REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
13-10-2014	Final Report	15-Aug-2011 - 14-Aug-2014

4. TITLE AND SUBTITLE
Multi-scale and Multi-physics Numerical Methods For Modeling Transport in Mesoscopic Systems (a proposal submitted to Numerical Analysis Program, Mathematical Sciences)

5a. CONTRACT NUMBER
W911NF-11-1-0364

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
57926-MA.13

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
In this project, we have accomplished in development of algorithms to model transport and eletromagnetic processes in mesoscopic systems such as nano-electronics and biological membrane, and layered inhomogeneous media.
Specifically, the following results have been obtained resulting in the publication of 6 peer-referred journal papers and a third part of a Cambridge University Press book.

15. SUBJECT TERMS
Transport, Electromagnetic Phenomena, nano-electronics, ion channels, layered media

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Wei Cai
					19b. TELEPHONE NUMBER
					704-687-0628

Report Title

Multi-scale and Multi-physics Numerical Methods For Modeling Transport in Mesoscopic Systems (a proposal submitted to Numerical Analysis Program, Mathematical Sciences)

ABSTRACT

In this project, we have accomplished in development of algorithms to model transport and eletromagnetic processes in mesoscopic systems such as nano-electronics and biological membrane, and layered inhomogeneous media.
Specifically, the following results have been obtained resulting in the publication of 6 peer-referred journal papers and a third part of a Cambridge University Press book.

(1) fast integral solver for quantum dots in 3-D layered media. The fast solver is based on a window accelerated method for computing the layered Green's function and wide band Fast multipole methods for Hankel waves.
(2) a new linear scaling discontinuous Galerkin density functional theory, which provide a brand new approach in combining physics-based orbitals
and piece-wise polynomial finite element basis in finding the ground state energy of the DFT for quantum systems.
(3) numerical methods for computation of electrostatics in ion-channel transport,
(4) a new parallel solver for elliptic PDEs by combining random walk Feynmann-Kac formula and local boundary integral equations for extreme computing,
(5) an improved device adaptive inflow boundary condition for Wigner quantum transport equations.

Also, a book titled "Computational Methods for Electromagnetic Phenomena: electrostatics in solvation, scattering and electron transport" was published by Cambridge University Press on Feb. 25, 2013. The work on electron transport (Part III of the book) results from this project.

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)

Received		Paper
08/07/2013	3.00	Tiao Lu, Wei Cai, Jianguo Xin, Yinglong Guo. Linear Scaling Discontinuous Galerkin Density Matrix Minimization Method with Local Orbital Enriched Finite Element Basis: 1-D Lattice Model System, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (08 2013): 276. doi: 10.4208/cicp.290212.240812a
08/15/2012	1.00	Wei Cai, Min Hyung Cho. A parallel fast algorithm for computing the Helmholtz integral operator in 3-D layered media, Journal of Computational Physics, (07 2012): 0. doi: 10.1016/j.jcp.2012.05.022
10/13/2014	7.00	Min Hyung Cho, Wei Cai. A parallel fast algorithm for computing the Helmholtz integral operatorin 3-D layered media, Journal of Computational Physics, (05 2012): 5910. doi:
10/13/2014	8.00	Tiao Lu,Wei Cai, Jianguo Xin,Yinglong Guo. Linear Scaling Discontinuous Galerkin Density MatrixMinimization Method with Local Orbital EnrichedFinite Element Basis: 1-D Lattice Model System, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (08 2013): 276. doi:
10/13/2014	11.00	CHANHAO YAN, WEI CAI, AND XUAN ZENG. A PARALLEL METHOD FOR SOLVING LAPLACEEQUATIONS WITH DIRICHLET DATA USING LOCALBOUNDARY INTEGRAL EQUATIONS AND RANDOMWALKS, SIAM J Scientific Computing, (08 2013): 868. doi:
10/13/2014	12.00	CHO Min Hyung & Wei Cai. Fast integral equation solver for Maxwell’s equationsin layered media with FMM for Bessel functions, Science China Mathematics, (12 2013): 2561. doi:

TOTAL: 6

Number of Papers published in peer-reviewed journals:

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

Received		Paper
10/13/2014	9.00	Huimin Lin, Huazhong Tang, Wei Cai. Accuracy and efficiency in computing electrostatic potentialfor an ion channel model in layered dielectric/electrolytemedia, Journal of Computational Physics, (12 2013): 488. doi:
10/13/2014	10.00	Haiyan Jiang, Tiao Lu, Wei Cai. A device adaptive inflow boundary condition for Wignerequations of quantum transport, Journal of Computational Physics, (11 2013): 773. doi:
TOTAL:		**2**

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):

Received	Paper
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
08/07/2013	5.00	Haiyan Jiang, Tiao Lu, Wei Cai. A device adaptive inflow boundary conditionfor Wigner equations of quantum transport, Journal of Computattional Physics (03 2013)
08/07/2013	4.00	Huimin Lin, Huazhong Tang, Wei Cai. Accuracy and efficiency in computingelectrostatic potential for an ion channelmodel in layered dielectric/electrolyte media, Journal of Computational Physics (06 2013)
08/07/2013	6.00	CHANHAO YAN, WEI CAI, XUAN ZENG. A PARALLEL METHOD FOR SOLVING LAPLACE EQUATIONSWITH DIRICHLET DATA USING LOCAL BOUNDARY INTEGRALEQUATIONS AND RANDOM WALKS, SIAM Journal on Scientific Computing (06 2013)
08/16/2012	2.00	Wei Cai, Jianguo Xin, Tiao Lu, Yinglong Guo. Linear scaling discontinuous Galerkin densitymatrix minimization method with localorbital enriched ¯nite element basis: 1-Dlattice model system, COMMUNICATIONS IN COMPUTATIONAL PHYSICS (04 2012)
TOTAL:		**4**

Number of Manuscripts:

Books

Received	Book
TOTAL:	

Received	Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Jian Wu	0.25	
Kathy Baker	0.25	
Yijing Zhou	0.25	
FTE Equivalent:	**0.75**	
Total Number:	**3**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Steven Xin	0.25
FTE Equivalent:	**0.25**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Wei Cai	0.17	
FTE Equivalent:	**0.17**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
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

NAME	
Total Number:	

Names of personnel receiving PHDs

NAME	
Kathy Baker	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

[1] On fast integral solver for quantum dots, we have developed a parallel fast algorithm for computing the product of the discretized Helmholtz integral operator in layered media and a vector in O(NqNz^2 Nx Ny logNx Ny) operations. Here Nx Ny Nz is the number of sources and Nq is the number of quadrature points used in the evaluation of the Sommerfeld integral in the definition of layered Green's function. The fast solver is based on two important techniques which reduce the cost of quadrature summations in the Sommerfeld contour integral for Green's functions in 3-D layered media.

The first technique is the removal of surface pole effects along the real axis integration contour by identifying the pole locations with a Discrete Wavelet Transform; In the second technique, we apply a window-based high frequency filter to shorten the contour length. As a result, the integral operator for the 3-D layered media can be efficiently written as a sum of 2-D Hankel cylindrical integral operators, and the latter can be calculated by either a tree-code or a 2-D wideband FMM in a fast manner.

[2] On the linear scaling quantum DFT algorithm, we have proposed a new framework using discontinuous Gakerlin method for linear scaling methods for density functional theory, which forms the fundamental approach for studying quantum system ground state energy. The salient feature of this framework is the flexibility of using hybrid physics-based local orbitals and accuracy-guaranteed piecewise polynomial basis in representing the Hamiltonian of the many body system. Such a flexibility is made possible by using the discontinuous Galerkin method to approximate the Hamiltonian matrix elements with proper constructions of numerical DG fluxes at the finite element interfaces.

[3] Computation of electrostatics in ion-channel transport.

Here we investigate the numerical accuracy and efficiency in computing the electrostatic potential for an ion channel model made of finite-height cylinder embedded in a layered dielectric/electrolyte medium representing a biological membrane and ionic solvents. Two numerical techniques, a specially designed boundary integral equation method and an image charge method, have been investigated and compared in terms of accuracy and efficiency for computing the electrostatic potential.

[4] A new parallel solver for elliptic PDEs for extreme computing.

In this result, a hybrid approach for solving the Laplace equation in general 3-D domains is proposed. The approach is based on a local method for the Dirichletto-Neumann (DtN) mapping of a Laplace equation by combining a deterministic (local) boundary integral equation (BIE) method and the probabilistic Feynman–Kac formula for solutions of elliptic partial differential equations. This hybridization produces a parallel algorithm where the bulk of the computation has no need for data communication between processors, therefore it has great potential for highly scalable solver for elliptic PDEs for extreme scale computing.

[5] An improved device adaptive inflow boundary condition for Wigner quantum transport equations.

An improved inflow boundary condition is proposed for Wigner equations in simulating a resonant tunneling diode (RTD), which takes into consideration the band structure of the device and the effect of the quantum interaction inside the quantum device. Numerical results on computing the electron density inside the RTD under various incident waves and non-zero bias conditions show much improvement by the new boundary condition over the traditional Frensley inflow boundary condition.

Technology Transfer