EFFICIENT SIMULATION OF SINGLE-ELECTRON DYNAMICS IN COUPLED QUANTUM DOTS

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ABSTRACT

The simulation and modeling of the tunneling dynamics between coupled quantum dots requires a numerical solution for the time dependent Schrödinger equation. This paper presents an optimization method for MATLAB code which implements an efficient simulation for real-time single-electron dynamics in cells with two coupled quantum dots.

1. INTRODUCTION

The time dependent Schrödinger equation is:

$$\left[-\frac{\hbar}{2m}\nabla^2 + eV(\mathbf{r})\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} \quad (1)$$

For the simulation of a one-dimensional Schrödinger equation, a discrete update rule, developed by Fredkin and Barton, that is reversible in time and guarantees energy conservation, as shown by Feyman [1], was used. The update rules are shown in Eqs. (2) - (5), where $m \in [0,M]$, m is the integer that represents the position, in discrete values, for one dimension and M is the array size. In all simulations the cell dimension was 10nm.

$$X_m = X_m - \left[\alpha\frac{\Delta t}{\Delta x^2}\left(Y_{m+1} - 2Y_m + Y_{m-1}\right) + \beta\cdot\Delta t\cdot V_m\cdot Y_m\right] \quad (2)$$

$$Y_m = Y_m - \left[\alpha\frac{\Delta t}{\Delta x^2}\left(X_{m+1} - 2X_m + X_{m-1}\right) + \beta\cdot\Delta t\cdot V_m\cdot X_m\right] \quad (3)$$

$$\alpha = \frac{\hbar}{2m} \quad (4)$$

$$\beta = \frac{-2}{\hbar} \quad (5)$$

The real (X) and imaginary (Y) of the psi wave function are calculated in sequence. The time step, Δt, of the simulation was chosen to guarantee stability and convergence of the algorithm for the available fundamental states of the simulated system. Current and charge probability densities, and a damping potential, are also calculated.

The self-capacitance effect, considered in the simulations, represents the influence of the redistribution of image charges in the proximities of each quantum dot in the cell. This effect uses a simple linear model, described by equation (6), where ΔE is the variation of energy potential between the wells. The charges q_1 and q_2 are fractions of the fundamental electron charge, which are present in each quantum dot. Finally, C_{eff} is the value of the effective self-capacitance, assuming that it is equal for both quantum dots.

$$\Delta E = e\frac{q_1 - q_2}{C_{eff}} \quad (6)$$

2. OPTIMIZATION METHODOLOGY

The initial, non-optimized code was written using the mathematical simulation software MATLAB [2] and its programming language, by M. V. Batistuta, *et. al* [3]. The ease of generating graphical interfaces in its environment and its numerous built in functions were determinant for the choice. On the other hand, the MATLAB programming language is parsed, where code is interpreted and translated into computer operations in real-time. This leads to a relatively slow and inefficient simulation program, if compared with other languages, like C and C++ for instance. Consequently, code optimization is crucial for an efficient real-time simulation of real-time single electron dynamics.

The first step towards optimization consisted in using vectorization techniques on the code that calculates the initial values of the vectors that represent the double quantum dot cell and the wave function of the excess electron. As a result, all loops that were used in this part of the code were eliminated, being substituted by vectorized functions, leading to a faster calculation of the initial state of the system.

Also, the update of the real and imaginary part of the wave function was done using only vector functions. Vectorization was applied, finally, to the calculations of the current, total energy and self-capacitance of the coupled quantum dot system. This optimization process resulted in a lighter and more efficient code with only a few loops.

3. SIMULATION RESULTS

To compare the original and optimized codes, an analysis of the iteration time, corresponding to one calculation of X and Y was made. For each different array size (M), the system was simulated for 1000 time-steps and the mean time for each simulation was measured. The results are shown in Fig. 1.

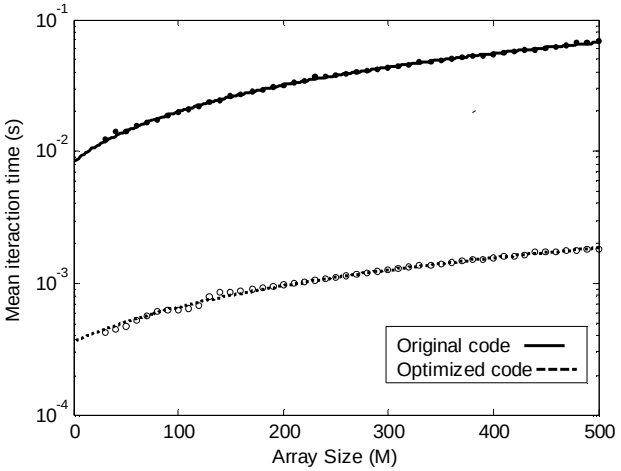

Figure 1: Mean iteration time for different array sizes (*M*).

It can be clearly observed that the iteration time varies linearly with the array size. Besides that, it can also be seen that the optimized code has a mean iteration time almost 20 times smaller than the original code. Consequently, a precise simulation of the behavior of the double quantum-dot cell can be obtained, within MATLAB, with reduced computational effort. It can also be seen that the optimized code has a mean iteration time almost 20 times smaller than the original code.

Therefore, a relatively simple optimization method reduced significantly the time to simulate the real-time single-electron dynamics in the cell, with two coupled quantum dots. Moreover, an efficient code allows the inclusion of complementary code, for more complex analysis.

4. CONCLUSIONS AND FUTURE WORK

In this paper, a methodology for optimizing the simulation of single-electron dynamics in cells with two coupled quantum dots was presented. The simulation of the time dependent Schrödinger equation was based on the discrete update rule, developed by Fredkin and Barton. The effects of simple optimization methods reduced significantly the iteration time of the original code. Moreover, the faster algorithm allows future inclusion of other physical effects and the simulation of large coupled quantum dot systems. Future work will include the creation of digital environment for modeling and simulation of electron dynamics in large-scale coupled quantum-dot systems.

4. ACKNOLEDGMENTS

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10. REFERENCES

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