REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
13-03-2018	Final Report	20-Jun-2014 - 19-Dec-2017

4. TITLE AND SUBTITLE
Final Report: Numerical Methods for Studying Optical Absorption of Random Media and Quantum Dots for Solar Cell Designs

5a. CONTRACT NUMBER
W911NF-14-1-0297

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

6. AUTHORS

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
University of North Carolina - Charlotte
9201 University City Boulevard

Charlotte, NC 28223 -0001

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)
65357-MA.9

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for public release; distribution is 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

15. SUBJECT TERMS

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

RPPR Final Report
as of 14-Mar-2018

Agency Code:

Proposal Number: 65357MA **Agreement Number: W911NF-14-1-0297**
INVESTIGATOR(S):

Name: Wei Cai
Email: wcai@uncc.edu
Phone Number: 7046870628
Principal: Y

Organization: **University of North Carolina - Charlotte**
Address: 9201 University City Boulevard, Charlotte, NC 282230001
Country: USA
DUNS Number: 066300096 EIN: 560791228
Report Date: 19-Mar-2018 Date Received: 13-Mar-2018
Final Report for Period Beginning 20-Jun-2014 and Ending 19-Dec-2017
Title: Numerical Methods for Studying Optical Absorption of Random Media and Quantum Dots for Solar Cell Designs
Begin Performance Period: 20-Jun-2014 **End Performance Period:** 19-Dec-2017
Report Term: 0-Other
Submitted By: Wei Cai Email: wcai@uncc.edu
Phone: (704) 687-0628
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 1 **STEM Participants:** 0

Major Goals: Our objective is to develop fast stochastic computational methods to optimize the optical absorption of solar cells.

We aim to find out the effect of randomness in absorber layer in solar cells on its ability to harvest light energy over the whole visible light spectrum. Both time domain and frequency domain methods for computing the optical absorption of random structures will be developed and efficient stochastic simulation methods will be used to study the correlation of randomness on the optical properties of absorbers.

Accomplishments: Several key scientific developments have been achieved during this project:

1. A de-singularized accurate volume integral equation (VIE) Nystrom method for the Maxwell equations in layered media

2. Accurate and economic quadratures for micro-structures of various shapes used in absorber layers for the solar cells

3. A high order discontinuous Galerkin method for time domain Maxwell equations using orthogonal polynomial basis on tetrahedron and a 3-D code for unstructured grid is also developed.

4. A well conditioned hyper-singular integral equation for electrostatics in in-homogeneous media

5. An efficient formulations of dyadic Green's functions for electric and magnetic fields in layered media

6. Developed high order hierarchical finite element H(div) basis for magnetic induction equations

7. Developed stochastic methods for abnormal diffusion.

Training Opportunities: Nothing to Report

Results Dissemination: Nothing to Report

RPPR Final Report
as of 14-Mar-2018

Honors and Awards: Offered Clements Endowed Chair of Applied Mathematics at Southern Methodist University.

Protocol Activity Status:

Technology Transfer: Once we have the codes ready, we plan to provide them to Dr. William Beck' group at ARL in Adelphi to optimize the optical absorption of rough surfaces in solar cells.

PARTICIPANTS:

Participant Type: Faculty
Participant: Duan Chen
Person Months Worked: 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Brian Zinser
Person Months Worked: 9.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Caylah Retz
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Richard Swanson
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Wenzhong Zhang
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

RPPR Final Report
as of 14-Mar-2018

Participant Type: Graduate Student (research assistant)
Participant: Yetong Zhou
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Final Project Report

(Period 6/20/2014-12/19/2017)

by Wei Cai

3/13/2018

1. Science

a. What is the mathematical objective of your project? What question are you trying to answer?

Our objective is to develop fast stochastic computational methods to optimize the optical absorption of solar cells.

We aim to find out the effect of randomness in absorber layer in solar cells on its ability to harvest light energy over the whole visible light spectrum.

b. What are the challenges in doing this? What makes it difficult?

Due to the large number of nano-structures (100k to millions) in the absorber layer and the stochastic variances of their shapes, it calls for fast solutions of the multiple electromagnetic wave scattering and efficient compression methods for the random variables so an efficient optimization of the absorber will be possible for ARL design scientists.

c. What is the scientific opportunity that is enabling you to make progress in this difficult area?

Several key scientific developments in our group enable us to achieve our objectives:

- **A de-singularized accurate volume integral equation (VIE) Nystrom method for the Maxwell equations**
- **Accurate and economic quadratures for micro-structures of various shapes used in absorber layers for the solar cells**
- **Fast solver for VIE linear systems in layered media**
- **Efficient generalized polynomial chaos representation of random variables in solar cell absorber.**

d. Please attach one (or a few if you wish) graphic that best represents what your project is about. People are visual; one graphic can help them grab onto your project much quicker.

Goal: Optimal optical absorption of rough surface for quantum dot solar cells @ ARL

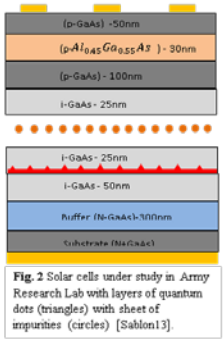
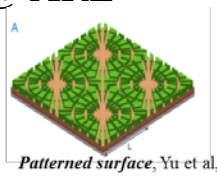
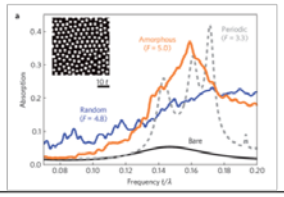


Fig. 2 Solar cells under study in Army Research Lab with layers of quantum dots (triangles) with sheet of impurities (circles) [Sablon13].

Top surface



Patterned surface, Yu et al, PNAS, 2010



Random surface: Increased absorption with Random Spheres, Vynck, Nature Material, 2012

Quantum solar cell (Sablon, et al, ARL, 2013)

EM Scattering of Random Structures Over Layered media by our VIE Code

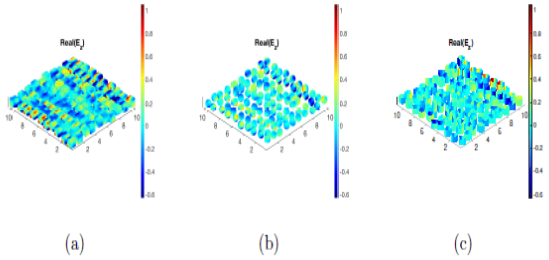
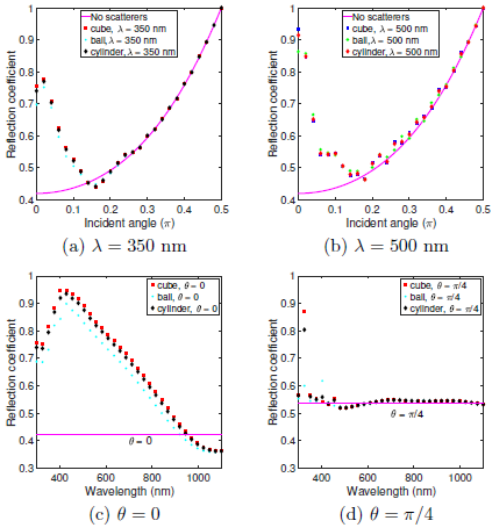


FIG. 13. *Electric field component E_z in 10×10 scatterer arrays with a TE incident wave in a half space. (a) Cubic scatterer with 27 collocation points in each; (b) spherical scatterer with 72 collocation points in each; (c) cylindrical scatterer with 72 collocation points.*



(Left) Scattering of meta-material (MM) over layered media, (Right) effects of layered media on the reflection of MM on the left.

Cited from work supported by ARO fund:

[1] Accurate And Efficient Nystrom Volume Integral Equation Method For Electromagnetic Scattering Of 3-D Meta-Materials In Layered Media, **SIAM J. on Scientific computing** Vol. 40, No. 1, pp. B259–B282.

2. Collaborations
a. Name and give organization of anybody in the Army/DoD/govt who you have collaborated with in the course of this project.

Dr. William Beck
Army Research Laboratory
EO/IR Materials and Devices Branch
Attn: RDRL-SEE-I
2800 Powder Mill Road
Adelphi, MD 20783-1197

b. Describe the nature of the collaboration. Include co-authoring with them, giving talks at their place, inviting them to your school, getting scenarios or data or ideas from them, conducting joint workshops or seminars, etc.

PI visited Dr. Beck and his group in the first year of the project to understand the need and specifications for the design of optical absorber in solar cells and has continued the communications via emails.

Our eventual goal is to provide his group a code which will allow researchers at his group or other ARLs to design optimal optical absorber for quantum dots solar cells or other photo-voltaic devices.

c. If any of your students, postdocs, or faculty were hired by the Army or DoD, please give details.

Five Ph.D. students (Brian Zinser, Caylah Retz, Richard Swanson, Wenzhong Zhang Yetong Zhou; caylah and yetong are female) are supported to study various numerical issues related to this project.

3. Transitions: Describe anything from this project that you transitioned to anybody else (whether Army, DoD, govt, commercial, or other).
a. Who did you give it to, and what is their organization?

Not yet, but we plan to provide a code to Dr. William Beck' group at ARL in Adelphi to optimize the optical absorption of rough surfaces in solar cells.

b. What did you give them? Code, papers, algorithms...

c. What eventual application might this enable?

d. What was your scientific accomplishment that enabled this?

4. Awards/honors: By you and anybody funded by this project: students, postdocs, faculty ...

Endowed Clements Chair Professor of Applied Mathematics at Southern Methodist University.

a. Include awards, prizes, Fellow/Society election, best paper prizes (especially student),elected positions, papers in Science or Nature, ...

5. Metrics related to your grant:
a. # peer-reviewed papers (related to this grant)

8 papers have been published in referred scientific journals.

1. Accurate and Efficient Nystrom Volume Integral Equation Method for Electromagnetic Scattering of 3-D Meta-materials in Layered Media, Duan Chen Min Hyung Cho Wei Cai, **SIAM J. on Scientific computing,** Vol. 40, No. 1, pp. B259–B282, (2018)**.**

2. Accurate and Efficient Volume Integral Equation Method for the Maxwell equations for Multiple 3-D Scatterers, D. Chen, Wei Cai, B. Zinser, and M.H. Cho, **Journal of Computational Physics,** 321 (2016), 303-320.

3. Quadrature Weights on Tensor-Product Nodes for Accurate Integration of Hypersingular Functions over Some Simple 3-D Geometric Shapes, B. Zinser, W. Cai, D. Chen, **the Communication in Computational Physics**, Vol. 20, No. 5, pp. 1283-1312, 2016.

4. A well-conditioned hypersingular boundary element method for electrostatic potentials in the presence of inhomogeneities within layered media, Brian Zinser, and Wei Cai, **Communication in Computational Physics**, Vol. 19, No. 4, pp. 970-997, 2016.

5. A high-order time domain discontinuous Galerkin method with orthogonal tetrahedral basis for electromagnetic simulations in 3-D heterogeneous conductive media, Jun Yang, Wei Cai, Xiaoping Wang, **Communications in Computational Physics**, Volume 21, Issue 4 April 2017 , pp. 1065-1089.

6. High Order Hierarchical Divergence-free Constrained Transport H(div) Finite Element Method for Magnetic Induction Equation, W. Cai, J. Hu, S.Y. Zhang, **Numerical Mathematics: Theory, Methods and Applications**, Volume 10, Issue 2 May 2017 , pp. 243-254.

7. Efficient and accurate computation of electric field dyadic Green's function in layered media, M.H. Cho, W. Cai, **Journal of Scientific Computing**, 71 (2017), pp. 1319-1350.

8. Discovering variable fractional orders of advection-dispersion equations from field data using multi-fidelity Bayesian optimization. Pang G, Perdikaris P, Cai W, Karniadakis GE. **Journal of Computational Physics**. 2017 Nov 1;348(C):694-714.

b. manuscripts (related to this grant)

c. presentations (related to this grant)

[1] Oct. 29, 2014, Research talk, Army Research Laboratory, EO/IR Materials and Devices Branch

[2] April, 22, 2015, invited talk at Dept. of Math, SMU

[3] May 29-30, 2015 invited talk at International Conference on Numerical Partial Differential Equations and Their Applications, Wuhan, China

[3] June 29-July 2, 2015, Invited talk at International Workshop on Computational Mathematics 2015, Qingdao, China

[4] Invited talk at 13th Workshop on Finite Elements (FEM2016), Florence, Italy, May 15-19, 2016.

[5] International Conference on Recent Advances in Computational and Applied Mathematics, Wuhan University, China on December 14-17, 2017

d. patents submitted (funded by this grant)

e. # grad students/yr (funded by this grant)

5 Ph.D. students by this grant

f. #postdocs/yr (funded by this grant)

g. PhD degrees awarded (funded by this grant)

1 American student (Brain Zinser) awarded in 2016, now works at Sandia National Lab.

1 American female student (Caylah Retz) has finished her thesis research work and will defend her Ph.D. in 2018.

h. MS degrees awarded (funded by this grant)

6. Anything else of note we should know about and tell the BOV about?