equations. It contains also a particle solver for the solution of the relativistic equations of motion[?] including particle localization and cell assignment. The DSMC solver contains a high fidelity solver for the following collisional processes: electron impact induced processes elastic scattering (including polarization), excitation, de-excitation, ionization, and non-radiative recombination. The embedded Monte Carlo based FP solver accounts for the Coulomb collisions such that, in essence, the DSMC solver in his current state solves *all* collisional processes typically relevant in highly rarefied plasmas. For a detailed description of the DSMC model and corresponding short and long range interaction models please refer to literature[12] and references therein.

The basic idea with respect to kinetic fusion modeling is to apply the same DSMC approach. This demands an implementation of the relevant fusion cross sections and an accurate Coulomb cross section model. However, first analysis shows that a kinetic modeling demands also an accurate definition of the Debye length λ_D or a quantity which is usually associated with λ_D: the scale, at which Coulomb collisions become (un)important. Typically, PIC codes which neglect Coulomb collisions are applied on scales larger than λ_D since on smaller scales Coulomb collisions need to be considered.

The standard definition of λ_D contains some definitions and assumptions. A brief re-examination of this well-established quantity in plasma physics shows that

- the definition of λ_D is based on equilibrium quantities like the temperature:

$$\lambda_D = \sqrt{\frac{\varepsilon_0 k_B T_e}{e^2 \left(n_e + T_e \sum_k \frac{n_k Z_k^2}{T_k} \right)}} \tag{2}$$

  with ε_0, k_B, T_e, e, Z, and k representing the vacuum permittivity, the Boltzmann constant, the electron temperature, the elementary charge, the charge number, and the k-th ion species. Equation (2) is often used for describing the damping of a charge's potential U surrounded by other charged particles:

$$U = \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{x} \exp\left(-\frac{x}{\lambda_D} \right). \tag{3}$$

  However, equilibrium quantities should generally be avoided in a fully kinetic approach as those quantities *reduce* the model to a fluid approach.

- λ_D can be derived making use of a one-dimensional equation of motion. In fact, the Debye length is defined as the distance at which the (shielded) charge decreases to U/e. The choice of this value is by no means physically justified, only mathematically.

III. DSMC Considerations

In this section we limit ourselves to the basic algorithms which are of relevance for the following sections. For a wide introduction to DSMC the reader should refer to proper reference.[16]

A. Spatial Resolution

If we consider a fully ionized hydrogen plasma than we have no short range interactions - all ions are stripped. This simplifies the resolution considerations to the PIC and FP solver.

PIC solvers represent the physics on scales above the Debye length λ_D and FP solvers on scales below λ_D. In DSMC the mean free path λ is supposed to be resolved such that the cells are smaller than λ. In fact, in most cases $\lambda \neq \lambda_D$. But as mentioned before, the short range interactions can be omitted in a fully ionized plasma. However, in case of fusion processes we have

$$\frac{\sigma_{fus}}{\sigma_{cou}} \to 0 \tag{4}$$

such that λ_{fus} is *practically* infinite. Therefore, treating nuclear fusion processes with DSMC embedded in a PIC-DSMC-FP solver allows to consider only *one* spatial scale.

B. Temporal Resolution

Again, all three solver types have to be discussed in order to identify temporal resolution needs.

The applied PIC solver is an explicit full Maxwell solver.[13] This implies that numerical stability depends on the CFL criterion with the vacuum speed of light c_0 representing the speed at which information is transported. Therefore, this PIC solver imposes time step sizes of the order $\triangle t \sim \triangle x/c_0$ where $\triangle x$ is a measure of the smallest cell size.

The Fokker-Planck solver resolves the Coulomb collisions. Generally, the characteristic time scales for collisional processes can be aligned as follows: $\tau_{ee} < \tau_{ie} < \tau_{ii} < \tau_{ne} < \tau_{ni} < \tau_{nn}$. The indices in this order correspond to electron-electron, electron-ion, ion-ion, neutral-electron, neutral-ion, and neutral-neutral collisions. Given that the implemented FP approach[12] contains no stability related constraints with respect to the choice of $\triangle t$ the basic time constraint originates from the chosen PIC solver.

Moreover, since classical short range interactions do not occur in the kinetic simulation of fully ionized hydrogen plasmas and $\sigma_{fus} << \sigma_{cou}$ - no certain temporal resolution needs to be taken into account in the DSMC model.

C. Collision Probability Evaluation

DSMC was originally developed for the kinetic simulation of rarefied (neutral) gases with well defined total cross sections σ_T. Hence, inter-particle collisions were treated as binary interactions. The underlying probabilistic methodology reduces the N^2 dependency to a linear dependency of the computational effort on the simulated particle number N by simply aiming for the reproduction of the correct collision rate. This is realized by building $N_{cell}/2$ random pairs in a spatial cell which contains N_{cell} particles and evaluating each pair regarding its individual collision probability P_c. In our DSMC model,[14] collision evaluation is treated on basis of the Natural Sample Size (NSS) method.[17] The resulting collision probability equals

$$P_c = \frac{n_\alpha n_\beta}{1+\delta_{\alpha\beta}} \frac{V_{cell} \triangle t}{Q_{\alpha\beta}} \sigma_T g \tag{5}$$

where n, V_{cell}, $\triangle t$, and $Q_{\alpha\beta}$ represent particle densities, cell volume, time step size, and the number of possible collision pairs. The Kronecker symbol $\delta_{\alpha\beta}$ accounts for possible double counts. A collision occurs if $P_c > R \in [0,1]$ where R is an equally distributed random number. The loop goes over all particles in the currently evaluated cell.

D. Reaction Probability Evaluation

Only those particle pairs with $P_c > R$ are evaluated further regarding their individual interaction probability P_i of the interaction type i following the simple equation

$$P_i = \frac{\sigma_i}{\sigma_T} = \frac{\sigma_i}{\sum_j \sigma_j}. \tag{6}$$

The total cross section covers *all* potentially occurring interactions j for a given pair of particle types. In case of e.g. two naked light nuclei it would be elastic scattering (Coulomb scattering) and fusion, i.e. $\sigma_T = \sigma_{cou} + \sigma_{fus}$.

E. Impact of Diverging Coulomb Cross Section

The (electrostatic) long range interaction potential decays very slowly ($\sim 1/x$) such that a charge interacts with all charges in its vicinity at the same time. Therefore, Coulomb scattering is not a binary collision but a multi-body collision which usually prohibits a treatment with standard DSMC methods. The mathematically diverging Coulomb cross section induces two *major* problems which can be circumvented in the following way:

1. $P_c \to \infty$. However, by spatially resolving the Debye length in each cell computation of P_c becomes obsolete as, by definition, every charge interacts with every other charge in the same cell.

2. $P_{fus} \to 0$. This can be circumvented by introducing a sub-cycling in DSMC with $\triangle t_{fus} >> \triangle t_{sim}$ where the latter represents the global simulation time step size. The increased fusion probability scales according to $\triangle t_{fus}/\triangle t_{sim} \cdot P_{fus}$.

These proposed approaches are not comprehensive, they just transform the problems in a way that simplified expressions of σ_{cou} can be applied now.

In order to prevent the divergence of σ_{cou}, integration limits are introduced like a cut-off angle or an effective action distance. The latter is often associated with the Debye length. But as shown in the previous section, λ_D as effective acting distance is of arbitrary nature and, strictly speaking, a mathematical definition. Nevertheless, it is often used in order to express the Coulomb cross section,

$$\sigma_{cou} = \pi \lambda_D^2. \tag{7}$$

By using equilibrium relations it is possible to express Eq. (7) as a function of energy, however, the underlying assumptions might be too crude for the application to kinetic particle codes. In fact, literature contains different expressions for σ_{cou} which implies that there are different definitions or derivations for the same physical quantity, leading to different numbers. However, in numerics the application of exact physical quantities might be crucial to the result or to the simulation stability as such. To emphasize this in the context of kinetic simulations of IEC devices we consider in the following the *minor* problems which result from the transformation of the two major problems as described above.

1. The consequences of an inaccurately resolved spatial cell in plasma kinetic simulations are complex. Spatial resolution affects numerical heating and stability of the PIC solver.[10] Moreover, numerically caused violation of the energy conservation due to improper cell resolution depends on different aspects, e.g. on the way how charges are assigned to cell nodes and on the particle discretization. The interrelationship between these simulation and model properties is non-linear and case dependent.

2. Introducing sub-cycling in DSMC still demands a finite, non-vanishing, and accurate P_{fus} model as every inaccuracy in σ_{cou} is multiplied by the factor $\triangle t_{fus}/\triangle t_{sim}$.

Evidently, for numerical purposes Eq. (7) is not accurate enough as long as the standard definition of λ_D (represented by Eq. (2)) is applied. Therefore, an alternative expression for σ_{cou} needs to be identified. In the following section we derive a pathway to a numerical identification of a potentially accurate σ_{cou} expression.

IV. Proposition of a Numerical Experiment

The rate coefficient $\langle \sigma_i g \rangle$ of a certain interaction i is the energy averaged product of the corresponding cross section σ_i and the relative velocity between both particles,

$$\langle \sigma_i g \rangle = \int_{-\infty}^{\infty} \sigma_i g f(g) \mathrm{d}g. \tag{8}$$

In Eq. (8), $f(g)$ is the well known Maxwellian distribution function of the relative velocity g. Given that

$$P_{fus} = \frac{\sigma_{fus}}{\sigma_{fus} + \sigma_{cou}} \tag{9}$$

the fusion rate coefficient

$$\langle \sigma_{fus} g \rangle = \int_{-\infty}^{\infty} P_{fus} \sigma_T g f(g) \mathrm{d}g \tag{10}$$

can be obtained via numerical integration once the cross sections are known. Using Eq. (9) in Eq. (10) leads to Eq. (8) with $i = fus$. However, this implies that Eq. (10) cannot be applied for the determination of σ_{cou} without further modification. Hence, we introduce a small perturbation, yielding a small inconsistency with two variations:

1. $P_{fus} \approx \frac{\sigma_{fus}}{\sigma_{cou}}$ and $\sigma_T = \sigma_{cou} + \sigma_{fus}$. From this follows

$$P_{fus}\sigma_T = \frac{\sigma_{fus}^2 + \sigma_{fus}\sigma_{cou}}{\sigma_{cou}} \equiv \sigma_{f,1}. \tag{11}$$

   Since $\sigma_{fus} << \sigma_{cou}$ the inconsistency drops out if one neglects σ_{fus}^2 such that Eq. (10) is reproduced, showing that the induced error is of higher order.

2. $P_{fus} = \frac{\sigma_{fus}}{\sigma_{cou} + \sigma_{fus}}$ and $\sigma_T \approx \sigma_{cou}$. Here we obtain

$$P_{fus}\sigma_T = \frac{\sigma_{fus}\sigma_{cou}}{\sigma_{fus} + \sigma_{cou}} \equiv \sigma_{f,2} \tag{12}$$

   which has similarity with the concept of the reduced mass. Again, due to $\sigma_{fus} << \sigma_{cou}$ the reference value Eq. (10) is approximated.

The introduced perturbations might allow for identifying an alternative and more accurate expression for σ_{cou} by numerical high fidelity integration[18] of Eq. (10).

V. Conclusions

The spherical IEC principle was briefly introduced and discussed in terms of the numerical applicability of kinetic particle codes. Numerical questions to answer regard in first place the microscopic processes leading to the jet extraction, in second place how nuclear fusion reactions affect this jet extraction process. Since jet extraction is believed to be electrostatic in nature the microscopic processes should be resolvable by coupled PIC-DSMC-FP simulations where the nuclear fusion reactions are considered to be treated in the frame of the DSMC solver.

We have discussed typical DSMC aspects related to the resolution of spatial and temporal scales. We have found that only one spatial scale would be of relevance in an fully ionized hydrogen plasma kinetic simulation which means that only one computational grid would be needed, i.e. $\triangle x_{PIC} = \triangle x_{FP} = \triangle x_{DSMC}$. However, in terms of time step size three different time scales ($\triangle t_{PIC} < \triangle t_{FP} < \triangle t_{DSMC}$) need to be accounted for, partly caused by the applied (time-accurate explicit) field solver within this research project. A reduction to two general time step sizes can be achieved by applying an electrostatic field solver which does not resolve electromagnetic wave propagation. Since the implemented FP solver has no stability related constraints on the choice of $\triangle t$ one would simplify the temporal resolution to $\triangle t_{PIC} = \triangle t_{FP} < \triangle t_{DSMC}$.

The kinetic simulation of fusion reactions in spherical IEC devices is computationally affordable only if sub-cycling algorithms for DSMC are implemented according to $\triangle t_{DSMC} \approx \triangle t_{ii} \cdot \frac{\sigma_{cou}}{\sigma_{fus}}$. Inaccuracies in σ_{cou} would thus be amplified such that future research activities will account for the identification of a high fidelity expression of σ_{cou} and the proposed numerical experiment. The fusion reaction modeling needs finalization, followed up by evaluating of the resolution criteria derived here for the DSMC module.

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