Modeling and Optimization in Science and Technologies

Mihnea Dulea · Aneta Karaivanova
Anastasis Oulas · Ioannis Liabotis
Danica Stojiljkovic · Ognjen Prnjat *Editors*

High-Performance Computing Infrastructure for South East Europe's Research Communities

Results of the HP-SEE User Forum 2012

HP-SEE
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Volume 2

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Preface

High-Performance Computing (HPC) is one of the key enablers of scientific research and of the development of Information Society in Europe. Enabling large-scale innovative research to be conducted through collaboration of distributed teams of scientists across the European Research Area paves the way towards a long-term vision of a sustainable, transparent, ubiquitous electronic infrastructure open to a wide range of scientific user communities. European Commission sees "strategic nature of High-Performance Computing as a crucial asset for the EU's innovation capacity, and calls on Member States, industry and the scientific communities, in cooperation with the Commission, to step up joint efforts to ensure European leadership in the supply and use of HPC systems and services by 2020." Pan-European PRACE infrastructure supports this strategy and currently provides the core of High-Performance Computing power for European research. In this context, the inclusion of less-developed regions of Europe, which suffer from the digital divide and brain-drain in all fields and especially high-technology, into the wider European Research Area is an aim closely aligned to this vision. HP-SEE project, co-funded by Framework Programme 7 of the European Commission, is currently advancing the computing infrastructures in South-East Europe (SEE), activating new user communities and enabling collaborative research across a number of fields, and thus contributes to closing the existing technological and scientific gap, and following the wider European HPC strategy.

The HP-SEE User Forum took place in Belgrade on October 17-19, 2012, at premises of National Library of Serbia and hosted by the Institutes of Physics Belgrade: this scientific conference gathered 65 participants from 16 countries in the region and beyond, with main focus on the fields of Computational Physics, Computational Chemistry, Life Sciences, Scientific Computing and HPC Systems and Network Operations. Conference programme comprised of seven invited lectures, both from related e-Infrastructure projects and HP-SEE scientific community, 26 contributed oral presentations and a poster session featuring 11 poster presentations. This edition of papers from the User Forum is comprised of 20 peer-reviewed papers: 7 from Computational Physics applications in HPC, 5 from Computational Chemistry, 3 from Life Sciences, and 5 from Scientific computing and HPC operations. The project as well as the wider SEE community has benefited greatly from the exchange of experiences of leading scientists in

the region in their use of High-Performance Computing technology to empower their research.

In my role of HP-SEE project manager, I would like to thank the authors, reviewers, editors, programme and organization committees and guest speakers for their contributions to this event.

April 2013

Dr. Ognjen Prnjat
HP-SEE Project Manager

Conference Topics

- Computational Physics
- Computational Chemistry
- Life Sciences
- Scientific Computing
- HPC Systems and Network Operation

Keynote Speakers

Regional eInfrastructure Development for South East Europes Research Communities
Ioannis Liabotis, GRNET, Greece

International HPC - Building bigger pyramide
Richard Kenway, NeSC, UK

LinkSCEEM2: Development of an HPC ecoSystem in the Eastern Mediterranean
Jens Wiegand, CaSToRC, Cyprus

The impact of GISELA Science Gateway (GSG) on the supported Latin America VRC's
Jesus Cruz Guzman, UNAM, Mexico

Numerical Study of Ultracold Quantum Gases: Formation of Faraday Patterns, Geometric Resonances, and Fragmentation
Antun Balaž, IPB, Serbia

Monte Carlo methods for Electron Transport: Scalability Study using HP-SEE infrastructure
Aneta Karaivanova, IICT-BAS, Bulgaria

Use of High Performance Computing in (Bio)Chemistry
Ivan Juranić, FCUB, Serbia

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E. Atanassov	D. Jakimovski	Lj. Pejov
A. Balaž	A. Karaivanova	B. Rybakin
V. Baran	P. Korosoglou	M. Spassova
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R. Gábor	K. Nikas	N. Vukmirović

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The Editors and the HP-SEE project would like to acknowledge valuable help and support by the National Library of Serbia which hosted the conference.

Contents

Simulation of Electron Transport Using HPC Infrastructure in South-Eastern Europe

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Abstract. In this work we present Monte Carlo simulation of ultrafast electron transport in semiconductors. We study the scalability of the presented algorithms using high-performance computing resources in South-Eastern Europe. Numerical results for parallel efficiency and computational cost are also presented. In addition we discuss the coordinated use of heterogeneous HPC resources for one and the same application in order to achieve a good performance.

Keywords: Electron transport, Monte Carlo algorithms, scalability, parallel efficiency, high-performance computations.

1 Introduction

The Monte Carlo Methods (MCMs) provide approximate solutions to a variety of mathematical problems by performing statistical sampling experiments on a computer [1–4]. They are based on the simulation of random variables whose mathematical expectations are equal to a given functional of the solution of the problem under consideration.

Many problems in a transport theory and related areas can be described mathematically by a second kind integral equation:

$$f = \mathbb{K}(f) + \phi, \tag{1}$$

where $\mathbb{K}$ is an integral operator. In general, the physical quantities of interest are determined by functionals of the type:

$$J_g(f) \equiv (g, f) = \int_G g(x) f(x) dx, \tag{2}$$

where the domain $G \subset \mathbb{R}^d$ and $\mathbb{R}^d$ is the d-dimensional Euclidean space. The functions $f(x)$ and $g(x)$ belong to any Banach space X and to the adjoint space X^*, respectively, and $f(x)$ is the solution of (1).

The mathematical concept of the MC approach is based on the iterative expansion of the solution of (1):

$$f_s = \mathbb{K}(f_{s-1}) + \phi, \;\; s = 1, 2, \ldots, \tag{3}$$

where s is the number of iterations. In fact (3) defines a Neumann series

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$$f_s = \phi + I\!K(\phi) + \ldots + I\!K^{s-1}(\phi) + I\!K^s(f_0), \qquad s > 1\,,$$

where $I\!K^s$ means the s-th iteration of $I\!K$. If the corresponding infinite series converges then the sum is an element f from the space X which satisfies (1).

The replacement of f by the Neumann series in (2), gives rise to a sum of consecutive terms which are evaluated by a MC method with the help of random estimators.

We define a random variable ξ such that its mathematical expectation is equal to $J(f)$: $E\xi = J(f)$.

Then we can define a MC method

$$\overline{\xi} = \frac{1}{N}\sum_{i=1}^{N} \xi^{(i)} \xrightarrow{P} J_g(f), \tag{4}$$

where $\xi^{(1)}, \ldots, \xi^{(N)}$ are independent values of ξ and $\xrightarrow{P}$ means stochastic convergence as $N \longrightarrow \infty$. The rate of convergence is evaluated by the "law of the three sigmas", [1, 3]:

$$P\left(|\overline{\xi} - J_g(f)| < 3\frac{\sqrt{Var(\xi)}}{\sqrt{N}}\right) \approx 0.997.$$

Here $Var(\xi) = E\xi^2 - E^2\xi$ is the variance of the MC estimator. Thus, a peculiarity of any MC estimator is that the result is obtained with a statistical error [1, 3, 7]. As N increases, the statistical error decreases proportionally to $N^{-1/2}$.

Thus, there are two types of errors – systematic (a truncation error) and stochastic (a probability error) [7, 8]. The systematic error depends on the number of iterations of the used iterative method, while the stochastic error is related to the the probabilistic nature of the MC method. From (1) and (3) one can get the value of the truncation error. If $f_0 = \phi$ then

$$f_s - f = I\!K^s(\phi - f).$$

The relation (4) still does not determine the computational MC algorithm: we must specify the modeling function (called sampling rule) for the random variable ξ.

$$\Theta = F(\beta_1, \beta_2, \ldots,), \tag{5}$$

where $\beta_1, \beta_2, \ldots,$ are uniformly distributed random numbers in the interval (0, 1). It is known that pseudorandom number generators are used to produce such sequences of numbers. They are based on specific mathematical algorithms. Now both relations (4) and (5) define a MC algorithm for estimating $J_g(f)$. The case when $g = \delta(x - x_0)$ is of special interest, because it is used for calculating the value of f at x_0, where $x_0 \in G$ is a fixed point.

Every iterative algorithm uses a finite number of iterations s. In practice we define a MC estimator ξ_s for computing the functional $J_g(f_s)$ with a statistical error. On the other hand ξ_s is a biased estimator for the functional $J_g(f)$ with

stochastic and truncation errors [7, 8]. The number of iterations can be a random variable when an ε-criterion is used to truncate the Neumann series or the corresponding Markov chain in the MC algorithm.

In order to compute the physical quantities of interest, we simulate a large number of trajectories, following the backward Monte Carlo algorithmic scheme. The trajectory is abolished when the time step becomes sufficiently small. All the physical quantities of interest are approximated as averages of random variables that are sampled in the Monte Carlo algorithm, so that one numerical trajectory contributes to all the quantities of interest, for better efficiency. Since the trajectories are independent, there is large amount of available parallelism that is exploited via MPI and, if possible, CUDA. In order to achieve accurate estimates, when the evolution time becomes large enough, we need billions of sampled trajectories. This requirements together with the high number of parallel processes or threads, puts a strain on the quality of the random number generator library. When quasi-random numbers are used, then one should be careful how to distribute the computations so that the desired error rate is attained.

The presented numerical results are obtained using HP-SEE computing infrastructure. The regional HPC infrastructure incorporates state of the art HPC clusters and two supercomputers BlueGene/P. The HP-SEE resources are located in 8 HPC resource centers in the countries: Bulgaria, Hungary, Romania, FYROM and Serbia. The total peak performance of the HP-SEE computing resources is about 120 Tflops in double precision. The GPU resources currently achieve 12 Tflops in single precision. More information can be found at www.hp-see.eu. In order to cope with the heterogeneity in the HP-SEE infrastructure and the evolution of the mathematical algorithms the application is built using a modular structure, containing several different modules/libraries. While we use standard libraries for random number generation like SPRNG and CUDA CURAND, we use our in-house libraries for scrambled quasi-random number generators, [4–6]. The main computations are organized in a library too, where we have different computational kernels for the case of CPU vs GPU computations. We also separate the parallelization part, based on MPI.

The paper is organized as follows. In Section 2 the quantum-kinetic equation is derived from a physical model describing electron transport in quantum wires. An integral form of the equation is obtained by reducing the dimensionality of space and momentum coordinates. The MC approach and corresponding MC algorithm are presented in Section 3. The numerical results using Bulgarian HPC resources are discussed in Section 4. Summary and directions for future work are given in Section 5.

2 The Quantum Kinetic Integral Equation

In the general case a Wigner equation for nanometer and femtosecond transport regime is derived from a three equations set model based on the generalized Wigner function [10]. The complete Wigner equation poses serious numerical

challenges. Two limiting versions of the equation corresponding to simplified physical conditions are considered in few works, namely, the Wigner-Boltzmann equation [11] and the homogeneous Levinson (or Barker-Ferry) equation [12, 13]. These equations are analyzed with various MCMs using spherical and cylindrical transformations to reduce the dimensions in the momentum space [14, 15]. The computer power of the European Grid infrastructure (EGI) in some cases is used to investigate above problems [16–18].

Here we consider a highly non-equilibrium electron distribution which propagates in a quantum semiconductor wire [19]. The electrons, which can be initially injected or optically generated in the wire, begin to interact with three-dimensional phonons. This is third limiting case, where the electron-phonon interaction is described on the quantum-kinetic level by the Levinson equation [20, 21], but the evolution problem becomes inhomogeneous due to the spatial dependence of the initial condition. The direction of the wire is chosen to be z, the corresponding component of the wave vector is k_z. The electrons are in the ground state $\Psi(\mathbf{r}_\perp)$ in the plane normal to the wire, which is an assumption consistent at low temperatures. The initial carrier distribution is assumed Gaussian both in energy and space coordinates, and an electric field can be applied along the wire.

The integral representation of the quantum kinetic equation for the electron Wigner function f_w in this case has the form [22]:

$$f_w(z,k_z,t) = f_w(z-\frac{\hbar k_z}{m}t+\frac{\hbar F}{2m}t^2,k_z,0)+ \tag{6}$$

$$\int_0^t dt'' \int_{t''}^t dt' \int d\mathbf{q}'_\perp \int dk'_z \left[S(k'_z,k_z,t',t'',\mathbf{q}'_\perp)\times\right.$$

$$f_w\left(z-\frac{\hbar k_z}{m}(t-t'')+\frac{\hbar F}{2m}(t^2-t''^2)+\frac{\hbar q'_z}{2m}(t'-t''),k'_z,t''\right)-$$

$$\left.S(k_z,k'_z,t',t''\mathbf{q}'_\perp)f_w\left(z-\frac{\hbar k_z}{m}(t-t'')+\frac{\hbar F}{2m}(t^2-t''^2)-\frac{\hbar q'_z}{2m}(t'-t''),k_z,t''\right)\right],$$

where

$$S(k'_z,k_z,t',t'',\mathbf{q}'_\perp) =$$

$$\frac{2V}{(2\pi)^3}|G(\mathbf{q}'_\perp)\mathcal{F}(\mathbf{q}'_\perp,k_z-k'_z)|^2\left[(n(\mathbf{q}')+1)\times\right.$$

$$\cos\left(\frac{\epsilon(k_z)-\epsilon(k'_z)+\hbar\omega_{\mathbf{q}'}}{\hbar}(t'-t'')+\frac{\hbar}{2m}Fq'_z(t'^2-t''^2)\right)+$$

$$\left.n(\mathbf{q}')\cos\left(\frac{\epsilon(k_z)-\epsilon(k'_z)-\hbar\omega_{\mathbf{q}'}}{\hbar}(t'-t'')+\frac{\hbar}{2m}Fq'_z(t'^2-t''^2)\right)\right].$$

Here, $f(z,k_z,t)$ is the Wigner function described in the $2D$ phase space of the carrier wave vector k_z and the position z, and t is the evolution time.

The electric force F depends on the electric field E as follows: $F = eE/\hbar$, where the electric field is along the direction of the wire, e being the electron charge and $\hbar$ - the Plank's constant.

$n_{\mathbf{q}'} = 1/(\exp(\hbar\omega_{\mathbf{q}'}/\mathcal{K}T) - 1)$ is the Bose function, where $\mathcal{K}$ is the Boltzmann constant and T is the temperature of the crystal, corresponds to an equilibrium distributed phonon bath.

$\hbar\omega_{\mathbf{q}'}$ is the phonon energy which generally depends on $\mathbf{q}' = \mathbf{q}'_\perp + q'_z = \mathbf{q}'_\perp + (k_z - k'_z)$, and $\varepsilon(k_z) = (\hbar^2 k_z^2)/2m$ is the electron energy.

$\mathcal{F}$ is obtained from the Fröhlich electron-phonon coupling by recalling the factor $i\hbar$ in the interaction Hamiltonian:

$$\mathcal{F}(\mathbf{q}'_\perp, k_z - k'_z) = -\left[\frac{2\pi e^2\omega_{\mathbf{q}'}}{\hbar V}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)\frac{1}{(\mathbf{q}')^2}\right]^{\frac{1}{2}},$$

where (ε_∞) and (ε_s) are the optical and static dielectric constants. The shape of the wire affects the electron-phonon coupling through the factor

$$G(\mathbf{q}'_\perp) = \int d\mathbf{r}_\perp e^{i\mathbf{q}'_\perp \mathbf{r}_\perp} |\Psi(\mathbf{r}_\perp)|^2,$$

where Ψ is the ground state of the electron system in the plane normal to the wire. If the cross-section of the wire is chosen to be a square with side a than we obtain:

$$|G(\mathbf{q}'_\perp)|^2 = |G(q'_x)G(q'_y)|^2 = \left(\frac{4\pi^2}{q'_x a\left((q'_x a)^2 - 4\pi^2\right)}\right)^2 4\sin^2(aq'_x/2)\times$$

$$\left(\frac{4\pi^2}{q'_y a\left((q'_y a)^2 - 4\pi^2\right)}\right)^2 4\sin^2(aq'_y/2).$$

3 Monte Carlo Approach

The equation (6) can be rewritten in the form:

$$f_w(z, k_z, t) = f_w(z - z(k_z, t), k_z, 0) + \tag{7}$$

$$\int_0^t dt'' \int_{t''}^t dt' \int_G d^3\mathbf{k}' K_1(k_z, \mathbf{k}', t', t'') \times f_w\left(z + h(k_z, q'_z, t, t', t'', F), k'_z, t''\right) +$$

$$\int_0^t dt'' \int_{t''}^t dt' \int_G d^3\mathbf{k}' K_2(k_z, \mathbf{k}', t', t'') \times f_w\left(z + h(k_z, -q'_z, t, t', t'', F), k_z, t''\right),$$

where

$$z(k_z, t) = \frac{\hbar k_z}{m}t - \frac{\hbar F}{2m}t^2,$$

$$h(k_z, q'_z, t, t', t'', F) = -\frac{\hbar k_z}{m}(t - t'') + \frac{\hbar F}{2m}(t^2 - t''^2) + \frac{\hbar q'_z}{2m}(t' - t''),$$

$$K_1(k_z, \mathbf{k}', t', t'') == S(k'_z, k_z, t', t'', \mathbf{q}'_\perp) = -K_2(\mathbf{k}', k_z, t', t''),$$

and

$$\int_G d^3\mathbf{k}' = \int d\mathbf{q}'_\perp \int_{-Q_2}^{Q_2} dk_z.$$

The values of the physical quantities are expressed by the following general functional of the solution of (7):

$$J_g(f) = \int_0^{\mathcal{T}} \int_D g(z, k_z, t) f_w(z, k_z, t) dz dk_z dt. \tag{8}$$

Here we specify that the phase space point (z, k_z) belongs to a rectangular domain $D = (-Q_1, Q_1) \times (-Q_2, Q_2)$, and $t \in (0, \mathcal{T})$.

The function $g(z, k_z, t)$ depends on the quantity of interest. Here, we are going to estimate by MC approach the Wigner function (6), the wave vector (and respectively the energy) $f(k_z, t)$, and the density distribution $n(z, t)$. The last two functions are given by the integrals

$$f(k_z, t) = \int \frac{dz}{2\pi} f_w(z, k_z, t) \text{ and, } n(z, t) = \int \frac{dk_z}{2\pi} f_w(z, k_z, t).$$

The MC estimator for evaluating the functional (8) using backward time evolution of the numerical trajectories can be constructed in the following way:

$$\xi_s[J_g(f)] = \frac{g(z, k_z, t)}{p_{in}(z, k_z, t)} W_0 f_w(., k_z, 0) + \frac{g(z, k_z, t)}{p_{in}(z, k_z, t)} \sum_{j=1}^{s} W_j^{\alpha} f_w\left(., k_{z,j}^{\alpha}, t_j\right). \tag{9}$$

Here

$$f_w\left(., k_{z,j}^{\alpha}, t_j\right) = \begin{cases} f_w\left(z + h(k_{z,j-1}, k_{z,j-1} - k_{z,j}, t_{j-1}, t'_j, t_j, F), k_{z,j}, t_j\right), \\ f_w\left(z + h(k_{z,j-1}, k_{z,j} - k_{z,j-1}, t_{j-1}, t'_j, t_j, F), k_{z,j-1}, t_j\right) \end{cases}$$

where $\alpha = 1$, in the first case, and $\alpha = 2$ in the second one;

$$W_j^{\alpha} = W_{j-1}^{\alpha} \frac{K_{\alpha}(k_{z\,j-1}, \mathbf{k}_j, t'_j, t_j)}{p_{\alpha} p_{tr}(\mathbf{k}_{j-1}, \mathbf{k}_j, t'_j, t_j)}, \text{ where } W_0^{\alpha} = W_0 = 1, \ \alpha = 1, 2, \ j = 1, \ldots, s.$$

The probabilities $p_{\alpha}, (\alpha = 1, 2)$ are chosen to be proportional to the absolute value of the kernels in (6). The initial density $p_{in}(z, k_z, t)$ and the transition density $p_{tr}(\mathbf{k}, \mathbf{k}', t', t'')$ are chosen to be tolerant[1] to the function $g(z, k_z, t)$ and the kernels, respectively. The first point (z, k_{z0}, t_0) in the Markov chain is chosen using the initial density, where k_{z0} is the third coordinate of the wave vector $\mathbf{k}_0$. Next points $(k_{z\,j}, t'_j, t_j) \in (-Q_2, Q_2) \times (t_j, t_{j-1}) \times (0, t_{j-1})$ of the Markov chain:

$$(k_{z0}, t_0) \to (k_{z1}, t'_1, t_1) \to \ldots \to (k_{z\,j}, t'_j, t_j) \to \ldots \to,$$

where $j = 1, 2, \ldots, s$ do not depend on the position z of the electrons. They are sampled using the transition density $p_{tr}(\mathbf{k}, \mathbf{k}', t', t'')$ as we take only the z-coordinate of the wave vector $\mathbf{k}$. Note the time t'_j conditionally depends on the

[1] $r(x)$ is tolerant to $g(x)$ if $r(x) > 0$ when $g(x) \neq 0$ and $r(x) \geq 0$ when $g(x) = 0$.

selected time t_j. The Markov chain terminates in time $t_s < \varepsilon_1$, where ε_1 is a fixed small positive number called a truncation parameter.

In order to evaluate the functional (8) by N independent samples of the estimator (9), we define a Monte Carlo method

$$\frac{1}{N}\sum_{i=1}^{N}(\xi_s[J_g(f)])_i \xrightarrow{P} J_g(f_s) \approx J_g(f), \tag{10}$$

where $\xrightarrow{P}$ means stochastic convergence as $N \to \infty$; f_s is the iterative solution obtained by the Neumann series of (7), and s is the number of iterations.

The relation (10) still does not determine the computational algorithm. To define a MC algorithm we have to specify the initial and transition densities, as well the modeling function (or sampling rule). The modeling function describes the rule needed to calculate the states of the Markov chain by using uniformly distributed random numbers in the interval $(0, 1)$. In our case we use SPRNG library [9].

Here, the following transition density is chosen:

$$p_{tr}(\mathbf{k}, \mathbf{k}', t', t'') = p(\mathbf{k}'/\mathbf{k})p(t, t', t''),$$

where

$$p(t, t', t'') = p(t, t'')p(t'/t'') = \frac{1}{t}\frac{1}{(t - t'')}$$

and

$$p(\mathbf{k}'/\mathbf{k}) = c_1/(\mathbf{k}' - \mathbf{k})^2$$

(c_1 is the normalized constant). Thus, if we know t, the next times t'' and t' are computed by using the inverse-transformation rule.

The wave vectors $\mathbf{k}'$ are sampled in the following algorithm:

1. **Sample** a random unit vector $\omega = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ as $\sin\theta = 2\sqrt{(\beta_1 - \beta_1^2)}$, $\cos\theta = 2\beta_1 - 1$, and $\varphi = 2\pi\beta_2$ where β_1 and β_2 are uniformly distributed numbers in (0, 1);
2. **Calculate** $l(\omega) = -\omega \cdot \mathbf{k} + (Q_2^2 + (\omega \cdot \mathbf{k})^2 - \mathbf{k}^2)^{\frac{1}{2}}$, where $\omega \cdot \mathbf{k}$ denotes a scalar product between two vectors;
3. **Sample** $\rho = l(\omega)\beta_3$, where β_3 is an uniformly distributed number in (0, 1);
4. **Calculate** $\mathbf{k}' = \mathbf{k} + \rho\omega$.

We note that we have to compute all three coordinates of the wave vector although we need only the third one. The choice of $p_{in}(z, k_z, t)$ depends on the function $g(z, k_z, t)$. The cases when

$$(i)\quad g(z, k_z, t) = \delta(z - z_0)\delta(k_z - k_{z,0})\delta(t - t_0),$$
$$(ii)\quad g(z, k_z, t) = \frac{1}{2\pi}\delta(k_z - k_{z,0})\delta(t - t_0),$$
$$(iii)\quad g(z, k_z, t) = \frac{1}{2\pi}\delta(z - z_0)\delta(t - t_0),$$

are of special interest, because they estimate the values of the Wigner function, wave vector and density distribution in fixed points.

4 Parallel Implementation and Numerical Results

The stochastic error for the (homogeneous) Levinson or Barker-Ferry models has order $O(\exp(c_2 t)\, N^{-1/2})$, where t is the evolution time and c_2 is a constant depending on the kernels of the obtained quantum kinetic equation [14, 15]. Using the same mathematical techniques as in [14], we can prove that the stochastic error of the MC estimator under consideration has order $O(\exp\left(c_3 t^2\right) N^{-1/2})$. The factor $\exp\left(c_3 t^2\right)$ contains the term t^2 because there is a double integration over the evolution time in the the quantum kinetic equation (6). The estimate shows that when t is fixed and $N \to \infty$ the error decreases, but for large t the factor $\exp\left(c_3 t^2\right)$ looks ominous. Therefore, the MC algorithm described above solves an NP-hard problem concerning the evolution time. The suggested importance sampling technique, which overcomes the singularity in the kernels, is not enough to solve the problem for long evolution time with small stochastic error. In order to decrease the stochastic error we have to increase N - the number of Markov chain realizations. For this aim, a lot of CPU power is needed for achieving acceptable accuracy at evolution times above 100 femtoseconds.

The suggested simulation was tested with new random number generators using permutations. Optimizations of transition density using genetic algorithm and acceptance-rejection methods were done. Initial scientific results for simulation of electron transport on quantum wires and are obtained.

It is known that the MC algorithms are perceived as computationally intensive and naturally parallel [23]. They can usually be implemented via the so-called dynamic *bag-of-work* model [24]. In this model, a large MC task is split into smaller independent subtasks, which are then executed separately. One process or thread is designated as "master" and is responsible for the communications with the "slave" processes or threads, which perform the actual computations. Then, the partial results are collected and used to assemble an accumulated result with smaller variance than that of a single copy. The inherent characteristics of MC algorithms and the dynamic *bag-of-work* model make them a natural fit for the parallel architectures.

Our numerical results are obtained using the following HPC platforms:

(i) The biggest HPC resource in Bulgaria is the supercomputer BlueGene/P which is deployed at the Executive Agency "Electronic Communications Networks and Information Systems". It has two racks with 2048 PowerPC 450 processors (32 bits, 850 MHz), 8192 processor cores and a total of 4 TB random access memory. The theoretical peak performance is 27.85 Tflops.

(ii) The other HPC platform is the HPC cluster deployed at the institute of information and communication technologies of the Bulgarian academy of sciences. This cluster consists of two racks which contain HP Cluster Platform Express 7000 enclosures with 36 blades BL 280c with dual Intel Xeon X5560 @ 2.8Ghz (total 576 cores), 24 GB RAM per blade. There are 8 storage and management controlling nodes 8 HP DL 380 G6 with dual Intel X5560 @ 2.8 Ghz and 32 GB RAM. All these servers are interconnected via non-blocking DDR Infiniband interconnect at 20Gbps line speed. The theoretical peak performance is 3.23 Tflops. The HPC cluster was upgraded with an HP SL390s G7 4U Lft Half