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14. ABSTRACT During this project, we have conducted development of numerical methods for various quantum mechanics models. Accomplishments have been made in the following areas: [1] Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations, [2] Effect of Boundary treatment on transport current in nano-MOSFETs. [3] Accuracy of Frensey inflow boundary conditions.					
15. SUBJECT TERMS quantum transport, nano-devices					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Wei Cai
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 704-687-4581

Report Title

Multi-scale and Multi-physics Numerical Methods For Modeling Transport in Mesoscopic Systems

ABSTRACT

During this project, we have conducted development of numerical methods for various quantum mechanics models. Accomplishments have been made in the following areas: [1] Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations, [2] Effect of Boundary treatment on transport current in nano-MOSFETs. [3] Accuracy of Frensley inflow boundary conditions.

Three journal publications have resulted from this effort.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
2011/08/26 1 2	Sihong Shao, Tiao Lu, Wei Cai. Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (3 2010): 0. doi: 10.4208/cicp.080509.310310s
2011/08/26 1 1	Wei Cai, Haiyan Jiang. Effect of boundary treatments on quantum transport current in the Green's function and Wigner distribution methods for a nano-scale DG-MOSFET, Journal of Computational Physics, (06 2010): 0. doi: 10.1016/j.jcp.2010.02.008
2011/08/26 1 3	Haiyan Jiang, Wei Cai, Raphael Tsu. Accuracy of the Frensley inflow boundary condition for Wigner equations in simulating resonant tunneling diodes, Journal of Computational Physics, (03 2011): 0. doi: 10.1016/j.jcp.2010.12.002

TOTAL: 3

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Haiyan Jiang	1.00
Steve Xin	0.25
Tiao Lu	0.25
FTE Equivalent:	1.50
Total Number:	3

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Wei Cai	0.25	
FTE Equivalent:	0.25	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

- The number of undergraduates funded by this agreement who graduated during this period: 0.00
- The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00
- The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00
- Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00
- Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00
- The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00
- The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

***Statement of the problem:

Due to the quantum nature of the electron transport in nanoscale devices, quantum transport models including Wigner equations and Non-equilibrium Green's functions are required to compute the current in those devices. Our main goal is to develop accurate and efficient numerical algorithms to compute these quantum transport models.

***Summary of Results:

We have made scientific progress in the following three areas of accomplishments:

In paper [1] on Conservative Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations. We designed and tested a new conservative adaptive spectral element method using cell-average formulation for the time dependent Wigner equations for non-equilibrium transport. The main challenge in this approach is the cost associated with the high dimensional problem in phase space variables (6 for 3-D device in addition to the time variable). To reduce this cost, we propose a Cell-Average representation of the Wigner distribution function $f(x; k; t)$ in the k -space, which allows exact enforcement of conservation of electron mass and adaptive meshing in the phase space using domain decomposition technique.

In paper [2] on effect of treatment of quantum device boundary on the transport current: A nano-scale Double gate MOSFET is investigated with both nonequilibrium Green's function (NEGF) and Wigner distribution methods, each with different treatment of the device boundaries. The NEGF handles the device-contact condition through a self energy term while the Wigner distribution function method employs inflow flux conditions using the Fermi-Dirac electron distribution inside the contact. Numerical results have shown higher transport current at a given gate voltage with the Wigner distribution approach. As the current-voltage (I-V curve) characteristic is the key measurement of a quantum device, correct current simulation will be important in quantum device modeling.

In paper [3] on Accuracy of Frensey inflow boundary conditions: Continuing the studies in [2] above, We carefully investigate the accuracy of the Frensey inflow boundary condition of the Wigner equation in computing the I-V characteristics of a Resonant Tunneling Diode (RTD). We found that the Frensey inflow boundary condition for incoming electrons holds only exactly infinite away from the active device region and its accuracy depends on the length of contacts included in the simulation. For this study, the non-equilibrium Green's function (NEGF) with a Dirichlet to Neumann mapping boundary condition is used for comparison. The I-V characteristics of the RTD are found to agree between self-consistent NEGF and Wigner methods at low biaspotentials only with sufficiently large GaAs contact lengths.

*** Bibliography

[1] Sihong Shao, Tiao Lu, Wei Cai. Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (3 2010): 0. doi: 10.4208/cicp.080509.310310s

[2] Wei Cai, Haiyan Jiang. Effect of boundary treatments on quantum transport current in the Green's function and Wigner distribution methods for a nano-scale DG-MOSFET, Journal of Computational Physics, (06 2010): 0. doi: 10.1016/j.jcp.2010.02.008

[3] Haiyan Jiang, Wei Cai, Raphael Tsu. Accuracy of the Frensey inflow boundary condition for Wigner equations in simulating resonant tunneling diodes, Journal of Computational Physics, (03 2011): 0. doi: 10.1016/j.jcp.2010.12.002

Technology Transfer