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SALUTE –GRID Application for problems in quantum transport

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Abstract body:
SALUTE (Stochastic ALgorithms for Ultra-fast Transport in sEmiconductors) is an MPI Grid application developed for solving computationally intensive problems in quantum transport.

Monte Carlo (MC) methods for quantum transport in semiconductors and semiconductor devices have been actively developed during the last decade. If temporal or spatial scales become short, the evolution of the semiconductor carriers cannot be described in terms of the Boltzmann transport [1] and therefore a quantum description is needed. We note the importance of active investigations in this field: nowadays nanotechnology provides devices and structures where the carrier transport occurs at nanometer and femtosecond scales. As a rule quantum problems are very computationally intensive and require parallel and Grid implementations.

SALUTE is a pilot grid application developed at the Department of Parallel Algorithms, Institute for Parallel Processing - BAS where the stochastic approach relies on the numerical MC theory applied to the integral form of the generalized electron-phonon Wigner equation. The Wigner equation for the nanometer and femtosecond transport regime is derived from a three equations set model based on the generalized Wigner function [2]. The full version of the equation poses serious numerical challenges. Two major formulations (for homogeneous and inhomogeneous cases) of the equation are studied using SALUTE.

The physical model in the first formulation describes a femtosecond relaxation process of optically excited electrons which interact with phonons in one-band semiconductor [3]. The interaction with phonons is switched on after a laser pulse creates an initial electron distribution. Experimentally, such processes can be investigated by using ultra-fast spectroscopy, where the relaxation of electrons is explored during the first hundreds femtoseconds after the optical excitation. In our model we consider a low-density regime, where the interaction with phonons dominates the carrier-carrier interaction. In the second formulation we consider a highly non-equilibrium electron distribution which propagates in a quantum semiconductor wire [4]. The electrons, which can be initially injected or optically generated in the wire, begin to interact with three dimensional phonons. The evolution of such process is quantum, both, in the real space due to the confinements of the wire, and in the momentum space due to the early stage of the electron-phonon kinetics. A detailed description of the algorithms can be found in [5, 6, 7].

Monte Carlo applications are widely perceived as computationally intensive but naturally parallel. The subsequent growth of computer power, especially that of the parallel computers and distributed systems, made possible the development of distributed MC applications performing more and more ambitious calculations. Compared to the parallel computing environment, a large-scale distributed computing environment or a Computational Grid has tremendous amount of computational power. Let us mention the EGEE Grid which today consists of over 18900 CPU in 200 Grid sites.

SALUTE solves an NP-hard problem concerning the evolution time. On the other hand, SALUTE consists of Monte Carlo algorithms which are inherently parallel. Thus, SALUTE is a very good candidate for implementations on MPI-enabled Grid sites. By using the Grid environment provided by the EGEE project middleware, we were able to reduce the computing time of Monte Carlo simulations of ultra-fast carrier transport in semiconductors. The simulations are parallelized on the Grid by splitting the underlying random number sequences.

Successful tests of the application were performed at several Bulgarian and South East European EGEE GRID sites using the Resource Broker at IPP-BAS. The MPI version was MPICH 1.2.6, and the execution was performed on clusters using both pbs and lcgpbs jobmanagers, i.e. with shared or non-shared home directories. The test results show excellent parallel efficiency. Obtaining results for larger evolution times requires more computational power, which means that the application should run on larger sites or on several sites in parallel. The application can provide results for other types of semiconductors like Si or for composite materials.

Figure 1. Distribution of optically generated electrons in a quantum wire.

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Summary

A Grid application developed for electron transport problems called SALUTE (Stochastic ALgorithms for Ultra-fast Transport in sEmiconductors) is presented. Monte Carlo algorithms for solving quantum-kinetic equations describing a bunch of problems are developed. A physical model of a femtosecond relaxation of optically excited electrons which interact with phonons in an one-band semicondoctor is considered. The electron-phonon interaction is switched on after a laser pulse creates an initial electron distribution. Two cases of this process are investigated - with and without an applied electric field.

We describe Grid implementation of the developed algorithms which are CPU-intensive. Using this application innovative results for different materials can be obtained. Here we present the first version of SALUTE which is used to obtain innovative results for GaAs materials.

The results from a number of tests on MPI-enabled Grids are shown and disscussed.

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