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Meshless Solution of the 3-D Semiconductor Poisson Equation

Z. Aksamija, and U. Ravaioli
Beckman Institute, University of Illinois, 405 N. Mathews, 61801 Urbana IL., U.S.A.
e-mail: aksamija@uiuc.edu

INTRODUCTION

The Poisson equation arises frequently from problems in applied physics, fluid dynamics and electrical engineering. We solve the Poisson equation in order to obtain the electric potential in a semiconductor device and find the electric field for electronic simulation. Finding a suitable solution mesh is complicated by the fact that there is usually a large region at the bottom of the device which has few particles and is of little interest. On the other hand, the channel region at the top of the device is small but the detailed solution in it is important. There are also numerous problems arising from assigning charge to a regular mesh [1], [2]. Therefore a regular rectangular mesh is the least desirable solution. An alternative approach is to treat each individual particle as a mesh point. Meshless methods have been proposed in the past [3], [4]. This work starts with a series expansion and aims at reaching a solution which is continuous and infinitely differentiable, and optimal in the least squares sense.

NUMERICAL APPROACH

In order to seek a solution, we expand the potential into sinusoidal components. Since we have fixed boundary conditions (the voltage at the edges/contacts is given), we know all solutions must be a super-position of sinusoidal harmonics, so we write the solution as in (1), where L_x, L_y and L_z are the lengths of the solution domain in each respective direction.

$$V(x, y, z) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \sum_{n=1}^{N_n} \Phi(l, m, n)$$
$$sin\left(\frac{\pi l}{L_x} x\right) sin\left(\frac{\pi m}{L_y} y\right) sin\left(\frac{\pi n}{L_z} z\right) \quad (1)$$

Now the Laplacian operator can be applied analytically to each of the terms above. This produces one equation for each particle. Taken together, we have a system of equations with $N_l \times N_m \times N_n$ terms in each row, and P rows, where $N_l, N_m,$ and N_n is the number of harmonic components in each direction and P is the total number of particles. This algebraic system can be expressed in matrix form as $A\Phi = \rho \setminus \epsilon$ and solved for Φ. In order to obtain an overdetermined system of equations, we must have more points than harmonic components. Then the system can be solved by standard lest-squares techniques or by fast iterative methods [5].

RESULTS

A test was performed by solving the system above for a rectangular region with zero boundary conditions and uniformly randomly distributed charges. The 3-D results in Fig. 2 shows good smoothness and precision. Fig. 3 compares the numerical solution to the analytical one we would expect from a uniform charge distribution.

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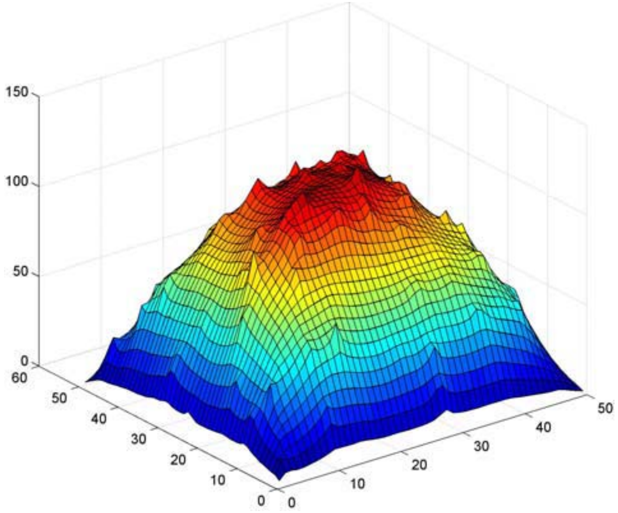

Fig. 1. Solution obtained finite differences with a CIC charge assignment. Only a horizontal cut through the 3-D computational domain is shown.

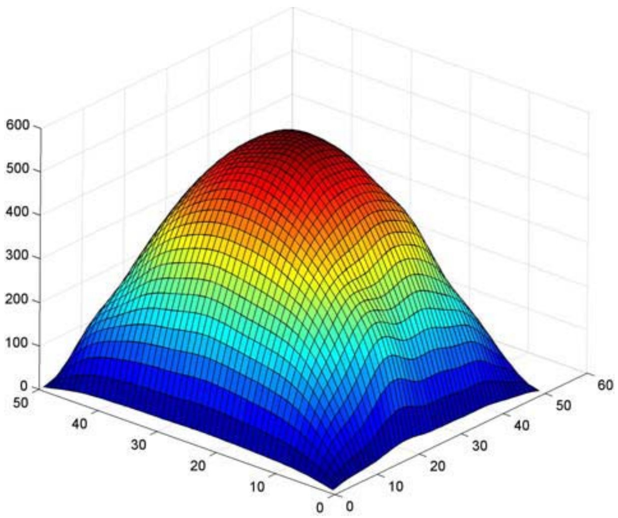

Fig. 2. Solution obtained from the meshless approach. Only a horizontal cut through the 3-D computational domain is shown.

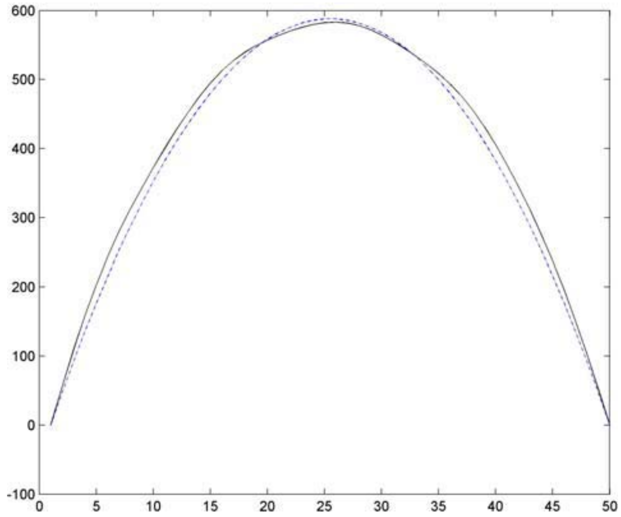

Fig. 3. Comparison of solutions. The solid line is the numerically computed solution, and the dashed line is the analytical quadratic solution which assumes a uniform distribution. The agreement is excellent and the small discrepancy is due to the random assignment of charge locations.

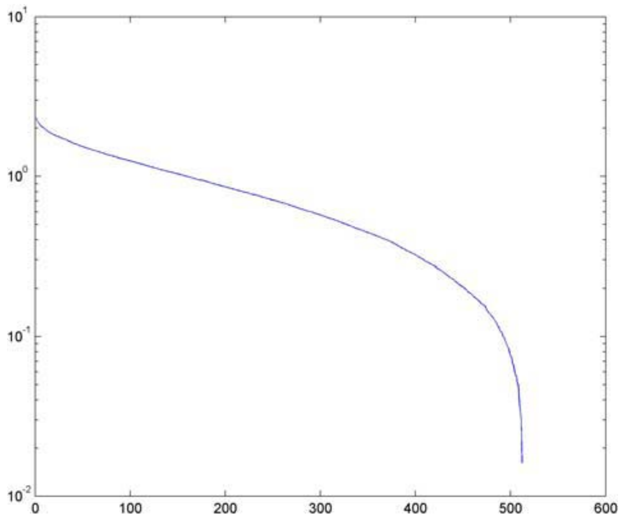

Fig. 4. Logarithmic plot of the singular values of the matrix A. The ratio of the largest to the smallest singular value is around 100, meaning that the solution is sufficiently well conditioned. Experience has shown that increasing the number of harmonics N beyond the number of points P drastically increases the condition number and makes the solution ill-conditioned.