

Massively Parallel Solution of Quantum Transport Problems

P. Balasingam and V. P. Roychowdhury
School of Electrical Engineering
Purdue University
West Lafayette, IN 47906

Abstract

A numerically intensive program used in the study of quantum transport has been implemented on a MasPar MP-1. Parallel solution of the problem, which possesses parallelism to varying degrees throughout the application, is described.

1 Introduction

The implementation of large application programs in a manner which efficiently utilizes a parallel computer, is a topic of considerable current interest. In the following, we discuss the implementation of a numerically intensive program on a MasPar MP-1, which is an SIMD machine consisting of a square array of 16,384 processing elements (PE).

The application considered in this work arises in the investigation of electron devices, an area which has historically relied heavily on computer simulations for the choice of optimal design parameters. As electron devices become smaller, the numerical models used for their simulation grow in complexity, since fundamental physical phenomena begin to influence device behavior. In particular, the investigation of transport in nanostructured semiconductor devices is numerically very intensive. In the following section we describe aspects of quantum transport in such devices, and establish the scope of the computational requirements. Methods adopted for effecting a parallel solution of the problem, are outlined in section 3.

2 Computational Quantum Transport

The theoretical treatment of coherent electron transport in semiconductor devices is usually carried out using the Landauer-Büttiker formalism [1], which allows the determination of measurable transport coefficients, in terms of scattering probabilities obtain-

able by solving the Schrödinger equation over planar geometries.

The scattering problem can be rendered as a complex-valued linear system $Ax = b$, where the coefficient matrix A is obtained by carrying out a finite-difference discretization of the Schrödinger equation, and imposing boundary conditions which permit the entry and emission of waves at the various ports. The discretization is carried out so that each mesh-point coincides with an atomic lattice site of the underlying semiconductor. The matrix A is sparse, with a typical size of 512×512 . In general for a given A solutions for multiple right-hand sides b will be needed, each b corresponding to different modes (indexed ν), or ports (indexed p) of incidence. Typically there will be several tens of modes incident from each of several ports. For systems maintained at non-zero temperatures, or operated at finite applied biases, linear system solutions are performed for a large number of different matrices A , each corresponding to a different electron energy ϵ . Computationally, this constitutes the most time consuming step.

Now, the complete device consists of the scattering region considered above, as well as long leads of width W_p and length L_p , connected to the scattering region at the various ports p . It is necessary to determine the local chemical potential $\mu(x, y)$, the electrostatic potential $\phi(x, y)$ as well as the local current density $\vec{J}(x, y)$ throughout these leads. The first step for the evaluation of these quantities is the reconstruction of the wavefunctions $\psi_{\nu,p}(\epsilon; x, y)$ throughout these leads, using the scattering amplitudes obtained from the linear system solution.

Numerical simulators developed on less powerful machines have been used for the investigation of transport under simplifying assumptions, which render the computed results only qualitatively comparable with experimental findings. More realistic simulations require the treatment of finite temperature as well as large applied bias conditions, on devices with large device dimensions. The high execution rates, as well

as the possibility of treating larger problem sizes on the MasPar MP-1 have permitted the exploration of realistic physical parameters.

3 Parallel Solution

Parallelization of this application can be separated into two different phases : (i) solution of the scattering problem represented by $Ax = b$, (ii) evaluation of the physical quantities, $\psi_{\nu,p}(\epsilon; x, y)$, $\mu(x, y)$, $\tilde{J}(x, y)$ and $\phi(x, y)$, within the leads. Experimentally measurable physical quantities can be determined with minimal computing once the above physical quantities are known. The program has been implemented in MPL, a version of the C language with parallel features suitable for the MasPar MP-1. The program manipulates complex valued quantities, and its performance, as well as its memory requirements are accordingly affected.

3.1 Scattering Problem

For a rectangular scattering region of length L and width W the matrix A corresponding to the scattering problem, consist of $W \times W$ submatrices, arranged in an $(L + 2) \times (L + 2)$ block matrix. The 128×128 PE array is then divided into subarrays of $[128/(L + 2)] \times [128/(L + 2)]$ PEs each, and the $W \times W$ blocks of the matrix A are assigned to each PE subarray. For sufficiently large problem sizes, each PE will be assigned several matrix elements. Since information transfer within a PE is more efficient than communication between PEs, the algorithm performs better as the problem size increases, before becoming bottlenecked by memory constraints. Although, the A matrices are sparse and regular, in general they fail to converge within iterative solution schemes, which are well suited for the MasPar architecture. Therefore, a direct Gaussian elimination algorithm has been used for most of the linear system solutions. However, the time-dependent scattering problem is amenable to be solved using an iterative algorithm. The advantage of the iterative approach is that much larger problems can be mapped to the PE array, since each equation of the linear system can be associated with a single PE.

3.2 Physical Quantities

The physical quantities of interest are evaluated within each of the current leads p , which are attached to the scatterer discussed above. The current leads

are rectangular, with the p^{th} lead having dimensions $W_p \times L_p$. Each grid point (x, y) within the p^{th} lead is associated with a single PE, and the electron state $\psi_{\nu,p}(\epsilon; x, y)$ for every mode ν is evaluated in parallel at each point. These functions are evaluated in terms of a linear combination of periodic functions defined on the mesh, an example of which is given below,

$$\psi_{\nu,p}(x, y) = \sum_{\mu=1}^{W_p} t_{\mu,p} e^{ik_{\mu}x} \sin\left(\frac{\pi\mu y}{W_p + 1}\right)$$

where the scattering amplitude $t_{\mu,p}$ is obtained from the linear system solution described in the preceding sub-section.

Once the quantities $\psi_{\nu,p}(x, y)$ are evaluated for every ν the local current density $\tilde{J}(x, y)$ as well as the local chemical potential $\mu(x, y)$ can be determined through highly parallel local operations, which require, at most, information from nearest neighbor PEs. The electrostatic potential $\phi(x, y)$ is determined by solving Poisson's equation $\nabla^2\phi = -\rho(x, y)$, where the charge density ρ is obtained as a weighted sum of $|\psi_{\nu,p}(\epsilon; x, y)|^2$, summed over ν and ϵ . The discretized version of Poisson's equation is efficiently solved in parallel using an iterative Jacobi method, which too requires only nearest neighbor communication patterns.

4 Conclusions

A numerically intensive program for the simulation of quantum transport in small structures has been implemented on a MasPar MP-1. The high degree of parallelism inherent in numerically intensive sections of the problem has been exploited, and devices with realistic dimensions and operating conditions have been investigated.

Acknowledgements

This work is supported by funds provided by a General Motors faculty fellowship provided by Purdue University.

References

- [1] M. Büttiker, Y. Imry, R. Landauer and S. Pinhas "Generalized Many-channel Conductance Formula with Application to Small Rings" *Phys. Rev. B*, Vol. 31, pp. 6207-6215, 1985.