Exact Correction of the Self-Force Problem in Monte Carlo Device Simulation

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***Abstract*—The self-force is a specific problem of self-consistent Monte Carlo-Poisson simulation resulting in an un-physical field component acting on a particle coming from the particle itself (the self-force). Several approaches have been proposed in literature to mitigate this problem, but all of them suffer to some extent of approximations and/or limitations. In this paper we propose a new and mathematically exact correction of the self-force problem based on a numerical approach. Although computationally expensive, it has no restriction and can be always applied. The new method has been tested on the difficult problem of plasma oscillation simulation providing the expected plasma energy from theory. Moreover, the same mathematical framework introduced here for the self-force correction can be readily applied also for the exact calculation of the reference force in the Particle-Particle-Particle-Mesh (P3M) method. The accuracy of such approach to P3M method is demonstrated by simulating the bulk low field mobility dependence on doping concentration.**

I. Introduction

Since the seminal work of Hockney and Eastwood [1] the self-force (SF) problem has been recognized as a critical problem for self-consistent Monte Carlo-Poisson simulation (SC-MC-P). It arises from mixing point-like particles (charges) with finite element solution of the Poisson Eq. for the potential/field profile. Typically, SC-MC-P includes the following steps: 1) charge assignment to the mesh; 2) solution of the Poisson Eq. for the potential; 3) interpolation of the resulting electric field back to particle position. The problem stems from the unavoidable displacement of the charge implicit in step 1) and the approximation involved in step 3).

In order to understand the origin of the SF problem, we can consider the simple case of a single particle with zero initial velocity/energy and no external field (the so called 'lone' particle case). Obviously, the particle should stay fixed where it is, but this is not the case for SC-MC-P, as explained in Fig. 1. Indeed, let's consider for convenience the simplest charge assignment method scheme at step 1), that is assigning the particle charge to the nearest grid point (NGP). Then the computed potential (solid line) will feature a finite deep at that grid point (whose amplitude depends on the grid spacing), and the corresponding field would be piece-wise constant (dotted line). The key point to notice is that the computed field is not zero at the particle position as it should be. Instead there is a fictitious field acting on the particle due to the particle itself that should not be there. This is caused by the displacement of the computed potential profile on the mesh with respect to the real one (Coulomb potential, dashed line) due to space discretization, and the interpolation of the electric field at the particle position that is not able to resolve the symmetry of the field around the particle position.

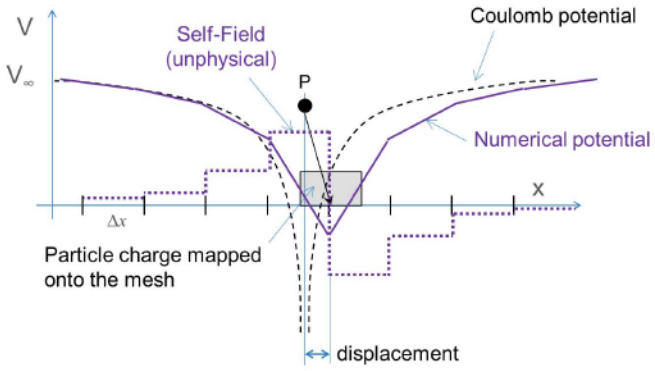

Fig. 1. Schematic description of the SF origin for a single particle P. Correct (Coulomb) potential: dashed line. Finite element solution of the Poisson Eq. (solid line) and corresponding field profile (dotted line).

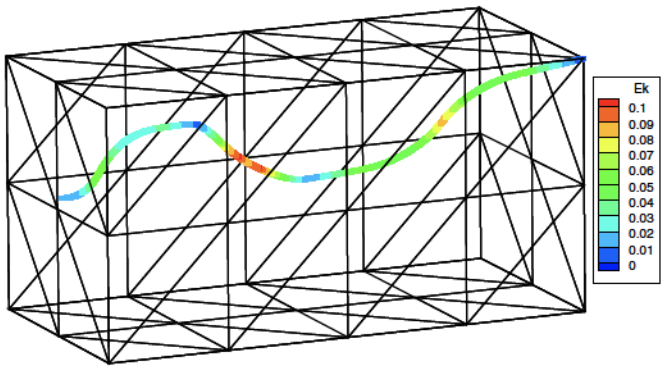

Fig. 2. Example of SC-MC-P simulation of the 'lone' particle case when the SF problem is not corrected. Color level represents the particle kinetic energy E_k in eV.

An example of such un-physical results is reported in Fig. 2. A particle with no kinetic energy (E_k) has been placed on a mesh node. Then a SC-MC-P simulation is carried out with only this unique particle. Because of the SF problem, the particle starts to move around, attaining also a significant kinetic energy, whereas it should stay fixed at the initial position. Followed trajectory and gained energy are un-predictable as they depend on the mesh topology, initial position, how often the potential profile is updated and so on.

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Clearly this problem is present only in SC-MC-P simulation, it worsens for decreasing mesh spacing, i.e mesh node distance (Δx), and it is more impacting where the external field is low.

Several methods have been proposed in the literature to mitigate the SF problem. Many of them are based on smoother charge assignment schemes such as Cloud-in-Cell (CIC) [1], nearest-element-center (NEC) [2], etc. Others, instead, are based on more complex field interpolation [3]. However, all of them suffer of some limitations, either imposing some constraint on the mesh (e.g. uniform spacing, or no interfaces, or equilateral triangles [2]), either not guaranteeing the consistency of potential and field, possibly leading to the not conservation of both momentum and energy [1].

In this paper we introduce a new approach to solve the SF problem in SC-MC-P simulation. It is based on a numerical correction of the potential profile. Although it might be computational expensive, it is mathematically exact, and does not suffer of any of the above-mentioned limitations, and thus can be generally applied.

Sect. II introduces the mathematical framework behind the new correction, whose results are then discussed in Sect. III. The same approach is leveraged in Sect. IV for an exact implementation of the P3M method. Finally Sect. V draws some conclusions.

II. Exact Self-Force Correction

In principle, the SF can be avoided if the potential caused by the *i-th* particle p_i (φ_i) is removed from the total potential ψ. In practice, this can be done by applying to p_i a corrected potential $\psi_i^{cor} = \psi - \varphi_i$. Here ψ is the solution of the Poisson Eq. that, in case of point-like charges, can be written as

$$\nabla \cdot (-\epsilon \nabla \psi) = q\Big(\sum_i w_i \delta\big(\vec{r} - \vec{r}_{NGP(p_i)}\big) + N_c(\vec{r})\Big) \quad (1)$$

with boundary conditions

$$\psi = \psi_a \quad \text{on electrodes} \quad (2)$$

$$\frac{d\psi}{d\vec{n}} = 0 \quad \text{on remaining boundary,} \quad (3)$$

where q is the elementary charge, ϵ the dielectric constant, N_c is any charge described by a continuous profile (e.g. doping), $\vec{r}_{NGP(p_i)}$ is the nearest grid point to p_i, and w_i is its statistical weight (with sign, i.e. positive for holes, negative for electrons). The difficulty lies in identifying φ_i.

The new method we are proposing calculates φ_i numerically, and, therefore, can be always applied, and it is mathematically exact within the framework of finite element calculation of ψ. To this purpose we follow the main idea in [4]. We start by noticing that ψ can be written as

$$\psi = \psi_c + \sum_i w_i \Phi_{NGP(p_i)}, \quad (4)$$

where ψ_c is the solution of

$$\nabla \cdot (-\epsilon \nabla \psi_c) = q N_c(\vec{r}) \quad (5)$$

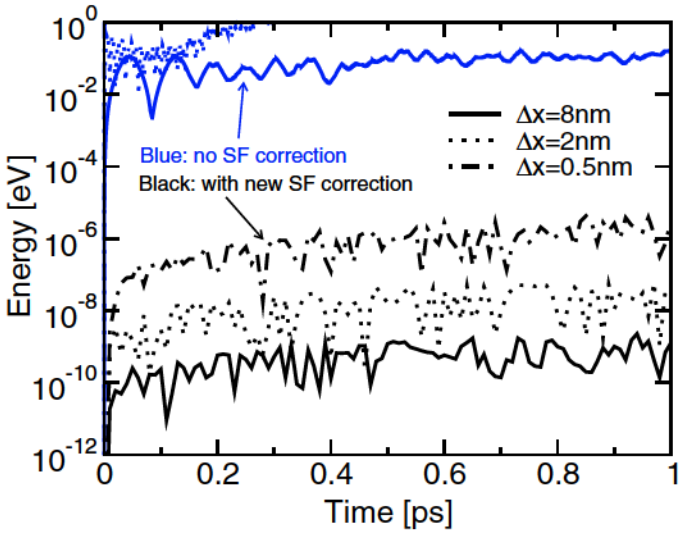

Fig. 3. 'Lone' particle energy SC-MC-P 3D simulation results for different mesh spacing Δx. Blue lines: no SF correction. Black lines: with exact SF correction. The correct value should be 0.

with boundary conditions (2) and (3), and $\Phi_{NGP(p_i)}$ is the solution of

$$\nabla \cdot \big(-\epsilon \nabla \Phi_{NGP(p_i)}\big) = q\delta\big(\vec{r} - \vec{r}_{NGP(p_i)}\big) \quad (6)$$

with boundary conditions (3) and

$$\Phi_{NGP(p_i)} = 0 \quad \text{on electrodes.} \quad (7)$$

Notice that: *i*) this method is somehow different from [4] because of the different form of (6) and the different boundary condition represented by (7) (compare them to (4) and (5) in [4] respectively); *ii*) (7) is mandatory in order for (4) to be true; *iii*) (7) sets a clear and unambiguous boundary condition regardless of the device structure.

From (4) it is clear that

$$\varphi_i = w_i \Phi_{NGP(p_i)}. \quad (8)$$

The new method then requires to compute and store the solution of (6) for all mesh nodes to be later used to correct the potential on a particle basis. This can be computationally expensive, but it can be speeded-up parallelizing the solution of (6), that are all independent on each other. Moreover, it also requires a lot of memory, but this is not a problem anymore for modern computers with hundreds of GB of memory.

III. Results and Discussion

First, we verified the new method on the case of the single particle with zero initial energy/velocity. In this particular case, ψ and φ_i coincide, except for the numerical error in their calculation. Thus $\psi_i^{cor} = 0$ always, and, consequently, the particle keeps its state. SC-MC-P 3D simulation results with and without the new correction are reported in Fig. 3 for different mesh spacing. Clearly, without any SF correction, the particle energy rapidly diverges. Only for the larger mesh spacing, the particle energy attains a finite value in the

range of hundreds of *meV*, which is anyway not acceptable (the correct one should be 0). On the contrary, the new SF correction always provides a particle energy below $10^{-6}eV$, i.e. comparable with the numerical precision with which ψ and φ_i have been computed.

Next, we tested the new SF correction on the 3D simulation of plasma oscillations. Plasma oscillations are a collective motion of a gas of free electrical particles. Let's consider the simple case of a gas of free electrons of density n on a uniform background of positive fixed charge. If an electron is displaced from its equilibrium position even by a small amount the Coulomb interaction with the other charges will tend to pull it back, resulting in an oscillation around the equilibrium configuration. These oscillations take place at a characteristics frequency

$$\omega_p = \sqrt{\frac{nq^2}{m^*\epsilon}}$$

where m^* is the carrier effective mass. In this process, the free electrons exchange energy with the Coulomb potential resulting in an increased average kinetic energy (ΔE_C) with respect to the thermal energy. Theory in [5] showed this extra energy to be

$$\Delta E_C = 1.451 \frac{q^2 n^{1/3}}{4\pi\epsilon_\infty} \left[1 + \left(\frac{1}{\omega_p \tau_m}\right)^2\right]^{-1/2} \quad (9)$$

where τ_m is the momentum relaxation time due to the other scattering mechanisms.

Plasma simulation is a very difficult task for SC-MC-P since it requires very short time step between Poisson Eq. solution ($\Delta t \ll 1/\omega_p$) to capture the potential oscillation, and very small grid spacing to accurately resolve the Coulomb force among particles according to the Particle-Mesh (PM) scheme [1]. We found that $\Delta x = 1/4\sqrt[3]{n}$ is as good trade-off between accuracy and computational time. Under these conditions SF becomes very important and thus must be avoided. In the simulation we adjust the size of the 3D cubic domain to hold approximately 1000 electrons at all densities, resulting in a mesh with $\approx$ 70K nodes. In this case, calculation of all $\Phi_{NGP(p_i)}$ takes approximately half of the simulation time, which is anyway dominated by the time spent solving (1), and $\approx$ 25GB of RAM.

Fig. 4 compares simulation results with and without the new SF correction against the theoretical value. Without SF correction the simulated average energy is much higher than expected, while the new and exact SF correction provides a good agreement with theory, demonstrating the validity of the approach.

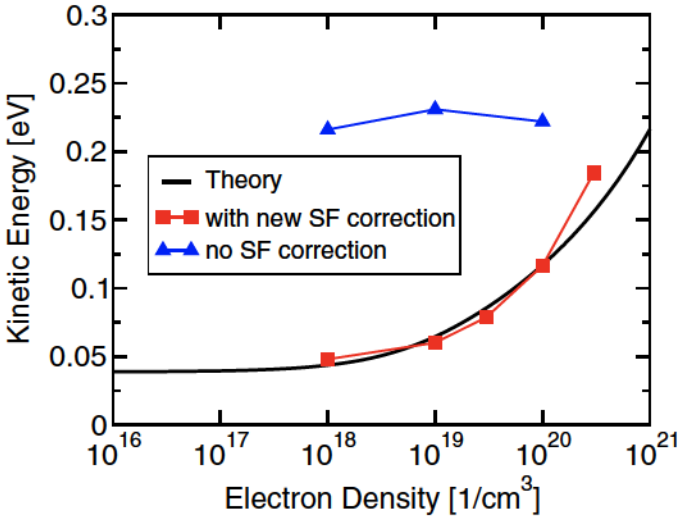

Fig. 4. Plasma energy simulation. Black line: theoretical value $1.5k_BT + \Delta E_C$. Blue triangles: no SF correction. Red squares: exact SF correction.

IV. Extension to P3M method

The calculation of φ_i (contribution of the particle p_i to the total potential ψ) is also required in the implementation of the Coulomb interaction among charges according to the Particle-Particle-Particle-Mesh (P3M) method [1]. In order to allow the use of coarser grid than needed by the PM method as discussed in the previous section, in the P3M method the Coulomb force exchanged with surrounding charges is explicitly added to the electric field acting on a particle. In this way, Coulomb scattering with fixed dopants (impurity scattering) and with other mobile carriers (electron-electron scattering) are not treated anymore as explicit localized scattering events with their own rates, but they are substituted by the continuous interaction exchanged via the Coulomb force during particle motion (a sort of molecular dynamics approach). However, in order not to double count the interaction with surrounding particles, since also included in the mesh potential, their contribution to ψ, that in the framework of P3M is called reference potential(force), must be removed [1], [6]–[8]. This contribution is, by definition, the same as derived in Sect. II and it is given again by (8). Therefore, in the P3M method, the potential profile 'seen' by the *i-th* particle, including also the SF correction introduced in this paper, is

$$\begin{aligned} \psi_i^{P3M} = \psi \quad &+ \sum_{j\neq i} \frac{q w_j}{4\pi\epsilon\,|\vec{r_j} - \vec{r_i}|} && \text{Coulomb potential} \\ &- \sum_{j\neq i} w_j \Phi_{NGP(p_j)} && \text{Reference potential} \\ &- w_i \Phi_{NGP(p_i)} && \text{SF correction.} \end{aligned} \quad (10)$$

The accuracy of such approach is demonstrated by simulating the bulk low field mobility dependence on doping (i.e. impurity) concentration. Usually, in the framework of MC device simulation, impurity scattering is treated as any other scattering mechanisms with its own scattering rate and after scattering state selection rules, provided by a number of models (Brook and Herring [9], Ridley [10], Conwell-Weisskopf [11], Kosina [12]), that are all depending on the doping concentration considered as a continuous profile. Often, these models have fitting parameters [13], as reproducing low field mobility doping dependence is a difficult task for MC.

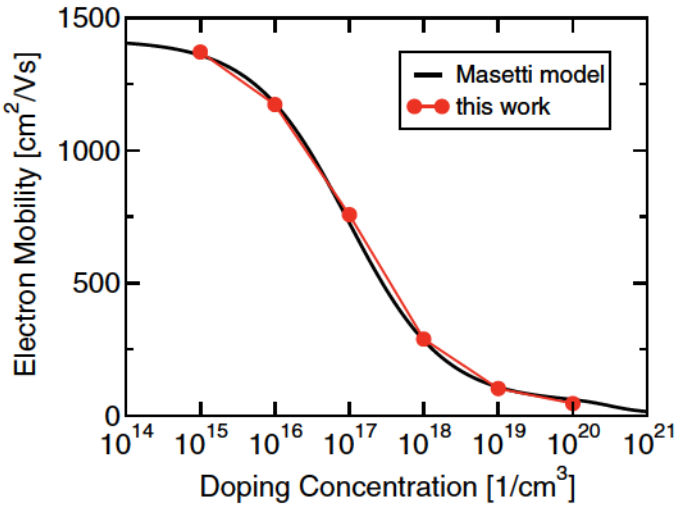

Fig. 5. Comparison of simulated low field electron bulk mobility in Silicon (symbols) with the analytical Masetti model [15].

However, with the restless shrinking of device physical dimension, nowadays only a few dopants are present in the channel of MOS transistors, and even in the source/drain extensions, mandating to treat them as discrete, and randomly placed, fixed particles [14]. Therefore, the aforementioned models cannot be applied anymore, whereas the P3M method is particularly suited for this as it was designed to handle Coulomb interaction with point-like particles.

SF correction and P3M method have been implemented in our MC code (MC++), which was then used to simulate the bulk low field mobility for several doping levels. These simulations are very similar to the ones in the previous section with the following differences: 1) background doping is described here by discrete particles placed randomly (no need to be located at mesh nodes though); 2) an external low field ($1KV/cm$) is applied to induce a detectable average drift velocity; 3) mesh spacing has been relaxed as allowed by P3M and adapted to doping level to include in the 3D simulation domain a large number of impurities in order to reduce the statistical variability associated with the random placement while keeping to a manageable level the number of mesh nodes.

Results of such simulations are compared in Fig. 5 to the reference Masetti model that is a good fit to experimental data [15]. The agreement is quite good demonstrating the soundness of P3M for this kind of problem, and the effectiveness of the proposed implementation. It is worth noticing that: 1) in the simulation of Fig. 5 there is no free parameter as the only phenomenon at play is the Coulomb force; 2) SF correction is again mandatory to get the correct kinetic energy and, hence, velocity.

V. Conclusion

In this paper we have introduced a new method for the correction of the self-force problem in SC-MC-P simulation. This method is based on the identification of the contribution of each particle to the potential/field profile, so that it can be easily removed from the driving forces of particle motion. This operation is done numerically on the simulation mesh and, although computationally expensive, is mathematically exact within the framework of finite element calculation of the potential profile, and it has no restriction. We demonstrated its effectiveness by showing that this new method allows to reproduce the average kinetic energy in plasma oscillation simulation.

Moreover we have proposed to use the same approach also to compute the reference force needed for the implementation of the Coulomb interaction among point-like charges (either fixed or mobile) via the P3M method. We verified the correctness of this new approach to P3M by reproducing the electron low field mobility dependence on doping concentration with no fitting parameter.

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