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# Numerical Methods of Computational Electromagnetics for Complex Inhomogeneous Systems

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## I. Executive Summary

Understanding electromagnetic phenomena is the key in many scientific investigation and engineering designs such as solar cell designs, studying biological ion channels for diseases, and creating clean fusion energies, among other things. Computational modeling with efficient numerical algorithm is indispensable for achieving this understanding. This project have developed novel numerical algorithms for solving Maxwell equations and electrostatics in inhomogeneous media occurring in those systems, which have advanced our capability in carrying out accurate and large scale computations for the benefit of cleaner energy and better medical treatment of the society.

## II. Accomplishments and Project Objectives

The technical objectives of the project are to develop high order numerical methods to simulate evanescent electromagnetic waves occurring in plasmon solar cells and biological ion-channels, where local field enhancement within random media in the former and long range electrostatic interactions in the latter are of major challenges for accurate and efficient numerical computations.

We have accomplished these objectives by developing high order numerical methods for solving Maxwell equations such as high order finite element basis for discontinuous Galerkin methods, well-conditioned Nedelec edge element method, divergence free finite element basis for MHD, and fast integral equation methods for layered media. These methods can be used to model the complex local field enhancement in plasmon solar cells. On the other hand, to treat long range electrostatic interaction in ion channels, we have developed image charge based method for a hybrid model in combining atomistic electrostatics and continuum Poisson-Boltzmann electrostatics. Such a hybrid model will speed up the molecular dynamics simulation of transport in biological ion-channels.

## III. Summary of Project Activities

Research results have been obtained in the following technical areas:

- Image charge approximations of reaction fields and FMM for charges inside a dielectric sphere or finite height cylinder model for ion-channels.

- A generalized discontinuous Galerkin (GDG) method based on split distributions for PDE for phase shift masks

- A parallel spectral method for high frequency complex Helmholtz and Maxwell equations in inhomogeneous media using generalized eigen-oscillations

- Wide band FMM for 2-D Helmholtz equations

- Hierarchical Nedelc H(curl) basis for Maxwell equations

- Divergence free H(div) basis for MHD equations

- Stochastic modeling of uncertainty in the VLSI design processes: the random roughness in the interconnect surfaces and its effect on their electrical property and polishing pads in the chemical mechanical polishing .

## IV. Publication List

The following summarizes the **26** peer-reviewed publications acknowledging the support of this grant and weblinks have been provided for downloading the papers.


1. S. Deng, W. Cai, Analysis and Application of an Orthogonal Nodal Basis on Triangles for Discontinuous Spectral Element Methods, **Applied Numerical Analysis and Computational Mathematics**, 2(3):311-330, 2005 http://math2.uncc.edu/~wcai/dengcaiNodal.pdf

2. T. Yu, W. Cai, FIFA - Fast Interpolation and Filtering Algorithm for Calculating Dyadic Green's Function in the Electromagnetic Scattering of Multi-layered Structures, the **Communication in Computational Physics**, Vol. 1, No. 2, pp. 228-258, 2006. http://math2.uncc.edu/~wcai/YuCai.pdf

3. S. Deng, W. Cai, A Fourth-Order Upwinding Embedded Boundary Method (UEBM) for Maxwell's Equations in Media with Material Interfaces: Part I, the Communication in Computational Physics, Volume 1, Number 4, June 2006, pp. 744-764. http://math2.uncc.edu/~wcai/uebm4final.pdf

4. W. Cai, S. Z. Deng, D. Jacobs, Extending the Fast Multipole Method to Charges Inside or Outside a Dielectric Sphere, the **Journal of Computational Physics**, 223 (2007), pp. 846-864. http://math2.uncc.edu/~wcai/fmmionic.pdf

5. S.Z. Deng, W. Cai, Extending the fast multipole method for charges inside a dielectric sphere in an ionic solvent: high order image approximations for reaction fields, the

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6. S.Z. Deng, W. Cai, Discrete Image Approximations of Ionic Solvent Induced Reaction Field to Charges, the **Communications in Computational Physics**, 2 (2007), p.1007-1026. http://math2.uncc.edu/~wcai/ionicfinal.pdf

7. Shaozhong Deng, Wei Cai, Donald Jacobs, A Comparable study of image approximations to the reaction fields, Computer Physics Communications, Vol. 177, 9, Nov. (2007), pp. 689-699. http://math2.uncc.edu/~wcai/CompareImage.pdf

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9. K. Fan, W. Cai, X. Ji, A Full Vectorial Generalized Discontinuous Galerkin Beam Propagatiom Method (GDG- BPM) for Inhomogeneous Optical Waveguide, **Journal of Computational Physics**, 227 (2008), pp. 7178.
http://math2.uncc.edu/~wcai/GDGBPM.pdf

10. W. Cai, X. Ji, J.G. Sun, S.H. Shao, A Schwarz Generalized Eigen-oscillation Spectral Element Method (GeSEM) for 2-D High Frequency Electromagnetic Scattering in Dispersive Inhomogeneous Media the **Journal of Computational Physics**, 227, 2008, 9933–9954. http://math2.uncc.edu/~wcai/GeSem.pdf

11. X. Ji, W. Cai, P.W.Zhang, Transmission and Dispersion Characteristic of a Discontinuous Galerkin Method for Maxwell's Equations in Dispersive Inhomogeneuos Media, the **Journal of Computational Mathematics,** 26, (2008), pp. 347-364. http://math2.uncc.edu/~wcai/TransDispFinal.pdf

12. P.H. Qin, Z.L. Xu, W. Cai and D. Jacobs,Image charge methods for a three-dielectric-layer hybrid solvation model of biomolecules, **Communications in Computational Physics**, vol. 6, No. 5, (2009) pp. 955-977.
http://math2.uncc.edu/~wcai/ImageLayer.pdf

13. K. Zong, X. Zeng, X. Ji and W. Cai, Highly Parallel Rigorous Simulation of Phase Shift Masks with a Generalized Eigen- oscillation Spectral Element Method (GeSEM), the **Journal of Micro/Nanolithography, MEMS, and MOEMS**, a special issue on Computational Lithography, 8(3), 1, (Jul–Sep 2009).
http://math2.uncc.edu/~wcai/psm.pdf

14. C. Y. Feng, X. Zeng, Changhao Yan , Jun Tao ,W. Cai, A contact mechanics based model for general rough pads in chemical mechanical polishing processes, the **Journal of The Electrochemical Society**, p. H601, vol. 156, (2009). http://math2.uncc.edu/~wcai/cmp.pdf

15. H.L. Zhu, X. Zeng, X. Luo, W. Cai, Generalized Stochastic Collocation Method for Variation-Aware Capacitance Extraction of Interconnects Considering Arbitrary Random Probability, the **IEICE transaction electron,** 508, vol. E92.C, 2009. http://math2.uncc.edu/~wcai/SCCMarbitrary.pdf

16. S. Xin, W. Cai, and J. Tichy, A fundamental model proposed for material removal in chemical mechanical polishing, **Wear**, 268 (2010) 837–844. http://math2.uncc.edu/~wcai/cmp_model.pdf

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18. M. Cho, W. Cai, A wideband fast multipole method for the two dimensional complex Helmholtz equation, the **Computer Physics Communications,** 181 (2010) 2086-2090. http://math2.uncc.edu/~wcai/WidebandFMM.pdf

19. Z. L. Xu, W. Cai, Fast analytical methods for macroscopic electrostatic models in biomolecular simulations, **SIAM review**, vol. 53, No. 4, pp. 683-720, 2011. http://math2.uncc.edu/~wcai/fastReviewFinal.pdf

20. J.Xin, W. Cai, A well-conditioned hierarchical basis for triangular H(curl)-conforming elements, **Communication in Computational Physics**, a special issue in the memory of David Gottlieb, vol. 9, No. 3, pp. 780-806, 2011. http://math2.uncc.edu/~wcai/Nedelec2d.pdf

21. J. Xin, N. Guo and W. Cai,On the construction of well-conditioned hierarchical bases for tetrahedral H(curl)-conforming Nedelec elements, **Journal of Computational Mathematics**, v29 (2011), No.5, pp.526-542. http://math2.uncc.edu/~wcai/Nedelec3d.pdf

22. Z. L. Xu, W. Cai, X.L. Cheng, Image Charge Method for Reaction Fields in a Hybrid Ion-Channel Model, **Communications in Computational Physics**, vol. 9, No. 4, pp. 1056-1070, 2011. http://math2.uncc.edu/~wcai/ImageIonChannel.pdf

23. J. Xin, W. Cai, Well-conditioned orthonormal hierarchical L2 bases on R^n simplicial elements, **Journal of scientific computing**, (2012) 50:446–461. http://math2.uncc.edu/~wcai/L2basis.pdf

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25. Wei Cai, Jian Wu and Jianguo Xin, Divergence-free H(div)-conforming hierarchical bases for Magnetohydrodynamics (MHD), **Communications in Mathematics and Statistics** (2013) 1:19-35. http://math2.uncc.edu/~wcai/divfreebasis.pdf

26. J Xin, W. Cai, and N.L. Guo, On the construction of well-conditioned hierarchical bases for H(div)-conforming R^n simplicial elements, **Communications in computational physics**, Vol. 14, No.3, (2013), pp. 621-638. http://math2.uncc.edu/~wcai/h_div.pdf