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Particle splitting in PIC-MCC codes

Usually, Particle In Cell-Monte Carlo Collisional (PIC-MCC) codes are equipped with technique aimed to reduce the total number of simulation particles in order to limit computation time. This approach is not always effcient from the point of view of both the Particle In Cell (PIC) and Monte Carlo (MC) modules. PIC methods are affected by charge spatial distribution on the grid; when this fluctuates rapidly, usually because of a not high enough number of particles per cell, the solution of the electric field introduces numerical noise. Moreover, it's widely known that Monte Carlo techniques effectiveness depends on the number of sample: the statistical approach of the method requires a representative enough ensemble. This means that a depletion of simulation particles due to adsorbing events or charge neutralization could compromise the correctness of the results, biasing the solution towards a casual direction. A splitting technique, succesfully emploied in Monte Carlo simulations, will be adapted to hybrid PIC-MCC codes in order to reduce noise and to improve representativeness in the phase-space domain.

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Abstract

Usually, Particle In Cell-Monte Carlo Collisional (PIC-MCC) codes are equipped with technique aimed to reduce the total number of simulation particles in order to limit computation time. This approach is not always effcient from the point of view of both the Particle In Cell (PIC) and Monte Carlo (MC) modules. PIC methods are affected by charge spatial distribution on the grid; when this fluctuates rapidly, usually because of a not high enough number of particles per cell, the solution of the electric field introduces numerical noise. Moreover, it's widely known that Monte Carlo techniques effectiveness depends on the number of sample: the statistical approach of the method requires a representative enough ensemble. This means that a depletion of simulation particles due to adsorbing events or charge neutralization could compromise the correctness of the results, biasing the solution towards a casual direction. A splitting technique, succesfully emploied in Monte Carlo simulations, will be adapted to hybrid PIC-MCC codes in order to reduce noise and to improve representativeness in the phase-space domain.

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1 Introduction

In many simulation of industrial plasma application a depletion of particles in certain domain regions is observed [1]. This phenomenon is essentially related to a too large weight of the simulation particles: typically $10^7 \div 10^8$ real charges are represented by one simulation particle, seeking a reduction of total computation time (proportional to the sum of the

number of particle N_p and $N_\mathrm{g}^D \log N_\mathrm{g}^D$, with N_g number of grid points in D dimensions, for the PIC module [2, 3], and proportional to N_p for the MCC one [4, 5]). Nevertheless, plasma dynamics simulations could lead to a not uniform distribution of simulation particles in the domain of interest; moreover, if weight-based technique are implemented to randomly reduce the number of simulation particles (i.e. *russian roulette*), some specific region (like the cathode-fall one [1]) could undergo a dramatic and dangerous depletion of particles. A situation of just one (or no) particle per cell could be reached causing a high fluctuation of the charge density in the region: the main consequence is a strong fluctuation of the electric field which could influence the behaviour of highly mobile electrons and the strength of the ionization avalanche.

The problem is not only related to the charge assignment and field calculation of the PIC module, since MC technique [4, 5, 6, 7, 8] requires a sufficiently high sampling to reduce the variance of the stochastic processes. For a classical MC model, the variance is proportional to inverse of the square root of the number of samples (if no variance reduction technique is used), which means that a the representativeness of the results is heavily influenced by the particles number N_p; on the other hand, as mentioned before, the cpu-time is directly proportional to N_p (in unbiased simulations). Moreover, the study of phenomena characterized by a threshold energy (i.e. ionization, anelastic scattering, ...) usually makes the statistics of high energy particles less representative with respect to that of bulk energy ones.

A logical approach of the problem is the development of weight-based variance and noise reduction techniques combined with conservation methods of the total number of simulation particles acting on the entire phase-space. In the present work, the first techniques will be dealt, while for the second ones the reader can refer to [9, 10].

In the past, few authors developed similar techniques [1] based on ions splitting at the interface between cathode-fall and bulk regions in glow discharges. The method presented can be extended and generalized to the whole phase space defining few basic rules not specific for a particular simulation.

2 Spatial splitting

Splitting technique are widely used in MC simulations. Here they will be briefly presented underlining the weight meaning and its importance for conservation rules.

The weight w_i of the i-th simulation particle is exactly the number (or fraction) of real charges it represents. During its motion the particle can be splitted into N_c^split; consequently its weigth have to be updated to the value

$$w_i^\mathrm{new} = \frac{w_i^\mathrm{old}}{N_c^\mathrm{split}}\,, \tag{1}$$

since the number of simulation particles increases articially while that of real charges isn't changed. Particles weight acts on both charge q and mass m of the species: it means that $q_i = q w_i$ and $m_i = m w_i$, while the ratio $q/m = q_i/m_i$ (related to the particle acceleration in the equations of motion) remains unchanged. As far as energy and momentum are considered, the new weighted particle is not to be intended as a particle of a different species with a

reduced energy and momentum, but as a particle of the same species of the original one with its energy and momentum properties but a reduced importance w_i. A rigorous weighting management assures the satisfaction of all conservation laws and the right values of tallied quantities.

After the splitting procedure, all the splitted particles will have the same velocity and position of the unsplitted original one: conservation laws of momentum, energy, mass and charge are all satisfied and no noise effect is artificially introduced. This implies that, at a first stage, all the reduced weight particles will move along the same trajectory; the collisions with the neutral gas is governed by the probability

$$P_{\text{coll}} = 1 - \exp(-n_{\text{b}} v \sigma_{\text{tot}}(E) t_{\text{coll}}) \,, \tag{2}$$

with n_{b} density of the background gas, v and E respectively velocity and energy of the incident particle, σ_{tot} total cross section and t_{coll} time to next collision; the randomness of P_{coll} will then separate the particles histories. In a collisionless system, the splitting technique wouldn't lead to any different result. The degree of homogenization, and thus the efficiency of the scheme, increases with L/λ, where L is the characteristic length of the low-density region and λ the mean free path of the charged particle in the background gas.

Inside the MCC module, the simulation particles will undergo collisions as real charged particles and not as simulation weighted particles. Consistently, a simulation particle with weight w_i generates w_i-weighted electrons and ions in an ionization event.

In MC simulations the splitting technique is applied when a particle undergoes an event or when it crosses an interface (real or virtual). The second criterion was followed in [1] by separation of the domain in a bulk and cathod-fall region. Nevertheless, in addition to MC models, PIC algorithms introduce time-dependence, letting the definition of a new time-based rule to call the splitting procedure. Every N_{t} time steps a check is made over the number of particles N_c per each cell; if it is less than a threshold value $N_c^{\min}$, the particles will be splitted in order to obtain an optimum number $N_c^{\text{opt}} > N_c^{\min}$ of simulation particles per cell; chosen a number of splitted particle N_c^{split} per each original one, they will gain new weights given by (1). In this way, mantaining a number of splitting particles greater than the threshold, the migration of some of them to adjacent cells in a time step will not necessarily imply a new splitting at the next check, which would lead to a highly time-consuming procedure. It is then necessary to define a value for N_{t} in order to optimize the splitting instants: the unknown is the time slot during which a cell undergoes a depletion of $N_c^{\text{depl}} > N_c^{\text{split}} - N_c^{\min}$ particles. The value of N_{t} is then very difficult to evaluate beacuse strictly dependent on the electric field strenght. If a uniform electric field is applied in a sufficiently large domain, under the hypothesis of isotropic scattering, the number of particles leaving a cell are, on average, replaced by particles from adjacent cells. The basic hypothesis aren't satisfied at boundaries of non-periodic domains and/or at the interface with low density regions; in these cases the replacing particles contribute is rather low, if not zero, and the depletion will progressively interest new cells. Roughly N_{t} can be estimated as the number of time steps necessary on average to have a particle leaving a cell. Since, usually, the time-step is mantained sufficiently short to avoid particle velocities which would imply a length of flight greater than two grid cells, then the condition $N_{\text{t}} > 1$ is automatically satisfied. Moreover, it would be useless to split a just-splitted particle if it's velocity hasn't been yet raondomized

in direction and modulus; this means that the particle should undergo few collisions before being splitted a second time: by comparison of the collisional frequency $\nu_{\rm coll}$ and time-step length, a new condition for $N_{\rm t}$ is obtained.

Another check is necessary to avoid the creation of negligible weighted particles: once a cell with a too low number of particles N_c is found, the weight of them is evaluated and compared with a minimum acceptable weight $w_{\rm min}$, under which the splitting must be avoided; in this way, only $N_c^{w_i>w_{\rm min}}$ particles, with weight $w_i > w_{\rm min}$, will be splitted in $N_c^{\rm split}$ new particles. Since $N_c^{w_i>w_{\rm min}}$ will remain unsplitted, only

$$N_c^{\rm res} = N_{\rm c}^{\rm opt} - (N_c - N_c^{w_i>w_{\rm min}}) = N_{\rm c}^{\rm opt} - N_c^{w_i<w_{\rm min}}$$

particles have to be splitted, and so $N_c^{\rm split}$ is immediately given by

$$N_c^{\rm split} = {\rm int}\left(\frac{N_c^{\rm res}}{N_c^{w_i>w_{\rm min}}}\right),$$

and, consequently, the weights of the splitted particles will be updated to

$$w_i^{\rm new} = w_i^{\rm old}\frac{1}{N_c^{\rm split}}.$$

The function ${\rm int}(x)$ has to be intended as that function which gives the nearest integer to x. If the truncation to the first integer less than x (${\rm floor}(x)$) was used, it can be pointed out that the particles would be splitted only if

$$\frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}} \geq 2 \qquad \text{and} \qquad N_c < N_c^{\rm min};$$

on the contrary, if the first integer greater than x (${\rm ceiling}(x)$) was used, new particles would be generated every time

$$\frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}} > 1 \qquad \text{and} \qquad N_c < N_c^{\rm min}.$$

In the first case $N_{\rm c}^{\rm opt}$ wouldn't be achieved until the depletion of not too small weighted particles overcome a 50%, while in the second one $N_{\rm c}^{\rm opt}$ would be exceeded as soon as N_c decreases of just one unit under $N_c^{\rm min}$.

A precautionary choice is based on the use of the ceiling integer of $N_c^{\rm split}$,

$$\overline{N}_c^{\rm split} = {\rm ceiling}\left(\frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}}\right);$$

the total value $N_{\rm c}^{\rm opt}$ is not reached exactly in general, since an excess of

$$N_c^{\rm exc} = N_c^{w_i>w_{\rm min}}\left({\rm ceiling}\left(\frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}}\right) - \frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}}\right) < N_c^{w_i>w_{\rm min}}$$

particles would be generated. Generally, the optimum number of particle per cell $N_c^{\rm opt}$ could be overcome by splitting only $N_c^{\rm to-split}$ particles of the $N_c^{w_i>w_{\rm min}}$ splittable ones: $N_c^{\rm to-split}$ is then ginven by the lower integer satisfying the condition

$$N_c^{\rm to-split}\overline{N}_c^{\rm split} + (N_c^{w_i>w_{\rm min}} - N_c^{\rm to-split}) > N_{\rm c}^{\rm opt}\,.$$

Sorting the particles by decreasing weight inside each cell, then, at each splitting call, one or more particles between the lower weighted ensemble won't undergo the splitting procedure, but, at the next call, they will probabily be the first ones to be splitted, having become the heavier in importance. The main problem is that, if the threshold $N_c^{\rm max}$ is very close to $N_{\rm c}^{\rm opt}$, then the exceeding particles could imply the overcoming of $N_c^{\rm max}$, and then a merging procedure would be called.

A last alternative approach let to calculate how many particles in the cell ($\underline{N}_c$ of N_c) have to be splitted into $\underline{N}_c^{\rm split} = {\rm floor}(N_{\rm c}^{\rm res}/N_c^{w_i>w_{\rm min}})$ and how many ($\overline{N}_c$) in $\overline{N}_c^{\rm split} = \underline{N}_c^{\rm split} + 1 = {\rm ceiling}(N_{\rm c}^{\rm res}/N_c^{w_i>w_{\rm min}})$. The answer is given by the solution of the following system

$$\begin{aligned}
&\underline{N}_c\underline{N}_c^{\rm split} + \overline{N}_c\overline{N}_c^{\rm split} = N_{\rm c}^{\rm res}\\
&\underline{N}_c + \overline{N}_c = N_c^{w_i>w_{\rm min}}\,.
\end{aligned}$$

Combining the two equations, one obtains

$$\underline{N}_c = N_c^{w_i>w_{\rm min}}\overline{N}_c^{\rm split} - N_{\rm c}^{\rm res} \tag{3a}$$

$$\overline{N}_c = N_c^{w_i>w_{\rm min}} - \underline{N}_c\,. \tag{3b}$$

This method doesn't require a sorting of the particles on the base of their weight (even if it would be useful seeking maximum uniformity). Since the weights of the splitted particles are obtained by dividing the old weights by the number of particles in which the original has been splitted, they will vary of $1/\underline{N}_c^{\rm split} - 1/\overline{N}_c^{\rm split}$ ($1/2 - 1/3 \simeq 0,1667$ as maximum) between the two ensemble of $\underline{N}_c^{\rm split}$ and $\overline{N}_c^{\rm split}$ particles. It is easy to show that the number $\overline{N}_c$ is simply given by the remainder of the ratio between the number of particles wanted after the splitting, $N_c^{\rm res}$, and the number of splittable ones, $N_c^{w_i>w_{\rm min}}$: by substitution of (3a) in (3b) one obtains

$$\begin{aligned}
\overline{N}_c = N_c^{w_i>w_{\rm min}} - \underline{N}_c = N_c^{w_i>w_{\rm min}}(1 - \overline{N}_c^{\rm split}) + N_{\rm c}^{\rm res} =\\
= N_{\rm c}^{\rm res} - N_c^{w_i>w_{\rm min}}\underline{N}_c^{\rm split}
\end{aligned}$$

and by definition of remainder

$$\begin{aligned}
{\rm mod}(N_{\rm c}^{\rm res}, N_c^{w_i>w_{\rm min}}) = N_{\rm c}^{\rm res} - {\rm floor}\left(\frac{N_{\rm c}^{\rm res}}{N_c^{w_i>w_{\rm min}}}\right)N_c^{w_i>w_{\rm min}} =\\
= N_{\rm c}^{\rm res} - N_c^{w_i>w_{\rm min}}\underline{N}_c^{\rm split}
\end{aligned}$$

the same result is obtained.

Future implementations of both merging [9] and splitting techniques require caution to avoid alternating application of the two methods, with a consequent increase of computational time and a descrease of sampling goodness. Subordinating the merging call to the overcoming of a maximum number $N_c^{\max}$ of particles per cell, this number must be set sfficiently greater than $N_c^{\min}$ and an optimum number $N_c^{\rm opt}$ of macro-particles per cell has to be created properly merging $N_c^{\rm merge}$ simulation particles. The thresholds $N_c^{\max}$ and $N_c^{\min}$ have to be fixed in order to avoid a periodic variation of N_c to values less than $N_c^{\min}$ and greater than $N_c^{\max}$ in few timesteps.

3 Energetic splitting

Plasma electron component in rapidly varying and highly intense electric fields is usually characterized by maxwellian-shaped Electron Energy Distribution Functions (EEDF) with a more populated energetic tail. Notwithstanding this, the number of particles with high energies is sensitively lower than that of the bulk ones. In plasma simulations with particle-code, this affects the outcoming EEDF with increasing oscillations amplitude towards higher energies. The effect is substantially due to the bad sampling of high energy processes. A way to reduce the arising fluctuations is the artificial increase of energetic paricles, achievable by particle splitting based on an energetic-check.

While, in real space, the grid helps the splitting technique by definition of cells, PIC codes treat energy in continuum. Then, the first step is the disctretization of energy in proper bins $\Delta E_b(E)$ and the definition of the optimum number of particles per bin $N_b^{\rm opt}$. While, spatially, the technique is used to avoid numerical noise related to the electric field solution, the energetic splitting is aimed to obtain uniformly distributed simulation particles in energy. This means that bigger is the energetic bin lager has to be the total number of particles it contains. The total number of particles should be substituted by their density $\rho_b^{\rm opt} = N_b^{\rm opt}/\Delta E_b$ in the energetic bin b of width ΔE_b: asking for a constant $\rho_b^{\rm opt}$, it follows that $N_b^{\rm opt}$ varies over b. Following a strategy similar to that of spatial splitting, a minimum acceptable density $\rho_b^{\min}$ is defined as a threshold and $N_b^{w_i>w_{\min}}$ is the number of particles to be splitted into $N_b^{\rm split}$ new particles, for each energetic bin. Since $N_b^{\rm opt}$ must be an integer, it has to be defined as

$$N_b^{\rm opt} = {\rm int}(\rho_b^{\rm opt}\Delta E_b)\,,$$

where the choice of the int(x) seems here the best one. Note that $N_b^{w_i<w_{\min}}$ particles cannot be splitted having a too low weight; then the number of particles to be obtained from the splitting is given by

$$N_b^{\rm res} = N_b^{\rm opt} - N_b^{w_i<w_{\min}} = {\rm int}(\rho_b^{\rm opt}\Delta E_b) + N_b^{w_i>w_{\min}} - N_b\,.$$

If an energy bin results completely devoided of particles, then the constant density $\rho_b^{\rm opt}$ cannot be achieved over it. To avoid this, the void bins should be merged together adjacent ones until they contain at least one particle: broadening the width of the energy bin, the optimum number of particles $N_b^{\rm opt}$ increases. Note that the splitted particles will have the same energy of the original one and only after few collisions they will be distributed in space and velocity fields.

A higher sampling rate for energetic particles improves the representativeness of high energy events, like ionization and inelastic scattering. If a particle of weight w_i has an ionization probability $P_{\rm ion}$ in a timestep Δt, in mean $2P_{\rm ion}w_i$ particles are created in Δt; if the particle is splitted in $N^{\rm split}$ particles with weight $w_i^{\rm new} = w_i^{\rm old}/N^{\rm split}$, each of them has the same probability $P_{\rm ion}$ to ionize a background atom and generate two particles with weight $w_i^{\rm new}$: in all, the same number $2NP_{\rm ion}w_i/N$ of particles is obtained, but a better statistics is achived, due to the increased number of samples N. Consequently, collisions will redistribute energies with no influence on the exponential growth due to ionization phenomenon. From the collisional point of view, there is no reason to discretize the whole velocity field, since cross sections depend only on the incident particle energy (see (2)). A complete 2D-3V merging procedure, instead, has to be performed to satisfy energy and conservation laws.

4 Spatial and energetic splitting

The procedures presented in section 2 and 3 are not mutually excluding. On the contrary, it's reasonable to apply both of them. If the spatial splitting is applied as first, the energetic splitting could modify the number of particles per cell increasing it over $N_c^{\rm opt}$, or, also, over $N_c^{\rm max}$; the reverse order would modify the optimum choice for $\rho_b^{\rm opt}$. This means that a coupled technique has to be developed.

The three dimensional space of coordinates (x_1, x_2, E) can be easily meshed by composition of the spatial grid and of an energetic binning. The possible strategy is based on the definition of an optimal density $\rho_{c,b}^{\rm opt}$ of simulation particles per each 3D $\Delta x_1 \Delta x_2 \Delta E_b$ element of the virtual phase space, which conrresponds to an optimal varying total number $N_{c,b}^{\rm opt}$. The same strategy followed in the energetic splitting should be followed locally for each grid cell.

The new number of particles per spatial cell is obtained as the projection of the particles of each bin under the same cell in the spatial plane or, in other terms, as the summation of $N_{c,b}^{\rm opt}$.

Since the preservation of an optimum number of particles per cell $N_c^{\rm opt}$ is the task in the PIC economy for noise reduction in electric field solution, the density of particle per 3D element has to be defined in order to obtain

$$N_c^{\rm opt} = \sum_b \rho_{c,b}^{\rm opt} \Delta x_1 \Delta x_2 \Delta E_b = \rho_b^{\rm opt} \sum_b \Delta E_b = \rho_b^{\rm opt} (E_{\rm max} - E_{\rm min}) \,,$$

since $\Delta x_1 \Delta x_2$ is independent of b: $\rho_b^{\rm opt} = \rho_{c,b}^{\rm opt} \Delta x_1 \Delta x_2$; this means

$$\rho_b^{\rm opt} = \frac{N_c^{\rm opt}}{E_{\rm max} - E_{\rm min}} \,,$$

known for a fixed $N_c^{\rm opt}$.

The splitting procedure has to be applied to each 3D element, producing the total number of particle $N_{c,b}^{\rm opt}$, given by

$$N_{c,b}^{\rm opt} = {\rm int}(\rho_{c,b}^{\rm opt} \Delta x_1 \Delta x_2 \Delta E_b) = {\rm int}(\rho_b^{\rm opt} \Delta E_b) \,.$$

The choice of the function int(x), instead of floor(x) or ceiling(x), modifies the number of $N_{c,b}^{\rm opt}$ of ± 1 and, then, could drastically modify the total value of $N_c^{\rm opt}$ or produce a compensation of the effects. If the energetic bins are equally spaced, the local effect is always the same, being $\rho_b^{\rm opt}$ constant, and so the total effect (in excess or defect) is equal to the total number of energetic bins. To artificially avoid this, one could assign an exceding particle every two energetic bins, which means to use alternatively the floor(x) and ceiling(x) function varying the index b. This can be mathematically translated in

$$N_{c,b}^{\rm opt} = {\rm floor}(\rho_b^{\rm opt}\Delta E_b) + \frac{1+(-1)^b}{2}\,,$$

where the second addendum gives an exceding particle when b is even and no exceding particle when it is odd.

Once $N_{c,b}^{\rm opt}$ is known, the number of particles $N_{c,b}^{\rm res}$ to be obtained by splitting, per each bin b over the cell c, is given by

$$N_{c,b}^{\rm res} = N_{\rm c,b}^{\rm opt} - N_{c,b}^{w_i<w_{\rm min}} = {\rm floor}(\rho_b^{\rm opt}\Delta E_b) + \frac{1+(-1)^b}{2} - N_{c,b}^{w_i<w_{\rm min}}\,,$$

where subscripts and superscripts have the usual meaning. Following a strategy similar to the one presented in the spatial case, one could define the number of particle $N_{c,b}^{\rm split}$ in which each particle of the 3D element with indexes b, c have to be splitted, as

$$N_{c,b}^{\rm split} = {\rm int}\left(\frac{N_{c,b}^{\rm res}}{N_{c,b}^{w_i>w_{\rm min}}}\right)\,,$$

or, even better, the couple of values $\underline{N}_{c,b}$ and $\overline{N}_{c,b}$ can be obtained starting from $N_{c,b}^{w_i>w_{\rm min}}$ and $N_{c,b}^{\rm res}$ and defining $\underline{N}_{c,b}^{\rm split} = {\rm floor}(N_{\rm c}^{\rm res}/N_c^{w_i>w_{\rm min}})$ and $\overline{N}_{c,b}^{\rm split} = \underline{N}_c^{\rm split}+1 = {\rm ceiling}(N_{\rm c}^{\rm res}/N_c^{w_i>w_{\rm min}})$, as presented in equations (3).

5 Implicit splitting and forced generation

Another MC technique which could be superimposed to the just described splitting procedure, is the implicit splitting. Usually the depletion of particles arises in the cathode-fall region; right here secondary electrons are produced by interaction of CF ions with the cathode boundary. Then, whenever an ion hits the cathod, it can be supposed as composed of $N^{\rm split}$ ions of weight $1/N^{\rm split}$ increasing artificially the number of samples on which the secondary electron emission test will be made by comparison of its probability γ with a random number R.

Alternatively, the forced generation can be implemented: everytime an ion hits the cathod boundary it will produce a secondary electron with weight given by the product of the ion weight and the secondary emission probability. In this way a secondary electron able to sustain the discharge will be certainly produced but with a reduced weight proportional to the real probability associated to its production. Even without increasing the samples number, the statistics is improved acting on particle weight.

6 Concluding remarks

A new splitting technique is proposed for PIC-MCC codes. After a preliminar analysis of the separate spatial and energetic cases, a comprehensive method is developed in order to obtain a constant simulation particle density over the energetic binning and a spatially uniform number of particles per cell. The technique, coupled with a merging one based on the collapse of particles in the 2D-3V phase space, allows to obtain a uniform distribution of simulation particles over the domain reducing numerical noise in electric field solution and, at the same time, increases drastically the representativeness of MC stochastic events.

A great advantage arises in parallelization of the algorithm. Generally, PIC codes require an Adaptive Mesh Refinement (AMR) in more densly populated regions in order to distribute more uniformly the load over each node in the cluster (load-balancing). Artificial redistribution of simulation particles over the grid assures the same aim simplifying the parallelization procedures: the portion of the grid associated to each node is always the same; consequently, only interface conditions are passed during field solution, and only particles crossing grid portions are transfered during particles advancing.

It is evident that the code must treat in a continuum form the weight of each particle. This means a double precision variable (8 bytes) for each particle to be stored in memory. Moreover, a particle array manipulation is useful to avoid the position and energy testing to find the cell and energy bin containing the particle. Storing the number of particle per cell and the number of particles per energy bin and sorting the particle array would be enough to solve the problem. Linked lists may be of help in this procedure, allowing a sort by pointer manipulation with no memory transfer; the drawbacks are that advantages in cache trashing [11] with sorted arrays is lost using linked lists and pointer management requires a higher memory storage than classical arrays.

References

[1] P. Meyer and G. Wunner. Unified particle simulation technique for the plasma bulk and the cathode sheath of a dc glow discharge. *J. Appl. Phys.*, 77:992–1000, 1995.

[2] C. K. Birdsall and A. B. Langdon. *Plasma Physics via computer simulation*. McGraw-Hill, 1976.

[3] R. W. Hockney and J. W. Eastwood. *Computer Simulation using Particles*. Adam Hilger, 1988.

[4] A. F. Bielajew. *Fundamentals of the Monte Carlo method for neutral and charged particle transport*. The University of Michigan, 2001.

[5] L. L. Carter and E. D. Cashwell. *Particle transport simulation with the Monte Carlo method*. Los Alamos Laboratory, 1975.

[6] X-5 Monte Carlo Team. *MCNP, A General Monte Carlo N-Particle Transport Code system, Version 5*. Oak Ridge National Laboratory, 2003. managed by UT-BATELLE, LLC for the U.S. DEPARTMENT OF ENERGY (RSICC computer code collection).

[7] F Salvat J M Fernndez-Varea and J Sempau. *PENELOPE – A Code System for Monte Carlo Simulation of Electron and Photon Transport*. Facultat de Fisica (ECM), Universitat de Barcelona, Spain, 2003.

[8] I Kawrakow and D W O Rogers. *The EGSnrc Code System: Monte Carlo Simulation of Electron and Photon Transport*. Ionizing Radiation Standards – National Research Council of Canada.

[9] M. Frignani and G. Grasso. Spatial particles merging in 2D PIC codes. Technical Report LIN-R02.2006, LIN, 2006.

[10] H. J. Lee C. H. Shon and J. K. Lee. Method to increase the simulation speed of particle-in-cell (PIC) code. *Comp. Phys. Comm.*, 141:322–329, 2001.

[11] J. K. Bowers. Accelerating a Particle-In-Cell simulation using a hybrid counting sort. *J. Comp. Phys.*, 173(2):393–411, 2001.