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A Boundary-Element/Multipole Algorithm for Self-Consistent Poisson Calculations in Monte-Carlo Simulation

J. Lloyd, J. Phillips, J. White

Research Laboratory of Electronics and the
Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology
Cambridge, MA 02139

I. Introduction

Simulation of small geometry devices by particle simulation or Monte-Carlo techniques is becoming increasing popular, even though the method is computationally much more expensive than numerically solving the standard or modified drift-diffusion equations[2][3][4]. This popularity is mostly due to the ease in which physical phenomenon, particularly scattering mechanisms, can be directly incorporated into Monte-Carlo simulations. In the past, the primary use of Monte-Carlo simulation has been to investigate the physics of semiconductors, and the numerical algorithms used were kept as simple as possible. The recent more widely spread use of Monte-Carlo simulation has focused investigations on more sophisticated numerical algorithms to try to reduce the simulation time and to improve accuracy.

In this paper we address the problem of computing the self-consistent electric fields for Monte-Carlo simulation of physical devices. The approach used in many existing programs involves solving Poisson's equation by first constructing a mesh over the device and discretizing the potential using finite-difference methods. Then, the discrete space charge in the device, represented by the many thousands of particles, is associated with points in the mesh by a cloud-in-a-cell approach. The forces on the individual particles are computed from the discretized representation of the potential[2]. The short-coming of this approach is that when there are few particles in any particular region of the mesh, the interaction of nearby particles may not be calculated accurately, and may jump as a particle crosses boundaries from one region of the mesh to another. In addition, nearby and far-field Coulomb interaction can not be easily separated, making accurate electron-electron scattering calculations difficult.

II. Separation Approach

It is possible to derive an alternative that avoids some of these difficulties by separating the Poisson equation into two pieces, one that represents potential due to doping and potential boundary conditions, and the other due to the discrete electron concentration. Specifically, consider the Poisson equation for a device in which hole concentration is ignored as

$$\nabla \epsilon \nabla \psi + q\,(N - n) = 0, \tag{1}$$

where ψ is the electrostatic potential, q is the magnitude of electronic charge, n is the, in this case discrete, electron concentration, and N is continous net doping concentration. The potential due to the continous doping and the discrete electron concentrations can be separated as

$$\nabla \epsilon \nabla \psi_a + qN = 0, \tag{2}$$

and

$$\epsilon \nabla^2 \psi_b + qn = 0. \tag{3}$$

where $\psi_a + \psi_b = \psi$, and in (3) we are assuming that the electron concentration is contained in a uniform dielectric material.

The forces on each particle due to the gradients in ψ_a can be calculated using standard finite-difference methods, as the charge due to doping can be modeled as being continously distributed in the device. Since the final goal is to compute the forces on each particle, the forces due to gradients in ψ_b on each particle can computed directly by summing the Coulomb force due to all the other particles, and then handling the boundary conditions with a boundary element approach. This combination of techniques has the appealing features handling nearby interactions accurately, and allowing for nearby and far-field interactions to be easily separated. The summation of the Coulomb forces can be performed in time that grows linearly with the number of particles using the recently developed fast multipole algorithm[1].

III. Conclusions

Once a discretized version of the surface charge density has been computed, the forces on each of the charged particles due to the gradient of ψ_b in Eqn. (3) can be computed using the multipole algorithm mentioned above. Preliminary experiments indicate that this computation can be completed in less than 30 cpu seconds on a SUN4 workstation for a problem with 5000 particles where the contacts have been broken up into 400 tiles. Additional work is needed to improve the speed of the calculation, and to extend it to the case where the hole contribution to the forces are considered.

References

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