Parallel-Platform Based Numerical Simulation of Instabilities in Nanoscale Tunneling Devices

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***Abstract* — This paper presents theoretical results on instability processes in nanoscale tunneling structures that were obtained from a computationally improved physics-based simulator. The results were obtained from a numerical implementation of the Wigner-Poisson electron transport model upon a parallel-computing platform. These investigations considered various forms of multi-barrier resonant tunneling structures (RTSs) and they were used to test the robustness of the new modeling code. This improved modeling tool is shown to be fast and efficient with the potential to facilitate complete and rigorous studies of this time-dependent phenomenon. This is important because it will allow for the study of RTSs embedded in realistic circuit configurations. Hence, this advanced simulation tool will allow for the detailed study of RTS devices coupled to circuits where numerical simulations in time and iterative numerical optimization over the circuit parameters are required. Therefore, this work will enable the future study of RTS-based circuits operating at very high frequencies.**

I. Introduction

The accurate study of instability processes in nanoscale tunneling structures presents new and formidable theoretical challenges. A complete and rigorous study of electronic instabilities in nanostructures requires a detailed consideration of time-dependent quantum mechanical effects and this leads to computationally intensive numerical simulation. These investigations utilize a Wigner-Poisson model to study electron transport and intrinsic oscillations within double- and triple-barrier resonant tunneling structures (RTSs). Studies of time-dependent processes in nanostructures are important because it is believed that if the dynamics surrounding intrinsic oscillations can be understood and controlled then resonant tunneling structures have the potential to supply significant levels of output power at very high frequencies [1]. Here, an advanced and fast numerical algorithm is developed and implemented on a parallel-computing platform to facilitate these time-dependent investigations.

This paper presents the details of that numerical algorithm which allows for scientific investigations of the underlying origins of the quantum-based fluctuations. This fast solver is based on a complete restructuring of an original Wigner-Poisson simulator that was the first to theoretically demonstration intrinsic oscillations within resonant tunneling diodes. This improved solver also employs a new higher-order Runge-Kutta method and utilizes efficient programming constructs that encourage parallelization and the effective use of modern multi-level caches. This simulator allows for detailed investigations of the complex quantum-mechanical coupling within the multi-quantum-well systems. These scientific studies reveal fundamental insight into new methods for generating and enhancing intrinsic oscillations within multi-barrier quantum-well systems. Most importantly, the parallel-platform-based numerical simulator developed here will allow for the efficient study and advanced design of novel nanostructures that have the potential for functioning as very high frequency electronic sources. Here, practical design studies will require the detailed analysis of RTSs that are embedded within optimized circuit configurations. Hence, numerical optimization iterations are required for each time-domain simulation and this mandates the need for a fast and efficient electron transport simulator.

II. Wigner-Poisson Electron Transport Model

The Wigner function formulation of quantum mechanics was selected for these investigations into RTSs because of its many useful characteristics for the simulation of

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quantum-effect electronic devices, including the natural ability to handle dissipate and open-boundary systems. The Wigner function can be combined with the Poisson equation to provide for an adequate quantum mechanical description of the electron transport through tunneling nanostructures. The Wigner-Poisson (WP) model has been used by many groups in the past [2] and we have applied it to isolated RTSs to provide a qualitative explanation for the origins of the intrinsic oscillation [3] and to reveal techniques for enhancing the effect [4]. The focus of this work is towards improving the computational aspects related to numerically solving the WP model systems equations subject to the necessary and sufficient boundary conditions. Details regarding the derivation can be found elsewhere [2], but the model is a two equation system with the basic mathematical form

$$\frac{\partial f(x,k,t)}{\partial t} = W(f) \tag{1}$$

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{q^2}{\varepsilon}\left[N_d(x) - n(x)\right] \tag{2}$$

where the last term in Eq. (1) is given by

$$W(f) = C_1 k \frac{\partial f}{\partial x} - K_0(f) + \left.\frac{\partial f}{\partial t}\right|_{coll} \tag{3}$$

with the physical constant $C_1 = -h/(2\pi m^*)$ and the integral expression defined by

$$K_0(f) = \frac{1}{h}\int_{-\infty}^{\infty} dk' f(x,k') T(x,k')$$
$$T(x,k') = \int_0^L dy \left[U(x+y) - U(x-y)\right]\sin\left(2y(k-k')\right) \tag{4}$$

where L is the length of the tunneling structure under consideration. The last term in Eq. (3) is due to scattering dissipation and is modeled using the relaxation time approximation [1]. The boundary conditions on $f(x,k')$ at the emitter ($x = 0$) and collector ($x = L$) are specified to approximate flat-band transport. Here, equilibrium electron-distribution conditions are prescribed for values of the Wigner function at $x = 0$ that correspond to injection from the left (i.e., $k > 0$) and at $x = L$ that correspond to injection from the right (i.e., $k < 0$) according to the mathematical relations [1]

$$f(0, k>0) = \frac{4\pi m^* k_B T}{h^2}\ln\{1 + \mathrm{E}(\mu_0)\}$$
$$f(L, k<0) = \frac{4\pi m^* k_B T}{h^2}\ln\{1 + \mathrm{E}(\mu_L)\} \tag{5}$$
$$\mathrm{E}(z) = \exp\left[-\frac{1}{k_B T}\left(\frac{h^2 k^2}{8\pi^2 m^*} - z\right)\right]$$

where μ_0 and μ_L are the known Fermi energies at the source and collector, respectfully. The total potential energy function of the structure is given by

$$U(x) = u(x) + \Delta_c(x) \tag{6}$$

where $\Delta_c(x)$ is the band offset function the defines the barriers and wells within the RTS. The total potential energy is dependent on the Wigner function through

$$n(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ f(x,k) \tag{7}$$

which defines the electron density function *n(x)*. Once the electron density profile is defined *u(x)* can be determined by solving the Poisson equation in Eq. (2) using a specified doping profile function $N_d(x)$ and the applied bias boundary conditions

$$u(0) = 0, \text{ and } \quad u(L) = -V_{bias}. \tag{8}$$

Finally, the electron current density through the RTS is given by the relation

$$j(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ \frac{\hbar k}{m^*} f(x,k) \tag{9}$$

where m* is the free electron mass.

III. Parallel Code Development

A. Basic Goals

Many structural changes to the original code from [5] were needed to enable parallelism, conserve storage, and allow for the use of modern algorithms for temporal integration and solution of linear and nonlinear equations. The structural changes included,

- the reordering of loops to enhance locality of references to memory,
- the elimination of banded matrix storage to conserve memory and facilitate distributed memory computation, and
- the replacement of basic vector and matrix-vector loops with calls to hand-tuned computational kernels [6].

B. Development Steps & Details

The parallelization of the basic code has been done on a four-processor node of an IBM-SP3 at the North Carolina Supercomputing Center (NCSC). The shared memory environment is sufficiently powerful and has ample memory for simulations like those considered here [3]. Further work in more than one space dimension or the use of these models for optimization and design will require distributed memory platforms such as the SP or a Beowulf cluster.

The parallel results we report in this paper are based on loop-level parallelism using the OPEN-MP programming environment. In this mode of parallel programming the outermost loops of the few most computationally intensive components of the code are divided between a small number (2--16) of processors.

The critical part of the code is the computation of the integral in Eq. (4). Our approach to parallelism was to use OPEN-MP directives to obtain four-way parallelism of the outer loop and to use calls to LAPACK [6] to speed up the inner integrals.

C. Temporal Error Control

The original code from [3] used a semi-implicit form of the Euler methods. This method required the solution of a large linear system at each time step. The solve was performed with a direct solver for banded matrices. The expense of this linear solve was, according to our execution profiler, nearly 90% of the execution time and required most of the storage during the simulation.

We have replaced this algorithm with ROCK4 [7,8] an advanced Runge-Kutta code. ROCK4 uses varying orders and stages to maximize the intersection of the stability region and the negative real axis. In this way the disadvantages of an explicit method with respect to stability are reduced. An explicit method of this type incurs no linear algebra costs, either in computation or storage. A disadvantage of the ROCK4 code is that many more function evaluations must be computed at each time step to obtain the desired accuracy than would be necessary with a standard fourth order Runge-Kutta code [9]. The savings in linear algebra costs from the old code are significant, i.e., being at least a factor of five.

A fully implicit integrator such as VODEPK [10,11] which uses iterative methods for the large linear systems that are needed to compute Newton steps might be even more efficient if good preconditioners can be found [12]. The authors are investigating this option.

D. Simulation Results and Statistics

In the studies reported here, the simulation performance of the modified code was considered for three different types of RTSs. Namely, the modified simulator was applied to the following basic RTS types,

(i) the basic double-barrier RTS that originally demonstrated intrinsic oscillation behavior [3],
(ii) a modified double-barrier RTS that utilizes emitter engineering of the doping profile to enhance the intrinsic oscillations, and
(iii) a new double-well RTS that is being consider as a alternative methodology for realizing subband-coupling induced oscillatory behavior.

In the previous studies, time-domain simulations were performed at a discrete set of applied bias that were slowly sweep forward from zero to some maximum value and then backwards to zero. Examples of the average current-voltage (I-V) characteristic across a forward voltage sweep that were obtained from this previous study on a type-(ii) RTS are given in Fig. 1.

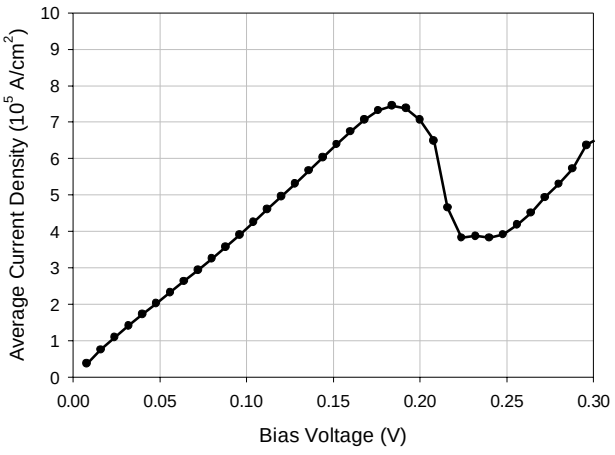

Fig. 1 Averaged I-V results from a type-(ii) RTS.

At certain values of applied bias near the bottom of the negative-differential-region, the RTS will demonstrate intrinsic oscillations due to quantum subband-coupling and this process is illustrated in Figure 2.

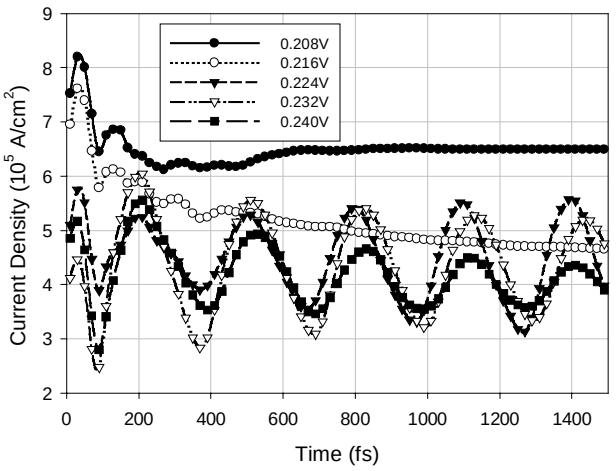

Fig. 2 Current verses time from a type-(ii) RTS.

The results obtained from the parallel simulator are both qualitatively and quantitatively similar to the earlier work. Most importantly, the new code reduces the total simulation times from days to hours. Table I presents a comparison of the simulation times on one and four processors using the IBM SP-3 at the NCSC. The performance of the code was estimated with a profiler and we found that the one critical loop took 80-90% of the execution time (ET) when in serial

Table I. CPU time in seconds.

RTS Type	1 processor	4 processors	Efficiency
(i)	16784	6515	0.64
(ii)	21145	7748	0.68
(iii)	32138	13025	0.62

mode. A single OPEN-MP directive was applied to parallelize this same critical loop and efficiencies of 60-70% were obtained using four processors. Here, parallel efficiency is defined by the relation:

$$\frac{ET\ on\ One\ \mathrm{Pr}ocessor}{ET\ on\ Four\ \mathrm{Pr}ocessors \times 4}$$

This is very good performance and is consistent with almost perfect speedup for a block that takes 80-85% of the CPU time for the serial code.

IV. Conclusion

The results of these computational studies have demonstrated that parallel-platforms offer considerable speedup in the simulation of instabilities in resonant tunneling structures (RTSs). Hence, this work suggests that modern scalable computer architectures and loop-level parallelism may be exploited to facilitate the future study of nanoelectronic-based circuits operating at very high frequencies.

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