Charged Particle Collisions for Particle Simulation Methods

D.D'Andrea [1], W. Maschek [1], R. Schneider [2]

[1] Institut für Kern- und Energietechnik -- Karlsruher Institut für Technologie
[2] Institut für Hochleistungsimpuls- und Mikrowellentechnik -- Karlsruher Institut für Technologie

Email contact of main author: danilo.dandrea@iket.fzk.de

Abstract. The modelling of Coulomb collisions is an important item for a deeper understanding of pulsed plasma propulsion accelerators. The Fokker-Planck formulation of this problem allows a particle treatment of the long range inter- and intra-species interactions in the frame of a Particle-In-Cell, self-consistent approach. The particles are advanced in velocity space according to the stochastic differential equation (the probabilistic dual of the Fokker-Planck equation) so that the distribution function can be reconstructed and its moments evaluated at each time step. In particular, the time evolution of the first and second moment is the object of this study since it contains precious information about the so-called time scales. Results concerning the slowing-down time and deflection time are presented for electron- electron and electron-ion collisions separately and together.

1. Introduction

Of the many existing particle accelerators, electric thrusters for space applications represent a peculiarity for their simpleness and highly effectiveness. They successfully make use of the long lifetime when significant thrust is not needed especially when this includes orbit transfers, attitude adjustments, drag compensation for low earth orbits, and ultra fine adjustments for specific scientific missions. Ion thrusters can also be used for interplanetary and deep space missions where time is not crucial. Continuous thrust over a very long time can potentially build up a larger velocity than traditional chemical rockets. Obviously the numerical simulation of plasma devices must include a model for the Coulomb collisions which mainly determine the shape of the electron energy distribution function which again determines to some extent the plasma chemistry. The temporal evolution of the electrons and ions distribution function and its moments - as a consequence of the repeated small angle encounters - contains the most important information of the physics of the phenomenon. An important aspect of the whole collision process is the time needed by collisions to produce large variations in the original velocity distribution. It might be important for instance, to know how rapidly any initial distribution function changes into a Maxwellian one, because of collisions. The time required for it is known as ``relaxation time", although in literature not clearly defined. Starting from the pioneer studies of Chandrasekhar and Spitzer, the intent of this paper is to provide an analysis of the slowing-down time and deflection time performed by means of self-consistent calculations of electron-electron (e-e) collisions alone and coupled with electron-ion collisions (e-X).It follows a short introduction of the governing equations and the numerical framework, the results are described in the subsequent section and an outlook on the future planned activities completes this work.

2. Mathematical Modelling

To model elastic intra-species, like electron-electron, and inter-species, like electron-ion, Coulomb collisions in a plasma, an appropriate start is the Fokker-Planck collision operator (see for instance [2])

$$\left(\frac{\partial f_e}{\partial t}\right)_{coll} = \frac{\partial}{\partial v_q}\left[F_q^{(e)} f_e\right] + \frac{\partial^2}{\partial v_q \partial v_r}\left[D_{qr}^{(e)} f_e\right] \tag{1}$$

which is the lowest order approximation of the Boltzmann collision integral and describes the temporal evolution of the electron distribution function f_e due to the mutual interactions of the charged particles. The components of the drift vector $\mathbf{F}^{(e)}(\mathbf{v},t)$ and the diffusion tensor $\mathsf{D}^{(e)}(\mathbf{v},t)$ are given by

$$F_q^{(e)} = \sum_\sigma n_\sigma \Gamma_P^{(eq)} \frac{m_e}{\mu_{e\sigma}} \frac{\partial H}{\partial v_q} \quad \text{and} \quad D_{qr}^{(e)} = \sum_\sigma n_\sigma \Gamma_P^{(eq)} \frac{\partial^2 G}{\partial v_q \partial v_r} \tag{2}$$

where the sum runs over the types of field particles, μ is the reduced mass and $\Gamma_P^{(\sigma e)}$ is the plasma parameter which contains the charge e the mass m of the electron, the vacuum permittivity ε_0 and finally the classical Coulomb logarithm $\ln(\Lambda)$ [2]. The key-quantities to determine the coefficients in (1) are the Rosenbluth potentials

$$H^{(\sigma)}(\mathbf{v},t) = \int_{R^3} d^3w |\mathbf{g}|^{-1} f_\sigma(\mathbf{w},t) \quad \text{and} \quad G^{(\sigma)}(\mathbf{v},t) = \int_{\mathrm{R}^3} d^3w |\mathbf{g}| f_\sigma(\mathbf{w},t) \tag{3}$$

where $\mathsf{g} = \mathsf{v} - \mathsf{w}$ is the relative velocity between the scattered and the field velocity particle, namely the scatterer. For the construction of a particle method it is essential to exploit the equivalence of the Fokker-Planck equation (FPE) for the evolution of f_e with the stochastic differential equation. By means of Itô calculus it is possible to write [3]

$$d\mathbf{V}(t) = \mathbf{F}^{(e)}(\mathbf{V},t) + \mathsf{S}^{(e)}(\mathbf{V},t) d\mathbf{W}(t) \tag{4}$$

in which a quantitative analogy with the FPE can be immediately recognized through the drift vector $\mathbf{F}^e$ and the relation between the matrix $\mathsf{S}^{(e)}$ and the diffusion tensor $\mathsf{D}^{(e)}$, being $\mathsf{D}^{(e)} = \mathsf{S}^{(e)}\mathsf{S}^{(e)T}$. $\mathbf{V}$ is in general a stochastic variable which depends on the time and whose distribution function is f_e; it will be later identified with the single charged particle velocity, while $\mathbf{W}$ is a three dimensional Wiener process.

2.1. Intra-species Collisions

In a self-consistent analysis of (e-e) collisions no apriori knowledge of f_e is available and furthermore no simplyfing approximation is possible, therefore some observations concerning the quantities in (3) can be helpful: despite their complicated aspect they are nothing else than convolutions of the distribution function with $|\mathbf{g}|$ or its inverse, a formulation that recalls Fourier transform technique for the evaluation of these three dimensional integrals for which a quadrature formula would be far too expansive. Also the derivatives of the Rosenbluth potentials, i.e. directly the drift and diffusion components, can be readily obtained as follows:

$$\frac{\partial H}{\partial v_q} = 8\pi i F^{-1}\left\{\frac{k_q}{k^2}\hat{f}(\mathbf{k})\right\} \quad \text{and} \quad \frac{\partial G}{\partial k_q k_r} = 8\pi i F^{-1}\left\{\frac{k_q k_r}{k^4}\hat{f}(\mathbf{k})\right\}, \tag{5}$$

where $\hat{f}_e(\mathbf{k})$ is the Fourier transform of f_e and F^{-1} denotes the inverse Fourier transformation of the argument in the brackets.This is the last piece of the puzzle whose picture represents the solution of the FPE. The sequence in which all the bricks will be mounted is described in the next section.

3. Numerical Framework

The mathematical formalism sketched in the previous section can be nicely organized in a Particle-In-Cell (PIC) based numerical solution [4] as schematically illustrated in the block diagram below. The analogy with the classical PIC concept is immediately evident. One part of the computational cycle is situated in a mesh-free zone (*Langevin Solver*), while another one needs a discretization grid (*Rosenbluth Solver*). Two interfaces procedures (*Reconstruction* and *Interpolation*) couples mesh-free and grid space and vice versa and close the whole calculation.

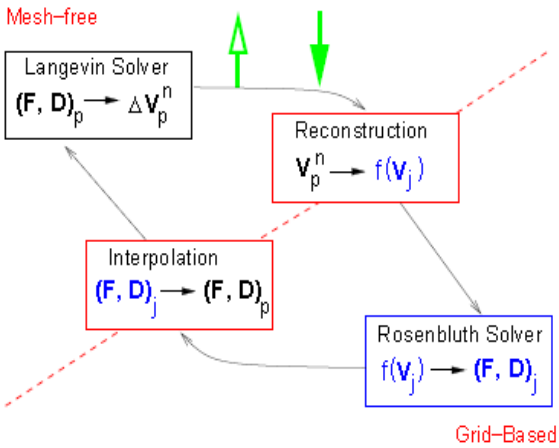

FIG. 1. Building blocks of the PIC-based approach for the FPE.

In the following, a short description of the single building blocks of the Fokker-Planck solver is given; for details see Ref [5].

Reconstruction. From the actual location of the charged plasma particles in the three-dimensional mesh-free velocity space, the distribution function $f_e(\mathbf{v},t)$ is resolved on the Cartesian velocity grid. For that, the volume-weighting technique is used to compute relative weighting coordinates for each charge ``p" from which individual particle weights $g^{(p)}$ can be determined. These particle weights then contain the necessary information to assign each particle to the corresponding grid cell of the velocity mesh. ***Rosenbluth Solver***. Afterwards, for the grid-based computations a FFT method similar to the Cooley \& Tukey algorithm is applied to calculate the Fourier transform $\hat{f}_e(\mathbf{k},t)$ of the distribution function $f_e(\mathbf{v},t)$. Subsequent multiplications of $f_e(\mathbf{k},t)$ with $1/k^2$ k_q/k^2, etc. and a final inverse transformation yields the grid-based Rosenbluth potentials (3) and their derivatives with respect to velocity. With these information the components of the drift vector and the diffusion matrix (2) can immediately be determined. Bear in mind that the use of Fourier approach allows the first principle computation of the relevant quantities arising in Langevin-type equation (4) which leads to a self-consistent modeling of the collisional relaxation. ***Interpolation.*** The ``Langevin forces", which are the deterministic drift and the stochastic

diffusion, have to be computed at the actual position of each particle in grid-free velocity space. Since interpolation is nothing else than the inverse operation of assignment, the particle weights $g^{(p)}$ are once again used to interpolate the Langevin forces at the position of particle ``p" in continuous velocity space. ***Langevin Solver***. Under the action of the velocity-dependent Langevin forces, each plasma particle is moved in the velocity space according to the SDE (4), where appropriate numerical methods are required. On the purpose, weak approximations [6]} of equation (4) is used. For instance, the simplest multi-dimensional weak Taylor expansion leads to the Euler scheme

$$\mathbf{V}^{n+1} = \mathbf{V}^n + \mathbf{F}\left(\mathbf{V}^n, t^n\right)\Delta t + \sum_{\alpha=1}^{3} \mathbf{b}_\alpha^{(e)}\left(\mathbf{V}^n, t^n\right)\Delta \mathbf{W}_n^\alpha \tag{6}$$

Here, $\mathbf{b}_\alpha^{(e)} = \mathsf{S}^{(e)}\mathbf{e}_\alpha$, with unit vector $\mathbf{e}_\alpha$ and the Wiener increment ΔW_n^α is defined according to $\Delta W_n^\alpha = \sqrt{\Delta t}\eta_\alpha$, where Δt is the time step size and $\eta_\alpha = N(0,1)$ denotes a Gaussian distributed random number with mean $\mu = 0$ and variance $\sigma = 1$. This step closes the self-consistent computation cycle, which have to be run through at each time step. The introduced PIC-based computation strategy admits a self-consistent description of the collisional relaxation process which seems to be very important, for instance, in the context of the thermalization of an electron (ion) beam in an electron (ion) gas (see below).

4. Inter-species Collisions

In the case of electron-ion collision the electron speed is so much larger than the ions one and the mass ratio between the two species is so small that a simplifying hypothesis can be introduced in the evaluation of the drift and diffusion coefficients. With this in mind a Taylor expansion up to the second order in (3) and hand-differentiation yields:

$$\begin{aligned} \mathbf{F}^{(e)} &= \frac{n_x \Gamma_P^{(eX)}}{v^2}\left(1 - \frac{9}{4}\frac{\bar{v}_x^2}{v^2}\right)\hat{\mathbf{v}} \\ \mathsf{D}^{(e)} &= \frac{n_x \Gamma_P^{(eX)}}{v}\left[\mathsf{H} - \frac{3}{4}\frac{\hat{v}_x^2}{v^2}\left(\mathsf{I} - 3\hat{\mathbf{v}}\hat{\mathbf{v}}^T\right)\right] \end{aligned} \tag{7}$$

Where $\mathsf{H} = \mathsf{I} - \hat{\mathbf{v}}\hat{\mathbf{v}}^T$, $\bar{v}_x$ is the thermal velocity of the ions and $\hat{\mathbf{v}} = \mathbf{v}/v$ denotes the unit vector of the sines and cosines of the scattering and azimuthal angles. Then S can be immediately derived as:

$$\mathsf{S}^{(e)} = \sqrt{\omega_s^{(eX)}}v\mathsf{H} \tag{8}$$

where the introduced quantity $\omega_s^{(eX)} = n_X \Gamma_{(ex)}^P v^{-3}$ is usually referred as momentum transfer collision frequency.
The SDE can now be rearranged as:

$$d\hat{\mathbf{V}}(t) = -\omega_s^{(eX)}\hat{\mathbf{V}}(t)dt + \sqrt{\omega_s^{(eX)}}\mathsf{H}d\mathbf{W}, \tag{9}$$

which is now an equation in the directions of the velocities. On the basis of the zero expectation property of the Itô integral and the use of the Itô formula a solution for the first and second moment of the components of $\hat{\mathbf{V}}$ can be written as [7]:

$$\left\langle \hat{V}_{//}^{2}(t) \right\rangle = \frac{1}{3}\left[1-\exp\left\{3-\omega_s^{(eX)}(t-t_0)\right\}\right]+\left[\exp\left\{-3\omega_s^{(eX)}(t-t_0)\right\}-\exp\left\{2-\omega_s^{(eX)}(t-t_0)\right\}\right] \quad (10)$$

and

$$\left\langle \hat{V}_{y}^{2}(t) \right\rangle = \left\langle \hat{V}_{z}^{2}(t) \right\rangle = \frac{1}{3}\left[1-\exp\left\{-3\omega_s^{(eX)}(t-t_0)\right\}\right] \quad (11)$$

where $V_{//}$ is identified **as** V_x and the total transversal variance can be expressed as $\left\langle \hat{V}_{\perp}^{2}(t) \right\rangle = \left\langle \hat{V}_{z}^{2}(t) \right\rangle + \left\langle \hat{V}_{x}^{2}(t) \right\rangle$

5. Results

The characteristic time in which a system changes to an equilibrium condition from a non-equilibrium state has an impact on the temporal evolution of the chemistry in the interior of the pulsed plasma propulsion accelerators. In this section a sequence of results and considerations in this sense are presented: the relaxation dynamics of the (e-e) and (e-X)collision is discussed separately and then a more realistic simulation in which both mechanisms are operating is run. One way to obtain estimations of such parameter is to consider the scattering of one particle and try to get information about the time scaling of a distribution of particles with the same initial velocity conditions. This classical method known as test-particle approach was developed by Chandrasekhar [8] and Spitzer [9], and a variation can be found, for instance, in Montgomery & Tidman [2] and Trubnikov [8]. One relaxation time investigated by the test-particle method is the so-called slowing down time. \textit{slowing down time}. This time scale gives the rate at which collisions decrease the mean velocity of the test particles. These particles are initially ``injected`` into the plasma as a monochromatic ``beam`` which has only a constant V_z velocity component and are ``tracked`` up to the time where they are stopped. Note that it can be shown [2] that the slowing down time is only related to the friction force coefficients of the FPE. Another relaxation time of interest in the test-particle approach is the so-called deflection time, which may be considered as the typical time scale for an initially anisotropic distribution becoming isotropic [3]. Per construction this time scale is associated with the transverse velocity components of the test particles which are zero initially and is a measure of gradual deflection of the test particles by 90 degrees caused by the cumulative effects of collisions. Simple considerations reveal that the rate of increase of the transversal velocities is only due to the diffusion term of the FPE [2]. In the context of the present work the self-consistent dynamical evolution of the velocity distribution is studied, where both friction and diffusion forces are similarly important. Clearly, to switch off one of the dynamical aspects seems to be ideal but would contradict our self-consistent approach. In order to filter out characteristic times required by a whatever distribution function to reach an equilibrium state, because of collisions, the following procedure is proposed.The particles in the numerical experiments are subdivided in two groups: The first one consists of the background (abbreviated by BG) particles (constant number $N_{BG} = 3 \cdot 10^5$) which are initially Maxwellian distributed (that is Gaussian distributed in each velocity component; $\mu_{BG} = 0$, $\sigma_{BG} = 0$) , and the second group

is the beam particles (labelled as b). In the numerical experiments discussed below, the latter group represent an ideal monochromatic beam that hits initially the background particles with velocity only in the z-direction $\left(V_z^{(b)}(t=0)=5\right)$. To get an intuition of the complex non-linear dynamics resulting from the self-consistent computations, the simulations will be compared with a reference experiment, where the Maxwellian distributed BG-particles are not affected by the beam particles. In this sense the distribution function changes only because of the beam particles, which are advanced according to (4), where the non-linear velocity-dependent friction force and diffusion coefficients are obtained exactly by the background characteristics (see [6]). In fact, this experiment can be considered as an interface between the pure test-particle approach, where the coefficients are held constant for all the particles all the time (namely, at the initial values), and a real simulation. Also in the style of the test-particle approach, the mean value $\langle V_Z \rangle$ and the ``transversal`` variance σ_y^2 of the beam particles are used as measurable quantities which are recorded as function of time and seen in Figures 2 and 3 as full lines.

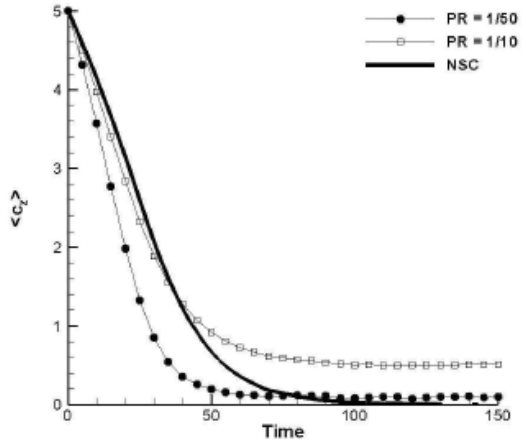

FIG. 2.Velocity mean value of the beam particles as a function of time of the self-consistent simulations with pr=1/50 (line with circle) and pr=1/10 (line with open squares) and the non self-consistent reference experiment

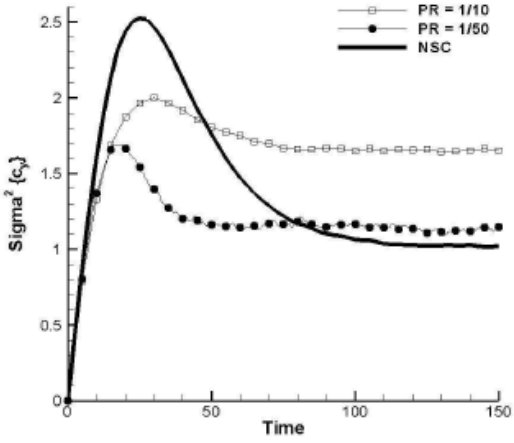

FIG. 3.Temporal evolution of the transversal variance. Full line: reference simulation; line with filled circles pr=1/50 and line with open squares pr=1/10 .

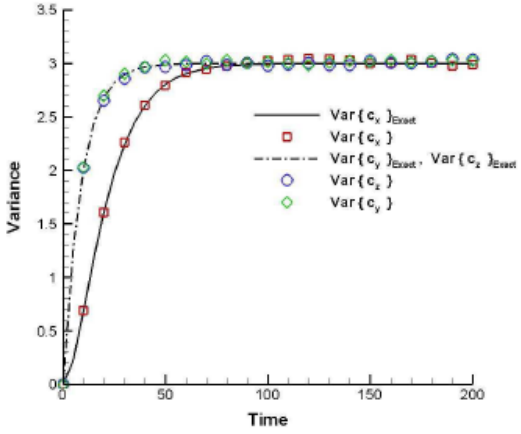

FIG. 4. Variances time values (symbols) and comparison with exact curves (full lines)

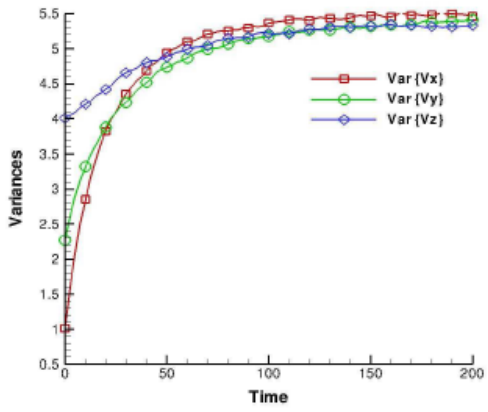

FIG. 5.Variances time evolution of the three velocity distribution functions during a (e-e) collision process. The thermal energy increases at expenses of the initial kinetic energy in the x-direction (see also FIG. .6)

Moreover, in these Figures the results of two self-consistent simulations ($3\cdot10^3$ cycles with $\Delta t = 5\cdot10^{-2}$) are depicted, where the beam to background particle ratios (pr) are fixed to pr=1/50 (lines with filled circles) and pr=1/10 (lines with open squares). Finally, we remark that in both self-consistent simulations the global velocity distribution functions established by the beam and background particles are highly non-Gaussian up to $t \leq\approx 35$ (not shown here).The equations (10) and (11) represent a natural benchmark for the inter-species collision case: a beam of electrons entering the ions reservoir with $\mathbf{V}(t_0) = (3,0,0)^T$ is considered and the event dynamics is monitored through the distribution functions and its moments. Figure 4 plots the exact variances of $f_e(V_q)$ (full line: σ_x^2 dash-dotted line: σ_y^2) with respect to time for the said initial conditions and the numerical solutions that are in very good agreement. Finally the above discussed phenomena are both taken into account for a more realistic simulation. The velocity of the electrons is now initialised with three Gaussian with different variances, respectively, $\sigma_x^2(t_0) = 1, \sigma_y^2(t_0) = 2.25$ and $\sigma_z^2(t_0) = 4$, and the electrons impact the ion reservoir with an additional stream velocity $V_x(t_0) = 3$ in the x- direction. Note that if in the same experiment the (e-X) collisions were inactive the mean value of $V_x(t_0) = 3$ would stay constant at the initial velocity $V_x(t_0) = 3$ since no mechanism is available to convert the initial kinetic energy into the thermal internal energy; i.e to turn ``coherent flow`` into ``disordered motion``. The result of the coupled intra-inter-species simulation is seen in Fig. 5.The inter-species collision part provides a mechanism which re-distributes the initial velocity uniformly in each direction resulting in the ``decay`` of the mean velocity (see Fig. 6) while the variances (thermal energy) are to reach a common value. Consequently, in the coupled numerical experiment the initial kinetic energy is transformed in thermal energy (due to inter-species interaction) and it is clear from Fig. 5 that in this case the distribution in each direction will posses a value which is one third of the sum of that achieved for the intra-species case for the same initial condition plus one third of the square of the initial flow velocity. Moreover, it is obvious from Fig. 5 that the coupled calculation is slower than the two independent processes: The difference in the time needed by $\langle V_{//} \rangle$ to reach the asymptotic final value with respect to the (e-e) case is huge: a rough estimation would indicate ≈ 100 and ≈ 500 time units for the intra- and inter-species respectively. This observation may be traced back to the fact that the parameter α^2 in eq. (9) is no longer a constant (as it is assumed there) during the simulation. In fact, a comparison of the curves seen in Fig. 6 admits the conclusion that α^2 is smaller in the coupled simulation.

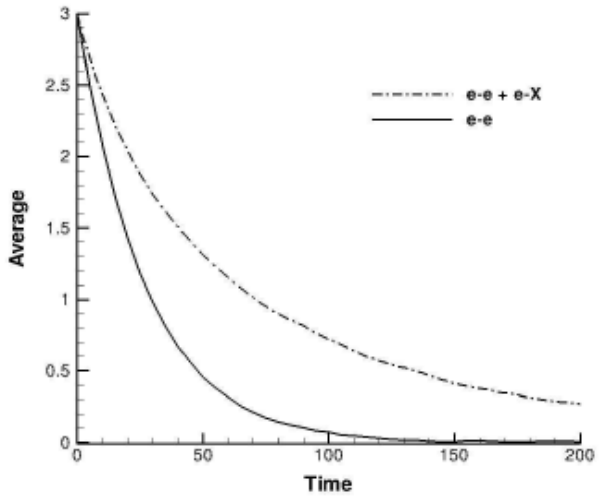

FIG. 6. Comparison between the mean value decay for the x-direction of the velocity in the (e-X) case(full line) and the coupled case (e-e)+ (e-X) (dashed-dotted lines).

Outlook

Inspired by the classical test-particle approach, a first study of the characteristic time constants in self-consistent collisional relaxation has been presented. A future intensive experimental campaign is planned to get a better understandings of the parameters which can have a stronger impact on the characteristic scale. Since it represents the closest approximation of the reality, the simultaneous operation of (e-e) and (e-X) mechanism will be the object of deeper analysis for example in the case of higher ionized ions. The influence of the electromagnetic fields (external and self-generated) will be also examined by coupling the present code with a Maxwell solver. Plasmas like polytetrafluoroethylene (commercially known as Teflon) or Argon plasmas will also be investigated for their wide applications, the former being used as fuel in pulsed plasma thrusters.

References

[1] MONTGOMERY, D., and TIDMAN, D., Plasma Kinetic Theory, McGraw-Hill, New York (1964)
[2] DIVER, D. A Plasma Formulary for Physics, Technology and Astrophysics Wiley-VCH Verlag, Berlin, (2001)
[3] GARDINER, C. Handbook of Stochastic Methods. Springer Verlag, Berlin Heidelberg, New York (1985)
[4] HOCKNEY, R. and EASTWOOD J. Computer Simulation using Particles, McGraw-Hill, New York (1981)
[5] D'ANDREA D., Modelling of Intra and Inter-Species Charged Particle Collisions for Flow Simulation in Pulsed Plasma Thruster, PhD Thesis, Fakultät Luft und Raumfahrtsysteme und Geodesie, Universität Stuttgart, Germany (2008)
[6] KLOEDEN,P. and PLATEN, E. Numerical Solution of Stochastic Differential Equations, Springer Verlag Berlin Heidelberg, New York (1999)
[7] TRUBNIKOV, B. Particles Interactions in a fully ionised Plasma; in Reviews of Plasma Physics, M.A. Leontovich (ed). Consultants Bureau, New York, (1965)
[8] CHANDRASEKHAR, S. Principles of stellar Dynamics, University of Chicago, (1942)
[9] SPITZER L., Physics of Fully Ionised Gases, Interscience Publishers, Inc., New York, (1956)