Spectral Element Method for the Schrödinger-Poisson System

Candong Cheng, Qing Huo Liu, *Senior Member, IEEE,* and Hisham Z. Massoud, *Fellow, IEEE*
Electrical and Computer Engineering, Duke University, Durham, NC 27708
Email: ccheng@ee.duke.edu

A novel fast spectral element method (SEM) with exponential accuracy for the self-consistent solution of the Schrödinger-Poisson system has been developed for the simulation of semiconductor nanodevices. Gauss-Lobatto-Legendre polynomials were used to represent the unknown fields in the Schrödinger and Poisson equations. The model allows arbitrary potential energy and charge distributions. The predictor-corrector algorithm is applied to solve the outer loop of the self-consistent iteration. The nonlinear Poisson equation is solved by Newton's method to increase the efficiency of the system. Numerical results confirm the spectral accuracy of this method. The method can achieve high accuracy with a low sampling density, thus significantly lowering the computer memory and computational time compared to conventional methods. Our typical examples show that, compared with the second-order finite-difference (FD) method to reach 1% and 0.1% accuracy, this method is about 125 and 778 times faster in CPU time with only 0.25% and 0.0085% of memory usage, respectively. The high efficiency and the flexibility on the geometry make this method a promising method in large-scale nanodevice simulation problems.

In this paper, the spectral element method is first applied on an infinite quantum well under an external bias to solve the Schrödinger equation. Table I shows the comparison of the CPU time and memory requirements of this method and a 2nd-order finite-difference method for a three-region quantum well system under external bias. To reach 1% of accuracy, the spectral element method is 125 times faster with only 1/397 of the memory required by the FD method. Similarly, to reach 0.1% of accuracy, the spectral element method is 778 times faster with 1/11741 of the memory required by the FD method. This efficiency improvement can be understood by plotting the error with the number of discretization points, as shown in Figure 1. From this figure, we observe that the spectral element method has an exponential accuracy, while the finite-difference method only has a 2nd order accuracy.

Next, the same method is applied to solve the Poisson equation for a MOSFET. As shown in Figure 2, the exponential accuracy is also observed, implying the similar efficiency and accuracy as the Schrödinger's solver.

The coupled Schrödinger-Poisson system is currently under investigation. As both the Schrödinger and Poisson solvers have exponential accuracy and are independent, an exponential accuracy is expected for the coupled solver, and will have the similar efficiency. Numerical results will be reported shortly.

Table I. Comparison of the computational efficiency of the SEM and FD method for the eigenenergy of a GaAs/Al$_{0.3}$Ga$_{0.7}$As quantum well under bias (f$_0$=55). The central region has width of d=30 um with the outer boundaries x$_L$=-0.8d and x$_R$=0.8d truncated by infinite potential walls. The results show that to reach the same accuracy, the spectral element method is far more efficient than the finite-difference method in the CPU time and the memory usage.

Error			≤1%		
	N$_1$, N$_2$, N$_3$	Actual Error	ε$_3$	CPU	Memory
FD	29,68,29	0.996%	6.46428	0.2s	57188
SEM	4,9,4	0.683%	6.48474	0.0016s	144
Efficiency	--	--	--	125	397

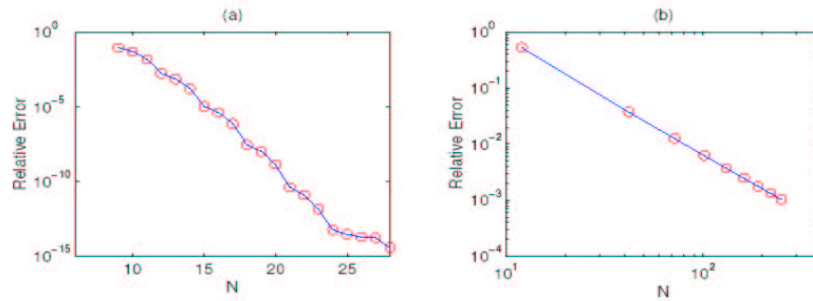| Error			≤0.1%		
	N$_1$, N$_2$, N$_3$	Actual Error	ε$_3$	CPU	Memory
FD	99,230,99	0.099%	6.52278	1.40s	2254230
SEM	4,12,4	0.0347%	6.53157	0.0018s	192
Efficiency	--	--	--	778	11741

Figure 1: The relative error of the third normalized eigenenergy as a function of N in an infinite quantum well under normalized bias f$_0$=90 in (a) the spectral element method (SEM) and (b) finite-difference (FD) method. The results show that the error of eigenenergy decreases exponentially for the SEM, and only quadratically for the FD method.
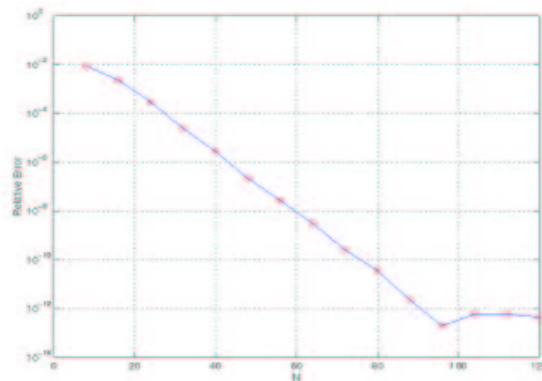

Figure 2: The relative error of the electrical potential at the interface of the bulk as a function of N in the SEM Poisson solver for the MOSFET.