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Particle-Based Simulation: An Algorithmic Perspective

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INTRODUCTION

This talk reviews some of the latest advances of the algorithmic aspects of particle-based methods for the simulation of both solid-state devices and biological systems. After a brief historical introduction, a discussion will be offered about the recent evolution of numerical methods used by both Full-Band Ensemble Monte Carlo (EMC) and Molecular Dynamics (MD) algorithms. A discussion of some relevant applications of both simulative approaches will be accompanied by a critical analysis of the main limitations of the methods. Several needed improvement will be discussed as well, and the potential of the algorithms for modelling systems of higher complexity.

FULL-BAND SIMULATION

The idea of using a k-space tabulated representation of the electronic structure and scattering rates of a semiconductor material rather than an analytical representation of portions of the first Brillouin Zone (BZ1) was introduced by K. Hess and coworkers in 1981 [1], [2]. The subsequent work of M. Fischetti and S. Laux [3] set the algorithmic standard for EMC simulation in 1988. In 2000, M. Saraniti and S. Goodnick revised the basic EMC algorithm by introducing the Cellular Monte Carlo (CMC) method [4], based on the tabulation of the probability of transition between different regions of BZ1, rather than the probability of scattering out of an initial momentum "state". The growing availability of large amounts of fast storage (RAM) and the introduction of efficient data compression techniques allowed the extremely fast CMC to reach accuracy comparable to the traditional EMC. From the viewpoint of force-field schemes, the implementation of state-of-the-art Poisson solvers [5], [6], [7] allowed longer simulation times and extremely complex (and large) 3D devices [8]. The self-consistent coupling of the charge transport simulation with time-domain Maxwell solvers [9] allowed the resolution of the radiation field generated by a device. As a consequence of these improvements, the characterization of the dynamic behavior of devices, as well as study of device noise became realistic. The recent introduction in the consumer market of fast 64bit processors based on dedicated memory bus architecture extended dramatically the addressable memory space and its efficiency, and allowed the implementation of more sophisticated physical models in particle-based full-band simulation codes. Recent applications of such algorithmic improvements will be discussed, such as the simulation of spin transport and the modeling of self-consistent non-equilibrium electron-phonon interactions.

MOLECULAR DYNAMICS

The evolution of the computing hardware discussed above had an even more dramatic impact on the application of molecular dynamics algorithms to the simulation of complex biological systems. Basing on simulation tools developed by the whole community [10], [11] and on the intensive use of parallel computing, MD algorithms made possible the atomistic simulation of macromolecules [12] and even small viruses [13]. While these advances are extremely encouraging, much work needs to be done on the algorithmic development of the force-fields schemes [14], [15] used in MD. The talk will review some state-of-the-art algorithms for polarizable force-fields [16], [17], and will discuss their development. Applications to the simulation of

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both solid- and liquid-state systems will be shown as well.

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