Nanoscale Electromagnetic Elements: Computational Aspects

by

Brenton Thomas

A thesis presented to the University of Technology Sydney in fulfillment of the requirement for the degree of Master of Science 2007

Sydney, New South Wales, Australia, 2007

© Brenton Thomas 2007

CERTIFICATE OF AUTHORSHIP/ORIGINALITY

I certify that the work in this thesis has not previously been submitted for a degree nor has it been submitted as part of requirements for a degree except as fully acknowledged within the text. I also certify that the thesis has been written by me. Any help that I have received in my research work and the preparation of the thesis itself has been acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

Signature

Production Note: Signature removed prior to publication.

I further authorize the University of Technology Sydney to reproduce this thesis by photocopying or by other means, in total or in part, at the request of other institutions or individuals for the purpose of scholarly research.

Signature

Production Note: Signature removed prior to publication.

Abstract

The use of the Finite Difference Time Domain (FDTD) and the Transmission Line Matrix (TLM) algorithm to model nanoscale electromagnetic elements is investigated. It is found that comparable accuracy of the TLM algorithm to the FDTD algorithm combined with significant practical reductions in computation time render TLM a superior algorithm for nanoscale optoelectronic problems. It is also found that as the as the TLM algorithm implicitly incorporates "split fields" into its definition that it lends itself to a natural and simple implementation of the Berenger Perfectly Matched Layer from FDTD that appears not to have been reported in the literature. In the course of the research an extension to the Drude Lorentz complex permittivity model of gold is developed that provides coverage across the entire optical spectrum. This extended model is then used to validate the TLM algorithm against known the known optical response of a variety of objects including gold films, nano spheres and nano rods. The effect of coupling between elements of an array of nano scale objects is investigated with a consistent blue shift in the extinction spectra for arrays of closely spaced nanoscale objects observed.

Acknowledgements

I would like to thank my supervisors Mike Ford and Geoff Anstis as well as the Institute for Nanoscale Technology at the University of Technology Sydney for providing me with the opportunity to return to study after a long hiatus. Many thanks also to Matthew Arnold for reminding me that the universe is causal and for pointing me at Vial et al's gold model. Also thanks to Nadine Harris and Mike Cortie for producing DDScat nano rod results at short notice.

Table of Contents

Abstract	iii
Acknowledgements	iv
Table of Contents	. v
List of Figures	vii
List of Tables	ix
Chapter 1 Introduction	. 1
1.1 Objectives	. 1
1.2 Strategy	. 1
Chapter 2 Time Domain Nanoscale Electromagnetic Modeling Suite	3
2.1 Application Framework	3
2.2 Front End Application	5
2.3 Backend Application	8
Chapter 3 Basic Time Domain Algorithms	9
3.1 Time Domain Algorithm Overview	9
3.2 Yee Finite Difference Time Domain	10
3.3 Transmission Line Matrix Algorithm	13
3.3.1 A Fundamental Difference in Time Stepping	22
3.4 Absorbing Boundary Conditions	23
3.4.1 FDTD ABC's	23
3.4.2 A New TLM Absorbing Boundary Condition	24
3.5 Absorbing Boundary Performance	27
Chapter 4 General Complex Material Models	32
4.1 Complex Material Modeling	32
4.2 Auxiliary Differential Equation	34
4.3 Recursive Convolution	36
4.4 Z Transform	42
4.4.1 Lookup Table Z Transform	43
4.4.2 Z Transform via Bilinear Transform	44
Chapter 5 Complex Material-Time Domain Algorithm Implementation	46
5.1 FDTD Complex Material Implementation	47
5.1.1 Auxiliary Differential Equation FDTD Implementation	47
5.1.2 Recursive Convolution FDTD Implementation	48
5.1.3 Z Transform FDTD Implementation	51

:

5.2 TLM Complex Material Implementation	58
Chapter 6 Optical Frequency Gold Validation and Extension	63
6.1 Gold at Optical Frequencies	63
6.2 Model Validation	69
6.3 Algorithm Validation	70
Chapter 7 Computation Time	74
Chapter 8 Gold Nano-Spheres	79
Chapter 9 Nanorod Absorption	90
Chapter 10 Conclusion and Future Directions	93

List of Figures

Figure 1 High Level System Architecture
Figure 2 Modeling View
Figure 3 Job Creation Screen
Figure 4 Data Display View7
Figure 5 Yee Cell Position Offset
Figure 6 TLM Port Voltage Geometry
Figure 7 One Dimensional Absorbing Boundary Test Space
Figure 8 Three Dimensional Absorbing Boundary Test Space
Figure 9 Comparison of TLM and FDTD Absorbing Boundaries on a one dimensional space 29
Figure 10 Comparison of TLM and FDTD Absorbing Boundaries on a three dimensional space 30
Figure 11 Energy Flow into the TLM grid from the absorbing boundaries
Figure 12. Single Term Drude Gold Model
Figure 13. Single Term Drude + Single Term Lorentz Gold Model65
Figure 14. Single Term Drude + Dual Term Lorentz, Gold Model
Figure 15. Mie Theory comparison of the new gold model extinction with actual
Figure 16 Thin Film Validation Space and Interacting Pulse
Figure 17 FDTD Auxiliary Differential Equation 10nm Gold Film
Figure 18 FDTD Z Transform via Tables 10nm Gold Film
Figure 19 FDTD Recursive Convolution 10nm Gold Film73
Figure 20 TLM Z Transform 10nm Gold Film
Figure 21 Run Time Comparison – Main Grid - Same Number Of Iterations
Figure 22 Run Time Comparison - ABC – Same Number Of Iterations
Figure 23 ABC Run Time Comparison – Same Effective Duration – Time Step Half CFL77
Figure 24 Run Time Comparison – Same Effective Duration – Time Step Half CFL77
Figure 25 Run Time Comparison – Same Effective Duration
Figure 26 ABC Run Time Comparison – Same Effective Duration
Figure 27 Gold Nanosphere Extinction Experiment Problem Geometry
Figure 28 Mie Extinction Efficiency Curves – New Model81
Figure 29, Experimental space containing a150nm sphere
Figure 30, Stair casing effects on a 60nmSphere
Figure 31 Calculated Extinction Efficiency – Various Sphere Diameters
Figure 32 Calculated Extinction Efficiency – 150nm Sphere Various Sphere Separation
Figure 33 Attenuation within an absorbing boundary enclosed space

Figure 34 Extinction within an absorbing boundary enclosed space	86
Figure 35 Electric Field Surrounding a 120nm Sphere	87
Figure 36 Poynting Field Surrounding a 120nm Sphere	88
Figure 37 Electric Field Surrounding a 120nm sphere a few time steps after pulse interaction	89
Figure 38. Experimental space containing a 100nm gold rod	90
Figure 39. TLM extinction of an array of gold rods compared to DDScat	91
Figure 40. FDTD extinction of an array of gold rods compared to DDScat	92

List of Tables

Table 1 Time, Fourier and Z Transform domain function correspondence	41
Table 2 Gold Model Coefficients Traditional Format	67
Table 3 Gold Model Coefficients, Model Independent Format	68