Simulations of optical radiation pressure on deformable media

by

Cael Warner

B.ASc., The University of British Columbia, 2019

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF APPLIED SCIENCE

in

THE COLLEGE OF GRADUATE STUDIES

(Electrical Engineering)

THE UNIVERSITY OF BRITISH COLUMBIA

(Okanagan)

December 2021

© Cael Warner, 2021
The following individuals certify that they have read, and recommend to the College of Graduate Studies for acceptance, a thesis/dissertation entitled:

**Simulations of optical radiation pressure on deformable media**

submitted by Cael Warner in partial fulfilment of the requirements of the degree of Master of Applied Science

Kenneth J. Chau, School of Engineering
Supervisor

Loïc Markley, School of Engineering
Co-Supervisor

Joshua Brinkerhoff, School of Engineering
Supervisory Committee Member

Sunny Li, School of Engineering
University Examiner

Additional Committee Members include:

Jonathan Holzman, School of Engineering
Supervisory Committee Member
Abstract

Multiple electrodynamic theories have existed for over a century, which has led to controversy over a field-based description of light-matter interactions. Experiments that aim to support or disprove an electrodynamic theory benefit from accurate numerical simulation of each theory’s predictions of light-matter interactions. However, most experiments and their numerical simulations are limited to cases of rigid-body translation or elastic deformation, which are equivalently predicted by each electrodynamic theory. Alternative experiments that investigate the continuous deformation of fluids subjected to optical radiation pressure may benefit from multi-physics simulation based on statistical mechanics, which are locally non-linear and rigorously conserve momentum. This thesis applies the lattice-Boltzmann method to describe both the electrodynamic and kinetic sub-systems in a multi-physics simulation of a quasi-stationary multiphase fluid subjected to optical radiation pressure. The simulations are used to model multiple electrodynamic formalisms, which yield distinct predictions of microscale fluid deformation. Multiphysics simulations based in statistical mechanics may assist in realizing a single theory for electrodynamics.
Lay Summary

This thesis begins with a review of theoretical and experimental investigations into light-matter interactions, and the development of analytical and numerical approaches for their prediction. Classical light can be described as a population of interacting waves, while classical matter can be described as a population of interacting particles. This thesis applies a discrete numerical method for describing the most likely interaction between these populations of light waves and mass particles. In particular, lattice-Boltzmann numerical methods which invoke Boltzmann’s equation from statistical mechanics. Lattice-Boltzmann numerical methods are used to fulfill the key goals and contributions of this thesis, which include:

1. Comparing the accuracy and computational time of the Yee-lattice finite-difference method and the electrodynamic lattice-Boltzmann method in predicting a force caused by light;

2. Implementing a multi-scale simulation of interactions between light and a fluid in two and three dimensions; and

3. Simulating several varying theoretical predictions for how light can move or reshape fluids in two and three dimensions.

While this thesis attempts to develop a general approach for predicting the interaction of light and matter, it only provides an initial framework. Further adaptation is required to describe a specific fluid used in a real-world experiment. Nonetheless, the framework is simple to implement and adapt for different experiments given adequate computational resources. The numerical method or approach used in this thesis illustrates cases where multiple theories predict either similar or distinct light-matter interactions. Predicting light-matter interactions on deformable media may help guide experiments that aim to identify a single theory for light-matter interactions. Predicting light-matter interactions is also important for a number of emerging technologies which use optical trapping and optical acceleration for micro-assembly or micro-assays.
Preface

Chapters 3, 4, and 5 include paraphrased information from co-authored manuscripts with intended submission to peer-reviewed journals. Throughout this thesis, theories, analytical and numerical methods developed by numerous authors are utilized. The original authors are appropriately cited where their methods are used or described. The combination of these methods and their use for a particular dynamic system are original to this work.
# Table of Contents

Abstract ........................................................................ iii  
Lay Summary ................................................................. iv  
Preface ........................................................................... v  
Table of Contents ........................................................... vi  
List of Tables ................................................................. x  
List of Figures ............................................................... xi  
List of Acronyms ........................................................... xix  
Acknowledgements ....................................................... xxi  
Dedication ........................................................................ xxii  

## Chapter 1: Introduction ............................................... 1  
1.1 Brief history of optical radiation pressure ................. 1  
1.2 Simulations of optical radiation pressure ................. 5  
1.3 The goals and contributions of this thesis ............... 6  
1.4 The organization of this thesis ............................... 6  

## Chapter 2: Theory ....................................................... 8  
2.1 Multi-physics energy and momentum conservation .... 8  
2.2 Electrodynanmic sub-system theory ....................... 12  
2.3 Kinetic sub-system theory ...................................... 16  
2.3.1 Mass and momentum conservation .................. 18  
2.4 Numerical methods .............................................. 19  
2.4.1 The central difference equation....................... 20  
2.4.2 Lattice stencils ............................................... 20
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4.3 Discrete spatial operators for the lattice-Boltzmann equation</td>
<td>23</td>
</tr>
<tr>
<td>2.4.4 The lattice-Boltzmann equation</td>
<td>24</td>
</tr>
<tr>
<td>2.4.5 Collision and propagation operators in the lattice-Boltzmann equation</td>
<td>25</td>
</tr>
<tr>
<td>Chapter 3: Comparing finite-difference methods and lattice-Boltzmann methods solutions of kinetic force density</td>
<td>27</td>
</tr>
<tr>
<td>3.1 Initial condition</td>
<td>27</td>
</tr>
<tr>
<td>3.1.1 Hermite Gaussian wave-functions</td>
<td>28</td>
</tr>
<tr>
<td>3.2 The Yee-lattice finite-difference time-domain method</td>
<td>31</td>
</tr>
<tr>
<td>3.2.1 Electric and magnetic fields</td>
<td>31</td>
</tr>
<tr>
<td>3.2.2 Energy density and momentum density</td>
<td>33</td>
</tr>
<tr>
<td>3.2.3 Force density</td>
<td>34</td>
</tr>
<tr>
<td>3.2.4 Boundary conditions</td>
<td>37</td>
</tr>
<tr>
<td>3.2.5 Limitations</td>
<td>37</td>
</tr>
<tr>
<td>3.3 The electrodynamic lattice-Boltzmann method</td>
<td>40</td>
</tr>
<tr>
<td>3.3.1 Electric and magnetic fields</td>
<td>40</td>
</tr>
<tr>
<td>3.3.2 Two-dimensional lattice-matrices</td>
<td>42</td>
</tr>
<tr>
<td>3.3.3 Three-dimensional lattice-matrices</td>
<td>44</td>
</tr>
<tr>
<td>3.3.4 Ponderable media</td>
<td>44</td>
</tr>
<tr>
<td>3.3.5 Energy density and momentum density</td>
<td>45</td>
</tr>
<tr>
<td>3.3.6 Force density</td>
<td>46</td>
</tr>
<tr>
<td>3.3.7 Dimensional conversions</td>
<td>47</td>
</tr>
<tr>
<td>3.3.8 Limitations</td>
<td>47</td>
</tr>
<tr>
<td>3.4 Comparative simulation configuration</td>
<td>48</td>
</tr>
<tr>
<td>3.5 Comparative analysis</td>
<td>50</td>
</tr>
<tr>
<td>3.6 Computational time and accuracy comparison</td>
<td>50</td>
</tr>
<tr>
<td>3.6.1 Time-averaged force density</td>
<td>53</td>
</tr>
<tr>
<td>Chapter 4: Multi-physics simulation of optical radiation pressure on a multi-phase fluid</td>
<td>54</td>
</tr>
<tr>
<td>4.1 Review of multi-physics simulation methods</td>
<td>54</td>
</tr>
<tr>
<td>4.2 The pseudopotential lattice-Boltzmann method</td>
<td>56</td>
</tr>
<tr>
<td>4.2.1 Initial condition</td>
<td>56</td>
</tr>
<tr>
<td>4.2.2 Mass and momentum</td>
<td>58</td>
</tr>
<tr>
<td>4.2.3 The pseudopotential force density</td>
<td>58</td>
</tr>
<tr>
<td>4.2.4 The kinetic force density</td>
<td>60</td>
</tr>
<tr>
<td>4.2.5 Collision operation and operators</td>
<td>61</td>
</tr>
</tbody>
</table>
# TABLE OF CONTENTS

4.2.6 Equilibrium probability mass function ............... 65
4.2.7 Propagation operation .................................. 66
4.2.8 Boundary conditions ..................................... 67
4.2.9 Dimensionless numbers ................................. 70
4.2.10 Dimensional conversion ................................. 71
4.3 Algorithm .................................................. 72

Chapter 5: Two- and three-dimensional optical acceleration and deformation of multi-phase fluids ....... 73
5.1 Two-dimensional simulation ................................. 74
5.1.1 Methodology ............................................. 74
5.1.2 Flat liquid-vapor interface ............................... 77
5.1.3 Circular liquid-vapour interface ......................... 79
5.1.4 Conclusion .............................................. 80
5.2 Three-dimensional simulation ............................... 81
5.2.1 Methodology ............................................. 81
5.2.2 The linearly-polarized Hermite-Gaussian beam ........ 83
5.2.3 The circularly-polarized Hermite-Gaussian beam ....... 85
5.2.4 Kinetic momentum transfer and electric field polarization .............................................. 87
5.2.5 Conclusion .............................................. 89

Chapter 6: Conclusion ........................................... 90
6.1 Recommendations ........................................... 93

Bibliography ..................................................... 94

Appendices ......................................................... 108
Appendix A: Analytical methods ................................. 108
A.1 Coordinate systems ......................................... 108
A.2 Matrix operations ........................................... 109
A.3 Polynomials and functions ................................ 111
Appendix B: Momentum flux density tensors expanded .... 113
B.1 Abraham’s momentum flux density tensor ................. 113
B.2 Minkowski’s momentum flux density tensor ............... 113
B.3 Einstein & Laub’s momentum flux density tensor ......... 114
B.4 Chu’s momentum flux density tensor ....................... 114
B.5 Ampere’s momentum flux density tensor ................. 114
B.6 Helmholtz momentum flux density tensor ................. 115
B.7 Divergence of a stress-tensor .............................. 115
TABLE OF CONTENTS

B.7.1 Two-dimensional Minkowski stress-tensor divergence . 116
B.7.2 Two-dimensional Chu stress-tensor divergence . . . . . 116
Appendix C: Dimensional Conversions . . . . . . . . . . . . . . 117
Appendix D: Program Implementations . . . . . . . . . . . . . . 118
D.1 Electrodynamic lattice-Boltzmann method force density . . 118
D.2 Shan-Chen force density with applicable equation of state . . 120
D.3 Periodic boundary conditions . . . . . . . . . . . . . . . . . . 121
D.4 Collision operation . . . . . . . . . . . . . . . . . . . . . . . . 121
D.5 Propagation operation . . . . . . . . . . . . . . . . . . . . . . . 123
List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Minkowski formulation of electrodynamics</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Einstein &amp; Laub formulation of electrodynamics</td>
<td>13</td>
</tr>
<tr>
<td>2.3</td>
<td>The E-H formulation of electrodynamics</td>
<td>13</td>
</tr>
<tr>
<td>2.4</td>
<td>Electrodynamic Momentum and Power Density</td>
<td>14</td>
</tr>
<tr>
<td>2.5</td>
<td>Electrodynamic Momentum Flux Density Tensors</td>
<td>15</td>
</tr>
<tr>
<td>2.6</td>
<td>Moments of the particle population, $n(x,v,t)$</td>
<td>16</td>
</tr>
<tr>
<td>2.7</td>
<td>Properties of lattice-stencils used in this thesis</td>
<td>22</td>
</tr>
<tr>
<td>3.1</td>
<td>Conversion of dimensionless electrodynamic sub-system variables</td>
<td>47</td>
</tr>
<tr>
<td>4.1</td>
<td>Conversion of dimensionless kinetic sub-system variables</td>
<td>71</td>
</tr>
<tr>
<td>A.1</td>
<td>Hermite polynomials</td>
<td>112</td>
</tr>
<tr>
<td>C.1</td>
<td>Dimensional conversion of system variables</td>
<td>117</td>
</tr>
</tbody>
</table>
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Electrodynamics of rigid bodies</td>
<td>11</td>
</tr>
<tr>
<td>2.2</td>
<td>Illustration of lattice stencils</td>
<td>21</td>
</tr>
<tr>
<td>2.3</td>
<td>The collision process</td>
<td>26</td>
</tr>
<tr>
<td>3.1</td>
<td>The two-dimensional Yee-lattice</td>
<td>32</td>
</tr>
<tr>
<td>3.2</td>
<td>Visual comparison of YL-FDTDM and ELBM numerical dispersion</td>
<td>39</td>
</tr>
<tr>
<td>3.3</td>
<td>Discrete lattice-vectors representing a p-polarized electric field</td>
<td>42</td>
</tr>
<tr>
<td>3.4</td>
<td>Discrete lattice-vectors representing an s-polarized electric field</td>
<td>43</td>
</tr>
<tr>
<td>3.5</td>
<td>Illustration of the spatial domain comparing Yee-lattice and lattice-Boltzmann methods</td>
<td>49</td>
</tr>
<tr>
<td>3.6</td>
<td>Computational time of the YL-FDTDM and the ELBM</td>
<td>51</td>
</tr>
<tr>
<td>3.7</td>
<td>Numerical accuracy of the YL-FDTDM and the ELBM</td>
<td>52</td>
</tr>
<tr>
<td>3.8</td>
<td>Ratios of errors and computational times with respect to spatial units per wavelength</td>
<td>52</td>
</tr>
<tr>
<td>3.9</td>
<td>Chu time-averaged force density in the YL-FDTDM and the ELBM</td>
<td>53</td>
</tr>
<tr>
<td>4.1</td>
<td>Liquid-vapor phase coexistence</td>
<td>60</td>
</tr>
<tr>
<td>4.2</td>
<td>Illustration of periodic boundary conditions</td>
<td>67</td>
</tr>
<tr>
<td>4.3</td>
<td>Bounce-back boundary conditions</td>
<td>68</td>
</tr>
<tr>
<td>4.4</td>
<td>Non-equilibrium bounce-back boundary conditions</td>
<td>70</td>
</tr>
<tr>
<td>4.5</td>
<td>Multi-physics simulation algorithm</td>
<td>72</td>
</tr>
<tr>
<td>4.1</td>
<td>Two-dimensional simulation configuration used to examine the deformation of a flat liquid-vapour interface</td>
<td>75</td>
</tr>
<tr>
<td>4.2</td>
<td>Two-dimensional simulation configuration used to examine the deformation of a circular liquid-vapour interface</td>
<td>76</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>5.3</td>
<td>Two-dimensional dielectric liquid-vapor interface deformation from a p-polarized electric field</td>
<td>77</td>
</tr>
<tr>
<td>5.4</td>
<td>Two-dimensional dielectric liquid-vapor interface deformation from an s-polarized electric field</td>
<td>78</td>
</tr>
<tr>
<td>5.5</td>
<td>Two-dimensional dielectric droplet deformation</td>
<td>79</td>
</tr>
<tr>
<td>5.6</td>
<td>Two-dimensional magnetic droplet deformation</td>
<td>80</td>
</tr>
<tr>
<td>5.7</td>
<td>Three-dimensional simulation configuration used to examine the deformation of a spherical liquid-vapour interface</td>
<td>82</td>
</tr>
<tr>
<td>5.8</td>
<td>Three-dimensional deformation of an incompressible spherical droplet from a linearly-polarized Gaussian beam</td>
<td>84</td>
</tr>
<tr>
<td>5.9</td>
<td>Three-dimensional deformation of an incompressible spherical droplet from a circularly-polarized Gaussian beam</td>
<td>86</td>
</tr>
<tr>
<td>5.10</td>
<td>Polarization-dependent momentum transfer according to the Chu and Amperian/Lorentz formalisms</td>
<td>87</td>
</tr>
<tr>
<td>5.11</td>
<td>Polarization-independent momentum transfer according to the Abraham, Minkowski, Einstein &amp; Laub, and Helmholtz formalisms</td>
<td>88</td>
</tr>
<tr>
<td>A.1</td>
<td>Difference between the position vector and displacement vector</td>
<td>109</td>
</tr>
</tbody>
</table>
# List of Symbols

- $(x_0, y_0, z_0)$: Position of the beam-waist on the beam-axis, page 29
- $[\mathbf{n}], [\hat{n}]$: Population density as a vector in velocity space and moment space, page 63
- $[\mathbf{\Lambda}], [\hat{\mathbf{\Lambda}}]$: Collision matrix in velocity space and moment space, page 63
- $[\mathbf{M}]$: Transformation matrix, page 63
- $\Re$: Refractive index, page 28
- $\alpha, \beta, \gamma, \mu, \nu$: Order and dimensional indices, page 18
- $\mathbf{G}$: Momentum density, page 8
- $\mathbf{S}$: Power per cross-sectional area, page 8
- $\Delta t$: Dimensional time unit, page 36
- $\delta t$: Dimensionless time unit, page 25
- $\Delta x$: Dimensional spatial unit, page 33
- $\delta x$: Dimensionless spatial unit, page 25
- $\epsilon$: Permittivity of a non-vacuum medium, page 14
- $\epsilon_0$: Free-space permittivity, page 12
- $\epsilon_r$: Relative permittivity, page 14
- $\eta$: Impedance of the source medium, page 30
- $\hat{n}_i$: Normal unit vector at an interface, page 57
- $\iota$: Interface thickness, page 57
- $\lambda_0$: Free-space wavelength, page 28
### LIST OF SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbb{R}^2$</td>
<td>Determination coefficient</td>
<td>79</td>
</tr>
<tr>
<td>k</td>
<td>Wave vector</td>
<td>11</td>
</tr>
<tr>
<td>T</td>
<td>Torque</td>
<td>11</td>
</tr>
<tr>
<td>B</td>
<td>Magnetic flux density</td>
<td>12</td>
</tr>
<tr>
<td>D</td>
<td>Electric flux density</td>
<td>12</td>
</tr>
<tr>
<td>E</td>
<td>Electric field intensity</td>
<td>12</td>
</tr>
<tr>
<td>e</td>
<td>Discrete electric field lattice vector</td>
<td>41</td>
</tr>
<tr>
<td>f</td>
<td>Force density</td>
<td>8</td>
</tr>
<tr>
<td>$f_{SC}$</td>
<td>Shan-Chen force density</td>
<td>59</td>
</tr>
<tr>
<td>H</td>
<td>Magnetic field intensity</td>
<td>12</td>
</tr>
<tr>
<td>h</td>
<td>Discrete magnetic field lattice vector</td>
<td>41</td>
</tr>
<tr>
<td>i</td>
<td>Imaginary unit</td>
<td>29</td>
</tr>
<tr>
<td>$J_E$</td>
<td>Electric current density</td>
<td>12</td>
</tr>
<tr>
<td>$J_M$</td>
<td>Magnetic current density</td>
<td>12</td>
</tr>
<tr>
<td>$M^{eq}$</td>
<td>Magnetization density equilibrium state</td>
<td>44</td>
</tr>
<tr>
<td>$P^{eq}$</td>
<td>Polarization density equilibrium state</td>
<td>44</td>
</tr>
<tr>
<td>r</td>
<td>Displacement vector</td>
<td>57</td>
</tr>
<tr>
<td>$r_i$</td>
<td>Locus of the interface with respect to the origin</td>
<td>57</td>
</tr>
<tr>
<td>s</td>
<td>Two-dimensional axis vector for a Hermite-Gaussian beam</td>
<td>29</td>
</tr>
<tr>
<td>$s_\perp$</td>
<td>Two-dimensional curvature vector for a Hermite-Gaussian beam</td>
<td>29</td>
</tr>
<tr>
<td>u</td>
<td>Mean velocity of a particle population</td>
<td>13</td>
</tr>
<tr>
<td>v</td>
<td>Random velocity of a particle population with reference to a stationary absolute space</td>
<td>16</td>
</tr>
<tr>
<td>x</td>
<td>Vector position</td>
<td>16</td>
</tr>
</tbody>
</table>
### LIST OF SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{R}$</td>
<td>Gas constant</td>
<td>16</td>
</tr>
<tr>
<td>$\mathcal{T}$</td>
<td>Mean temperature field</td>
<td>16</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Permeability of a non-vacuum medium</td>
<td>14</td>
</tr>
<tr>
<td>$\mu_0$</td>
<td>Free-space permeability</td>
<td>12</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Relative permeability</td>
<td>14</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic viscosity</td>
<td>71</td>
</tr>
<tr>
<td>$\bigodot$</td>
<td>Into page</td>
<td>43</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Collision operator</td>
<td>17</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Angular frequency</td>
<td>28</td>
</tr>
<tr>
<td>$\otimes$</td>
<td>Out of page</td>
<td>43</td>
</tr>
<tr>
<td>$\mathbf{T}$</td>
<td>Momentum flux density tensor</td>
<td>8</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Power density</td>
<td>8</td>
</tr>
<tr>
<td>$\phi_{nm}$</td>
<td>Hermite-Gaussian wave-function</td>
<td>28</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Mean mass density</td>
<td>16</td>
</tr>
<tr>
<td>$\rho_c$</td>
<td>Two-phase critical point mass density</td>
<td>60</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>Electric charge density</td>
<td>12</td>
</tr>
<tr>
<td>$\rho_{\text{init.}}$</td>
<td>Initial mass density</td>
<td>57</td>
</tr>
<tr>
<td>$\rho_{\text{liq.}}$</td>
<td>Liquid mass density</td>
<td>57</td>
</tr>
<tr>
<td>$\rho_{\text{vap.}}$</td>
<td>Vapour mass density</td>
<td>57</td>
</tr>
<tr>
<td>$\sigma_E$</td>
<td>Electric conductivity</td>
<td>12</td>
</tr>
<tr>
<td>$\sigma_M$</td>
<td>Magnetic conductivity</td>
<td>12</td>
</tr>
<tr>
<td>$\sigma_{\alpha\beta}$</td>
<td>Stress tensor</td>
<td>19</td>
</tr>
<tr>
<td>$\sigma_{k,xx},\sigma_{k,xy}$</td>
<td>Diagonal and off-diagonal components of the Cauchy stress-tensor in two dimensions</td>
<td>64</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Discrete relaxation time</td>
<td>25</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>Ma</td>
<td>Mach number</td>
<td>77</td>
</tr>
<tr>
<td>$p_{k,x}$</td>
<td>Net dimensionless kinetic momentum in the $\hat{x}$ direction</td>
<td>87</td>
</tr>
<tr>
<td>$p_{k,y}$</td>
<td>Net dimensionless kinetic momentum in the $\hat{y}$ direction</td>
<td>87</td>
</tr>
<tr>
<td>$p_{k,z}$</td>
<td>Net dimensionless kinetic momentum in the $\hat{z}$ direction</td>
<td>87</td>
</tr>
<tr>
<td>$\theta(z)$</td>
<td>Divergence angle of the Hermite-Gaussian beam</td>
<td>29</td>
</tr>
<tr>
<td>$\vartheta$</td>
<td>Angle between the beam-axis and the source-axis</td>
<td>29</td>
</tr>
<tr>
<td>$\bar{v}$</td>
<td>Random velocity of a particle population relative to its mean velocity</td>
<td>16</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Bulk viscosity</td>
<td>63</td>
</tr>
<tr>
<td>$\tau$</td>
<td>The transpose operation</td>
<td>64</td>
</tr>
<tr>
<td>$a, b, R$</td>
<td>Constants used in the Carnahan-Starling equation of state</td>
<td>59</td>
</tr>
<tr>
<td>$c$</td>
<td>Speed of light in a vacuum</td>
<td>28</td>
</tr>
<tr>
<td>$c_0$</td>
<td>Dimensionless speed of light</td>
<td>45</td>
</tr>
<tr>
<td>$c_s$</td>
<td>The lattice speed of sound</td>
<td>25</td>
</tr>
<tr>
<td>$e$</td>
<td>Local energy density per mass density</td>
<td>16</td>
</tr>
<tr>
<td>$E_0$</td>
<td>Peak electric field intensity</td>
<td>30</td>
</tr>
<tr>
<td>$f$</td>
<td>Generic function</td>
<td>20</td>
</tr>
<tr>
<td>$G$</td>
<td>Interaction potential (constant)</td>
<td>59</td>
</tr>
<tr>
<td>$g_m$</td>
<td>Electrodynamis pseudoparticle probability mass function</td>
<td>40</td>
</tr>
<tr>
<td>$g^*_m$</td>
<td>Post-collision pseudo-particle population</td>
<td>40</td>
</tr>
<tr>
<td>$g^e_m$</td>
<td>Equilibrium electrodynamis pseudoparticle probability mass function</td>
<td>40</td>
</tr>
</tbody>
</table>
### LIST OF SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>Spatial index representing a column element in a discrete field, page 23</td>
</tr>
<tr>
<td>$j$</td>
<td>Spatial index representing a row element in a discrete field, page 23</td>
</tr>
<tr>
<td>$k$</td>
<td>Wave-number, page 28</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant, page 17</td>
</tr>
<tr>
<td>$l \in {s, k, e}$</td>
<td>Index for thermodynamic ($s$), kinetic ($k$), or electrodynamic ($e$) sub-system, page 8</td>
</tr>
<tr>
<td>$m_p$</td>
<td>Particle mass, page 17</td>
</tr>
<tr>
<td>$n$</td>
<td>Particle population density, time-index, or modal index, page 16</td>
</tr>
<tr>
<td>$n_{eq}$</td>
<td>Equilibrium particle population density, page 16</td>
</tr>
<tr>
<td>$n_\lambda$</td>
<td>Number of spatial units per wavelength, page 50</td>
</tr>
<tr>
<td>$N_m$</td>
<td>Number of collision outcomes for the particle population probability mass function, page 24</td>
</tr>
<tr>
<td>$n_m$</td>
<td>Particle population as a probability mass function, page 24</td>
</tr>
<tr>
<td>$n_m^*$</td>
<td>Post-collision particle population, page 25</td>
</tr>
<tr>
<td>$n_{eq}$</td>
<td>Equilibrium particle population as a probability mass function, page 24</td>
</tr>
<tr>
<td>$N_T$</td>
<td>Number of time-periods, page 36</td>
</tr>
<tr>
<td>$N_t$</td>
<td>Number of time steps, page 36</td>
</tr>
<tr>
<td>$N_x$</td>
<td>Number of spatial lattice units in the $\hat{x}$-direction, page 39</td>
</tr>
<tr>
<td>$N_y$</td>
<td>Number of spatial lattice units in the $\hat{y}$-direction, page 39</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure derived from an equation of state, page 59</td>
</tr>
<tr>
<td>$q(z)$</td>
<td>Complex beam parameter, page 29</td>
</tr>
<tr>
<td>$R(z)$</td>
<td>Beam radius of curvature, page 29</td>
</tr>
</tbody>
</table>
### LIST OF SYMBOLS

- $s$: Polar axis coordinate, page 29
- $S_m$: Forcing term used in the collision operation, page 61
- $s_m$: Relaxation parameters in a multi-relaxation approach, page 63
- $T$: Time period, page 28
- $t$: Time, page 16
- $V$: Generic variable representing a scalar field, page 12
- $W$: Energy density, page 8
- $w(z)$: Beam-waist of Hermite-Gaussian beam, page 29
- $w_{e,m}$: Lattice weights for an electrodynamic sub-system, page 22
- $w_{k,m}$: Lattice weights for a kinetic sub-system, page 22
- $x$: Dimension that is horizontal on the page in this thesis, page 23
- $y$: Dimension that is vertical on the page in this thesis, page 23
- $z$: Out-of-plane dimension (2D), vertical dimension (3D), page 29
- $z_R$: Rayleigh range, page 29
- $d$: Number of dimensions, page 16
## List of Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AB</td>
<td>Abraham. 14, 15, 77–80, 83–86, 88, 89, 92</td>
</tr>
<tr>
<td>AMP</td>
<td>Amperian. 14, 15, 77–80, 83–87, 89</td>
</tr>
<tr>
<td>BE</td>
<td>Boltzmann's equation. 17</td>
</tr>
<tr>
<td>BGK</td>
<td>Bhatnagar-Gross-Krook. 25, 61, 65, 66, 71</td>
</tr>
<tr>
<td>BPML</td>
<td>Berenger perfectly matched layer. 37, 48</td>
</tr>
<tr>
<td>CET</td>
<td>Chapman-Enskog theory. 19</td>
</tr>
<tr>
<td>CHU</td>
<td>Chu. 14, 15, 77–80, 83–87, 89</td>
</tr>
<tr>
<td>CS-EOS</td>
<td>Carnahan Starling equation of state. 60</td>
</tr>
<tr>
<td>D1Q3</td>
<td>one-dimensional three lattice vector. 19, 22, 23, 46</td>
</tr>
<tr>
<td>D2Q5</td>
<td>two-dimensional five lattice vector. 19–23, 42, 43, 46</td>
</tr>
<tr>
<td>D2Q9</td>
<td>two-dimensional nine lattice vector. 19, 21–23, 25, 26, 62–64, 69, 71, 75, 76</td>
</tr>
<tr>
<td>D3Q27</td>
<td>three-dimensional twenty-seven lattice vector. 19, 21–23, 25, 71</td>
</tr>
<tr>
<td>D3Q7</td>
<td>three-dimensional seven lattice vector. 19–23, 40, 46</td>
</tr>
<tr>
<td>EL</td>
<td>Einstein &amp; Laub. 14, 15, 77–80, 83–86, 88, 89</td>
</tr>
<tr>
<td>ELBM</td>
<td>electrodynamic lattice-Boltzmann method. xi, 7, 19, 27, 38–40, 44–54, 56, 72, 73, 81, 118</td>
</tr>
<tr>
<td>EOS</td>
<td>equation of state. 16, 19</td>
</tr>
<tr>
<td>EPMF</td>
<td>equilibrium probability mass function. 56, 61, 65, 66</td>
</tr>
<tr>
<td>FDTD</td>
<td>finite-difference time-domain. xxi, 5, 54</td>
</tr>
</tbody>
</table>
### List of Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEM</td>
<td>finite-element method. 5</td>
</tr>
<tr>
<td>HLM</td>
<td>Helmholtz. 14, 15, 77–80, 83–86, 88, 89</td>
</tr>
<tr>
<td>KBC</td>
<td>Karlin-Boltzmann Collision. 65, 66</td>
</tr>
<tr>
<td>LBE</td>
<td>lattice-Boltzmann equation. 19, 20, 24, 66</td>
</tr>
<tr>
<td>LBM</td>
<td>lattice-Boltzmann method. 20, 55, 59, 65–67, 70</td>
</tr>
<tr>
<td>MDW</td>
<td>mass-density wave. 4</td>
</tr>
<tr>
<td>MRT</td>
<td>multi-relaxation time. 62, 64–66, 76</td>
</tr>
<tr>
<td>NEBB</td>
<td>non-equilibrium bounce-back. 75</td>
</tr>
<tr>
<td>NSE</td>
<td>Navier-Stokes Equation. 55, 66</td>
</tr>
<tr>
<td>PBC</td>
<td>periodic boundary conditions. 82</td>
</tr>
<tr>
<td>PLBM</td>
<td>pseudopotential lattice-Boltzmann method. 7, 19, 55, 56, 59, 61, 65, 66, 70, 73–81, 118</td>
</tr>
<tr>
<td>PMF</td>
<td>probability mass function. 56, 58, 59, 61, 63, 66, 67</td>
</tr>
<tr>
<td>SEM</td>
<td>stress-energy-momentum. 4, 8, 15</td>
</tr>
<tr>
<td>SRT</td>
<td>single-relaxation time. 64–66, 75, 76, 81</td>
</tr>
<tr>
<td>TE</td>
<td>transverse electric, s-polarized. 32, 43</td>
</tr>
<tr>
<td>TEM</td>
<td>transverse Hermite-Gaussian. 28–30</td>
</tr>
<tr>
<td>TM</td>
<td>transverse magnetic, p-polarized. 32, 35, 42</td>
</tr>
<tr>
<td>YL-FDTDM</td>
<td>Yee-lattice finite-difference time-domain method. xi, 7, 19, 27, 31, 34, 36–40, 44, 47–53, 72, 73, 81</td>
</tr>
</tbody>
</table>
Acknowledgements

I would like to extend my deep appreciation to the Natural Sciences and Engineering Research Council (NSERC) of Canada and the University of British Columbia (UBC) College of Graduate Studies for their generous support in the form of the NSERC Canadian Graduate Scholarship - Masters (CGSM), the NSERC Discovery Grant (DG), and the UBC Graduate Deans Entrance Scholarship (GDES). This work was also made possible with the assistance of Dr. Loïc Markley and Dr. Kenneth J. Chau, who were available for bi-weekly discussions on the topic of optical radiation pressure throughout the COVID-19 pandemic. Loïc provided helpful suggestions for the electrodynamic sub-system, including improvements to the initial simulation methodology that increased its performance. He also brought a healthy skepticism to the methodology that helped it mature. Kenneth, with the assistance of his former student Max Bethune-Waddell, also provided the initial framework for computational electrodynamics that has enabled this thesis. In particular, the finite-difference time-domain (FDTD) methods of solving kinetic force density, and extensive testing of the force density of various electrodynamic formalisms on rigid and deformable media. I would further like to thank Brock Legentil for his time as an undergraduate research assistant, whose quick learning, impressive attention to detail and computational resources assisted our simulations of two-dimensional FDTD force-densities. Andreas Hauser and Dr. Chun-Sheng Wang, thank-you for your guidance and suggested practices with the electrodynamic and multi-phase lattice-Boltzmann methods. Special thanks to all anonymous reviewers and editors who helped clarify this work. Finally, I would like to thank Vincent Loi for showing me how to script acronyms and symbols in the thesis template.
I dedicate this work to all researchers who endeavoured to investigate light-matter interactions; your theories have stood the test of time. In particular, James C. Maxwell, who formulated much of the fundamental theory for both the electrodynamic and kinetic sub-systems explored in this thesis. Among Maxwell were Ludwig Boltzmann, William Thomson (Lord Kelvin), Hendrik Lorentz, John Henry Poynting, Albert Einstein, Jakob Laub, Max Abraham, Hermann Minkowski, Lan Jen Chu, Robert Fano, and Hermann von Helmholtz among many other scientists whose theories fundamentally contribute to this thesis. Further, I dedicate this work to those who have provided support to researchers who investigate optical radiation pressure; thank-you for appreciating the significance, challenges and value of understanding these ubiquitous forces acting at a distance.

More personally, I dedicate this thesis to Alice Jaquish for her kind words of encouragement as I pursued a university education; you may be gone, but you will be remembered. I also dedicate this thesis to Jan Cyganik; he was a good man who cared much for the well-being of others. I further dedicate this thesis to Josh, Brandon, Aspen and Joe; thank-you for the good times.
Chapter 1

Introduction

This chapter discusses the brief history of optical radiation pressure, from its discovery to its present theoretical debate. This brief history is followed by the computational methods used to predict optical radiation pressure, and how such methods are used to understand the phenomenon. Last, this chapter discusses the organization of subsequent chapters in this thesis with a short description of their content.

1.1 Brief history of optical radiation pressure

The first recorded observation of optical radiation pressure was made by James Kepler in 1679, when he observed a comet's tail directed away from the sun [1, 2]. It was almost two centuries later, in 1845, when electrostatic and magnetostatic forces on ponderable media were predicted and measured by Lord Kelvin [3]. In 1865, a dynamic relationship between electric and magnetic fields was discovered by Michael Faraday and developed into a classical theory of electromagnetism by James C. Maxwell [4]. James C. Maxwell's classical theory of electromagnetism describes the coupling of electric and magnetic fields as electromagnetic waves that manifest as light. Maxwell's equations imply that light can exert force on matter and therefore, it lets us conclude that light carries momentum. In 1881, Helmholtz defined electric and magnetic forces that satisfy Lord Kelvin's measurements, and in 1895, Lorentz derived electric and magnetic forces from Maxwell's equations [5, 6]. Although Helmholtz and Lorentz had introduced unique expressions for an electromagnetic force density, the former based on a polarization density and the latter based on free-charge, these force density expressions describe the same net force acting on a ponderable medium [7, 8]. In 1901, Lebedew confirmed the existence of optical radiation pressure by measuring the displacement of a solid dielectric [9]. In 1905, Poynting proposed that optical radiation pressure acts normal to a boundary [10].
1.1. Brief history of optical radiation pressure

Multiple electrodynamic formalisms were developed shortly after the theory of special relativity. The theory of special relativity, which was developed by Albert Einstein in 1905, suggests that mass, length, and time are velocity-dependent variables that change with respect to a universally constant vacuum speed of light [11]. Lorentz discovered that Maxwell’s equations also satisfy special relativity, given the appropriate Lorentz transformations for electric and magnetic fields in an arbitrary frame of reference [12]. Special relativity established the need for a frame-invariant, or Lorentz invariant, electrodynamic formalism capable of conserving energy and momentum in all frames of reference. In 1908 and 1909, Hermann Minkowski, Max Abraham, and Albert Einstein & Jakob Laub derived unique electrodynamic formalisms from the relativistic Maxwell’s equations, energy and momentum continuity [13–15]. Each formalism satisfies energy and momentum continuity, and therefore predicts the same net optical force on a rigid body [7, 8]. Minkowski and Abraham’s formalisms also describe the Lorentz force density, despite their distinct forms of momentum [13, 14]. Einstein & Laub presented a unique force density in their formalism, such that the torque density includes light-matter interactions exclusive of the force density [15, 16].

Early experiments with optical radiation pressure made definitive conclusions in favour of a single electrodynamic formalism that were later criticized and found inconclusive [7, 8, 17]. Theoretical controversy intensified given that each electrodynamic formalism has been supported in experiment [7, 17, 18]. Many experiments analyzed the deformation of elastic solids such as cantilevers, torsion beams, spectral mirrors, and optical fibers [17]. While the conclusions of these studies argue in favour of a single electrodynamic theory, the net forces and kinematics measured in each study have been identically predicted by each electrodynamic formalism in numerical analyses [7, 8].

Alternative electrodynamic theories were developed in the 1960’s in an attempt to resolve the ensuing controversy that had lasted for over half a century [5, 19, 20]. Lan Jen Chu developed the E-H formulation of Maxwell’s equations in the 1960’s, which is a microscopic formulation that depends only on external electric and magnetic field intensity [20]. Using the E-H formulation, with principles of energy and momentum conservation, Chu developed an electrodynamic formalism that describes the Lorentz force density and Abraham momentum density from electric and magnetic field
1.1. Brief history of optical radiation pressure

intensities alone. Since Chu’s formalism does not explicitly include the elec-
tric and magnetic dipoles of ponderable media, it is philosophically distinct
from the Abraham, Minkowski, and Einstein & Laub formalisms. Alter-
atively, the Lorentz/Amperian formalism described by Robert Fano only
differs from Chu’s formalism in describing magnetic dipoles in magnetic me-
dia [19].

Hidden momentum became a topic of the controversy following its
discovery by Shockley in 1967 [21]. Mansuripur demonstrated that the Chu
and Lorentz/Amperian formalisms for a dielectric neglect the influence of
“hidden momentum,” in favour of the Lorentz force density [16, 21]. Conse-
quently, there may exist additional terms for light-matter interactions in an
electromagnetic torque density that are exclusive of an electromagnetic force
density [16]. Although Einstein may have considered these additional terms
erroneous in the formalism he developed with Laub, Mansuripur demon-
strates that these additional terms may account for the “hidden momentum”
discovered by Shockley in 1967 [16, 21]. Plotting the Lorentz force density
throughout a dielectric medium, Mansuripur also predicted that it may cause
def ormation opposite to earlier experiments on fluids performed by Ashkin
& Dziedzic [22]. Such a conclusion was also drawn by Bethune-Waddell &
Chau who demonstrated that the Lorentz/Amperian and Chu formalisms, in
addition to predicting electric-field polarization-dependent optical radiation
pressure, can predict opposite interface deformation and optical trapping
compared with experiment [7, 8]. Given that the re-interpreted Einstein
& Laub formalism may accurately predict the deformation of generic fluids
subjected to optical radiation pressure, its predictions for the electrodynam-
ic of elastic media have also been explored [8, 16, 23].

Modern experiments with optical radiation pressure investigate its
def ormation of microscopic fluids or nanometric solids. Optical radiation
pressure on ponderable fluids was first studied by Ashkin & Dziedzic in 1973,
who subjected an air-water interface to a focused Gaussian laser beam [22].
Highly deformable toluene-water interfaces have also been investigated, and
suggested as a means of discriminating between the predictions of electrody-
namic formalisms [8, 24–27]. Ashkin & Dziedzic’s experiment was repeated
in 2014 by Astrath et al., with improved measurement sensitivity and preci-
sion, and demonstrated agreement between the measured deformation and
the simulated prediction of the Helmholtz formalism [5, 28]. However, As-
strath et al.’s study did not compare measurements of the fluid-fluid inter-
1.1. Brief history of optical radiation pressure

face deformation with the predicted deformation of other electrodynamic formalisms [23]. Zhang et al. demonstrated that fluid depth is also an important consideration in experiments deducing the Minkowski or Abraham momenta, since the trivial solution of the Laplace pressure becomes dominant in the Navier-Stokes equation with decreasing fluid depth [29]. However, Zhang et al.’s study approximates pressure at an interface according to Abraham and Minkowski momenta alone, while there exist alternative formalisms that were not compared and that may provide an alternative explanation for the downward interface deflection [7]. Pozar et al. compared predictions of acoustic vibrations from multiple electrodynamic formalisms with their piezoelectric measurement from pulsed optical radiation pressure on an elastic dielectric mirror [23]. Comparisons between the measured and simulated acoustic waves demonstrate that Chu and Amperian formalisms predict significantly less vibration than had been measured [23]. However, Pozar et al. noted that increased measurement precision may be required to discriminate between the remaining formalisms [23].

The theoretical foundation of electrodynamics remains contested, especially in studies where the frame invariance of multiple electrodynamic formalisms are re-examined. While each electrodynamic formalism was originally derived to satisfy Lorentzian and Lagrangian invariance, to ensure their independence from a particular frame of reference, their invariance with the frame of reference remains a subject of controversy [30, 31]. Partanen and Tulkki performed experiments of radiation pressure on thin films and developed a mass-polariton theory which remedies the Lagrangian variance in Minkowski’s stress-energy-momentum (SEM) tensor [30]. In the mass-polariton theory, mass-polaritons are quasi-particles which travel at the speed of sound within a medium, and represent interactive coupling between photons and atoms. Mass-polaritons produce an atomic mass-density wave (MDW) with acoustics described by Minkowski’s momentum [30]. Including the MDW and the rest energy of a material system in the energy continuity equation modifies the Minkowski SEM tensor to satisfy Lorentzian and Lagrangian invariance [30]. The mass-polariton theory also explains the difference in center-of-mass translation predicted by Minkowski and Abraham momenta, and how Minkowski’s momentum density satisfies Hamiltonian mechanics [32, 33]. In response, Kemp et al. emphasized the non-causality of the Minkowski SEM tensor [31]. Sheppard & Kemp also argue that the Abraham, Einstein & Laub, and Lorentz/Amperian SEM tensors are Lagrangian variant, such that Chu’s SEM tensor is the only formalism which
is Lagrangian invariant [31]. Therefore, the theoretical foundations of optical radiation pressure remain a topic of debate since there exist multiple theoretical interpretations of each electrodynamic formalism’s frame-invariance, energy and momentum conservation [34]. Resolving the debate will require either increased precision and accuracy measurement or more experiments elucidating distinct predictions from each of the formalisms [23]. Such experiments may benefit from the simulated deformation of quasi-stationary media in a laboratory frame of reference [7, 8, 23, 28].

1.2 Simulations of optical radiation pressure

Simulations of optical radiation pressure using finite-difference time-domain (FDTD) methods have been successful in representing multiple electrodynamic experiments on rigid media [7, 8, 33, 35]. FDTD has also been combined with front-tracking or the finite-element method (FEM) to simulate the deformation of liquids and viscoelastic media in optical radiation pressure experiments [7, 8, 23, 28]. Alternative numerical methods include the boundary-integral-element method with ray tracing to approximate optical radiation pressure [25]. Recently, there has been increased interest in lattice-Boltzmann methods for electrodynamics and multi-phase fluids [36–40]. Not only are electrodynamic and kinetic lattice-Boltzmann methods simpler to implement than FDTD or solvers of Maxwell’s equations or the Navier-Stokes equation, but they can more easily represent natural interfaces and mesoscopic phenomena [41]. Mesoscopic phenomena occur at a mesoscopic scale of condensed matter physics. The mesoscopic scale lies between the microscopic scale (which considers individual interacting atoms and molecules) and the macroscopic scale (which considers continuous materials). In addition, the kinetic lattice-Boltzmann method can simulate non-linear hydrodynamics locally, by-passing the need for iterative solutions of hyperbolic differential equations that are assumed linear in finite-element methods [41–43]. While inefficient for modeling steady flow, kinetic lattice-Boltzmann methods are more efficient for modeling weakly compressible flows [44]. The lattice-Boltzmann method has also been adapted to represent acoustics and high-Reynolds number, compressible, thermal and relativistic fluid flows [45–50].
1.3 The goals and contributions of this thesis

The goals and contributions of this thesis are to:

1. Develop a simple, accurate, and fast electrodynamic simulator of time-averaged optical force density in two and three dimensions.

2. Develop a simple, accurate, and re-configurable multi-physics simulator of optical radiation pressure on continuously deformable media in two and three dimensions.

3. Simulate optical radiation pressure on a spherical liquid droplet suspended in its own vapor to illustrate distinct deformations of a mesoscopic fluid predicted by multiple electrodynamic formalisms.

Numerically simulating the mesoscopic optical deformation of ponderable media may help guide future experiments aiming to contrast the predictions of multiple electrodynamic formalisms [22, 28]. Such simulations may benefit predictions of micro-assembly with optical tweezers [51], optical manipulation of cells and vesicles for their analysis in non-invasive surgery [52], or other microfluidic assays [36, 38, 53]. With further description of photothermal absorption, additional applications include the prediction of fluid deformation from plasmonic heating [54], nitrogen bubble nucleation and cavitation in liquid cryogenics [55, 56], or laser focusing [57]. Given adaptation for arbitrary frames of reference [50, 58, 59], such simulation methodology may benefit secondary applications in orbital debris removal [60], and interstellar space travel [2].

1.4 The organization of this thesis

This thesis uses formal classification to organize its content into chapters. The following chapters are organized in order of the thesis goals and contributions:

- Chapter 2, Theory: Describes classical electrodynamic theory, momentum and energy conservation. General conclusions for the electrodynamics of rigid bodies, the advantage of a statistical mechanics approach for mesoscopic analysis, and general/fundamental numerical methods and approaches are presented.

- Chapter 3, Comparing finite-difference methods and lattice-Boltzmann methods solutions of kinetic force density:
1.4. The organization of this thesis

Yee-lattice finite-difference time-domain method (YL-FDTDM) and a single-lattice electrodynamic lattice-Boltzmann method (ELBM) are compared for their numerical modeling of kinetic force densities in non-dispersive media.

– **Chapter 4, Multi-physics simulation of optical radiation pressure on a multi-phase fluid:** The pseudopotential lattice-Boltzmann method (PLBM), with a Carnahan-Starling equation of state, is integrated with the ELBM for two-dimensional and three-dimensional simulations of multiphase fluid optical acceleration and trapping.

– **Chapter 5, Two- and three-dimensional optical acceleration and deformation of multi-phase fluids:** Simulations of optical radiation pressure on mesoscopic liquid droplets suspended in vapor are explored in both two and three dimensions for multiple electrodynamic formalisms.

– **Chapter 6, Conclusion:** This thesis concludes with a description of the general observations from purely kinetic approaches which conserve momentum, and general properties of a quasi-stationary experiment or simulation thereof, which may benefit present understanding of optical radiation pressure. Limitations to the study and recommendations for future work are emphasized.

– **Appendix:** Contains the relevant mathematical operations and derivations in this thesis and some MATLAB functions for the numerical methods employed.
Chapter 2

Theory

This chapter describes the interaction between electrodynamic and kinetic sub-systems that conserve energy and momentum in the rest-frame. This chapter omits descriptions of Lagrangian-invariance or Lorentz-covariance of SEM tensors, which are outside the scope of this thesis [30, 31]. Maxwell’s equations and six popular electrodynamic formalisms are described in the quasi-stationary or “near-rest” frame in a discussion of the electrodynamic sub-system. Boltzmann’s equation and the discrete lattice-Boltzmann equation are detailed for the kinetic sub-system. Finally, this chapter concludes with a general description of discrete numerical methods employed in this thesis. Refer to “analytical methods,” Appendix A, for a discussion of the relevant mathematical operators, polynomials and functions.

2.1 Multi-physics energy and momentum conservation

In the rest-frame, a physical system can be separated into three sub-systems indexed by $l \in \{s, k, e\}$: thermodynamic ($l = s$), kinetic ($l = k$), and electrodynamic ($l = e$) sub-systems. These sub-systems interact according to the continuous conservation of their total energy density, $W$, and momentum density, $G$,

$$\nabla \cdot \mathbf{S} + \frac{\partial}{\partial t} W = \sum_l \Phi_l, \quad (2.1)$$

$$\nabla \cdot \mathbf{T} + \frac{\partial}{\partial t} G = \sum_l f_l, \quad (2.2)$$

where $\mathbf{S}$ is the power per cross-sectional area and $\mathbf{T}$ is momentum flux density tensor which defines the state of stress at a point for a stationary medium [8, 20]. In an isolated system, the net power density, $\sum_l \Phi_l$, is zero and the net force density, $\sum_l f_l$, is a null vector. Energy and momentum are
2.1. Multi-physics energy and momentum conservation

conserved in their transfer between sub-systems [20],

\[ \sum l \Phi_l = \Phi_e + \Phi_k + \Phi_s = 0, \quad \sum l f_l = f_e + f_k + f_s = 0. \] (2.3)

In this thesis, the thermodynamic sub-system is neglected such that \( \Phi_s = 0 \) and \( f_s = 0 \) to represent ideal light-matter interactions in an isolated isothermal system. Modern experiments investigating optical radiation pressure on deformable liquids are often designed to achieve such conditions, for example, the case of green laser light transmitted through pure liquid water [28]. Consequently, Newton’s third law states that the force density acting on the electrodynamic sub-system must be equal and opposite to the force density acting on the kinetic sub-system, such that \( f_k = -f_e \) [7, 8, 20]. The result is a single momentum continuity equation describing the kinetic force density acting on an isothermal kinetic sub-system in terms of an electromagnetic momentum flux density tensor, \( T_e \), and an electromagnetic momentum density, \( G_e \),

\[ \nabla \cdot T_e + \frac{\partial}{\partial t} G_e = -f_k. \] (2.4)

Multiple theoretical formulations of \( T_e \) and \( G_e \) have been proposed to satisfy this relation, particularly in the rest-frame. To limit comparative studies in the rest-frame, only a subset of six mathematically debatable frame-invariant electrodynamic formalisms are compared.

In typical optical radiation pressure experiments on macroscopic media, the velocity of the laboratory frame and/or the medium under consideration is negligible in comparison to the speed of light. The medium can then be considered quasi-stationary and Lorentz transformation unnecessary [8, 23]. The simulations in this thesis assume the medium is quasi-stationary and continuously deformable. This is a necessary development for distinguishing between electrodynamic formalisms as previous work has shown that they yield identical rigid-body motion [7, 8]. Previous studies reveal some general conclusions for the dynamics of magnetodielectric bodies subjected to quasi-stationary optical radiation pressure:

1. In one dimension, only linear pressure acting along the direction of propagation is accessible. Neither shear stress nor torque can be analyzed in one dimension.

2. In one dimension, each electrodynamic formalism predicts distinct force density but identical time-averaged time-harmonic pressure. Each formalism therefore predicts identical rigid-body kinematics in most experiments [8].
2.1. *Multi-physics energy and momentum conservation*

3. In two dimensions, the net line force density acts in the direction of propagation [10]. Each formalism predicts unique transverse shear stress resulting from electric and magnetic field attenuation. The transverse shear stress can be distinct for each electric field polarization.

4. Consistent net force on a body consisting of heterogeneous or homogeneous media can be evaluated when; (i) a source of radiation is external to the body, and (ii) the body is fully bounded by free space. Omitting a free-space/medium boundary, and/or initializing a source internal to the body, will result in an inconsistent evaluation of net force from a distributed force density.

5. Given a source of radiation with a symmetric transverse profile, forces acting orthogonal to the direction of propagation are balanced in each direction. Electromagnetic torque is generally non-zero and depends on the electric field polarization and isotropy of the media. Birefringent media will be subjected to electromagnetic torque [61].

6. If the body is distributed asymmetrically with respect to an external source of radiation, it can be subjected to a net force and/or torque from scattering transverse to the direction of incidence.

Figure 2.1 illustrates the general conclusions for the dynamics of magnetodielectric bodies subjected to quasi-stationary optical radiation pressure that were described in the previous list.
2.1. Multi-physics energy and momentum conservation

Figure 2.1: [Color online] Electrodynamics with different source and object configurations in one, two, and three dimensions. In the top left-hand corner of each box is a number representing each general conclusion. Dashed black lines are major axes, while solid black arrows represent propagation directions and wave-vectors, \{k_x, k_y, k_z\}. Solid black lines represent dielectric or system boundaries. (1) Neither transverse force density nor shear stress (solid blue arrow) can be evaluated in one dimension. Electrodynamnic torque, \(\mathbf{T}\), cannot be evaluated in one dimension. (2) Force density and optical radiation pressure (solid green arrows) can be evaluated in one dimension. The same time-averaged time-harmonic radiation pressure is predicted by each electrodynamic formalism. (3) Transverse force density or shear stress can be evaluated in two dimensions. (4) Net line-force density can only be evaluated using a source of electromagnetic radiation positioned in free-space (along the green dashed line for example). Net line force density cannot be evaluated using a source of electromagnetic radiation positioned within the medium (along the red dashed line for example). (5) Optical acceleration and direction of net force (green arrow) in a ponderable sphere subject to optical radiation with a symmetric transverse profile. (6) Net force and/or torque on a body asymmetrically distributed with respect to the transverse symmetric profile in (5).
2.2 Electrodynamic sub-system theory

The electrodynamic sub-system in a rest frame is typically represented by the Minkowski formulation of Maxwell’s equations, where the dot notation, i.e. “\( \dot{V} \)”, is a shorthand for the partial derivative of a field \( V \) with respect to time \( (\partial V/\partial t) \) [4].

\[
\begin{array}{|c|c|}
\hline
\text{Name of Law} & \text{Vector calculus form} \\
\hline
\text{Gauss’s Law} & \nabla \cdot \mathbf{D} = \rho_v \\
 & \nabla \cdot \mathbf{B} = 0 \\
\text{Faraday’s Law} & \nabla \times \mathbf{E} = -\dot{\mathbf{B}} - \mathbf{J}_M \\
\text{Ampere’s Law} & \nabla \times \mathbf{H} = \dot{\mathbf{D}} + \mathbf{J}_E \\
\hline
\end{array}
\]

In the Minkowski formulation of Maxwell’s equations, electric and magnetic field intensities are \( \mathbf{E} \) and \( \mathbf{H} \), while electric and magnetic flux densities are \( \mathbf{D} \) and \( \mathbf{B} \), respectively. Dimensional constants \( \epsilon_0 \) and \( \mu_0 \) represent the free-space permittivity and permeability, respectively. Gauss’s law predicts the electric charge density, \( \rho_v \), while free electric and magnetic current densities

\[
\mathbf{J}_E = \sigma_E \mathbf{E} \quad \text{and} \quad \mathbf{J}_M = \sigma_M \mathbf{H},
\]

are represented by electric conductivity \( \sigma_E \), and magnetic conductivity \( \sigma_M \). Although a magnetic current density has yet to be discovered, it serves as a useful analytical tool that satisfies Maxwell’s equations, energy and momentum conservation [62].

Alternative formulations for Maxwell’s equations, which differ philosophically from the Minkowski formulation, lead to alternative predictions of microscopic light-matter interactions. Einstein & Laub’s formulation describes a dependence between \( \mathbf{E} \) and an electric polarization density \( \mathbf{P} \), and \( \mathbf{H} \) and a magnetic polarization density \( \mathbf{M} \), in a magnetodielectric medium. According to Einstein & Laub’s formulation, electric and/or magnetic fields always exist in magnetodielectric media, even in the absence of external electric and magnetic fields [15, 16, 63]. In the latter case, the electric and/or magnetic forces are at equilibrium from the orientation of electric and/or magnetic dipoles. Einstein & Laub’s formulation (Tab. 2.2) is mathematically identical to Minkowski’s formulation (Tab. 2.1) given constitutive relations \( \mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} \) and \( \mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M}) \). However, Einstein & Laub’s formulation establishes a local dependence between field intensity and polarization.
2.2. Electrodynamic sub-system theory

density, such that \( \mathbf{P} \) and \( \mathbf{M} \) may describe the internal electric and magnetic field intensity distributed throughout a magnetodielectric medium.

<table>
<thead>
<tr>
<th>Name of Law</th>
<th>Vector calculus form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauss’s Law</td>
<td>( \nabla \cdot \epsilon_0 \mathbf{E} = -\nabla \cdot \mathbf{P} + \rho_v )  ( \nabla \cdot \mu_0 \mathbf{H} = -\nabla \cdot \mu_0 \mathbf{M} )</td>
</tr>
<tr>
<td>Faraday’s Law</td>
<td>( \nabla \times \mathbf{E} = -\mu_0(\mathbf{H} + \mathbf{M}) - \mathbf{J}_M )  ( \nabla \times \mathbf{H} = (\epsilon_0 \mathbf{E} + \mathbf{P}) + \mathbf{J}_E )</td>
</tr>
<tr>
<td>Ampere’s Law</td>
<td></td>
</tr>
</tbody>
</table>

Another formulation of Maxwell’s equations that considers the general case of polarization and magnetization density in fluids moving at relativistic velocities is called the E-H formulation. Although the E-H formulation of Maxwell’s equations is consistent with the Minkowski formulation [20], it directly includes the velocity of the polarization and magnetization density with respect to only external electric and magnetic fields.

<table>
<thead>
<tr>
<th>Name of Law</th>
<th>Vector Calculus Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauss’s Law</td>
<td>( \nabla \cdot \epsilon_0 \mathbf{E} = -\nabla \cdot \mathbf{P} + \rho_v )  ( \nabla \cdot \mu_0 \mathbf{H} = -\nabla \cdot \mu_0 \mathbf{M} )</td>
</tr>
<tr>
<td>Faraday’s Law</td>
<td>( \nabla \times \mathbf{E} = -\mu_0(\mathbf{H} + \mathbf{M}) - \nabla \times(\mu_0 \mathbf{M} \times \mathbf{u}) - \mathbf{J}_M )  ( \nabla \times \mathbf{H} = (\epsilon_0 \mathbf{E} + \mathbf{P}) + \nabla \times(\mathbf{P} \times \mathbf{u}) + \mathbf{J}_E )</td>
</tr>
<tr>
<td>Ampere’s Law</td>
<td></td>
</tr>
</tbody>
</table>

In the E-H formulation, \( \mathbf{E} \) and \( \mathbf{H} \) are generally different in polarizable or magnetizable media, as compared with their definition in the Minkowski formulation, which is an important consideration for their Lorentz covariance [20]. The relationship between the field intensities and field densities in the two formulations is

\[
\begin{align*}
\mathbf{E}_{\text{Min.}} &= \mathbf{E} + \mu_0 \mathbf{M} \times \mathbf{u}, & \mathbf{D}_{\text{Min.}} &= \epsilon_0 \mathbf{E} + \mathbf{P}, \\
\mathbf{H}_{\text{Min.}} &= \mathbf{H} - \mathbf{P} \times \mathbf{u}, & \mathbf{B}_{\text{Min.}} &= \mu_0(\mathbf{H} + \mathbf{M}),
\end{align*}
\]  

(2.6)

where \( \mathbf{u} \) is the mean velocity of particles in the medium, and subscript “\( \text{Min.} \)” designates the Minkowski formulation [20]. According to Eq. 2.6, local relative velocity of \( \mathbf{P} \) and \( \mathbf{M} \) are responsible for variation of \( \mathbf{E}_{\text{Min.}} \) and \( \mathbf{H}_{\text{Min.}} \) from \( \mathbf{E} \) and \( \mathbf{H} \) in the free-space Maxwell flux-density tensor. Should the mean velocity of particles in a medium have a magnitude that is negligible with respect to the speed of light \((|\mathbf{u}| \ll c)\), \( \mathbf{E} \) and \( \mathbf{H} \) are the same.
2.2. Electrodynamic sub-system theory

in both the E-H and Minkowski formulations of Maxwell’s equations [20].
This condition is satisfied by the quasi-stationary deformation of media from
time-averaged time-harmonic electromagnetic waves [8, 23]. Each formu-
lation of Maxwell’s equations can be expanded via dyadic products in the
rest-frame to recover an electrodynamic momentum flux density tensor and
momentum density [8]. Poynting’s theorem is applied to recover the power
and energy density which are similar if not the same for the majority of for-
malisms [10]. Electromagnetic energy density has both microscopic, \( W_{e,0} \),
and macroscopic, \( W_{e,1} \), forms

\[
W_{e,0} = \frac{1}{2}(\varepsilon_0 \mathbf{E} \cdot \mathbf{E} + \frac{1}{\mu_0} \mathbf{B} \cdot \mathbf{B}) \quad \text{and} \quad W_{e,1} = \frac{1}{2}(\varepsilon \mathbf{E} \cdot \mathbf{E} + \mu \mathbf{H} \cdot \mathbf{H}). \quad (2.7)
\]

While energy density and Poynting’s vector, \( \mathbf{S}_e \), have rarely been disputed,
six debated electrodynamic formalisms present unique momentum density
and/or momentum flux density tensors, as shown in Tables 2.4-2.5 [5, 8, 23].
In these tables, the variables \( E = (\mathbf{E} \cdot \mathbf{E})^{\frac{1}{2}} \), \( D = (\mathbf{D} \cdot \mathbf{D})^{\frac{1}{2}} \), \( H = (\mathbf{H} \cdot \mathbf{H})^{\frac{1}{2}} \),
and \( B = (\mathbf{B} \cdot \mathbf{B})^{\frac{1}{2}} \). The Helmholtz formalism also includes permittivity
and permeability of a Clausius Mossotti medium, such that polynomial expres-
sions represent the permittivity, \( \epsilon = \epsilon_r \epsilon_0 \), and permeability, \( \mu = \mu_r \mu_0 \), of a
magnetodielectric medium [5].

Table 2.4: Electrodynamic Momentum and Power Density.

<table>
<thead>
<tr>
<th>Name</th>
<th>Momentum Density</th>
<th>Power Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>G_e</td>
<td></td>
<td>S_e</td>
</tr>
<tr>
<td>Minkowski (MN) [13]</td>
<td>( \mathbf{D} \times \mathbf{B} )</td>
<td>( \mathbf{E} \times \mathbf{H} )</td>
</tr>
<tr>
<td>Abraham (AB) [14]</td>
<td>( (\mathbf{E} \times \mathbf{H})/c^2 )</td>
<td>( \mathbf{E} \times \mathbf{H} )</td>
</tr>
<tr>
<td>Einstein &amp; Laub (EL) [15]</td>
<td>( (\mathbf{E} \times \mathbf{H})/c^2 )</td>
<td>( \mathbf{E} \times \mathbf{H} )</td>
</tr>
<tr>
<td>Helmholtz (HLM) [5]</td>
<td>( ((\mu_r - 1)(2\epsilon_r + 1) + 3)(\mathbf{E} \times \mathbf{H})/(3c^2) )</td>
<td>( \mathbf{E} \times \mathbf{H} )</td>
</tr>
<tr>
<td>Chu (CHU) [19, 20]</td>
<td>( (\mathbf{E} \times \mathbf{H})/c^2 )</td>
<td>( \mathbf{E} \times \mathbf{H} )</td>
</tr>
<tr>
<td>Amperian (AMP) [19]</td>
<td>( \epsilon_0(\mathbf{E} \times \mathbf{B}) )</td>
<td>( \mathbf{E} \times \mathbf{B}/\mu_0 )</td>
</tr>
</tbody>
</table>
2.2. Electrodynamic sub-system theory

Table 2.5: Electrodynamic Momentum Flux Density Tensors.

<table>
<thead>
<tr>
<th>Name</th>
<th>Momentum Flux Density Tensor, $\mathbf{T}_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minkowski (MN) [13]</td>
<td>$(\mathbf{D} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{H})\hat{I}/2 - \mathbf{DE} - \mathbf{BH}$</td>
</tr>
<tr>
<td>Abraham (AB) [14]</td>
<td>$[(\mathbf{D} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{H})\hat{I} - \mathbf{DE} - \mathbf{BH} - \mathbf{ED} - \mathbf{HB}]/2$</td>
</tr>
<tr>
<td>Einstein &amp; Laub (EL) [15]</td>
<td>$(\epsilon_0 E^2 + \mu_0 H^2)\hat{I}/2 - \mathbf{DE} - \mathbf{BH}$</td>
</tr>
<tr>
<td>Helmholtz (HLM) [5]</td>
<td>$(\epsilon_0(2 + 2 \epsilon_r - \epsilon_r^2)E^2 + \mu_0(2 + 2 \mu_r - \mu_r^2)H^2)\hat{I}/6 - \epsilon\mathbf{EE} - \mu\mathbf{HH}$</td>
</tr>
<tr>
<td>Chu (CHU) [19, 20]</td>
<td>$(\epsilon_0 E^2 + \mu_0 H^2)\hat{I}/2 - \epsilon_0\mathbf{EE} - \mu_0\mathbf{HH}$</td>
</tr>
<tr>
<td>Amperian (AMP) [19]</td>
<td>$(\epsilon_0 E^2 + B^2/\mu_0)\hat{I}/2 - \epsilon_0\mathbf{EE} - \mathbf{BB}/\mu_0$</td>
</tr>
</tbody>
</table>

Each of the electrodynamic formalisms can be classified according to the formulation of Maxwell’s equations invoked in their derivation:

- **Class 1**: AB and MN formalisms, constructed from the Minkowski formulation of Maxwell’s equations (Tab. 2.1).
- **Class 2**: EL and HLM formalisms, constructed from the Einstein & Laub formulation of Maxwell’s equations (Tab. 2.2).
- **Class 3**: CHU and AMP formalisms, constructed from the E-H formulation of Maxwell’s equations (Tab. 2.3).

Each formulation of Maxwell’s equations is consistent with a Lorentz transformation of the reference frame [20], which is a necessary condition for the kinetic force density, momentum density, and stress predicted by a theoretical electrodynamics formalism. Recently, both the form of the electromagnetic momentum density and the relativistic frame-invariance of the stress-energy-momentum (SEM) tensor have been actively debated. Sheppard & Kemp contend that the symmetric Abraham and Einstein & Laub SEM tensors are Lagrangian-variant, while the asymmetric Minkowski SEM tensor is non-causal [64]. Partannen & Tulikki note that the energy continuity equation used by Sheppard & Kemp, which omits the momentum and rest energy of the kinetic sub-system, is incomplete [30]. Present theoretical debates for a single electrodynamic theory may benefit from general numerical methods capable of modeling their observable kinetics [8, 23, 28].
2.3 Kinetic sub-system theory

While James C. Maxwell is most often credited as the founder of classical electromagnetics, he also founded a dynamical theory of gases [65]. Alternative to the phenomenological description of fluids presented by the Navier-Stokes equation, James C. Maxwell’s theory considers an ideal gas as a population of colliding particles that conserve both energy and momentum. Within Maxwell’s description, a probability density function, \( n(x, v, t) \), describes the post-collision continuous random velocity, \( v \), of a particle population in a multi-dimensional particle velocity space at time \( t \) and vector position \( x \). In velocity space the zeroth, first, second and third moments of the probability density function describe the mean mass-density field, \( \rho(x, t) \), kinetic momentum-density field, \( G_k(x, t) = \rho(x, t)u(x, t) \), kinetic energy density field, \( W_k(x, t) = \rho(x, t)e(x, t) \), and the kinetic momentum flux density tensor, \( T_k(x, t) \), of an ideal gas, respectively. The vector field \( u(x, t) \) represents the local mean velocity and the scalar field \( e(x, t) \) represents the local energy density per mass density. Each of these moments are listed in Table 2.6, where \( \int d^3v \equiv \int \int \int d^3v_1d^3v_2d^3v_3 \).

<table>
<thead>
<tr>
<th>Moment</th>
<th>State-Variable</th>
<th>Expression at ((x, t))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Mass Density</td>
<td>( \rho = \int n d^3v )</td>
</tr>
<tr>
<td>1</td>
<td>Momentum Density</td>
<td>( G_k = \int n v d^3v )</td>
</tr>
<tr>
<td>2</td>
<td>Energy Density</td>
<td>( W_k = \frac{1}{2} \int n</td>
</tr>
<tr>
<td>3</td>
<td>Momentum Flux Density Tensor</td>
<td>( T_k = \int n (v \cdot v) v d^3v )</td>
</tr>
</tbody>
</table>

Maxwell also defined a probability density function describing the particle population of an ideal gas in a state of equilibrium [65],

\[
n_{eq}(x, |\vec{v}|, t) = \rho \left( \frac{1}{2\pi R T} \right)^{d/2} e^{-|\vec{v}|^2/(2RT)} \bigg|_{(x,t)}, \tag{2.8}
\]

where \( \vec{v}(x, t) \) is the random relative-velocity space, \( d \) is the number of dimensions, \( R \) is a gas constant, and \( T(x, t) \) is the mean temperature field derived from an equation-of-state (EOS). Relative velocity is the difference between the random particle population velocity, \( v(x, t) \), and the local mean velocity, \( u(x, t) \),

\[
\vec{v}(x, t) = v(x, t) - u(x, t). \tag{2.9}
\]
Given an ideal gas, \( R = k_B/m_p \), where \( k_B \) is the Boltzmann constant, and \( m_p \) is the particle mass. Maxwell’s equilibrium population density, \( n_{eq}(x, |\vec{v}|, t) \), demonstrates the following properties:

1. It is isotropic in velocity space around \( \mathbf{v}(x, t) = \mathbf{u}(x, t) \),

2. It is separable as the product of one-dimensional equilibrium distributions \([65]\), and

3. It has the same moments of density and energy as \( n(x, |\vec{v}|, t) \).

Maxwell’s dynamical theory of gases has a philosophical advantage over phenomenological theories of gases; it uses probability axioms to conserve mass, energy and momentum while describing their local relative likelihood at different velocities. Shortly after, Ludwig Boltzmann developed a kinetic theory of gases by considering the stochastic interactions of ideal-gas particle populations in velocity space as they approach the equilibrium population described by Maxwell \([66]\). With incorporation of a kinetic force density, \( f_k(x, t) \), representing an equation of state for a non-ideal gas (liquid), and/or the interaction of external sub-systems (electrodynamic and thermodynamic), it has proved useful in the numerical lattice-Boltzmann methods which simulate the kinetics of generic fluids \([67]\). According to Boltzmann’s theory, the kinetic sub-system can be described by Boltzmann’s equation (BE),

\[
\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + \frac{f_k}{\rho} \cdot \frac{\partial n}{\partial \mathbf{v}} \bigg|_{(x,t)} = \left( \frac{dn}{dt} \right)_{coll} \bigg|_{(x,t)} = \Omega \bigg|_{(x,t)}. \tag{2.10}
\]

Boltzmann’s equation can be derived from the total differential of the particle population density with respect to time, or using the Liouville operator or Hamiltonian. The subscript “coll” stands for a collision process as the ordinary derivative of the particle population with respect to time, \( D_t = dn/dt \), and is typically described using a collision operator \( \Omega(x, t) \) \([68]\). Integration of the collision operator throughout the entire velocity space is zero, \( \int \Omega(x, t) d^3v = 0 \), which conserves both particle populations and their momentum. In general, a collision operator must satisfy the second law of thermodynamics or Boltzmann’s \( \mathcal{H} \)-theorem \([46]\). In Boltzmann’s \( \mathcal{H} \)-theorem, the quantity

\[
\mathcal{H}(x, t) = \int n \ln n d^3v \bigg|_{(x,t)}, \tag{2.11}
\]
2.3. Kinetic sub-system theory

can only decrease, and reaches its minimum value when \( n(x, t) = n^\text{eq}(x, t) \) [66]. In Boltzmann’s kinetic theory, as opposed to continuum theory, conservation of mass and momentum are related to the collision and movement of particle populations via the total probability axiom. In Chu’s E-H formulation of electrodynamics and the mass-polariton theory [20, 30], such particle populations are used to describe a classical kinetic sub-system. However, in general, Boltzmann’s equation is non-relativistic and its traditional form may not account for Lorentz transformation or inertial frames of reference approaching the speed of light. Development of the relativistic Boltzmann’s equations and lattice-Boltzmann methods for relativistic hydrodynamics are an active area of research outside the scope of this thesis [49, 50].

2.3.1 Mass and momentum conservation

In order to demonstrate mass and momentum conservation, vector-space moments of a particle-population density are substituted into Boltzmann’s equation to represent particle collisions as a stochastic process. This can be accomplished by distinguishing zero and non-zero moments of the particle-population density and its derivatives [68]. All moments listed in Table 2.6 are non-zero, while any moments of the collision operator, \( \Omega \), are zero. Therefore, the equation of mass-conservation,

\[
\frac{\partial}{\partial t} \int n d^3v + \frac{\partial}{\partial x_\alpha} \int v_\alpha n d^3v + \frac{F_\alpha}{\rho} \int \frac{\partial n}{\partial v_\alpha} d^3v = \int \Omega d^3v
\]

\[
\frac{\partial}{\partial t} + \frac{\partial p}{\partial x_\alpha} = 0, \tag{2.12}
\]

can be derived given that

\[
\int n d^3v = \int \frac{dn}{dt} d^3v = 0 \quad \text{and} \quad \int \frac{\partial n}{\partial v_\alpha} d^3v = 0. \tag{2.13}
\]

Similar derivations can be used for the momentum and energy conservation equations [68],

\[
\frac{\partial G_{k,\alpha}}{\partial t} + \frac{\partial T_{k,\alpha\beta}}{\partial x_\beta} = f_{k,\alpha},
\]

\[
\frac{\partial W_k}{\partial t} + \frac{\partial S_{k,\alpha}}{\partial x_\alpha} = \Phi_k, \tag{2.14}
\]

where \( G_{k,\alpha} = \rho u_\alpha \) are components of momentum density, and \( \Phi_k = f_{k,\alpha} u_\alpha \) is the power flux density described using index notation for vector components.
If the particle velocity is described using the mean and relative velocity, \( \mathbf{v} = \mathbf{u} + \tilde{\mathbf{v}} \), the momentum flux density tensor is

\[
T_{k,\alpha\beta} = \rho u_\alpha u_\beta + \int \tilde{v}_\alpha \tilde{v}_\beta n d^3v,
\]

where the second term describes the stress tensor,

\[
\sigma_{\alpha\beta} = -\int \tilde{v}_\alpha \tilde{v}_\beta n d^3v.
\]

Since the stress tensor is unknown, the momentum conservation equation is not closed, such that an approximation of \( n \) is required by establishing a relation to hydrodynamics via Chapman-Enskog theory (CET). CET is a framework for deriving constitutive relations, such as the Navier-Stokes equation for hydrodynamics, from the molecular parameters described by Boltzmann’s equation. CET establishes a direct relationship between macroscopic phenomena and microscopic phenomena such as inter-particle collisions using an equation-of-state (EOS) [68, 69].

### 2.4 Numerical methods

Several numerical methods are used in this thesis including the Yee-lattice finite-difference time-domain method (YL-FD TDM), the electrodynamic lattice-Boltzmann method (ELBM) and the Shan-Chen pseudopotential lattice-Boltzmann method (PLBM). Each of these numerical methods discretize the phenomenological equations, or the lattice-Boltzmann equation (LBE), by using central differences or multi-range lattice-stencil operations. While the discretization of a phenomenological equation is specific to the represented sub-system, the LBE operations and their discretization are general and can be applied to multiple sub-systems. However, alternative lattice stencils and their weighted operations are required to maintain the stability and rotational isotropy of Boltzmann’s equation for a kinetic sub-system [45]. First this section describes the central difference equation, followed by one-dimensional three-vector (D1Q3), two-dimensional five-vector (D2Q5), two-dimensional nine-vector (D2Q9), three-dimensional seven-vector (D3Q7) and three-dimensional twenty-seven vector (D3Q27) spaces and their general operators. Finally, this section concludes with a description of the LBE and its generic algorithm using a two-dimensional kinetic sub-system as an example.
2.4. Numerical methods

2.4.1 The central difference equation

The central difference equation is a second-order-accurate numerical solution for the first derivative, \( f'(x) \), of a function \( f(x) \). Central differences can be derived by subtracting the backward difference Taylor series from the forward difference Taylor series of the first derivative of a function. The forward difference Taylor series is

\[
f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2 f''(x)}{2!} + \frac{\Delta x^3 f'''(\zeta_+)}{3!}, \quad \zeta_+ \in (x, x+\Delta x),
\]

while the backward difference Taylor series is

\[
f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2 f''(x)}{2!} - \frac{\Delta x^3 f'''(\zeta_-)}{3!}, \quad \zeta_- \in (x, x-\Delta x).
\]

The subtraction of these two Taylor series leads to a second-order \( O(\Delta x^2) \) central difference approximation of \( f'(x) \),

\[
f'(x) \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} - \frac{\Delta x^2}{12} (f'''(\zeta_+) + f'''(\zeta_-)). \tag{2.17}
\]

The error of the central difference equation is proportional to \( \Delta x^2 \). The one-dimensional central difference equation can approximate partial derivatives in multiple independent/orthogonal dimensions.

2.4.2 Lattice stencils

While an infinite vector space describes the random relative-velocity in Boltzmann’s equation, only a finite vector set, \( \mathbf{v}_m \), can exist on a lattice described by the LBE [70–72]. Consequently, the lattice-Boltzmann method (LBM) is a finite-difference method in a vector space, as opposed to a scalar space. Each lattice stencil is described by its number of orthogonal spatial dimensions, and its number of independent discrete lattice-vectors. These two properties of the lattice stencil determine its order of accuracy, its order-of-isotropy and the phenomena it can describe. In the case of inviscid flow, two-dimensional five lattice vector (D2Q5) and three-dimensional seven lattice vector (D3Q7) lattice stencils are sufficient for describing the vector space. However, there are general conditions a lattice stencil must satisfy to describe viscous interactions [45, 73]. In addition to mass and momentum conservation, rotational isotropy of the lattice is required. In a kinetic sub-system describing viscous flow, all moments of the lattice-vector weights, \( w_m \equiv w(|\mathbf{v}_m|) \), require isotropy up to the fifth order (as described
2.4. Numerical methods

by Maxwell’s theory) [45, 65, 73]. In this thesis, two-dimensional nine lattice vector (D2Q9) and three-dimensional twenty-seven lattice vector (D3Q27) stencils are used for their increased stability and accuracy. Both the D2Q9 and D3Q27 have the greatest number of lattice vectors that can be represented in a single square lattice unit. Each lattice stencil is illustrated in Fig. 2.2.

Figure 2.2: (a) Two-dimension five-velocity (D2Q5) lattice; (b) Two-dimension nine-velocity (D2Q9) lattice; (c) Three-dimension seven-velocity (D3Q7) lattice; (d) Three-dimension twenty-seven velocity (D3Q27) lattice. The black dot represents the present position on the lattice and the null vector.
Given a kinetic sub-system (subscript $k$), the weight for each discrete velocity in each lattice-stencil, $w_{k,m} \equiv w_k(|v_m|)$, can be derived from the following conditions [45, 65, 73],

$$\begin{align*}
\sum_{m=1}^{N_m} w_{k,m} &= 1, \\
\sum_{m=1}^{N_m} w_{k,m}v_{m\alpha} &= 0, \\
\sum_{m=1}^{N_m} w_{k,m}v_{m\alpha}v_{m\beta} &= c_s^2 \delta_{\alpha\beta}, \\
\sum_{m=1}^{N_m} w_{k,m}v_{m\alpha}v_{m\beta}v_{m\gamma} &= 0, \\
\sum_{m=1}^{N_m} w_{k,m}v_{m\alpha}v_{m\beta}v_{m\gamma}v_{m\mu} &= c_s^4 \left( \delta_{\alpha\beta} \delta_{\gamma\mu} + \delta_{\alpha\gamma} \delta_{\beta\mu} + \delta_{\alpha\mu} \delta_{\beta\gamma} \right), \\
\sum_{m=1}^{N_m} w_{k,m}v_{m\alpha}v_{m\beta}v_{m\gamma}v_{m\mu}v_{m\nu} &= 0,
\end{align*}$$

(2.18)

where $c_s$ is the lattice speed of sound representing an isothermal equation of state, and $N_m$ is the number of lattice vectors. Given an electrodynamic sub-system (subscript $e$), the weight for each non-zero lattice-vector in each lattice-stencil is $w_{e,m} \equiv w_e(|v_m| > 0) = 1/4$, while the weight for the null lattice-vector is zero ($w(|0|) = 0$), which is derived from the constraints of Eq. (3.37) in Chapter 3 [39]. Table 2.7 describes the lattice stencils in terms of their lattice-vectors (with magnitudes $|v_m|$), their lattice-vectors corresponding weights, and whether they are applied in a kinetic ($k$) or electrodynamic ($e$) sub-system.

| Lattice | $v_m$ | # | $|v_m|$ | $w_{k,m}$ | $w_{e,m}$ |
|---------|-------|---|--------|-----------|-----------|
| D1Q3[39] | $\langle 0 \rangle$ | 1 | 0 | - | 0 |
| | $\langle \pm 1 \rangle$ | 2 | 1 | - | 1/4 |
| D2Q5[39] | $\langle 0, 0 \rangle$, $\langle 0, \pm 1 \rangle$ | 1 | 0 | - | 0 |
| | $\langle \pm 1, 0 \rangle$, $\langle 0, \pm 1 \rangle$ | 4 | 1 | - | 1/4 |
| D2Q9[74] | $\langle 0, 0 \rangle$, $\langle 0, \pm 1 \rangle$ | 1 | 0 | 4/9 | - |
| | $\langle \pm 1, \pm 1 \rangle$ | 4 | $\sqrt{2}$ | 1/36 | - |
| D3Q7[39] | $\langle 0, 0 \rangle$, $\langle 0, \pm 1, 0 \rangle$, $\langle 0, 0, \pm 1 \rangle$ | 1 | 0 | - | 0 |
| | $\langle \pm 1, 0, 0 \rangle$, $\langle 0, \pm 1, 0 \rangle$, $\langle 0, 0, \pm 1 \rangle$ | 6 | 1 | - | 1/4 |
| D3Q27[74] | $\langle 0, 0, 0 \rangle$, $\langle 0, \pm 1, 0 \rangle$, $\langle 0, 0, \pm 1 \rangle$ | 1 | 0 | 8/27 | - |
| | $\langle \pm 1, 0, 0 \rangle$, $\langle 0, \pm 1, 0 \rangle$, $\langle 0, 0, \pm 1 \rangle$ | 6 | 1 | 2/27 | - |
| | $\langle \pm 1, \pm 1, 0 \rangle$, $\langle \pm 1, 0, \pm 1 \rangle$, $\langle 0, \pm 1, \pm 1 \rangle$ | 12 | $\sqrt{2}$ | 1/54 | - |
| | $\langle \pm 1, \pm 1, \pm 1 \rangle$ | 8 | $\sqrt{3}$ | 1/216 | - |
2.4. Numerical methods

2.4.3 Discrete spatial operators for the lattice-Boltzmann equation

Discrete spatial operators used in the lattice-Boltzmann method can be derived from the lattice stencil, including the velocities and their weights listed in Table 2.7 [75]. Two common operators used throughout this thesis include the gradient and divergence operators,

\[ \nabla \psi(x) = \sum_{m=1}^{N_m} w(|v_m|) \psi(x + v_m)v_m \]

\[ = \sum_{m=1}^{N_m} w_m \psi(x + v_m)v_m, \]

\[ \nabla \cdot u(x) = \sum_{m=1}^{N_m} w(|v_m|) u(x + v_m) \cdot v_m \]

\[ = \sum_{m=1}^{N_m} w_m u(x + v_m) \cdot v_m, \]

which reduce to the typical one-dimensional central difference equations given a D1Q3, D2Q5, or D3Q7 lattice. Other lattice stencils used, such as the D2Q9 and D3Q27 lattice stencils, will have more general central difference equations accounting for more directions in the lattice. Multi-range operations may also be used on the lattice, and can be accounted for by increasing the velocity space to D2Q9\(^r\) or D3Q27\(^r\), where \( r = 2, 3, \ldots \) represents the lattice range [40]. Below is an expansion of Eq. (2.19) for a D2Q9 lattice where \( i \) and \( j \) are the spatial indices in \( x \) and \( y \),

\[ \left( \frac{\partial \psi}{\partial x} \right)_i^j = \frac{1}{3} \left( \psi_{i,j+1} - \psi_{i,j-1} \right) + \frac{1}{12} \left( \psi_{i+1,j+1} - \psi_{i-1,j-1} + \psi_{i+1,j-1} - \psi_{i-1,j+1} \right), \]

\[ \left( \frac{\partial \psi}{\partial y} \right)_i^j = \frac{1}{3} \left( \psi_{i+1,j} - \psi_{i,j} \right) + \frac{1}{12} \left( \psi_{i+1,j+1} - \psi_{i-1,j-1} + \psi_{i-1,j+1} - \psi_{i+1,j-1} \right). \]

(2.21)

Given a single lattice and general operators such as Eqs. (2.19) and (2.20) available for lattice-Boltzmann methods, it is rare to find discrete representations such as Eq. (2.21). It is likely such notation is even discouraged, especially since it does not aid in implementing generic lattice-Boltzmann programs. MATLAB functions that use the notation of Eq. (2.19) for an arbitrary nearest-neighbour lattice-stencil are provided in Appendix D.
2.4. Numerical methods

2.4.4 The lattice-Boltzmann equation

The lattice-Boltzmann equation (LBE) with no external forces considers the case of an ideal particle population with a finite number of discrete collision velocities, \( N_m \) [76],

\[
\frac{\partial}{\partial t} n_m(x, t) + v_{ma} \frac{\partial}{\partial x_\alpha} n_m(x, t) = \Omega(n_m(x, t)), \quad m = 1, \ldots, N_m, \quad (2.22)
\]

where \( v_{ma} \) is component \( \alpha \) of the lattice vector \( v_m \), while

\[
n_m(x, t) \equiv n(x, v|v \in \{v_m\}, t) \quad (2.23)
\]

is a discrete probability mass function equivalent to the conditional probability that the continuous particle population \( n(x, v, t) \) collides and propagates with a finite number of velocities, \( v \in \{v_m\} \), that can be represented on a discrete lattice. The LBE is generic, such that it can be applied to represent multiple physical sub-systems, such as electrodynamic and kinetic sub-systems [37, 39, 76]. However, traditionally it was designed for the kinetic sub-system. There are a number of schemes that have been developed for incorporating an external force density, and different formulations of the collision operator, which will be described for the kinetic sub-system in Chapter 4. Moments of \( n_m(x, t) \) or its equilibrium condition, \( n_{eq}^m(x, t) \), represent different macroscopic state variables in each sub-system. One example is for a kinetic sub-system, where the zeroth moment is mass density, \( \rho(x, t) \), and the first moment is the momentum density, \( \rho(x, t)u(x, t) \), which are obtained using sums as opposed to continuous integrals [71],

\[
\rho(x, t) = \sum_{m=1}^{N_m} n_m(x, t) = \sum_{m=1}^{N_m} n_{eq}^m(x, t), \quad (2.24)
\]

\[
\rho(x, t)u(x, t) = \sum_{m=1}^{N_m} n_m(x, t)v_m = \sum_{m=1}^{N_m} n_{eq}^m(x, t)v_m.
\]

At each discrete time step, \( n_m(x, t) \) is relaxed as it approaches its equilibrium state, \( n_{eq}^m(x, t) \), proportional to the numerical order of accuracy. Given a kinetic sub-system, orthogonal Hermite polynomials are used to derive and approximate Maxwell’s equilibrium particle population density to a second order of accuracy [76],

\[
n_{eq}^m(x, t) = w_m \rho \left( 1 + \frac{v_{ma}u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta (v_{ma}v_{m\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} \right) \bigg|_{(x, t)}, \quad (2.25)
\]
where
\[ c_s = \frac{1}{\sqrt{3}} \frac{\delta x}{\delta t} \] (2.26)
is the lattice speed of sound for dimensionless spatial unit $\delta x$ and dimensionless time unit $\delta t$ in D2Q9 and D3Q27 lattices. Otherwise, if all higher-order terms are included in a generic form of the Maxwell equilibrium particle population, an entropic relaxation approach is required to accurately represent Boltzmann’s $H$-theorem [46].

### 2.4.5 Collision and propagation operators in the lattice-Boltzmann equation

The lattice-Boltzmann equation is represented in a discrete velocity space, although its implementation is represented in discrete space and time. Typically, this requires dimensionless spatial unit $\delta x = 1$, and a lattice-stencil dependent time unit $\delta t$. Particle population $n_m(x,t)$ is forced to approach $n_m^{eq}(x,t)$ in population collision and propagation operations.

**The collision operation** represents the perturbation of $n_m(x,t)$ as it approaches a state of equilibrium, $n_m^{eq}(x,t)$, during interparticle collisions at time $t$ and vector position $x$. Given a finite number of lattice velocities and single relaxation, the discrete Bhatnagar-Gross-Krook (BGK) collision operator has been used to represent the relaxation of the particle population $n_m(x,t)$ as it approaches $n_m^{eq}(x,t)$ according to the discrete Navier-Stokes equation [77],

\[ \Omega_m(x,t) = \frac{\delta t}{\tau} (n_m^{eq}(x,t) - n_m(x,t)) , \] (2.27)

where $\tau$ is the discrete relaxation time and $\delta t = 1$ for a kinetic lattice-Boltzmann method. In practice, the collision operator is added as a difference to $n_m(x,t)$ from the previous time step [71], such that

\[ n_m^*(x,t) = n_m(x,t) + \Omega_m(x,t), \]

\[ = n_m(x,t) + \frac{\delta t}{\tau} (n_m^{eq}(x,t) - n_m(x,t)) . \] (2.28)

Following its elastic collision, post-collision particle population $n_m^*(x,t)$ is assigned to adjacent lattice node $m$ in the propagation operation.
2.4. Numerical methods

The propagation operation represents the redistribution of \( n^*_m(x, t) \) to adjacent lattice node \( m \) for particle and momentum conservation \([76]\), such that

\[
n_m(x + v_m \delta t, t + \delta t) := n^*_m(x, t),
\]

where “:=” is an assignment operator. The collision and consecutive propagation process is illustrated in Fig. 2.3. Chapter 4 later discusses entropic and multi-relaxation approaches.

![Figure 2.3: Illustration of the collision process on a D2Q9 lattice. (a) The particle population outcomes stream toward each lattice node, indexed \( m = 9 \), from their respective adjacent lattice nodes, indexed \( m = 1, \ldots, 8 \), and collide elastically. (b) Following the collision, the particle population’s post-collision outcomes propagate to their respective adjacent lattice nodes.](image)
Chapter 3

Comparing finite-difference methods and lattice-Boltzmann methods solutions of kinetic force density

In considering light as a collisionless gas of pseudo-particles, Maxwell’s equations can be recovered from Boltzmann’s equation [37, 39, 49, 78]. This chapter demonstrates how such a construction provides time-domain simulations of electric and magnetic fields at the same location and time, increasing the numerical accuracy while decreasing the computational time of an electrodynamic simulation compared with the Yee-lattice finite-difference time-domain method (YL-FDTDM). First, the initial condition of the electrodynamic sub-system, a continuous Hermite-Gaussian wave-function, is described in detail. Second, the YL-FDTDM and discretization of Maxwell’s equations for computing central difference force density are described. Third, the formulation of central difference force-densities is described for Hauser & Verhey’s electrodynamic lattice-Boltzmann method (ELBM) [39]. These descriptions are followed by the implementation methodology of Hauser & Verhey’s ELBM for solving central difference force densities in uniform dielectric media [39], and a comparison between the computational time and numerical accuracy of force densities evaluated in the YL-FDTDM and the ELBM at the same spatial resolution.

3.1 Initial condition

Only monochromatic Hermite-Gaussian beams are used in this thesis because: (1) they can be modeled using a paraxial approximation, (2) they have finite cross-sectional area, (3) they mimic experimental conditions as-
3.1. Initial condition

associated with focused laser beams. The source condition is constrained to a single wavenumber and angular time-frequency

\[ k = \frac{2\pi \alpha}{\lambda_0} \quad \text{and} \quad \omega = \frac{2\pi}{T}, \]  

(3.1)

where \( \alpha \) is the refractive index of the source medium for free-space wavelength \( \lambda_0 \) and time-period \( T \). Free-space wavelength and time-period are linearly related by the vacuum speed of light, \( c = 299792458 \text{ m/s} \), such that

\[ \lambda_0 = cT. \]  

(3.2)

Unless otherwise stated, the source has a refractive index of \( \alpha = 1 \) such that the wavenumber \( k = k_0 = 2\pi/\lambda_0 \).

3.1.1 Hermite Gaussian wave-functions

Hermite-Gaussian wave-functions have an amplitude envelope described by a Gaussian function with a mode order of \( m \) along the primary axis, and \( n \) along the secondary axis in a transverse plane [79]. In this thesis, the fundamental TEM\(_{00}\) mode is explored since it represents the output of lasers used in optical radiation pressure experiments which focus the electric field to a maximum intensity for maximum optical radiation pressure [22]. The Hermite-Gaussian wave-functions are initialized as periodic and monochromatic sources, such that they require the minimum number of time samples for calculating a time-averaged kinetic force density. The complete Hermite-Gaussian wave-function also has a defined focal position without the use of optical lenses [7]. Explicit Hermite-Gaussian solutions can be derived from the paraxial Helmholtz equations in Ref. [79], where the wave-function

\[ \phi_{mn}(r) = \sqrt{\frac{2}{\pi w^2(z)}} H^{(m)}(\sqrt{2}x/w(z)) H^{(n)}(\sqrt{2}y/w(z)) \ldots \times \exp \left[ -i(m + n + 1)\theta(z) + \frac{iks^2}{2q(z)} \right] \]  

(3.3)

can represent the field components of both linearly and circularly-polarized Gaussian beams using “physicist’s form” Hermite polynomials \( H^{(m)} \) or \( H^{(n)} \), which have orders \( m \) and \( n \) for each transverse dimension. In the general case of a three-dimensional Gaussian beam, displacement from the beam-axis along the direction of propagation is represented by \( z - z_0 \), while \( s^2 = (x - x_0)^2 + (y - y_0)^2 \), \( i \) is the imaginary unit, \( \theta(z) = \tan^{-1}(z-z_0)/z_R) \) is
the Gouy phase, and \( w(z) = w_0 \sqrt{1 + \left( \frac{z - z_0}{z_R} \right)^2} \) is the beam-waist for a Rayleigh range \( z_R = kw_0^2/2 \). The corresponding beam radius, \( R(z) \), and complex beam parameter, \( q(z) \), are defined as

\[
R(z) = z - z_0 + \frac{z_R}{z - z_0} \quad \text{and} \quad \frac{1}{q(z)} = \frac{1}{R(z)} + \frac{2}{kw_0^2(z)}. \tag{3.4}
\]

In three dimensions, displacement is represented by \( r = (x - x_0) \hat{x} + (y - y_0) \hat{y} + (z - z_0) \hat{z} \), where the position of the beam-axis at the beam-waist is \((x_0, y_0, z_0)\). The authors of Ref. [79] used the properties of Hermite polynomials to derive Hermite-Gaussian functions for the electric field components describing linearly and circularly-polarized transverse Hermite-Gaussian, or TEM\(_{mn}\), modes.

The linearly-polarized TEM\(_{mn}\) Hermite-Gaussian functions for each of the electric field components are

\[
E_1^{(mn)}(r) = A_{mn} \phi_{mn}(r),
\]
\[
E_2^{(mn)}(r) = \frac{A_{mn}}{(kw_0)^2} \left[ 4mn\phi_{m-1,n-1}(r) - 2m\phi_{m-1,n+1}(r) \right] - 2m\phi_{m+1,n-1}(r) + \phi_{m+1,n+1}(r), \tag{3.5}
\]
\[
E_3^{(mn)}(r) = \frac{iA_{mn}}{2kw_0} \left[ 2m\phi_{m-1,n}(r) - \phi_{m+1,n}(r) \right].
\]

In three-dimensions the \( \hat{x} \)-polarized TEM\(_{00}\) Gaussian beam can be initialized using the \( x \)-component

\[
E_x^{(00)}(s,\theta,z) = \frac{A_{00}}{w(z)} \sqrt{\frac{2}{\pi}} \exp \left( -i\theta(z) + \frac{i ks^2}{2q(z)} \right) \exp(-i\omega t). \tag{3.6}
\]

However, in two dimensions the direction of propagation is in-plane, such that further considerations are necessary. One useful modification is an arbitrary in-plane direction of propagation given by the axial vector \( s = (x - x_0) \cos \vartheta \hat{x} + (y - y_0) \sin \vartheta \hat{y} \), such that the in-plane curvature of the beam is represented by the perpendicular vector \( s_\perp = (x - x_0) \sin \vartheta \hat{x} - (y - y_0) \cos \vartheta \hat{y} \), where \( \vartheta \) is the angle of the beam-axis with respect to \( x \). Therefore, in two-dimensional simulations it is appropriate to initialize the Hermite-Gaussian function using \( H_2 \) for a p-polarized simulation as

\[
H_2^{(00)}(s,\theta) = \frac{1}{\eta w(s)} A_{00} \sqrt{\frac{2}{\pi}} \exp \left( -i\theta(s) + \frac{i ks^2}{2q(s)} \right) \exp(-i\omega t), \tag{3.7}
\]
3.1. Initial condition

or $E_z$ for an s-polarized simulation,

$$E_z^{(00)}(s, \theta) = \frac{A_{00}}{w(s)} \sqrt{\frac{2}{\pi}} \exp \left( -i\theta(s) + \frac{iks^2}{2q(s)} \right) \exp(-i\omega t), \quad (3.8)$$

where $\eta$ is the impedance of the source medium. Although a Hermite-Gaussian wave-function of a single component only approximates a solution to Maxwell’s equations, its initialization satisfies the discrete Maxwell’s equations at each consecutive time step to represent a monochromatic source of focused electromagnetic radiation. Therefore, simulating beam focusing from a lens is not required, such that computational cost and time can be reduced compared with previous studies [7]. Cross-polarization of a linearly-polarized Gaussian beam occurs naturally in three dimensions, such that a three-dimensional simulation of optical radiation pressure from a linearly-polarized Gaussian beam simultaneously represents both predominantly p-polarized and s-polarized electric fields depending on the plane of incidence [79].

The circularly-polarized Hermite-Gaussian functions for each of the electric field components are,

$$E_1^{(mn)}(r) = \frac{A_{mn}}{\sqrt{2}} \phi_{mn}(r),$$

$$E_2^{(mn)}(r) = i\frac{A_{mn}}{\sqrt{2}} \phi_{mn}(r),$$

$$E_3^{(mn)}(r) = i\frac{A_{mn}}{2kw_0} \left[ 2m\phi_{m-1,n}(r) - \phi_{m+1,n}(r) \
+ 2in\phi_{m,n-1}(r) - i\phi_{m,n+1}(r) \right], \quad (3.9)$$

for a general TEM$_{mn}$ mode. The circularly-polarized TEM$_{00}$ mode Hermite-Gaussian beam that propagates in the $\hat{z}$ direction can only be represented in three dimensions, and requires the initialization of the $\hat{x}$ and $\hat{y}$ electric field components,

$$E_x^{(00)}(s, \theta, z) = \frac{A_{00}}{\sqrt{\pi}w(z)} \exp \left( -i\theta(z) + ik\frac{s^2}{2q(z)} \right) \exp(-i\omega t),$$

$$E_y^{(00)}(s, \theta, z) = \frac{iA_{00}}{\sqrt{\pi}w(z)} \exp \left( -i\theta(z) + ik\frac{s^2}{2q(z)} \right) \exp(-i\omega t). \quad (3.10)$$

This thesis typically defines the field intensity using its peak value, $E_0$, as the maximum electric field solved throughout the spatial domain and temporal duration of the simulation.
3.2 The Yee-lattice finite-difference time-domain method

The Yee-lattice finite-difference time-domain method (YL-FDTDM) has been implemented in one, two and three dimensions for solving a wide range of electrodynamic phenomena [8, 33, 80]. It is one of the most common and popular numerical methods in electrodynamics [23, 80]. The YL-FDTDM has been applied in two dimensions for solving kinetic force densities in ponderable media, which has enabled predictions of optical radiation pressure [23]. This section describes the construction of central difference force densities in the YL-FDTDM, beginning with the evaluation of the electric and magnetic fields, the space and time interpolation, and the momentum density and stress tensor [7, 8]. It concludes with a description of numerical dispersion in the YL-FDTDM [80].

3.2.1 Electric and magnetic fields

In a 2D plane of incidence, there is only an in-plane spatial variation of Maxwell’s equations in Tab. 2.1. Eliminating the third dimension enables independent treatment of p- and s-polarized electric fields. The 2D p-polarized (transverse-magnetic) Faraday and Ampere’s laws are

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \left( -\sigma E E_x + \frac{\partial H_y}{\partial x} - \frac{\partial H_z}{\partial y} \right), \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left( -\sigma E E_y - \frac{\partial H_z}{\partial x} \right), \\
\frac{\partial H_z}{\partial t} &= -\frac{1}{\mu} \left( \sigma_M H_z + \frac{\partial E_y}{\partial y} - \frac{\partial E_x}{\partial x} \right),
\end{align*}
\]

(3.11)

while the s-polarized (transverse-electric) Faraday and Ampere’s laws are

\[
\begin{align*}
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left( -\sigma E E_z + \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right), \\
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu} \left( \sigma_M H_x + \frac{\partial E_z}{\partial y} \right), \\
\frac{\partial H_y}{\partial t} &= -\frac{1}{\mu} \left( \sigma_M H_y - \frac{\partial E_z}{\partial x} \right).
\end{align*}
\]

(3.12)

central differences of these partial-differential equations can be implemented by half-grid space and time offsets of the electric and magnetic field components. This results in the Yee-lattice structure, which allows numerical solutions for electric and magnetic fields in tandem [80]. The two-dimensional
3.2. The Yee-lattice finite-difference time-domain method

Yee-lattices representing p- or s-polarized planes of incidence are illustrated in Figure 3.1.

![Yee-lattice diagram](image)

(a) TM, p-polarized Yee-Lattice  (b) TE, s-polarized Yee-Lattice

Figure 3.1: In (a), the Yee-lattice representing a p-polarized electric field is illustrated, while in (b), the Yee-lattice representing an s-polarized electric field is illustrated.

The p-polarized partial-differential equations in Eq. (3.11) can be discretized using central differences in space and time to represent the following central difference equations

\[
E_{x,i,j+\frac{1}{2}}^{n+1} = e_{1x} E_{x,i,j+\frac{1}{2}}^n + \frac{\Delta t}{\Delta y e_{i,j+\frac{1}{2}}} \left( \frac{1}{2} \left( H_{z,i,j+1}^{n+\frac{1}{2}} - H_{z,i,j}^{n+\frac{1}{2}} \right) \right),
\]

\[
E_{y,i+\frac{1}{2},j}^{n+1} = e_{2y} E_{y,i+\frac{1}{2},j}^n - \frac{\Delta t}{\Delta x e_{i+\frac{1}{2},j}} \left( \frac{1}{2} \left( H_{z,i+1,j}^{n+\frac{1}{2}} - H_{z,i,j}^{n+\frac{1}{2}} \right) \right),
\]

\[
H_{z,i,j}^{n+\frac{1}{2}} = h_{1z} H_{z,i,j}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_{i,j} h_{2z}} \left( \frac{E_{y,i+\frac{1}{2},j}^n - E_{y,i-\frac{1}{2},j}^n}{\Delta x} \right),
\]

with coefficients

\[
e_{1x} = 1 - \left( \frac{\Delta t \sigma E_{i,j+\frac{1}{2}} / 2 \epsilon_{i,j+\frac{1}{2}}}{2} \right), \quad e_{2x} = 1 + \left( \frac{\Delta t \sigma E_{i,j+\frac{1}{2}} / 2 \epsilon_{i,j+\frac{1}{2}}}{2} \right),
\]

\[
e_{1y} = 1 - \left( \frac{\Delta t \sigma E_{i+\frac{1}{2},j} / 2 \epsilon_{i+\frac{1}{2},j}}{2} \right), \quad e_{2y} = 1 + \left( \frac{\Delta t \sigma E_{i+\frac{1}{2},j} / 2 \epsilon_{i+\frac{1}{2},j}}{2} \right),
\]

\[
h_{1z} = 1 - \left( \frac{\Delta t \sigma M_{i,j} / 2 \mu_{i,j}}{2} \right), \quad h_{2z} = 1 + \left( \frac{\Delta t \sigma M_{i,j} / 2 \mu_{i,j}}{2} \right).
\]
3.2. The Yee-lattice finite-difference time-domain method

Similarly, the s-polarized partial differential equations in Eq. (3.12) are discretized in space and time to represent the following central difference equations:

\[ H_{x,i,j}^{n+\frac{1}{2}} = \frac{h_{1x}}{h_{2x}} H_{x,i,j}^n - \frac{\Delta t}{\Delta y \mu_{i,j+\frac{1}{2}}} \frac{1}{h_{2x}} \left( E_{z,i,j+1}^{n} - E_{z,i,j}^{n} \right), \]

\[ H_{y,i+\frac{1}{2},j}^{n+1} = \frac{h_{1y}}{h_{2y}} H_{y,i+\frac{1}{2},j}^n + \frac{\Delta t}{\Delta x \mu_{i+\frac{1}{2},j}} \frac{1}{h_{2y}} \left( E_{z,i+1,j}^{n} - E_{z,i,j}^{n} \right), \]

\[ E_{z,i,j}^{n+\frac{1}{2}} = \frac{e_{1z}}{e_{2z}} E_{z,i,j}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i,j}} \left( \frac{H_{y,i+\frac{1}{2},j}^n - H_{y,i-\frac{1}{2},j}^n}{\Delta x} - \frac{H_{x,i+\frac{1}{2},j}^n - H_{x,i-\frac{1}{2},j}^n}{\Delta y} \right), \]  

(3.15)

with coefficients

\[ h_{1x} = 1 - \left( \Delta t \sigma_{M,i,j+\frac{1}{2}} / 2 \mu_{i,j+\frac{1}{2}} \right), \quad h_{2x} = 1 + \left( \Delta t \sigma_{M,i,j+\frac{1}{2}} / 2 \mu_{i,j+\frac{1}{2}} \right), \]

\[ h_{1y} = 1 - \left( \Delta t \sigma_{M,i+\frac{1}{2},j} / 2 \mu_{i+\frac{1}{2},j} \right), \quad h_{2y} = 1 + \left( \Delta t \sigma_{M,i+\frac{1}{2},j} / 2 \mu_{i+\frac{1}{2},j} \right), \]

\[ e_{1z} = 1 - \left( \Delta t \sigma_{E,i,j} / 2 \epsilon_{i,j} \right), \quad e_{2z} = 1 + \left( \Delta t \sigma_{E,i,j} / 2 \epsilon_{i,j} \right), \]  

(3.16)

where \( \Delta x \) is the dimensional spatial unit and \( \Delta t \) is the dimensional time unit.

3.2.2 Energy density and momentum density

Interpolation in space and time is required in order to evaluate energy density and momentum density from the electric and magnetic fields, due to their offset components in an orthogonal Yee-lattice. The number of averages and their construction depends on the number of dimensions in the Yee-lattice [7, 8]. In a two-dimensional Yee-lattice representing p-polarized electromagnetic fields, interpolation of the electric field components in space and time are required to situate these components on the magnetic field component to calculate the energy density and momentum density. At time step \( n+\frac{1}{2} \), this is given by

\[ E_{x,i,j}^{n+\frac{1}{2}} = \frac{1}{4} \left( E_{x,i,j+\frac{1}{2}}^{n+1} + E_{x,i,j-\frac{1}{2}}^{n+1} + E_{x,i,j+\frac{1}{2}}^{n} + E_{x,i,j-\frac{1}{2}}^{n} \right), \]

\[ E_{y,i,j}^{n+\frac{1}{2}} = \frac{1}{4} \left( E_{y,i+\frac{1}{2},j}^{n+1} + E_{y,i-\frac{1}{2},j}^{n+1} + E_{y,i+\frac{1}{2},j}^{n} + E_{y,i-\frac{1}{2},j}^{n} \right), \]  

(3.17)
The corresponding energy density is

\[ W_{i,j}^{n+\frac{1}{2}} = \frac{1}{2} \left( \epsilon_{i,j} E_{x_{i,j}}^{n+\frac{1}{2}} E_{x_{i,j}}^{n+\frac{1}{2}} + \epsilon_{i,j} E_{y_{i,j}}^{n+\frac{1}{2}} E_{y_{i,j}}^{n+\frac{1}{2}} + \mu_{i,j} H_{z_{i,j}}^{n+\frac{1}{2}} H_{z_{i,j}}^{n+\frac{1}{2}} \right), \]  

(3.18)

while the momentum density is represented as

\[ G_{e,x_{i,j}}^{n+\frac{1}{2}} = E_{y_{i,j}}^{n+\frac{1}{2}} H_{z_{i,j}}^{n+\frac{1}{2}}, \]
\[ G_{e,y_{i,j}}^{n+\frac{1}{2}} = -E_{x_{i,j}}^{n+\frac{1}{2}} H_{z_{i,j}}^{n+\frac{1}{2}}. \]  

(3.19)

In a two-dimensional Yee-lattice representing s-polarized electromagnetic fields, interpolation of the magnetic field components in space and time are required to situate these components on the electric field component to calculate the energy density and momentum density. At time step \( n+\frac{1}{2} \), this is given by

\[ H_{x_{i,j}}^{n+\frac{1}{2}} = \frac{1}{4} \left( H_{x_{i,j}+\frac{1}{2}}^{n+1} + H_{x_{i,j}-\frac{1}{2}}^{n+1} + H_{x_{i,j}+\frac{1}{2}}^{n} + H_{x_{i,j}-\frac{1}{2}}^{n} \right), \]
\[ H_{y_{i,j}}^{n+\frac{1}{2}} = \frac{1}{4} \left( H_{y_{i,j}+\frac{1}{2},j}^{n+1} + H_{y_{i,j}-\frac{1}{2},j}^{n+1} + H_{y_{i,j}+\frac{1}{2},j}^{n} + H_{y_{i,j}-\frac{1}{2},j}^{n} \right). \]  

(3.20)

The corresponding energy density is,

\[ W_{i,j}^{n+\frac{1}{2}} = \frac{1}{2} \left( \epsilon_{i,j} E_{x_{i,j}}^{n+\frac{1}{2}} E_{x_{i,j}}^{n+\frac{1}{2}} + \mu_{i,j} H_{z_{i,j}}^{n+\frac{1}{2}} H_{z_{i,j}}^{n+\frac{1}{2}} + \mu_{i,j} H_{y_{i,j}}^{n+\frac{1}{2}} H_{y_{i,j}}^{n+\frac{1}{2}} \right), \]  

(3.21)

while the momentum density is represented as,

\[ G_{e,x_{i,j}}^{n+\frac{1}{2}} = -E_{x_{i,j}}^{n+\frac{1}{2}} H_{y_{i,j}}^{n+\frac{1}{2}}, \]
\[ G_{e,y_{i,j}}^{n+\frac{1}{2}} = E_{x_{i,j}}^{n+\frac{1}{2}} H_{y_{i,j}}^{n+\frac{1}{2}}. \]  

(3.22)

While these interpolations minimize numerical error in the YL-FDTDM, they still contain numerical error from the dispersion of electric and magnetic fields in free space. Offset electric and magnetic field components also represent a non-exact magnetodielectric boundary, and introduce numerical reflections. In three-dimensions, they become more involved.

### 3.2.3 Force density

Optical force density in the YL-FDTDM requires intricate spatio-temporal interpolation and central difference equations that are unique for each electric field polarization. This section is limited to a description of a p-polarized
3.2. The Yee-lattice finite-difference time-domain method

(TM) electric field Yee-lattice evaluation of force density. The transverse magnetic field solved at time step \( n + \frac{1}{2} \) is averaged in time and the in-plane electric-field components at time step \( n \) are averaged in space,

\[
H_{zi,j}^n = \frac{1}{2} \left( H_{zi,j}^{n+\frac{1}{2}} + H_{zi,j}^{n-\frac{1}{2}} \right),
\]

\[
E_{xi,j}^n = \frac{1}{2} \left( E_{xi,j+\frac{1}{2}}^n + E_{xi,j-\frac{1}{2}}^n \right),
\]

\[
E_{yi,j}^n = \frac{1}{2} \left( E_{yi,j+\frac{1}{2}}^n + E_{yi,j-\frac{1}{2}}^n \right).
\]

(3.23)

The divergence of the momentum flux density tensor,

\[
\nabla \cdot \mathbf{T}_{e,i,j}^n = \hat{x} \Delta T_{e,x,i,j}^n + \hat{y} \Delta T_{e,y,i,j}^n,
\]

(3.24)

is then solved using a central difference method in space with the interpolated field-quantities from Eq. (3.23). Divergence of the Chu momentum flux density tensor in the \( \hat{x} \)-direction is

\[
(\nabla \cdot \mathbf{T})_{e,xi,j}^n = \ldots
- \frac{\varepsilon_0}{2\Delta x} \left( \left( E_{xi+1,j}^n \right)^2 - \left( E_{xi-1,j}^n \right)^2 \right) \ldots
+ \frac{\varepsilon_0}{2\Delta x} \left( \left( E_{yi+1,j}^n \right)^2 - \left( E_{yi-1,j}^n \right)^2 \right) \ldots
+ \frac{\mu_0}{2\Delta x} \left( \left( H_{zi+1,j}^n \right)^2 - \left( H_{zi-1,j}^n \right)^2 \right) \ldots
+ \frac{\varepsilon_0}{2\Delta y} \left( E_{xi,j+1}^n E_{yi,j+1}^n - E_{xi,j-1}^n E_{xi,j-1}^n \right),
\]

(3.25)

while divergence of the Chu momentum flux density tensor in the \( \hat{y} \)-direction is

\[
(\nabla \cdot \mathbf{T})_{e,yi,j}^n = \ldots
\]

\[
\frac{\varepsilon_0}{2\Delta x} \left( E_{xi+1,j}^n E_{yi+1,j}^n - E_{xi-1,j}^n E_{xi-1,j}^n \right) \ldots
+ \frac{\varepsilon_0}{2\Delta y} \left( \left( E_{xi,j+1}^n \right)^2 - \left( E_{xi,j-1}^n \right)^2 \right) \ldots
- \frac{\varepsilon_0}{2\Delta y} \left( \left( E_{yi,j+1}^n \right)^2 - \left( E_{yi,j-1}^n \right)^2 \right) \ldots
+ \frac{\mu_0}{2\Delta y} \left( \left( H_{zi,j+1}^n \right)^2 - \left( H_{zi,j-1}^n \right)^2 \right) \ldots
\]

(3.26)
The derivation for the divergence of each formalisms momentum flux density tensor is provided in the Appendix B. Appendix D also describes a program implementation of conventional central difference equations used to evaluate these force densities. The transfer of kinetic momentum density at time step \( n + \frac{1}{2} \) is then calculated via a re-arranged central difference equation of Eq. (2.2),

\[
\begin{align*}
    g_{x,i,j}^{n+\frac{1}{2}} &= g_{x,i,j}^{n-\frac{1}{2}} - (\Delta T_{e,x,i,j}^n)\Delta t - (G_{e,x,i,j}^{n+\frac{1}{2}} - G_{e,x,i,j}^{n-\frac{1}{2}}), \\
    g_{y,i,j}^{n+\frac{1}{2}} &= g_{y,i,j}^{n-\frac{1}{2}} - (\Delta T_{e,y,i,j}^n)\Delta t - (G_{e,y,i,j}^{n+\frac{1}{2}} - G_{e,y,i,j}^{n-\frac{1}{2}}),
\end{align*}
\]

followed by the force density at time step \( n \), \( f_{k,y,i,j}^n \), using a central difference in time

\[
\begin{align*}
    f_{k,x,i,j}^n &= \frac{1}{\Delta t} (g_{e,x,i,j}^{n+\frac{1}{2}} - g_{e,x,i,j}^{n-\frac{1}{2}}), \\
    f_{k,y,i,j}^n &= \frac{1}{\Delta t} (g_{e,y,i,j}^{n+\frac{1}{2}} - g_{e,y,i,j}^{n-\frac{1}{2}}).
\end{align*}
\]

The force density is then averaged over a number of time-periods \( N_T \). Given an angular frequency, \( \omega \), the number of computational time steps averaged is \( N_t = 2\pi N_T/\omega \Delta t \) and therefore

\[
\begin{align*}
    \langle f_{k,x,i,j} \rangle &= \frac{1}{N_t} \sum_{n=0}^{N_t} f_{k,x,i,j}^n, \\
    \langle f_{k,y,i,j} \rangle &= \frac{1}{N_t} \sum_{n=0}^{N_t} f_{k,y,i,j}^n.
\end{align*}
\]

In order to reduce discrete-time error from the irrational time-period, this thesis recommends \( N_T > 5 \) [7, 8]. After time-averaging the kinetic force density over \( N_T > 5 \), there is less than 3% difference in the net force evaluated. This thesis uses \( N_T = 25 \) to mitigate time-averaging error in the YL-FDTDM.
3.2.4 Boundary conditions

Absorbing/radiating boundary conditions are ideal for a time-averaged electrodynamic simulation. Several different types of these boundary conditions exist based on the principle of attenuating free-space matched electric and magnetic field intensity in a small layer of several spatial units. One such layer in the YL-FDTDM is the Berenger perfectly matched layer (BPML) [62]. The BPML attenuates both the electric field and the magnetic field in a medium using electric and magnetic conductivity with relative magnitudes equivalent to the free-space impedance, $\eta_0$,

$$\frac{\sigma_M}{\mu_0} = \frac{\sigma_E}{\epsilon_0} \quad \text{and} \quad \sigma_M = \eta_0^2 \sigma_E. \quad (3.30)$$

The BPML is designed to absorb obliquely incident electromagnetic waves by attenuating transverse electric and magnetic field components which are oriented tangent to its boundary. Longitudinal field components are not explicitly attenuated, but indirectly from the transverse field components, which results in numerical reflections from the boundary of the BPML. Numerical reflections and dispersion can also occur within the BPML. While Berenger had minimized these reflections, a typical BPML requires a thickness of at least 3-4 spatial units [62].

3.2.5 Limitations

The YL-FDTDM can solve accurate electric and magnetic fields in the time-domain in a staggered Yee-lattice provided appropriate space and time-discretization. Since it has well-understood sources of numerical error, the YL-FDTDM can be quickly applied to achieve accurate numerical solutions for a wide variety of electromagnetic problems [80]. However, the YL-FDTDM demonstrates several limitations for electrodynamics:

− Numerical dispersion in free space, which leads to spurious time-averaged force densities where there are no electric charges or dipoles,

− Space and time offsets between electric and magnetic fields which must be interpolated for calculating momentum density and energy density,

− Space and time offsets at boundaries, which cause errors in local momentum conservation, leading to numerical reflection and asymmetry,

− Indirect relation between electric and magnetic fields to their energy and momentum conservation, which can introduce numerical instability.
The Yee-lattice finite-difference time-domain method

The limitations of the YL-FDTDM, and its implementation complexity, has limited most simulations of kinetic force density from electric and magnetic fields to one or two dimensions [7, 8]. However, natural electromagnetic radiation is three or four-dimensional (space and time), which has been considered in only a few studies to date [16, 23, 81]. This is largely due to the implementation complexity and computational time required from a Yee-lattice configuration.

Numerical dispersion can be described as any deviation of a numerical value from its analytical value for a particular frequency bin in a discrete frequency domain. Numerical dispersion occurs naturally in all electromagnetic finite-difference methods as a consequence of finite-difference approximations. In the one-dimensional conventional YL-FDTDM, numerical dispersion is represented by

\[
\sin\left(\frac{1}{2}\omega \Delta t\right) = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} \sin\left(\frac{1}{2}k \Delta x\right),
\]

which can satisfy \(\omega = kc\) in free space for the condition \(\Delta t = \Delta x/c\), which prevents numerical dispersion. In dielectric media or in higher dimensions, however, numerical dispersion cannot be avoided [80]. For example, the two-dimensional numerical dispersion relation

\[
\left(\frac{1}{c\Delta t} \sin\frac{1}{2} \omega \Delta t\right)^2 = \left(\frac{1}{\Delta x} \sin\frac{1}{2} k_x \Delta x\right)^2 + \left(\frac{1}{\Delta y} \sin\frac{1}{2} k_y \Delta y\right)^2
\]

(3.32)
cannot directly satisfy \(k_x^2 + k_y^2 = \omega^2 c^2\) in free space [39, 80]. The consequence of this numerical dispersion in the YL-FDTDM is distortion of the time and spatial periodicity of electromagnetic waves at further distances from the source, even in the absence of ponderable media. It is necessary that kinetic force density is evaluated everywhere with similar spatial periodicity and accuracy, a condition that cannot be satisfied with the frequency-distortion of electromagnetic waves. While bandwidth can be increased using a decreased time unit [82], spatial unit, higher-order finite-difference [83, 84], or model order reduction and eigenvalue perturbation [85, 86], these approaches offer a compromise between computational time and accuracy or vice versa. Alternatively, the electrodynamic lattice-Boltzmann method (ELBM) avoids free-space numerical dispersion in multiple dimensions by including additional degrees of freedom [39].

Fig. 3.2 illustrates the propagation of an electromagnetic pulse from a point source initialized in both YL-FDTDM and the ELBM. The initial electric field condition

\[
E_y(x, y) = 2e^{-0.05[(x-N_x/10)^2+(y-N_y/2)^2]}
\]

(3.33)
is re-used from Ref. [39] to demonstrate the successful implementation of
the method and the comparative numerical dispersion of the YL-FDTDM.
In the ELBM, δt = 1/2, while in the YL-FDTDM, δt = 1/√2. Eq. 3.33
generates an electromagnetic pulse that propagates through a lattice with
N_x lattice units in the x-direction and N_y lattice units in the y-direction.
Fig. 3.2 compares the cross-section of the dimensionless electric field along
its propagation axis, as evaluated in the (a) YL-FDTDM and the (b) ELBM.
Spatial distortion in the YL-FDTDM is visible as high-frequency transients
at the end of the pulse which increase over time in Fig. 3.2(a). No such spa-
tial distortion is visible in the ELBM Fig. 3.2(b) [39]. The spatial distortion
is an effect of numerical dispersion in the YL-FDTDM.

![Figure 3.2](image)

(a) YL-FDTDM  
(b) ELBM

Figure 3.2: Comparison of the electric field from an electromagnetic pulse
in (a) the YL-FDTDM, and (b) the ELBM during its propagation through
free space in a dimensionless spatial domain. The plot is a cross-section
of the two-dimensional simulation along the center of the pulse. Numerical
dispersion is evident in (a), yet absent in (b). These simulations were
conducted by Cael Warner and mimic the simulations described by Hauser
& Verhey, 2019 [39].
3.3 The electrodynamic lattice-Boltzmann method

Alternative to the YL-FDTDM is the recent electrodynamic lattice-Boltzmann method (ELBM) [37, 39, 49, 78]. The ELBM uses a single lattice in which electric and magnetic field components all share a common discrete position and discrete time. The ELBM derived by Hauser & Verhey uses a single-lattice configuration accomplished by mapping all orthogonal propagation outcomes of electric and magnetic fields to a single probability mass function [39]. The ELBM uses more degrees of freedom to represent the electric and magnetic fields, which provides numerical solutions with greater accuracy and stability than the YL-FDTDM [39]. Since interparticle collisions do not occur, and there is zero viscosity, a simple D3Q7 lattice is sufficient to represent all field propagation outcomes [39]. Collision and propagation operations in the stochastic Boltzmann process also preserve the space and time period of the electromagnetic waves, with less numerical dispersion which only manifests as a decrease in the field amplitude beyond the Courant condition. The following sections will describe the advantages of the ELBM over the YL-FDTDM for electrodynamic simulation.

3.3.1 Electric and magnetic fields

The ELBM assumes electric and magnetic fields can be represented by an inviscid, collision-less pseudo-particle population density, \( g_m(x, t) \), as a local probability mass function which has set of \( N_m \) outcomes, where each outcome \( (m = 1, \ldots, N_m) \) represents a discrete direction of propagation on the lattice [37, 39, 49, 78]. Moments of \( g_m(x, t) \) in terms of orthogonal lattice vectors \( v_m \), \( h_m \), and \( e_m \) represent the power density, magnetic field intensity, and electric field intensity in free space [39]. The ELBM operates at the limit of inviscid flow, \( \tau = 1/2 \), to represent the linear Ampere and Faraday laws [37, 49]. Given this constraint, the dimensionless time unit is \( \delta t = 1/2 \), and the dimensionless spatial unit is \( \delta x = 1 \). The collision and propagation operations occur at dimensionless time \( t \) and vector position \( x \) according to

\[
\begin{align*}
g^*_m(x, t) &= 2g^0_m(x, t) - g_m(x, t) \\
g_m(x + v_m\delta t, t + \delta t) &:= g^*_m(x, t),
\end{align*}
\]

where “:=” is the assignment operator and \( g^*_m(x, t) \) is the post-collision pseudo-particle population [39]. The equilibrium pseudo-particle population
density, \( g_{eq}^m(x,t) \), has been derived using suitable Lyapunov functions to guarantee stability [39, 78]. The equilibrium psedo-particle population density is represented by

\[
g_{eq}^m(x,t) = \frac{1}{4}(E(x,t) \cdot e_m + H(x,t) \cdot h_m), \tag{3.35}
\]

where \( E(x,t) \) and \( H(x,t) \) are the dimensionless electric and magnetic field intensity, which are calculated as moments of \( g_m(x,t) \),

\[
E(x,t) = \sum_{m=1}^{N_m} g_m(x,t)e_m \quad \text{and} \quad H(x,t) = \sum_{m=1}^{N_m} g_m(x,t)h_m. \tag{3.36}
\]

The possible lattice vectors depend on the number of dimensions, and in two dimensions, the polarization of the electric field. The lattice vectors can be organized into matrices, which are referred to as a lattice-matrices in this thesis. The elements of the lattice-matrix can be derived from the following conditions for orthogonality in the Chapman-Enskog expansion,

\[
\begin{align*}
\sum_{m=1}^{N_m} v_{\alpha m} &= \sum_{m=1}^{N_m} h_{\alpha m} = \sum_{m=1}^{N_m} e_{\alpha m} = 0, \\
\sum_{m=1}^{N_m} h_{\alpha m} h_{\beta m} &= \sum_{m=1}^{N_m} e_{\alpha m} e_{\beta m} = 4\delta_{\alpha\beta}, \\
\sum_{m=1}^{N_m} e_{\alpha m} h_{\beta m} &= 0, \\
\sum_{m=1}^{N_m} v_{\alpha m} e_{\beta m} h_{\gamma m} &= 2\epsilon_{\alpha\beta\gamma}, \\
\sum_{m=1}^{N_m} v_{\alpha m} e_{\beta m} e_{\gamma m} &= \sum_{m=1}^{N_m} v_{\alpha m} h_{\beta m} h_{\gamma m} = 0,
\end{align*}
\tag{3.37}
\]

where \( \{\alpha, \beta, \gamma\} \) are independent non-equivalent dimensional indices [39]. Hauser & Verhey’s method accounts for both left-handed and right-handed orthogonal propagation bases to maximize stability. However, the Minkowski formulation of Maxwell’s equations in Tab. 2.1 only represents right-handed propagation bases. Consequently, Hauser & Verhey’s Chapman-Enskog expansion requires a dimensionless time unit of \( \delta t = 1/2 \) [39], to represent Ampere and Faraday laws

\[
\frac{1}{2} \nabla \times H = \dot{E} \quad \text{and} \quad \frac{1}{2} \nabla \times E = -\dot{H}. \tag{3.38}
\]
3.3. The electrodynamic lattice-Boltzmann method

The factor of $1/2$ also manifests in the initial condition for the dimensionless electric and magnetic field intensity.

3.3.2 Two-dimensional lattice-matrices

Two-dimensional lattice-matrices represent $N_m = 8$ non-zero right-handed and left-handed orthogonal bases constructing the outcomes of $g_m(x, t)$. The two-dimensional lattice-matrices for a p-polarized, or transverse-magnetic (TM), electric field are

$$
\begin{align*}
\mathbf{v}_{\alpha m} &= \begin{bmatrix} 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 1 & 0 & -1 \end{bmatrix}, \\
\mathbf{e}_{\alpha m} &= \begin{bmatrix} 0 & -1 & 1 & 0 & 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 \end{bmatrix}, \\
\mathbf{h}_{\alpha m} &= \begin{bmatrix} -1 & -1 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}.
\end{align*}
$$

(3.39)

Fig. 3.3 illustrates the right-handed bases which represent half the propagation outcomes of a p-polarized electric field. The remaining left-handed bases have an opposite order and orientation. The polarization density, $\mathbf{P}(x, t)$, and magnetization density, $\mathbf{M}(x, t)$, are stationary outcomes of $\mathbf{E}(x, t)$ and $\mathbf{H}(x, t)$.

![Figure 3.3](image-url)

Figure 3.3: [Color online] Illustration of discrete lattice vectors forming right-handed propagation bases for a p-polarized electric field on a D2Q5 lattice. The remaining lattice vectors form the left-handed propagation bases which have an opposite order and orientation on the lattice. Polarization and magnetization density represent stationary electric and magnetic field outcomes. The symbol “⊗” is “into-the-page,” while the symbol “⊙” is “out-of-the-page.”
3.3. The electrodynamic lattice-Boltzmann method

The two-dimensional lattice-matrices for an s-polarized, or transverse-electric (TE), electric field are

\[
\begin{bmatrix}
\mathbf{v}_{am} \\
\mathbf{e}_{am} \\
\mathbf{h}_{am}
\end{bmatrix} =
\begin{bmatrix}
1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 \\
0 & -1 & 0 & 1 & 0 & 1 & 0 & -1 \\
1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 \\
0 & 1 & -1 & 0 & 0 & -1 & 1 & 0 \\
-1 & 0 & 0 & 1 & 1 & 0 & 0 & -1
\end{bmatrix}, \quad (3.40)
\]

Fig. 3.4 illustrates the right-handed bases as half the propagation outcomes of an s-polarized electric field. The remaining left-handed bases have an opposite order and orientation. The polarization density, \( \mathbf{P}(\mathbf{x},t) \), and magnetization density, \( \mathbf{M}(\mathbf{x},t) \), are stationary outcomes of \( \mathbf{E}(\mathbf{x},t) \) and \( \mathbf{H}(\mathbf{x},t) \).

Figure 3.4: [Color online] Illustration of discrete lattice vectors that form the right-handed propagation bases for an s-polarized electric field on a D2Q5 lattice. The remaining lattice vectors form the left-handed propagation bases which have an opposite order and orientation on the lattice. Polarization and magnetization density represent stationary electric and magnetic field outcomes. The symbol “⊗” is “into-the-page,” while the symbol “⊙” is “out-of-the-page.”
3.3.3 Three-dimensional lattice-matrices

The three-dimensional lattice-matrices represent $N_m = 12$ non-zero left-handed and right-handed orthogonal bases constructing the outcomes of $g_m(x, t)$.

$$[\mathbf{v}_{am}] = \begin{bmatrix} 1 & 0 & 0 &-1 & 0 & 0 &1 & 0 & 0 \\ 0 &-1 & 0 & 0 &1 & 0 &0 &-1 & 0 \\ 0 & 0 &-1 & 0 & 0 &1 & 0 & 0 &-1 \end{bmatrix},$$

$$[\mathbf{e}_{am}] = \begin{bmatrix} 0 & 0 &-1 & 0 & 0 &1 &-1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 &1 & 0 &-1 & 0 & 0 & 0 \\ 0 & 0 &-1 & 0 &-1 & 0 &0 & 0 & 1 \end{bmatrix},$$

$$[\mathbf{h}_{am}] = \begin{bmatrix} 0 & 1 & 0 & 0 &-1 & 0 &-1 & 0 & 0 & 1 \\ 0 & 0 &-1 & 0 & 0 &1 &-1 & 0 & 0 & 0 \\ -1 & 0 & 0 &-1 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}.$$  \hspace{1cm} (3.41)

These lattice-matrices are later used in a three-dimensional multi-physics simulation of optical radiation pressure. Two-dimensional and three-dimensional implementations of the ELBM are the same, except for their lattice-matrices. Therefore, a numerical method solving a three-dimensional force density is simpler to implement in the ELBM than in the YL-FDTDM.

3.3.4 Ponderable media

In ponderable media, the propagation of electric and magnetic fields are impeded by electric and magnetic dipoles at time $t$ and vector position $x$. The corresponding dimensionless polarization density, $\mathbf{P}(x, t)$, and magnetization density, $\mathbf{M}(x, t)$, manifest as the outcomes for electric and magnetic fields remaining at their present locations \[78\]. These outcomes are forced to approach their equilibrium conditions, $\mathbf{P}^{eq}(x, t) = (\epsilon_r(x) - 1)\mathbf{E}(x, t)$ and $\mathbf{M}^{eq}(x, t) = (\mu_r(x) - 1)\mathbf{H}(x, t)$, with a collision operation only (no propagation since they are stationary)

$$\mathbf{P}(x, t + \delta t) = 2\mathbf{P}^{eq}(x, t) - \mathbf{P}(x, t),$$

$$\mathbf{M}(x, t + \delta t) = 2\mathbf{M}^{eq}(x, t) - \mathbf{M}(x, t).$$  \hspace{1cm} (3.42)

In the presence of ponderable media, the electric and magnetic fields must have re-normalized moments of $g_m(x, t)$ to reflect the outcomes of polarization or magnetization density \[37, 39, 78\]. The dimensionless electric and
3.3. The electrodynamic lattice-Boltzmann method

Magnetic fields in lossless magnetodielectric media are therefore

\[
E(x, t) = \frac{1}{\epsilon_r(x)} \sum_{m=1}^{N_m} (g_m(x, t) e_m + P(x, t)),
\]

\[
H(x, t) = \frac{1}{\mu_r(x)} \sum_{m=1}^{N_m} (g_m(x) h_m + M(x, t)).
\]

(3.43)

While Eq. (3.43) provides a natural and accurate description of a ponderable medium’s magnetization and polarization density, the description requires additional operations to represent a point charge within a single lattice unit [39].

3.3.5 Energy density and momentum density

The energy density is the same for each of the electrodynamic formalisms, and can therefore be represented as the centred moment of \( g_m^{eq,2}(x, t) \),

\[
W_e(x, t) = \sum_{m=1}^{N_m} g_m^{eq,2}(x, t).
\]

(3.44)

When the dimensionless velocity is chosen as \( c_0 = 1 \), both the dimensionless power density and the momentum density are the first moment of \( g_m^{eq,2}(x, t) \) in terms of \( v_m \),

\[
G_e(x, t) = \sum_{m=1}^{N_m} g_m^{eq,2}(x, t) v_m.
\]

(3.45)

This suggests an energy continuity equation of the form \( \frac{1}{2} \nabla \cdot \mathbf{S}_e = -\dot{W}_e \) [39], which is true for uniform non-dispersive magnetodielectric media. Such an energy continuity condition requires that components of \( \mathbf{E}(x, t) \) or \( \mathbf{H}(x, t) \) are initialized at half their desired value to remain wholly consistent with Maxwell’s equations. Provided such a scaling in the initial condition, the dimensional conversions are \( W'_e(x', t') = W_e(x', t') \epsilon_0, \) \( S'_e(x', t') = S_e(x', t') / \eta_0, \) and \( G'_e(x', t') = G_e(x', t') / (c^2 \eta_0) \) remain consistent with the ELBM Faraday and Ampere laws in Eq. (3.38) and Tab. 2.1. Each of the electrodynamic dimensional conversions are summarized in Tab. 3.1.
3.3.6 Force density

The force density is the sum of time variation in momentum density and spatial variation in the momentum flux density tensor. The momentum flux density tensor divergence can be represented using a single-lattice divergence operator that is the same independent of the number of lattice dimensions. In the case of the D1Q3, D2Q5 and D3Q7 lattices used in Hauser & Verheý’s ELBM, the divergence of Chu’s momentum flux density tensor can be represented as

\[
\nabla \cdot \mathbf{T}_e(x, t) = \ldots
\]

\[
\frac{1}{8} \sum_{m=1}^{N_m} \left[ |\mathbf{E}(x + \hat{v}_m \delta x, t)|^2 + |\mathbf{H}(x + \hat{v}_m \delta x, t)|^2 \right] \hat{v}_m,
\]

where \( \hat{v}_m \) represents the unit vector of lattice velocity \( v_m \), and the dimensional scaling is

\[
\nabla \cdot \mathbf{T}'_e(x', t') = \frac{\epsilon_0}{\Delta x} (\nabla \cdot \mathbf{T}_e(x, t))
\]

since Eq. (3.46) reduces to a central difference equation in a D2Q5 or D3Q7 lattice. Meanwhile, the dimensional time-variation of energy density and momentum density can be respectively obtained using central difference equations

\[
\frac{\partial}{\partial t} W_e(x', t') = \frac{1}{2} \frac{1}{\delta t \Delta t} \left( W_e(x', t' + \delta t \Delta t) - W_e(x', t' - \delta t \Delta t) \right)
\]

and

\[
\frac{\partial}{\partial t} G_e(x', t') = \frac{1}{2} \frac{1}{\delta t \Delta t} \left( G_e(x', t' + \delta t \Delta t) - G_e(x', t' - \delta t \Delta t) \right).
\]

When calculated at each full time step, or every two iterations in the two-dimensional or three-dimensional ELBM, Eqs. (3.47) and (3.48) retain their second order of accuracy. The dimensional kinetic force density can then be calculated as the negative sum of Eqs. (3.47) and (3.48)

\[
f'_k(x', t') = -\nabla \cdot \mathbf{T}'_e(x', t') - \frac{\partial}{\partial t} G'_e(x', t').
\]

Since only a single lattice is used in the ELBM, space and time interpolation are no longer necessary to evaluate this kinetic force density.
3.3.7 Dimensional conversions

Tab. 3.1 provides the dimensional conversions for the ELBM. These dimensional conversions were derived from the equations provided by Hauser & Verhey in their method, and in the programmatic implementation of their method [39]. The dimensional conversions listed in Tab. 3.1 require that an electric or magnetic field component is initialized at one-half of its desired amplitude. Tab. 3.1 is a subset of the larger table of conversions provided in Tab. C.1 of Appendix C.

Table 3.1: Conversion of dimensionless electrodynamic sub-system variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Dimensionless ((x, t))</th>
<th>Dimensional ((x', t'))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>(t)</td>
<td>(t' = t\Delta t/2)</td>
</tr>
<tr>
<td>Position vector</td>
<td>(x)</td>
<td>(x = x\Delta x)</td>
</tr>
<tr>
<td>Electric field intensity</td>
<td>(E)</td>
<td>(E' = E)</td>
</tr>
<tr>
<td>Magnetic field intensity</td>
<td>(H)</td>
<td>(H' = H/\eta_0)</td>
</tr>
<tr>
<td>Energy density</td>
<td>(W_e)</td>
<td>(W'_e = W_e\epsilon_0)</td>
</tr>
<tr>
<td>Poynting’s vector</td>
<td>(S_e)</td>
<td>(S'_e = S_e/\eta_0)</td>
</tr>
<tr>
<td>Momentum density</td>
<td>(G_e)</td>
<td>(G'_e = G_e/(c^2\eta_0))</td>
</tr>
<tr>
<td>Momentum-flux tensor</td>
<td>(T_e)</td>
<td>(T'_e = T_e\epsilon_0)</td>
</tr>
</tbody>
</table>

3.3.8 Limitations

Unlike in the YL-FDTDM, the ELBM time- and spatial-units cannot be modified with respect to one another since the relaxation time is restricted to a single value, \(\tau = 1/2\). The consequence is that adaptive mesh refinement maybe impractical. Therefore, there maybe limited systems that benefit from the ELBM’s increased accuracy given its fixed space-time relation in a uniform lattice. However, static or sub-optimal dynamic mesh refinement in the YL-FDTDM can lead to late-time instability from increasing numerical error at interfaces between different spatial grids [87]. Therefore, the constraint of a uniform mesh with square lattice units is often used in electrodynamic simulations focused on predicting optical radiation pressure [7].
3.4 Comparative simulation configuration

Both the spatial unit, $\Delta x$, and the time unit, $\Delta t$, are simultaneously and proportionally varied to represent the same spatio-temporal domain. The source is time harmonic with a wavelength of $\lambda = 530 \text{ nm}$ and a time-period of $T = 1.77 \text{ fs}$ in free space. The instantaneous kinetic force densities are averaged over $N_T = 25$ optical periods. Two slightly different systems are required to compare the two methods. Fig 3.5 illustrates the $5\lambda \times 5\lambda$ YL-FDTDM spatial domain, and the $4\lambda \times 4\lambda$ ELBM spatial domain for evaluating force densities. The two domains cannot be exactly identical, since the YL-FDTDM requires additional spatial padding (shaded gray region) for its combined BPML ($\lambda/4$ thickness) and reflection buffer ($\lambda/4$ thickness). The reflection buffer is necessary to avoid time-averaged numerical reflections in free space from the source and BPML. However, in both illustrated systems, the black region is exactly the same size ($4\lambda \times 4\lambda$) with the same spatial resolution. It is within this region that the computational time and accuracy of the YL-FDTDM and ELBM time-averaged kinetic force densities are compared.

Although the YL-FDTDM requires less computational time than the ELBM for evaluating electric and magnetic fields at the same spatial resolution, the YL-FDTDM requires greater computational time for evaluating electric and magnetic fields of similar accuracy. Hauser & Verhey noted that the YL-FDTDM’s computational time is 18 times greater than the ELBM’s computational time in achieving solutions of the same numerical accuracy [39]. This thesis compares the additional computational time required for the YL-FDTDM and ELBM to solve time-averaged force density in the black region, which is the same spatial domain with the same spatial resolution for the two configurations illustrated in Fig. 3.5. Similarly, the numerical accuracy of the net force in the black region is compared between the YL-FDTDM and ELBM.
Figure 3.5: Illustration of the spatial domain used in (a) the YL-FDTDM, and in (b) the ELBM. Each spatial domain has an equivalent number of lattice units per wavelength (resolution), although a different size. Half-wavelength, $\lambda/2$, boundaries (gray regions) are included as a buffer in the YL-FDTDM for the quarter-wavelength $\lambda/4$ Berenger perfectly matched layer and its numerical reflections. The source condition is represented as a white dashed line near the bottom of each spatial domain. The black region represents where the force density is evaluated; this truncated spatial domain has the same size in the YL-FDTDM and the ELBM, with the same spatial resolution. The diameter of the dielectric cylinder cross-section is $D = 2\lambda$, and its refractive index is $\hat{n} = 1.333$ (where $\epsilon_r = 1.778$ and $\mu_r = 1$).
### 3.5 Comparative analysis

The Hermite-Gaussian beam is initialized using a magnetic field polarized in the \( \hat{z} \) direction and an electric field polarized in the \( \hat{x} \) direction, such that electromagnetic waves propagate in the \( \hat{y} \) direction on a two-dimensional \( xy \)-plane. Therefore, the electric field is p-polarized and parallel to the plane of incidence. The cylinder cross-section has a relative permittivity of \( \epsilon_r = 1.778 \) and permeability of \( \mu_r = 1 \), and is non-conductive. The accuracy of the YL-FDTDM and the ELBM are compared using a time-averaged net line-force density. The net time-averaged line-force density in two-dimensions can be calculated from

\[
\langle F \rangle = \int_A \langle f \rangle dA' \approx \sum_{i,j} \langle f_{i,j} \rangle \Delta x \Delta y \equiv \sum_{(x)=(i,j)} \langle f(x,t) \rangle \Delta x \Delta y,
\]

which is equivalent for each electrodynamic formalism, given horizontal and vertical spatial indices \( i \) and \( j \). In the ELBM, \( x = (i, j) \), since \( \delta x = 1 \) and \( \delta y = 1 \), such that the same numerical integration method is used to evaluate net time-averaged line-force density in the YL-FDTDM and the ELBM. Due to symmetry, the analytical solution for the \( \hat{x} \)-directed net time-averaged line-force density is \( \langle F_x \rangle = 0 \). The \( \hat{x} \)-directed net time-averaged line-force density is used to compare the YL-FDTDM and ELBM for its simplicity. The YL-FDTDM and the ELBM are compared in terms of computational time and absolute error with increasing spatial resolution from \( n_\lambda = 10 \) to \( n_\lambda = 80 \) spatial units per wavelength.

### 3.6 Computational time and accuracy comparison

Both the YL-FDTDM and the ELBM are used to predict central difference force densities according to multiple electrodynamic formalisms. Similar computational time is required by each electrodynamic formalism, with medium-independent formalisms requiring the least computational time. At the same spatial resolution, the YL-FDTDM is more efficient, such that it can compute a 50% greater sized array for the electric and magnetic fields in the same computational time. However, additional computational time is needed to evaluate the central difference time-averaged kinetic force density. Fig. 3.8(a) shows that, within the subset domain (black region), the space- and time-interpolated force densities in the YL-FDTDM require 4 to 8 times greater computational time than the single-lattice force densities evaluated...
3.6. Computational time and accuracy comparison

in the ELBM. Fig. 3.8(b) shows that the YL-FDTDM net time-averaged line-force density contains 11 to 35 times greater error than the ELBM’s at the same spatial resolution. This corroborates an earlier study, where it was shown that the ELBM evaluated more accurate electric and magnetic fields than the YL-FDTDM at the same spatial resolution [39].

Figure 3.6: [Color online] Computational time (C.T.) of the YL-FDTDM (a,b), and the ELBM (c,d) as the number of spatial units per wavelength, $n_\lambda$, increases. Surplus computational time required to evaluate central difference force densities are illustrated in (b) for the YL-FDTDM, and (d) for the ELBM. Simulations were performed in MATLAB using an Intel(R) Xeon(R) CPU E3-1225 v3 @ 3.20GHz processor having 7.80 GB RAM.
3.6. Computational time and accuracy comparison

Figure 3.7: The net time-averaged line-force density in the $x$-direction ($\rightarrow$), $\langle F_x \rangle$, plotted (a) in natural units and (b) on a semi-logarithmic scale. Analytically, $\langle F_x \rangle = 0 \text{ pN/m}$.

Figure 3.8: (a) Computational time ratio and (b) error ratio plotted with respect to the number of spatial units per wavelength, $n_\lambda$. When compared with the ELBM, the YL-FDTDM requires 4 to 8 times greater computational time for recovering solutions with 11 to 35 times greater error.
3.6. Computational time and accuracy comparison

3.6.1 Time-averaged force density

Chu’s formalism predicts time-averaged force densities throughout the cross-section of the dielectric cylinder. Comparing Chu’s time-averaged force densities in the ELBM and YL-FDTDM at \( n_\lambda = 10 \) and \( n_\lambda = 40 \), the YL-FDTDM predicts much greater non-physical time-averaged force densities in free space (which should not exist in the absence of electric dipoles).

Figure 3.9: [Color online] The Chu time-averaged force density in the \( x \)-direction (→) for a cylindrical cross-section in (a) the YL-FDTDM and (b) the ELBM, at \( n_\lambda = 10 \). Time-averaged force densities in free space are greater in the YL-FDTDM than in the ELBM. The YL-FDTDM time-averaged force densities in (c) approach the ELBM time-averaged force densities in (d) at \( n_\lambda = 40 \).
Chapter 4

Multi-physics simulation of optical radiation pressure on a multi-phase fluid

Since an analysis of deformation is required to discriminate between electrodynamic formalisms, this chapter describes an algorithm for the multi-phase multi-physics simulation of optical radiation pressure. In this chapter, we combine the ELBM from Chapter 3 with a lattice-Boltzmann method describing a multi-phase fluid. First this chapter provides a brief literature review of several different multi-physics simulations of optical radiation pressure on fluids and the advantages and disadvantages of the lattice-Boltzmann method. Following this literature review is a description of the different components of the kinetic lattice-Boltzmann method used in this thesis and how they comprise the fluid-solver algorithm. The algorithm requires a fluid relaxation time that is significantly greater than the time required for electromagnetic waves to propagate through the fluid medium. This assumption is typically true for optical radiation pressure on quasi-stationary media, where it has been successfully applied in previous electrodynamic simulations [7, 8, 23].

4.1 Review of multi-physics simulation methods

The multi-physics simulation of optical radiation pressure on fluids has been accomplished using an analytical approach with a boundary-integral-element method [26, 27], the finite-difference-time-domain (FDTD) method with front-tracking [7, 80, 88], and the finite-element method (FEM) [23, 28]. Each approach is philosophically similar in that it discretizes the phenomenological Navier-Stokes and Maxwell’s equations in space and/or time to numerically solve the deformation of a ponderable medium. Quantitative comparisons between experimentally measured and predicted deformation of a fluid-fluid interface are typically sufficient [27, 28]. However, these
previous studies analyzed a solution for the trivial Laplace-pressure, which may not distinguish between predictions of optical radiation pressure for several different formalisms [7, 8, 29]. Finite-element and front-tracking methods can also enforce the definition of an interface, which prevents a description of natural multiphase fluid separation, vaporization or coalescence under the influence of optical radiation pressure. Finite-element and front-tracking methods also solve the nonlinear advection term in the Navier-Stokes equation (NSE) non-locally, which requires implicit iterative solutions for hyperbolic differential equations [43]. Alternatively, the lattice-Boltzmann method (LBM) indirectly solves NSE via Boltzmann’s equation and solves the non-linear advection term locally. However, the greatest advantages of the LBM are its simplicity and achievement of direct mass and momentum conservation via a total probability axiom. Recently, entropic relaxation LBMs also have been developed for representing turbulent flow with increased stability [46], multi-range LBMs have been developed for compressible gases [89], and relativistic LBMs have been developed for describing gases with particle velocities approaching the speed of light [58].

Most multi-phase fluid simulations using an LBM invoke either a free-energy or interaction-potential (pseudopotential) approach for describing the phase separation. The pseudopotential approach was developed first [67], but its description of an effective mass density was found thermodynamically inconsistent [40]. Consequently, a thermodynamically consistent free-energy approach was developed [90]. However, the free-energy approach requires more computational operations, and its initial implementation exhibited Galilean invariance and instability for greater liquid-vapour density ratios [40]. While both the pseudopotential and free-energy approach have been modified to overcome their limitations, the pseudopotential approach is related to microscopic interactions while remaining simpler to implement. In its simplest form, the pseudopotential approach is also Galilean invariant and can approximate thermodynamic consistency provided a physical equation of state [40, 91], which is sufficient for a number of fluid experiments [40]. Thermodynamic inconsistency of the pseudopotential method is a consequence of second-order treatment of the third-order term in the Shan-Chen force density, the third-order term describing the phase separation [92]. Increased academic interest in the pseudopotential approach has provided greater information on adaptations overcoming its thermodynamic inconsistency [40, 92–94], and spurious velocities at an interface [40, 92]. Recently, the pseudopotential lattice Boltzmann method (PLBM) was applied to analyze the deformation of multi-phase fluids from an electrostatic field or continuous optical radiation pressure [36, 38]. Each study assumed
4.2. The pseudopotential lattice-Boltzmann method

The pseudopotential lattice-Boltzmann-method (PLBM) is a numerical solver of Boltzmann’s equation for multi-phase microscopic and macroscopic (mesoscopic) non-ideal fluids, which uses a non-ideal force density and equation of state to represent a vapour-liquid interface. The central parameter of the PLBM is a probability mass function (PMF), $n_m(x, t)$, representing a particle population in a random discrete-velocity space, $v_m$, at dimensionless time $t$ and vector position $x$, where $m = 1, ..., N_m$ as an index for the discrete velocities. The PMF, $n_m(x, t)$, is made to approach the Maxwell equilibrium probability mass function (EPMF), $n_{eq}^m(x, t)$, using either a single-relaxation, multi-relaxation, or entropic-relaxation process. Moments of the PMF in velocity space only represent the mass and momentum density of an ideal gas, and require the addition of an external force to represent their non-ideal state.

4.2.1 Initial condition

The initial condition for the multi-phase studies in this thesis is a distributed mass-density in the shape of a superellipse, a cylindrical cross-section, or a sphere with negligible velocity. Regardless of the initial density, the most stable interface is represented by a hyperbolic tangent function which serves as an analytical solution to Maxwell’s construction for an isothermal liquid vapor phase coexistence [95],

$$\rho_{init}(r, t) = \frac{1}{2} (\rho_{liq} + \rho_{vap}) \pm \frac{1}{2} (\rho_{liq} - \rho_{vap}) \tanh \left( \frac{2(r - r_i) \cdot \hat{n}_i}{l} \right), \quad (4.1)$$
4.2. The pseudopotential lattice-Boltzmann method

where \( \mathbf{r}_i \) is the locus of the interface with respect to the origin, \( \hat{n}_i \) is the normal unit vector, \( \iota \) is its thickness, and \( \mathbf{r} \) is the displacement vector from a common origin.

The superellipse is initialized as an approximate rectangle,

\[
\rho_{\text{init.}}(y, t) = \frac{1}{2} (\rho_{\text{liq.}} + \rho_{\text{vap.}}) \pm \frac{1}{2} (\rho_{\text{liq.}} - \rho_{\text{vap.}}) \tanh \left( \frac{2(y - h)}{\iota} \right),
\]

where \( y \) is the dimension in which mass density varies, and \( h \) represents the liquid depth. When initialized within one half of a macroscopic fluid domain, the superellipse can stabilize to represent an approximately flat interface. Flat interfaces are important since they have been used in former experiments and simulations of optical radiation pressure [7, 28]. However, a flat interface is thermodynamically unstable at the microscale according to Laplace’s law [96]. Even at millimetric scales, which exceed 1000 optical wavelengths, the steady-state water interface has a curved meniscus. Non-equilibrium oscillations from the unstable initial condition of a flat interface can contaminate the numerical solution. At the very least, additional computational time or specialized boundary conditions are required to stabilize a superellipse.

The cylinder cross-section or sphere is initialized as

\[
\rho_{\text{init.}}(r, t) = \frac{1}{2} (\rho_{\text{liq.}} + \rho_{\text{vap.}}) \pm \frac{1}{2} (\rho_{\text{liq.}} - \rho_{\text{vap.}}) \tanh \left( \frac{2(r - r_i)}{\iota} \right),
\]

where \( r \) is the radial distance from the center of the droplet, \( r_i \) is the radius of the interface representing a cylinder or sphere, and \( \iota \) is the thickness of the interface. Adding the second term represents a droplet, while subtracting the second term represents a bubble. The cylindrical cross-section or spherical droplet with negligible velocity has the minimum free surface energy and the greatest stability provided an ambient hydrostatic pressure. Therefore, it represents ideal microscopic light-matter interactions free from any external media. Droplets can also mimic cells which are analyzed in optical tweezing experiments [52]. Despite the challenges of accurately detecting such a system in experiment, it is convenient for testing an electrodynamic simulation method and its application.
4.2.2 Mass and momentum

Mass density, $\rho(x, t)$, and momentum density, $\rho(x, t)u(x, t)$, of an ideal gas can be computed as moments of the PMF, $n_m(x, t)$, in its discrete velocity space [71],

$$\rho(x, t) = \sum_{m=1}^{N_m} n_m(x, t), \quad \rho(x, t)u(x, t) = \sum_{m=1}^{N_m} n_m(x, t)v_m. \quad (4.4)$$

The momentum density of a non-ideal gas (or liquid), however, is perturbed by an external force density (such as the pseudopotential force density), which must be incorporated [67]. This thesis uses the Shan-Chen forcing scheme [40],

$$u(x, t) = \frac{1}{\rho(x, t)} \left( \sum_{m=1}^{N_m} n_m(x, t)v_m + \frac{\tau\delta t}{2}f(x, t) \right), \quad (4.5)$$

and the general Guo forcing scheme [97],

$$u(x, t) = \frac{1}{\rho(x, t)} \left( \sum_{m=1}^{N_m} n_m(x, t)v_m + \frac{\delta t}{2}f(x, t) \right), \quad (4.6)$$

to represent phase separation and external forces. Guo’s forcing scheme is used in single-relaxation and multi-relaxation approaches for two-dimensional fluid systems. Meanwhile, Shan-Chen’s forcing scheme is used in single-relaxation approaches for three-dimensional fluid systems.

4.2.3 The pseudopotential force density

The pseudopotential, or Shan-Chen, force density represents a third-order instability between a liquid and its vapor phase [40, 92]. While the instability has been criticized for its thermodynamic inconsistency, which may not allow explicit definition of surface tension, an equation of state may be used to indirectly approximate thermodynamic consistency and corresponding surface tension [40, 91]. In this case, the Shan-Chen force density based on an effective density is given by

$$f_{\text{SC}}(x, t) = -G\psi(x, t) \sum_{m=1}^{N_m} w(|v_m|) [\psi(x + v_m\delta t, t)], \quad (4.7)$$
4.2. The pseudopotential lattice-Boltzmann method

while the corresponding effective density approximating a thermodynamically consistent interface may be represented as

$$\psi(x, t) = \sqrt{\frac{2(p(x, t) - c_s^2)}{Gc_s^2}}, \quad (4.8)$$

where \(w(0) = 4/9, w(1) = 1/9, \) and \(w(2) = 1/36\) and the coefficient \(G = 1.\)

Given the effective mass, \(\psi(x, t),\) any arbitrary equation of state can be used to define \(p(x, t) [91].\) The Carnahan-Starling equation of state demonstrates the greatest thermodynamic consistency and stability [91],

$$p(x, t) = \rho RT \frac{1 + bp/4 + (bp/4)^2 - (bp/4)^3}{(1 - bp/4)^3} - a\rho^2 \bigg|_{(x,t)} \quad (4.9)$$

where \(a = 1, b = 4, \) and \(\mathcal{R} = 1\) are dimensionless versions of fundamental constants. However, it is also possible to generate a customized cubic equation of state [98]. Consequently, the PLBM has found wide application and adaptation for representing fluid phenomena including microscopic droplets and bubbles [40]. The Shan-Chen pseudopotential force density is also amenable to single-relaxation [40], multi-relaxation [93], and entropic-relaxation LBMs [99]. The Shan-Chen force density is essential to the pseudopotential approach and it has been applied in Guo and Lycett-Brown & Luo forcing schemes [92, 100] (among a variety of alternative forcing schemes) which perturb the PMF during the collision operation [40].
4.2. The pseudopotential lattice-Boltzmann method

Figure 4.1: [Color online] (a) The Carnahan-Starling equation of state (CS-EOS) liquid-vapor phase coexistence curve in terms of reduced temperature ($T = T'/T_c$) and reduced density ($\rho = \rho'/\rho_c$). The theoretical prediction is derived by equating chemical potentials in the liquid and vapor phases, similar to Ref. [91]. (b) Dimensionless “[]” mass density, $\rho$, plotted with its maximum liquid-vapour density ratio, $\rho_{\text{liq.}}/\rho_{\text{vap.}} = 1180$ at $T' = 0.531$, on a two-dimensional $128 \times 128$ grid.

4.2.4 The kinetic force density

Multiple force densities can be added to the Shan-Chen force density via the property of superposition, such that force densities can be incorporated between interacting sub-systems provided they have equivalent spatio-temporal dimensions. Since each system property is dimensionless, it is possible to linearly scale the multi-physics system to any physical dimensions provided that the mean-free-path of the fluid is smaller than the spatial unit. Regardless of the scale, dimensional conversion is required to represent physical system properties. In each sub-system, the dimensionless spatial unit is the fundamental unit of measure, $\delta x = 1$, by which mass density and time, $\rho$ and $\delta t = 1$, are secondary units of measure that can be scaled using the dimensional two-phase critical point mass density, $\rho'_c$, and physical time unit, $\Delta t$. The time-averaged kinetic force density is a component of external force density added to the Shan-Chen force density and incorporated within any of the forcing schemes described in this thesis.
4.2.5 Collision operation and operators

Collisions in the PLBM are locally non-linear, and bypass the Poisson equation with pseudo-compressibility, which enables their simple parallelization and adaptation for different scales and experiments [41, 42]. Given that the collision outcomes are linearly independent, the PLBM operations can be parallelized for greater computational efficiency in solving unsteady or incompressible fluid flows [42]. However, the original PLBM exhibits the greatest spurious liquid velocities at an interface [42]. Modifications to the collision operator include a third-order forcing term with an accurate equation of state [91, 92], multi-relaxation [40, 93], and/or entropic relaxation [46, 99].

The single relaxation method uses the Bhatnagar-Gross-Krook (BGK) collision operator [77], with the PMF, \( n_m(x, t) \), approaching the EPMF, \( n_m^{eq}(x, t) \), according to

\[
\begin{align*}
  n_m^*(x, t) &= n_m(x, t) - \frac{\delta t}{\tau} (n_m(x, t) - n_m^{eq}(x, t)) \\
  &\quad + \left(1 - \frac{\delta t}{2\tau}\right) S_m(x, t) \delta t.
\end{align*}
\]

(4.10)

The single-relaxation EPMF can be represented in the time-domain using Chapman Enskog expansion with Hermite polynomials [76]. The term \( S_m(x, t) \) is a non-ideal forcing term that modifies the collision operator for an external force density according to the forcing scheme. Multiple forcing schemes exist, but this thesis applies the Shan-Chen and Guo forcing schemes for their stability or accuracy [40, 97]. However, the Shan-Chen and Guo forcing schemes are limited compared with alternative forcing schemes, such as Lycett-Brown & Luo’s forcing scheme, which has tunable surface tension and interface width for increased stability and versatility [92]. In the Shan-Chen forcing scheme [40],

\[
S_m(x, t) = 0,
\]

(4.11)

which causes the density ratio between the liquid and vapor phases to change with relaxation time, \( \tau \), causing thermodynamic inconsistency and instability with deviation from \( \tau = 1 \) [93, 97]. This density-dependent relaxation time in the Shan-Chen forcing scheme severely limits the PLBM’s range of viscosity [93]. In this thesis, the Shan-Chen forcing scheme is only used in qualitative three-dimensional simulations for its stability given a relaxation time of \( \tau = 1 \). Alternatively, Guo’s forcing scheme can be used to
incorporate the Shan-Chen force density [97],

\[ S_m(x, t) = \left( 1 - \frac{1}{2\tau} \right) w_m \left[ \frac{v_m - u(x, t)}{c_s^2} + \frac{v_m \cdot u(x, t)}{c_s^4} v_m \right] \cdot f(x, t), \]  

(4.12)

and offers enhanced thermodynamic consistency with a greater range of relaxation time or viscosity. While the Shan-Chen forcing scheme compromises thermodynamic consistency for stability, Guo’s forcing scheme compromises stability for thermodynamic consistency. Regardless, both forcing schemes are only conditionally stable since they approximate the third-order Shan-Chen force density as second-order [92]. To represent the complete third-order Shan-Chen force density with tunable surface tension, the Lycett-Brown-Luo third-order forcing scheme is recommended [92].

The multi-relaxation method has a collision operation in moment space that is transformed to velocity space prior to the streaming/propagation operation [101]. The collision operation is the same in velocity space and moment space

\[ n^*_m(x, t) = n_m(x, t) - \sum_{q=1}^{N_q} \Lambda_{mq} (n_q(x, t) - n^*_{eq}(x, t)) \ldots \]  

(4.13)

\[ + \sum_{q=1}^{N_q} \left( \delta_{mq} - \frac{1}{2} \Lambda_{mq} \right) S_q(x, t) \delta t, \]

\[ \hat{n}^*_m(x, t) = \hat{n}_m(x, t) - \sum_{q=1}^{N_q} \hat{\Lambda}_{mq} (\hat{n}_q(x, t) - \hat{n}^*_{eq}(x, t)) \ldots \]  

(4.14)

\[ + \sum_{q=1}^{N_q} \left( \delta_{mq} - \frac{1}{2} \hat{\Lambda}_{mq} \right) \hat{S}_q(x, t) \delta t, \]

where \( \delta_{mq} \) is the Kronecker-delta symbol representing elements of the \( N \times N \) identity matrix for a DdQN lattice [93, 101]. This thesis implements the MRT collision operator on a D2Q9 lattice only [93, 102], although alternative implementations exist in three dimensions for D3Q15 and D3Q19 lattices [103, 104]. Multi-relaxation allows independent tuning of relaxation times for each element of \( \hat{n}^*_{eq}(x, t) \) based on bulk and kinematic viscosity, subject to constraints of hydrodynamics and stability [105]. The relaxation parameters are organized using a collision matrix in either velocity space,
4.2. The pseudopotential lattice-Boltzmann method

[Λ], or moment-space, [̂Λ]. However, the collision matrix in moment space can be defined as a diagonal (diag) matrix [105]

\[
[\hat{\Lambda}] = \text{diag}[s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9],
\]

where the relaxation parameters, \( s_1, \ldots, s_9 \), modify each component of \([\hat{n}]\), a matrix defining \( \hat{n}_m(x, t) \) [93]. When defined in a moment space, the collision matrix de-couples the physical quantities of \( \hat{n}^\text{eq}_m(x, t) \). Each parameter from \( s_1 \) to \( s_9 \) can be tuned independently, subject to stability constraints [105]. One such constraint is that \( s_1 = s_4 = s_6 = 1 \). The last two parameters, \( s_8 \) and \( s_9 \), are related to the single relaxation time and dimensionless kinematic viscosity via

\[
s_8 = s_9 = \frac{1}{\tau} \quad \text{and} \quad \nu = \left( \tau - \frac{1}{2} \right) c_s^2 \delta t.
\]

One additional parameter, \( s_2 \), is related to bulk viscosity, \( \zeta \),

\[
s_2 = \left( \frac{\zeta}{c_s^2 \delta t} + \frac{1}{2} \right)^{-1},
\]

while the remaining parameters \( s_3 = s_7 \) are independently tuned for stability [93]. The condition \( s_5 = s_7 \) is required to satisfy symmetry [93, 101]. Conversions between velocity space and moment space are accomplished using transformation matrix, \([M]\). Given a D2Q9 lattice, velocity-space to moment-space and moment-space to velocity-space transformations are

\[
[\hat{n}] = [M][n] \quad \text{and} \quad [n] = [M]^{-1}[\hat{n}],
\]

given transformation matrix [106]

\[
[M] = \\
\begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1
\end{bmatrix}.
\]

The vector representing the moment-space PMF, \([\hat{n}]\), is

\[
[\hat{n}] = [\rho, W_k, W_k^2, G_{k,x}, G_{k,y}, S_{k,x}, S_{k,y}, \sigma_{k,xx}, \sigma_{k,xy}]^T,
\]

63
4.2. The pseudopotential lattice-Boltzmann method

where \( \rho \) is the mass density, \( W_k \) is the kinetic energy density, \( G_{k,x} \) and \( G_{k,y} \) are the \( \hat{x} \) and \( \hat{y} \) components of the kinetic momentum density, \( S_{k,x} \) and \( S_{k,y} \) are similar components of the kinetic energy flux density, and \( \sigma_{k,xx} \) and \( \sigma_{k,xy} \) are the diagonal and off-diagonal components of the stress-tensor representing the kinetic sub-system [93]. In Eq. 4.20, the symbol “\(^\top\)” represents the transpose operation. In moment space, as opposed to velocity space, each of the outcomes have a physical meaning. Similarly, the equilibrium distribution and forcing term can be transformed to moment space using

\[
[\hat{n}_e] = [M][n_e] \quad \text{and} \quad [\hat{S}] = [M][S],
\]

which results in

\[
[\hat{n}_e] = \begin{bmatrix} \rho & -2\rho + G_k^2/9\rho & \rho - G_k^2/9\rho & G_{k,x} & -G_{k,x} & -G_{k,y} & (G_{k,x}^2 - G_{k,y}^2)/\rho & G_{k,x}G_{k,y}/\rho \end{bmatrix}
\]

and

\[
[\hat{S}] = \begin{bmatrix} 0 & 6(u_x f_{k,x} + u_y f_{k,y}) & -6(u_x f_{k,x} + u_y f_{k,y}) & f_{k,x} & -f_{k,x} & f_{k,y} & -f_{k,y} & 2(u_x f_{k,x} - u_y f_{k,y}) & u_x f_{k,y} + u_y f_{k,x} \end{bmatrix},
\]

when expanded for a D2Q9 lattice [93]. While independent tuning of each relaxation time allows the MRT approach to preserve a mass-density ratio over a greater range of kinematic viscosity than the SRT approach, the MRT forcing term requires minor adjustment for thermodynamic consistency and stability with increasing density ratio. Minor adjustment of \([\hat{S}]\) in Eq. (4.22) can tune the third-order instability of the Shan-Chen force density for increased thermodynamic consistency in the MRT approach [102],

\[
[\hat{S}] = \begin{bmatrix} 0 & 6(u_x f_{k,x} + u_y f_{k,y}) + \frac{12\sigma_{s,s_2}}{\psi^2\delta t(1-0.5s_2)}|f_k|^2 & -6(u_x f_{k,x} + u_y f_{k,y}) - \frac{12\sigma_{s,s_2}}{\psi^2\delta t(1-0.5s_2)}|f_k|^2 & f_{k,x} & -f_{k,x} & f_{k,y} & -f_{k,y} & 2(u_x f_{k,x} - u_y f_{k,y}) & u_x f_{k,y} + u_y f_{k,x} \end{bmatrix},
\]

(4.23)
4.2. The pseudopotential lattice-Boltzmann method

where $s_2$ and $s_3$ are relaxation parameters from Eq. 4.15, $\psi$ is the equivalent mass density from Eq. 4.8, $|f_k| = (f_{k,x}^2 + f_{k,y}^2)^{1/2}$ is the magnitude of the kinetic force density, and $\sigma_\gamma$ is a tuning parameter for the third-order instability [102]. Such adjustment is necessary to achieve high density ratios typical of the Carnahan-Starling equation of state. Since this thesis does not represent particular fluid experiments, it implements existing MRT relaxation parameters to demonstrate generic fluid behaviour [93, 102]. Further modifications to $[\hat{S}]$ are necessary to achieve an adjustable surface tension [103, 104, 107].

The entropic-relaxation method has a Karlin-Boltzmann-Collision (KBC) operator that represents the Boltzmann-$\mathcal{H}$ theorem [46]. The KBC collision operator is distinct from the BGK collision operator in that it maximizes entropy to represent a physical process. Recently, the KBC operator has been applied to free-energy and pseudopotential LBMs for multiphase fluids, with numerical solutions of increased accuracy compared with the BGK collision operator [99, 108]. Since negligible turbulence is demonstrated in the studies of this thesis, as per their momentum conservation, the KBC operator was found unnecessary. Nonetheless, this thesis recommends the KBC operator for future studies examining more general fluid behaviour [109].

4.2.6 Equilibrium probability mass function

The Maxwell equilibrium probability mass function (EPMF) is a discrete representation of the continuous Maxwell-Boltzmann distribution representing a population density of colliding ideal-gas particles [65]. EPMFs can be approximately derived for SRT or MRT methods using Hermite polynomials, or exactly derived for an entropic relaxation method using a separation of the EPMF in each orthogonal dimension [46, 76]. While each EPMF can be used to represent the equilibrium of the kinetic sub-system investigated in this thesis, entropic relaxation approaches were only recently developed for the PLBM and are still being refined for general implementation [99, 109]. Therefore, the kinetic second-order discrete Hermite-polynomial EPMF and the BGK collision operation were found to be sufficient as a proof of concept.
4.2. The pseudopotential lattice-Boltzmann method

Bhatnagar-Gross-Krook collision operators, either employing single or multi-relaxation, approximate the EPMF in a velocity space. The Hermite-polynomial EPMF was found to be stable with appreciable accuracy in both the two-dimensional and three-dimensional multiphase LBMs used in this thesis [76],

\[
n_{m}^{eq}(x, t) = w(|v_m|) \rho(x, t) \left\{ 1 + \frac{1}{c_s^2} v_m \cdot u(x, t) ... + \frac{1}{2c_s^2} (v_m \cdot u(x, t))^2 - \frac{1}{2c_s^2} u^2(x, t) \right\}.
\]  

However, KBC operators need an exact definition of the EPMF to represent entropic relaxation in three dimensions, which has increased stability for representing a wider range of viscosity in optical radiation pressure experiments [46, 109]. Such methods may be useful for investigating photothermal bubble nucleation or vaporization [54].

Karlin-Boltzmann collision operators have increased stability and accuracy by directly obeying the Boltzmann H-theorem. BGK SRT and MRT collision operators ignore entropy, as do classical methods representing the NSE, which assume that entropy is a higher-order numerical error. However, this assumption can cause both classical solvers of the NSEs and LBMs to become unstable or lose accuracy as time progresses. Karlin-Boltzmann collision (KBC) operators maximize entropy to minimize growth in numerical error, helping close the LBE for hydrodynamics and combat a loss in numerical accuracy with time [46]. Implementation of the KBC operator is beyond the scope of this thesis, although it has recently been applied to model multiphase liquid-vapor water using either a free-energy LBM or PLBM [99, 108].

4.2.7 Propagation operation

Following the collision operation in either the SRT or MRT approach, the post-collision PMF is re-distributed to adjacent lattice nodes, such that

\[
n_{m}(x + v_m \delta t, t + \delta t) := n_{m}^{*}(x, t),
\]  

where “:=” is an assignment operator. This propagation or “streaming” operation is similar to all LBMs.
4.2.8 Boundary conditions

Boundary conditions in kinetic LBMs redistribute outcomes \( n_m(x, t) \) at a boundary to represent a particular macroscopic fluid behaviour at that boundary. However, there exist more outcomes \( n_m(x, t) \) than macroscopic moments such that an inverse solution \( (n_m(x, t) \text{ as a function of macroscopic variables such as } \rho(x, t) \text{ or } G_k(x, t)) \) is not unique. Therefore, hundreds of boundary conditions exist for kinetic lattice-Boltzmann methods as of 2021. This thesis implements periodic, bounce-back, and non-equilibrium bounce-back boundary conditions. Each of these boundary conditions prevent particles from leaving the simulation domain. While periodic boundaries conserve momentum at each instant in time, the bounce-back boundaries do not.

**Periodic boundaries** allow the transfer of mass and momentum out of one boundary, where they simultaneously re-enter the system through the opposite boundary. Consequently, the entire simulation domain represents a single spatio-temporal period of an infinite periodic system. Such boundary conditions are advantageous for simulations of optical radiation pressure, since they conserve mass and momentum at all times. Periodic boundaries can be implemented in lattice Boltzmann methods by assigning the PMF on one boundary to its opposite boundary [110],

\[
n_m(x, t) := n_m(x + L, t),
\]

which is illustrated in Fig. 4.2. Virtual nodes on each boundary represent the boundary nodes on the opposite side of the simulation domain. Only outcomes of \( n_m(x, t) \) directed into the virtual space are assigned to \( n_m(x + L, t) \). In this thesis, periodic boundary conditions are used for simulating the deformation of droplets.

![Illustration of periodic boundary conditions](a) ![Illustration of periodic boundary conditions](b)

Figure 4.2: Illustration of periodic boundary conditions
4.2. The pseudopotential lattice-Boltzmann method

**Bounce-back boundaries** reflect particles as an opposite case to periodic boundaries, and are expressed as

\[ n_m(x, v_m, t) = n_m(x, -v_m, t + \delta t), \] (4.27)

along the boundary [110]. Fig. 4.3 illustrates the perfect reflection at the boundary, which does not move. Since the bounce-back boundary does not move following a collision, it does not necessarily conserve momentum [110]. Further, the bounce-back boundary is second order accurate with respect to space \([O(\delta x^2)]\) which can affect the solution of the third-order Shan-Chen force density and its instability everywhere. Additional momentum exchange algorithms have been developed to account for the transfer of momentum from the fluid to the boundary [111], however, these algorithms can be cumbersome compared with a higher-order bounce-back boundary scheme.

Figure 4.3: Particle with mass \(m\) and velocity \(v\) reflects from a rigid wall, such that its velocity is reversed. Since \(v(t + \delta t) = -v(t)\), the time-averaged particle momentum is \(\langle mv \rangle = (mv(t) + mv(t + \delta t))/2 = 0\). However, momentum transferred to the wall becomes \(2mv\), such that momentum is not conserved at each moment in time.
Non-equilibrium bounce-back boundary conditions  Alternatively, the non-equilibrium bounce-back boundary is a third order accurate $[O(\delta x^3)]$ boundary scheme for straight walls [112]. It uses the mass density and velocity of the fluid at the wall in order to enforce a no-slip condition. If an additional external force density is acting on the wall, it must also be included [113]. In a two-dimensional simulation using a D2Q9 lattice with velocities index $m = 1, ..., 9$, each with magnitude $|v_m| = 1$, the non-equilibrium bounce-back boundary conditions have a unique assignment at each boundary

- West boundary:

\[
\rho_w = \frac{1}{1 - u_{w,x}} \left[ n_9 + n_2 + n_4 + 2(n_3 + n_6 + n_7) - \frac{f_{w,x}}{2} \right],
\]
\[
n_1 = n_3 + \frac{2}{3} \rho_w u_{w,x} - \frac{f_{w,x}}{6},
\]
\[
n_5 = n_7 - \frac{1}{2} (n_2 - n_4) + \frac{1}{2} \rho_w u_{w,y} + \frac{1}{6} \rho_w u_{w,x} - \frac{f_{w,x}}{6} - \frac{f_{w,y}}{4},
\]
\[
n_8 = n_6 + \frac{1}{2} (n_2 - n_4) - \frac{1}{2} \rho_w u_{w,y} + \frac{1}{6} \rho_w u_{w,x} - \frac{f_{w,x}}{6} + \frac{f_{w,y}}{4}.
\]

(4.28)

- East boundary:

\[
\rho_w = \frac{1}{1 + u_{w,x}} \left[ n_9 + n_2 + n_4 + 2(n_1 + n_5 + n_8) + \frac{f_{w,x}}{2} \right],
\]
\[
n_3 = n_1 - \frac{2}{3} \rho_w u_{w,x} - \frac{f_{w,x}}{6},
\]
\[
n_7 = n_5 + \frac{1}{2} (n_2 - n_4) - \frac{1}{2} \rho_w u_{w,y} - \frac{1}{6} \rho_w u_{w,x} + \frac{f_{w,x}}{6} + \frac{f_{w,y}}{4},
\]
\[
n_6 = n_8 - \frac{1}{2} (n_2 - n_4) - \frac{1}{2} \rho_w u_{w,y} - \frac{1}{6} \rho_w u_{w,x} + \frac{f_{w,x}}{6} - \frac{f_{w,y}}{4}.
\]

(4.29)

- North boundary:

\[
\rho_w = \frac{1}{1 + u_{w,y}} \left[ n_9 + n_1 + n_3 + 2(n_2 + n_6 + n_5) + \frac{f_{w,y}}{2} \right],
\]
\[
n_4 = n_2 - \frac{2}{3} \rho_w u_{w,y} + \frac{f_{w,y}}{6},
\]
\[
n_7 = n_5 + \frac{1}{2} (n_1 - n_3) - \frac{1}{2} \rho_w u_{w,x} - \frac{1}{6} \rho_w u_{w,y} + \frac{f_{w,x}}{4} + \frac{f_{w,y}}{6},
\]
\[
n_8 = n_6 - \frac{1}{2} (n_1 - n_3) + \frac{1}{2} \rho_w u_{w,x} - \frac{1}{6} \rho_w u_{w,y} - \frac{f_{w,x}}{4} + \frac{f_{w,y}}{6}.
\]

(4.30)
4.2. The pseudopotential lattice-Boltzmann method

South boundary:

\[
\rho_w = \frac{1}{1 - u_{w,x}} \left[ n_9 + n_1 + n_3 + 2(n_4 + n_7 + n_8) - \frac{f_{w,x}}{2} \right],
\]

\[
n_2 = n_4 + \frac{2}{3} \rho_w u_{w,y} - \frac{f_{w,y}}{2},
\]

\[
n_5 = n_7 - \frac{1}{2} (n_1 - n_3) + \frac{1}{2} \rho_w u_{w,x} + \frac{1}{6} \rho_w u_{w,y} - \frac{f_{w,x}}{4} - \frac{f_{w,y}}{6},
\]

\[
n_6 = n_8 + \frac{1}{2} (n_1 - n_3) - \frac{1}{2} \rho_w u_{w,x} + \frac{1}{6} \rho_w u_{w,y} + \frac{f_{w,x}}{4} - \frac{f_{w,y}}{6}.
\]

In equations Eqs. (4.28)-(4.31), \( u_{w,x} \) and \( u_{w,y} \) represent the components of the local mean fluid velocity at the wall/boundary, \( \rho_w \) represents the mass density at the wall/boundary, and \( f_{w,x} \) and \( f_{w,y} \) represent the components of the force density at the wall/boundary.

\[
\text{Fluid} \quad \text{Wall} \quad \text{Solid}
\]

\[
\text{F}(t) \quad m\mathbf{v}(t) \quad m\mathbf{v}(t + \delta t)
\]

Figure 4.4: [Color online] The particle population with mass \( m \) and velocity \( \mathbf{v} \) reflects from the rigid wall, but its reflection is affected by non-equilibrium velocity and forces acting at the wall.

4.2.9 Dimensionless numbers

Dimensionless numbers have unique definitions in kinetic LBMs, such as the PLBM, compared with their definition for measured dimensional values. This is because the lattice speed of sound in two and three dimensions, \( c_s = (1/\sqrt{3}) \delta x/\delta t \) is distinct from the dimensional speed of sound. Consequently, the corresponding dimensionless numbers relevant to this thesis include

\[
\text{Re} = \frac{|\mathbf{u}| n_x \delta x}{c_s^2 (\tau - \delta t/2)} \quad \text{and} \quad \text{Ma} = \frac{|\mathbf{u}|}{c_s},
\]

which are the Reynolds number and Mach number, respectively. The simulations in this thesis distinguish between cases of incompressibility \( \text{Ma} < 0.1 \) and weak compressibility \( \text{Ma} \in (0.1, 0.3) \).
4.2. The pseudopotential lattice-Boltzmann method

4.2.10 Dimensional conversion

Table 4.1 provides a list of kinetic dimensional conversions used in this chapter. The dimensional conversions listed in Tab. 3.1 are a subset of the larger table of conversions provided in Tab. C.1 of Appendix C.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Dimensionless (x, t)</th>
<th>Dimensional (x', t')</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position vector</td>
<td>x</td>
<td>x' = xΔx</td>
</tr>
<tr>
<td>Time</td>
<td>t</td>
<td>t' = tΔt</td>
</tr>
<tr>
<td>Velocity</td>
<td>u</td>
<td>u' = u(Δx/Δt)</td>
</tr>
<tr>
<td>Mass density</td>
<td>ρ</td>
<td>ρ' = ρc</td>
</tr>
<tr>
<td>Force density</td>
<td>f_k</td>
<td>f_k' = f_k(ρcΔx/(Δt)^2)</td>
</tr>
<tr>
<td>Momentum density</td>
<td>G_k</td>
<td>G_k' = G_k(ρcΔx/Δt)</td>
</tr>
</tbody>
</table>

Similar conversions exist for kinematic viscosity, ν, or bulk viscosity, ζ, which can be derived from standard units. Given a BGK collision operation, the dimensional relationship between the spatial unit, Δx, and time unit, Δt, is often quadratic. The kinematic viscosity (and fluid velocity) for a particular Δt and Δx is decided by relaxation time or parameters. The relaxation time is related to both the time unit and the kinematic viscosity of the fluid for a single-relaxation method,

\[ \nu = \frac{c_s^2}{\nu'} \left( \tau - \frac{\delta t}{2} \right). \]  

Typically, the kinematic viscosity and velocity of the fluid are known, while the relaxation time is either \( \tau = 1 \) or tuned to a desired value to minimize second-order error. Therefore, a dimensional form of Eq. 4.27 is used to derive the dimensional time unit,

\[ \Delta t = \frac{(\Delta x)^2}{c_s^2 \nu'} \left( \tau - \frac{\delta t}{2} \right), \]  

where \( c_s = 1/\sqrt{3} \) in D2Q9 and D3Q27 lattice stencils. Using an example, if the dimensional spatial unit \( \Delta x = 26.5 \) nm, and the kinematic viscosity of water is \( \nu' = 1.0034 \times 10^{-6} \) m²/s, the corresponding time unit is approximately \( \Delta t = 1.05 \) ns. The bulk viscosity can be similarly defined to represent a physical fluid with increased stability for the multi-relaxation approach described in section 4.2.5.
4.3 Algorithm

Fig. 4.5 shows a schematic of the combined electrodynamic and kinetic lattice-Boltzmann method. While both the electrodynamic and kinetic sub-systems have an identical spatial unit, $\Delta x$, the electrodynamic sub-system has a negligible time unit compared with the kinetic sub-system, $\Delta t_e \ll \Delta t_k$, allowing a time-averaged kinetic force density to be computed. The time-averaged kinetic force density is imported into the kinetic sub-system, provided its dimensionless conversion. Perturbation of the fluid is allowed to occur until an appreciable deformation of the median fluid density by $\Delta x$, which is checked by the “shape change” condition in the kinetic sub-system. If “shape change” is “True”, then the electrodynamic sub-system is re-initialized, and the time-averaged force density is recomputed and re-applied to the kinetic sub-system to complete one algorithm cycle. The algorithm simulates the continuous deformation of a fluid subjected to a steady and continuous time-harmonic Gaussian beam. Time-averaged force densities existing in free space, which exist as an error of a finite time average in either the YL-FDTDM or ELBM, are set to zero to prevent numerical instability in the vapour phase.

![Diagram](image_url)

Figure 4.5: Multi-physics simulation algorithm for the combined interaction of an (a) electrodynamic sub-system, and (b) kinetic sub-system. In between the two sub-systems is the transfer of a time-averaged kinetic force density from the electrodynamic sub-system to the kinetic sub-system, given that $\Delta t_e \ll \Delta t_k$. 

72
Chapter 5

Two- and three-dimensional optical acceleration and deformation of multi-phase fluids

Numerical simulations have demonstrated that multiple electrodynamic formalisms predict identical rigid-body kinematics [7, 8]. However, such conclusions have not held for fluidic or viscoelastic media [7, 8, 23, 28, 114]. One significant difference established by the YL-FDTDM with front-tracking is that the Chu and Amperian/Lorentz formalisms predict concave fluid-fluid interface deformation from a p-polarized beam [7, 8]. Concave interface deformation was predicted by the Chu and Amperian/Lorentz formalisms regardless of surface tension. For example, similar interface deformations were predicted for illuminated air-water or toluene-water interfaces, even though their surface tensions differ by four orders of magnitude [7, 8]. Previous studies which investigated multiple electrodynamic formalisms predictions of optical radiation pressure on macroscopic fluids, which used either finite-element or front-tracking methods, omitted a study of the fluid’s momentum conservation [7, 28]. These studies were further restricted to conditions of axial symmetry in three dimensions [28], or the condition of low density ratio in two dimensions [7]. This chapter uses an alternative approach, the lattice-Boltzmann method, to represent the deformation of generic multiphase fluid-fluid interfaces subjected to optical radiation pressure in both two and three dimensions [36, 38]. Specifically, this chapter investigates the interaction between the electrodynamic lattice-Boltzmann method (ELBM) described in Chapter 3 and the pseudopotential lattice-Boltzmann method (PLBM) described in Chapter 4 according to the algorithm illustrated in Fig. 4.5. Multiphysics simulations are performed in two-dimensional and three-dimensional spatial configurations representative of the optical acceleration and trapping of microscopic quasi-stationary
5.1. Two-dimensional simulation

multi-phase fluid interfaces and droplets. This chapter demonstrates that, in support of theoretical arguments [115], there is identical interface deformation of dielectric fluids predicted by multiple electrodynamic formalisms in the rest frame. However, these formalisms fall within separate classes as discussed in Chapter 2, each class having a unique formulation of Maxwell’s equations [5, 7, 16, 20, 27, 115, 116]. If the classes are treated equivalently using the same multi-physics continuity equations [115], each class may predict distinct deformation of a dielectric fluid.

5.1 Two-dimensional simulation

In this section, two-dimensional deformation and optical acceleration from focused s- and p-polarized Hermite-Gaussian beams is investigated for the cases of both a flat liquid-vapour interface and a circular liquid-vapour interface.

5.1.1 Methodology

The multi-phase fluid is representative of water at 70 °C, with a liquid phase of dimensional mass density \( \rho'_{\text{liq.}} = 977 \text{ kg/m}^3 \) and kinematic viscosity \( \nu' = 1.0034 \times 10^{-6} \text{ m}^2/\text{s} \), but with a different surface tension which cannot be explicitly represented in the Guo or Shan & Chen forcing schemes. Each continuous-wave time-harmonic Gaussian beam is initialized with an optical wavelength of \( \lambda_0 = 530 \text{ nm} \), a vertical (\( \hat{y} \)) direction of propagation, and is focused to a beam-waist of \( w_0 = \lambda_0 \) at the center of the simulation domain. Refer to Chapter 3 “Initial condition” for a complete description of the Hermite-Gaussian beam profile. Two-dimensional simulation is sufficient for analyzing deformation along a single plane of incidence from either an s- or p-polarized Gaussian beam that propagates in the \( \hat{y} \) direction with its beam axis intersecting \( (x_0, y_0) \). While the choice of the electrodynamic lattice-Boltzmann method is invariant of the quasi-stationary multi-phase fluid investigated, the pseudopotential lattice-Boltzmann method must be adapted to satisfy constraints of stability, thermodynamic consistency, and numerical accuracy of a particular fluid system. Therefore, a different adaptation of the PLBM is described for each fluid simulation.
5.1. Two-dimensional simulation

The flat liquid-vapour interface, which is modeled using a single relaxation (SRT) PLBM with a multi-range lattice (D2Q92), is used to examine the incompressible and weakly compressible deformation of dielectric liquid with an optical index of water (\(N = 1.333\)) predicted by multiple electrodynamic formalisms. The flat liquid-vapour interface is initialized at \(y = 0\) nm in a spatial domain with a horizontal dimension \(x \in (-2120, 2120)\) nm and a vertical dimension \(y \in (-1060, 1060)\) nm. The dimensionless Shan-Chen surface tension of the liquid-vapour interface is measured as \(\gamma_{SC} = 0.235\) with determination coefficient \(\mathbb{R}^2 = 0.9647\). Non-equilibrium bounce-back (NEBB) boundary conditions are initialized along each of the walls (West, North, East, and South) in the spatial domain. Fig. 5.1 illustrates the simulation configuration representing a two-dimensional flat liquid-vapour interface.

**Figure 5.1:** [Color online] The configuration used in a two-dimensional simulation of optical radiation pressure on a flat interface. The dimensions of the simulation domain are \(8\lambda_0 \times 4\lambda_0\), bordered by a black line representing the non-equilibrium bounce-back (NEBB) boundaries. Black arrows from the boundary represent the reflection of particle populations. The thin gray line represents the interface, while the gray region represents the dielectric fluid. The white region is free space. The green dashed line is the source condition, which is a Hermite-Gaussian beam with a curvature represented by the thin dashed black lines, and a beam waist of \(w_0 = \lambda_0\) (not to scale) centred at the position \((0,0)\).
5.1. Two-dimensional simulation

The circular liquid-vapour interface, which is modeled using a multi relaxation (MRT) PLBM with a nearest-neighbour lattice (D2Q9), is used to examine weakly compressible optical deformation of a dielectric or magnetic droplet with an optical index of water ($n = 1.333$) predicted by multiple electrodynamic formalisms. Unlike the SRT PLBM, the MRT PLBM can be tuned for stability and thermodynamic consistency to model either droplets or bubbles of the same diameter with a liquid-vapor density ratio exceeding 1000 ($\rho_{\text{liq}}/\rho_{\text{vap.}} > 1000$) using the stability adjustment parameter $\sigma_\gamma = 0.195$. The circular liquid-vapour interface representing a “droplet” with a diameter of, $D = 1.5\lambda_0$, ($\lambda_0 = 530 \text{ nm}$) and refractive index $n = 1.333$ is centred in the $xy$-plane ($x_0, y_0) = (0, 0)$. Fig. 5.2 illustrates the simulation configuration representing a two-dimensional circular liquid-vapour interface.

Figure 5.2: [Color online] The configuration used in a two-dimensional simulation of optical radiation pressure on a circular interface (cylindrical cross-section). The size of the spatial domain is $4\lambda_0 \times 4\lambda_0$ and bordered by a black line representing periodic boundaries. Black arrows at the boundaries represent propagation of particle populations through the boundaries. The gray region represents the dielectric or magnetic fluid which has a diameter $D = 1.5\lambda_0$, and properties listed in the bottom right-hand corner. The white region is free space, with properties listed in the top right-hand corner. The green dashed line represents the position of the source, which is a Hermite-Gaussian beam with a curvature represented by the thin dashed black lines and a beam waist of $w_0 = \lambda_0$ (not illustrated to scale).
5.1. Two-dimensional simulation

5.1.2 Flat liquid-vapor interface

**Incompressible deformation** and flow occurs for a Mach number less than 0.1 (Ma < 0.1), as a figure of merit in kinetic lattice-Boltzmann simulations. Fig. 5.3(a) shows the deformation of an incompressible (Ma < 0.1) dielectric liquid (εr = 1.779) being subjected to optical radiation pressure from a p-polarized Hermite-Gaussian beam. The simulations were run up to 370 ns to represent the transient state of the liquid prior to its steady state, after which the liquid-vapour interface stabilizes within the Hermite-Gaussian beam and no longer exhibits steady deformation (but small periodic oscillations). The Abraham (AB), Minkowski (MN), Einstein & Laub (EL), and Helmholtz (HLM) electrodynamic formalisms predict an identical convex (outward) liquid-vapour interface deformation representative of a positive pressure. The Chu and Amperian/Lorentz (AMP/CHU) electrodynamic formalisms are identical in a dielectric, and predict the opposite case: a concave (downward) liquid-vapour interface deformation representative of a negative pressure. Chu and Amperian/Lorentz predictions of a concave interface deformation are consistent with Refs. [7, 8], which are the only distinction between electrodynamic formalisms predictions of time-harmonic time-averaged optical radiation pressure on a dielectric in two dimensions. Fig. 5.3(b) shows the maximum deformation over time, which is distinct between the cases of convex and concave deformation.

![Figure 5.3](https://example.com/figure5.3.png)

**Figure 5.3:** [Color online] Dielectric liquid-vapor (εr = ϵr and μr = 1) interface deformation simulated using PLBM given p-polarized incident radiation with peak intensity $E_0 = 0.875$ GV/m. The CHU/AMP formalisms are identical and opposite of the remaining formalisms, which are degenerate.
5.1. Two-dimensional simulation

Weakly compressible deformation and flow occurs for a Mach number in the range of $\text{Ma} \in (0.1, 0.3)$. Given weak compressibility, variations in mass density cause a medium to become inhomogeneous. In this study, the difference in mass density of the liquid phase from the vapor phase is linearly mapped to the difference in the relative permittivity of water from free space. Therefore, spatial variations in mass density of the liquid phase cause proportional spatial variations in dielectric permittivity. However, mass density and dielectric permittivity are uncorrelated at optical frequencies [117]. Their relation is described as electrostriction, which is a theoretical contribution to the deformation of the fluid nanoseconds after its illumination [27, 28]. Otherwise, electrostriction has balanced surface and volume contributions at optical frequencies [118]. Spatial variations in mass density and dielectric permittivity are similar to the spatial variation of the bulk force density, which predicts increased fluid deformation compared with a surface force density. Therefore, assuming dielectric permittivity is linearly proportional to mass density may lead to discrepancies in fluid deformation predicted by different electrodynamic formalisms. However, so can the assumption that dielectric permittivity remains homogeneous with variation in mass density. Although the source of differences in deformation predicted by bulk force density and surface force density requires further investigation, they may restrict the accuracy of the simulation method to the incompressible Mach flow regime ($\text{Ma} < 0.1$).

![Figure 5.4: Dielectric liquid-vapor ($\epsilon_r = k^2$ and $\mu_r = 1$) interface deformation simulated using the PLBM, given s-polarized incident radiation with peak intensity $E_0 = 1.125$ GV/m. Weak compressibility leads to differences in deformation predicted by the EL/HLM/CHU/AMP formalisms and by the MN/AB formalisms.](image-url)
5.1.3 Circular liquid-vapour interface

Fig. 5.5(a) shows the deformation of a two-dimensional weakly compressible (Ma < 0.3) dielectric droplet (\(\epsilon_r = 1.779\)), represented as a cylindrical cross section (or circular interface), subjected to a p-polarized Gaussian beam with a peak electric field intensity of \(E_0 = 0.98\) GV/m. The AB, MN, EL, and HLM electrodynamic formalisms predict similar elongation of the droplet longitudinal to the direction of propagation. CHU and AMP formalisms predict identical elongation of the droplet lateral to the direction of propagation. Fig. 5.5(b) shows the deformation of an identical two-dimensional incompressible dielectric droplet subjected to an s-polarized Gaussian beam with a peak electric field intensity of \(E_0 = 0.98\) GV/m. Each electrodynamic formalism predicts similar elongation of the droplet longitudinal to the direction of propagation.

![Diagram](image)

(a) p, \(\epsilon_r = \kappa^2, \mu_r = 1\)  
(b) s, \(\epsilon_r = \kappa^2, \mu_r = 1\)

Figure 5.5: [Color online] Dielectric droplet deformation simulated using PLBM. Given an s-polarized Hermite-Gaussian beam, each formalism predicts similar interface deformation after \(t = 157.5\) ns [t=150]. “REF” refers to the droplet’s initial shape.
5.1. Two-dimensional simulation

Fig. 5.6(a) shows the deformation of a two-dimensional weakly compressible (Ma < 0.3) magnetic droplet ($\mu_r = 1.779$), represented as a cylindrical cross section (or circular interface), subjected to an s-polarized Gaussian beam with a peak electric field intensity of $E_0 = 0.98 \text{ GV/m}$. While the AB, MN, EL, HLM and AMP electrodynamic formalisms predict similar elongation longitudinal to the direction of propagation, the CHU formalism predicts elongation lateral to the direction of propagation. Fig. 5.6(b) shows the deformation of an identical two-dimensional incompressible magnetic droplet subjected to a p-polarized Gaussian beam with a peak electric field intensity of $E_0 = 0.98 \text{ GV/m}$. Most electrodynamic formalisms predict similar elongation of the droplet longitudinal to the direction of propagation, except for the AMP formalism.

(a) s, $\epsilon_r = 1, \mu_r = N^2$

(b) p, $\epsilon_r = 1, \mu_r = N^2$

Figure 5.6: [Color online] Magnetic droplet deformation simulated using PLBM after $t = 157.5 \text{ ns}$ [t=150]. “REF” refers to the droplet’s initial shape.

5.1.4 Conclusion

In either the case of a flat interface or a circular interface, similar deformation of the fluid is predicted by multiple electrodynamic formalisms despite varying the lattice stencil range, the kinetic collision operator, the geometry of the fluid, the geometry of the simulation domain, and the boundary conditions utilized in the PLBM. Therefore, the simulations in this section represent the generic behaviour of dielectric or magnetic liquids with an optical index of water ($N = 1.333$) when subjected to optical radiation pressure from either s- or p-polarized Hermite-Gaussian beams.
5.2 Three-dimensional simulation

In two dimensions the Chu and Amperian/Lorentz electrodynamic formalisms predict a concave interface deflection from p-polarized optical radiation pressure, and a convex interface deflection from s-polarized optical radiation pressure. It is therefore necessary to simulate Chu’s formalism in three dimensions to properly analyze its polarization-dependent predictions of interface deformation. Three-dimensional simulation is also necessary for representing elliptically polarized Gaussian beams, for which linearly-polarized and circularly-polarized Gaussian beams are but a special case. Linearly-polarized Gaussian beams in three dimensions also exhibit cross-polarization, or the existence of electric field components orthogonal to the nominal polarization of the Gaussian beam [79]. Therefore, a three-dimensional simulation can represent both s- and p-polarized electric fields depending on an analyzed plane of incidence. Although the cross-polarized components of an electric field have less intensity, they are still present, necessary to satisfy Maxwell’s equations, and can contribute to material deformation. Therefore, three-dimensional simulations of optical radiation pressure are recommended for their consistency with experiment.

5.2.1 Methodology

ELBM and PLBM are simpler to implement in three dimensions than the YL-FDTDM and front-tracking, even with adaptations for surface tension and viscosity [92, 93]. The only difference between a two-dimensional and three-dimensional case for the ELBM and PLBM are the collision operator and the lattice vector set. Therefore, the deformation of spherical dielectric droplets from both linearly-polarized and circularly-polarized Gaussian beams are analyzed in three dimensions.

The spherical liquid-vapour interface, which is modeled using an SRT PLBM with a Shan-Chen forcing scheme, is used to predict the deformation of a “droplet” of refractive index $n = 1.333$ and diameter $D = 1.5\lambda_0$ subjected to optical radiation pressure from linearly-polarized and circularly-polarized Gaussian beams. Its spherical shape represents the most stable geometry for a microscopic liquid-vapour interface. When initialized in the center of the simulation domain, it can also be acted on by optical forces in all directions while avoiding kinetic interactions with the boundaries, which represent an external system. In each three-dimensional simulation, the liquid phase of the droplet is representative of water at 70 °C, and
5.2. Three-dimensional simulation

has a dimensional mass density \( \rho_{\text{liq.}}' = 977 \, \text{kg/m}^3 \) and kinematic viscosity \( \nu' = 1.0034 \times 10^{-6} \, \text{m}^2/\text{s} \). However, the surface tension is distinct from water: the dimensionless Shan-Chen surface tension was measured as \( \gamma_{\text{SC}} = 0.235 \) with determination coefficient \( R^2 = 0.9647 \). Fig. 5.7 shows an illustration of the three-dimensional simulation configuration.

Figure 5.7: [Color online] The configuration used in a three-dimensional simulation of optical radiation pressure on a spherical interface. The dimensions of the simulation domain are \( 4\lambda_0 \times 4\lambda_0 \times 4\lambda_0 \), bordered by a black line representing periodic boundary conditions (PBCs). The gray region represents the dielectric sphere, which has a diameter of \( D = 1.5\lambda_0 \) and a permittivity of \( \epsilon_r = 1.779 \). The white region is free space. The green dashed line is the source condition, which is a Hermite-Gaussian beam with a curvature represented by the thin dashed black lines, and a beam waist of \( w_0 = \lambda_0 \) (not to scale) centred at the position \((0,0,0)\).
5.2. Three-dimensional simulation

5.2.2 The linearly-polarized Hermite-Gaussian beam

The linearly-polarized Hermite-Gaussian beam is polarized in the \( \hat{x} \) direction, and propagates in the \( \hat{z} \) direction, causing a deformation of the spherical droplet which is predicted by multiple electrodynamic formalisms in Fig. 5.8. The electrodynamic formalisms can be divided into three classes depending on the deformation of the droplet, which is dictated by material parameters and their description within the momentum flux density tensor:

1. The AB and MN electrodynamic formalisms predict identical deformation, since time-averaged time-variation of the time-harmonic momentum density is zero. These two formalisms predict that the droplet deforms from a spherical shape to a smooth ellipsoid with a major axis aligned to the direction of propagation.

2. The EL and HLM electrodynamic formalisms predict identical deformation, since the medium is an isotropic dielectric. Similar to the AB/MN class, the EL/HLM class predicts that the droplet deforms from a sphere to an ellipsoid with a major axis aligned to the direction of propagation. However, the EL/HLM class predict time-averaged force density distributed throughout the dielectric, causing smaller spatially periodic ripples in the interface which are not predicted by the AB/MN class. This maybe an effect of electrostriction at the micro-scale.

3. The CHU and AMP electrodynamic formalisms predict identical ellipsoidal elongation of the droplet in the \( \hat{y} \) direction, which is transverse to the direction of propagation. The transverse fluid deformation was similarly predicted by Mansuripur, who suggested that a dielectric medium would form a “pancake” in his analysis of the Lorentz/Amperian time-averaged force density distribution [16].

Each class of electrodynamic formalism predicts that the droplet’s center of mass accelerates in the direction of propagation, with a distinct dimensionless momentum transfer on the order of \( 10^2 \) (Fig. 5.11). Each electrodynamic formalism also predicts zero dimensionless momentum transfer in lateral directions (\( 10^{-14} \)), validating the symmetry, isotropy, and momentum conservation of the simulation.
5.2. Three-dimensional simulation

Figure 5.8: Three-dimensional deformation of an incompressible spherical droplet from an $\hat{x}$-polarized Gaussian beam with a peak electric field intensity of $E_0 = 0.98$ GV/m (power $P_0 = 568$ W). The dimensional kinematic viscosity is $\nu' = 1.0034 \times 10^{-6}$ m$^2$/s, and the isosurface is plotted at dimensional time $t' = 157.5$ ns [$t = 150$] after the beam is turned on.
5.2. Three-dimensional simulation

5.2.3 The circularly-polarized Hermite-Gaussian beam

The circularly-polarized Hermite-Gaussian beam propagates in the \( \hat{z} \) direction, with a rotating transverse electric field vector, causing a deformation of the spherical droplet which is predicted by multiple electrodynamic formalisms in Fig. 5.9. The electrodynamic formalisms can be divided into three classes depending on the deformation of the droplet, which is dictated by material parameters and their description within the momentum flux density tensor:

1. The AB and MN electrodynamic formalism predict that the droplet deforms from a spherical shape to a smooth ellipsoid shape similar to the smooth ellipsoid caused by a linearly-polarized Hermite-Gaussian beam.

2. The EL and HLM electrodynamic formalisms predict that the droplet deforms from a spherical shape to a rippled ellipsoid shape similar to the rippled ellipsoid shape caused by a linearly-polarized Hermite-Gaussian beam.

3. The CHU and AMP electrodynamic formalisms identically predict an ellipsoidal elongation in the \( \hat{z} \) direction, which is the direction of propagation. Deformation in the direction of propagation is distinct from the CHU/AMP prediction of the droplet’s deformation from a linearly polarized Hermite-Gaussian beam. The electric-field polarization dependent deformation predicted by CHU and AMP formalisms results in polarization dependent momentum transfer to the kinetic sub-system over time. Given a circularly polarized Hermite-Gaussian beam, the CHU/AMP formalisms also predict significantly less deformation along the direction of propagation, \( \hat{z} \), compared with alternative electrodynamic formalisms. Polarization-dependent fluid deformation has yet to be observed in experiment.

Each class of electrodynamic formalism predicts that the droplet’s center of mass accelerates in the direction of propagation, with a distinct dimensionless momentum transfer on the order of \( 10^2 \) (Fig. 5.11). Each electrodynamic formalism also predicts zero momentum transfer in lateral directions \( (10^{-14}) \), validating the symmetry, isotropy, and momentum conservation of the simulation.
5.2. Three-dimensional simulation

Figure 5.9: Three-dimensional deformation of an incompressible spherical droplet from a circularly-polarized Gaussian beam with a peak electric field intensity of $E_0 = 0.98 \text{ GV/m}$ (power $P_0 = 568 \text{ W}$). The dimensional kinematic viscosity is $\nu' = 1.0034 \times 10^{-6} \text{ m}^2/\text{s}$, and the isosurface is plotted at dimensional time $t' = 157.5 \text{ ns}$ [$t = 150$] after the beam is turned on.
5.2. Three-dimensional simulation

5.2.4 Kinetic momentum transfer and electric field polarization

Due to their unique predictions of droplet deformation, each class of formalisms predicts a unique net dimensionless kinetic momentum along the longitudinal \( \hat{z} \) direction (\( p_{k,z} = \sum G_{k,z} \delta x^3 \)), and zero transfer of kinetic momentum in lateral directions \( \hat{x} \) or \( \hat{y} \), as illustrated in Figs. 5.10-5.11. The lateral kinetic momentum, \( p_{k,x} = \sum G_{k,x} \delta x^3 \) and \( p_{k,y} = \sum G_{k,y} \delta x^3 \), is theoretically zero. The numerical value of each lateral component illustrated in Figs. 5.10-5.11 is negligible \( (10^{-14}) \) relative to the dimensionless kinetic momentum in the direction of propagation, \( p_{k,z} \). While most formalisms predict the same momentum transfer independent of the electric field polarization (Fig. 5.11), the Chu and Amperian/Lorentz formalisms predict a momentum transfer that is dependent on the electric field polarization, as illustrated in Fig. 5.10.

![Figure 5.10: The CHU/AMP formalisms momentum transfer for an (a) linearly-polarized Gaussian beam, and (b) a circularly-polarized Gaussian beam. Each case predicts a distinct momentum transfer from the distinct shape of the droplet (\( p_{k,z,\text{lin.}} = 220 \) while \( p_{k,z,\text{circ.}} = 200 \) at \( t = 150 \)). Therefore, the Chu and Amperian/Lorentz formalisms are the only electric field polarization-dependent formalisms. There is no momentum transferred orthogonal to the direction of propagation, due to symmetry. Error is on the order of \( 10^{-14} \), and blue overlaps red.](image-url)
5.2. Three-dimensional simulation

Figure 5.11: Dimensionless kinetic momentum from [left] a linearly-polarized electric field and [right] a circularly-polarized electric field. AB, MN, EL, MN formalisms predict *polarization independent* longitudinal momentum. Transverse momentum is on the order of $10^{-14}$, and blue overlaps red.
5.2. Conclusion

Figs. 5.8 and 5.9 plot the deformation of a spherical droplet subjected to linearly-polarized and circularly-polarized Gaussian beams, respectively. Time-averaged force density causes most formalisms to predict that the droplet deforms along the direction of propagation, independent of electric-field polarization. The similar deformation predicted by the AB, MN, EL and HLM electrodynamic formalisms is illustrated by the paraboloid shape of the droplet after $t = 150$ lattice time units. However, the Chu and Amperean/Lorentz (CHU/AMP) formalisms can predict transverse polarization-dependent deformation instead. In each plot, the colorbar axis shows that the Mach number is below 0.3 ($Ma < 0.3$), such that the fluid remains incompressible. However, weak compressibility can still occur at this Mach number in lattice-Boltzmann simulations. The Helmholtz (HLM) and Einstein & Laub (EL) formalisms predict greater deformation of the droplet than Abraham (AB) and Minkowski (MN) formalisms. Regardless, momentum is conserved in each numerical simulation with a dimensionless error on the order of magnitude of $10^{-14}$, while the dimensionless net momentum transferred from the electrodynamic to kinetic sub-system is on the order of magnitude of $10^2$. 

5.2. Three-dimensional simulation
Chapter 6

Conclusion

Simulations attempting to isolate a single electrodynamic formalism benefit from alternative lattice-Boltzmann numerical methods which offer simpler implementation, potential increases in accuracy and precision, and decreased computational time for representing unsteady incompressible flow in two and three dimensions. Previous simulations of light-matter interactions investigated in either two or three dimensions were limited to either a low density ratio [7, 8], or linear approximations of a pressure at the interface [28]. In this thesis, Hauser & Verhey’s electrodynamic lattice Boltzmann method is integrated with both Shan & Chen single-relaxation time and Yu & Fan multi-relaxation-time pseudopotential lattice-Boltzmann methods to model the acceleration of generic two- and three-dimensional multi-phase fluids subjected to optical radiation pressure [39, 91, 93, 94]. When compared with the Yee-lattice finite-difference time-domain method, the electrodynamic lattice-Boltzmann method evaluates a time-averaged kinetic force density with greater accuracy in a decreased computational time. Single-component multi-phase fluids analyzed using the pseudopotential lattice-Boltzmann method achieve high density ratio and momentum conservation in two and three dimensions, while enabling the analysis of light-matter interactions at the mesoscopic scale. The sub-system interaction is in agreement with previous studies and conclusions regarding optical radiation pressure in either two or three dimensions [7, 8, 16, 38]. Simulation results can be scaled as necessary to represent experiments at characteristic lengths where the Navier-Stokes equation remains valid, and conditions for numerical stability and low Mach number are maintained. Additional modifications have also been suggested throughout this thesis for representing relativistic hydrodynamics or higher Mach number and Reynolds number flows. The methodology presented in this thesis shows that multiple electrodynamic formalisms can predict identical fluid-fluid interface deformation. However, this thesis finds that multiple electrodynamic formalisms predict distinct deformation of linear dielectric media, deformations that are in qualitative agreement with former studies and conclusions [7, 8, 16]. Therefore, this thesis satisfies the following objectives:
Chapter 6. Conclusion

1. Implement an alternative numerical approach for evaluating electrodynamic force density in uniform isotropic media that improves on former approaches.

2. Implement a multi-physics simulation of optical radiation pressure acting on unsteady mesoscopic multi-phase fluids in two and three dimensions.

3. Use the multi-physics simulation of optical radiation pressure to investigate two and three-dimensional systems capable of representing similarities or differences between electrodynamic formalism predictions in the near-rest (quasi-stationary) frame of reference.

Suitable numerical approaches in the literature were investigated, and the satisfaction of the former objectives lead to the following conclusions:

1. Lattice-Boltzmann methods, which consider particle population densities as opposed to phenomenological fields, are more accurate and simpler to implement for solving electromagnetic force density in two and three dimensions. Such methods have the same implementation regardless of the number of dimensions, and are devoid of lattice asymmetries or numerical dispersion in free space. At the same space and time resolution, the electrodynamic lattice-Boltzmann method is 11 to 35 times more accurate and 4 to 8 times faster than the Yee-lattice finite-difference time-domain method for evaluating a time-averaged kinetic force density.

2. The same lattice-Boltzmann algorithm can be applied to represent kinetic, electrodynamic and thermodynamic sub-systems by changing the collision operation, lattice stencil, equilibrium condition and interacting forces. It’s adaptability, portability and parallel operations are convenient for multi-physics simulation.

3. Lattice-Boltzmann methods provide similar predictions to former methodology, but their stability enables the simulation of greater density-ratio mesoscopic fluids with natural interface break-up, vaporization and coalescence.

4. Given a linearly-polarized Hermite-Gaussian beam transmitted through a quasi-stationary incompressible droplet, each electrodynamic formalism (besides the Chu and Amperian/Lorentz formalisms) predict that a spherical droplet suspended in its own vapor will form into a...
Chapter 6. Conclusion

paraboloid with its major axis oriented along the direction of propagation. Given a circularly-polarized Gaussian beam transmitted through a quasi-stationary incompressible droplet, each of the formalisms (including the Chu and Amperian/Lorentz formalisms) predict the formation of this paraboloid.

5. The Minkowski and Abraham formalisms predict time-averaged surface force densities that cause identical quasi-stationary isotropic magnetodielectric fluid interface deformation from time-harmonic electromagnetic waves. There is no difference in the time-averaged forces and fluid deformation occurring from the Abraham or Minkowski momentum density.

6. The Helmholtz and Einstein & Laub electrodynamic formalisms predict time-averaged bulk force densities that cause identical quasi-stationary isotropic magnetodielectric fluid interface deformation. Their prediction is distinct from the Abraham and Minkowski electrodynamic formalisms.

7. The Chu and Amperian/Lorentz formalisms predict identical force density in a dielectric medium, but distinct force density in a magnetic medium.

8. The Chu and Amperian/Lorentz electrodynamic formalisms predict that the deformation of a quasi-stationary isotropic magnetodielectric fluid interface depends on the polarization of the incident electric field, while alternative electrodynamic formalisms do not. Consequently, the Chu and Amperian/Lorentz electrodynamic formalisms also predict a polarization-dependent momentum transfer in a dielectric fluid over time.

9. Electrodynamic formalisms can be classified according to their interaction with a deformable medium. The cause of the distinct deformations predicted by each class of formalism may be attributed to the distinct formulation of Maxwell’s equations from which they are derived. Differences in the description of fields internal to a medium will require further investigation.

Besides Chu’s formalism, most other electrodynamic formalisms provide degenerate predictions of liquid-vapor interface deformation that are largely independent of the electric field polarization. Differences between the formalisms in each class may only exist in cases of compressible fluids and
6.1. Recommendations

with their photothermal expansion [23, 28, 53]. Developing a mesoscopic thermodynamic sub-system was beyond the scope of this thesis, which only considers the case of an isothermal fluid. Therefore, thermodynamic or photoacoustic effects were not investigated, but are recommended for future study.

The systems described in this thesis are also non-dimensional, such that they do not represent particular fluid-fluid optical radiation pressure experiments, and they may use fluid properties and dimensions that are difficult to realize in experiment. However, the method’s dimensionless nature may be scaled to a fluid system of arbitrary size when provided with the necessary computational resources.

6.1 Recommendations

In future studies, the incorporation of the thermodynamic sub-system and dimensional parameters would be useful for investigating experiments or applications of optical radiation pressure on general lossy multiphase and multi-component fluid systems. If performed as an academic research study, the scope of the development of this method for a particular experiment is recommended at the doctorate or post-doctorate level, preferably for a multi-disciplinary research group with independent members developing the independent systems based on their disciplines. Significant computational power may also be required to represent the electrodynamic sub-system for optically large simulation domains, but the resources necessary will depend on the system. The necessary computational resources require further investigation.
Bibliography


[8] Maximilien Bethune-waddell. *Simulations of Radiation Pressure Experiments*. Text, University of British Columbia, 2016. → pages 1, 2, 3, 5, 8, 9, 14, 15, 31, 33, 36, 38, 54, 55, 73, 77, 90


Bibliography

*Molecular, and Optical Physics*, 86(2), 2012. ISSN 10941622. doi: 10.1103/PhysRevA.86.025801. → pages 54


[42] R Robert Nourgaliev, Truc-Nam Dinh, Theo G Theofanous, and D Joseph. The lattice boltzmann equation method: theoretical inter-


[59] B. U. Felderhof. Relativistic hydrodynamics of magnetic and dielectric fluids in interaction with the electromagnetic field. *Journal


Bibliography


[104] Sami Ammar, Guillaume Pernaudat, and Jean-Yves Trépanier. A multiphase three-dimensional multi-relaxation time (mrt) lattice boltzmann model with surface tension adjustment. *Journal of Compu-


Appendix A

Analytical methods

In this thesis, a variety of mathematical operations and analytical approaches are used, including matrix operations, Taylor series expansion, and Chapman-Enskog analysis. Special functions such as Hermite-polynomials and/or Lyapunov functions are required to derive general equations or verify the stability of numerical models. This section briefly reviews the mathematical operations and analytical methods used in this thesis.

A.1 Coordinate systems

This thesis uses a Cartesian coordinate system with absolute space and time which are invariant with respect to one another. The coordinate system is also at rest. While the position vector, \( x \), depends on the origin’s location, \((x_0, y_0, z_0)\), the displacement vector, \( r \), does not. Fig. A.1 shows an illustration of position and displacement vectors.

**Position vector**

\[
x = \{x_1 \hat{x}_1 + x_2 \hat{x}_2 + x_3 \hat{x}_3\} \\
= \{x \hat{x} + y \hat{y} + z \hat{z}\}.
\]  

(A.1)

**Displacement vector**

\[
r = (x - x_0) \hat{x} + (y - y_0) \hat{y} + (z - z_0) \hat{z}.
\]  

(A.2)
A.2 Matrix operations

Matrix operations used in this thesis include the divergence, the dyadic product, and the scalar product. Special matrices include the Kronecker-Delta or unit matrix, and the Levi-Civita matrix.

Matrices can be used to describe a set of scalar components or orthogonal vectors in a multi-dimensional space. They may or may not describe physical quantities, being only a method for organizing and performing operations with sequences of numbers.

Tensors are multi-dimensional matrices describing a linear relationship between physical variables related to a vector space. Tensors are required to describe a state of stress at a point in two or three dimensions. Tensor elements can be represented with dimensional index $\alpha$ for a row, and dimensional index $\beta$ for a column. Written in matrix form, a three-dimensional tensor is

\[
T_{\alpha\beta} \in T, \quad \begin{bmatrix} T & T_{12} & T_{13} \\ T_{2} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}.
\]
A.2. Matrix operations

**Divergence** represents the outward flux of a vector or a tensor at a given point. In the case of a vector, the divergence is a scalar function,

\[ \nabla \cdot \mathbf{T} = \frac{\partial}{\partial x_1} T_1 + \frac{\partial}{\partial x_2} T_2 + \frac{\partial}{\partial x_3} T_3. \quad (A.4) \]

The divergence of a tensor is a vector that has both magnitude and direction,

\[ \nabla \cdot \mathbf{T} = \frac{\partial}{\partial x_\alpha} T_{\alpha\beta} \hat{x}_\alpha = \begin{bmatrix} \frac{\partial}{\partial x_1} T_{11} + \frac{\partial}{\partial x_2} T_{12} + \frac{\partial}{\partial x_3} T_{13} \\ \frac{\partial}{\partial x_1} T_{21} + \frac{\partial}{\partial x_2} T_{22} + \frac{\partial}{\partial x_3} T_{23} \\ \frac{\partial}{\partial x_1} T_{31} + \frac{\partial}{\partial x_2} T_{32} + \frac{\partial}{\partial x_3} T_{33} \end{bmatrix}, \quad (A.5) \]

where \( \hat{x}_\alpha \) represents a unit vector, pointed in the direction of an increasing dimension \( x_\alpha \). In this thesis, \( x_1 = x, \ x_2 = y, \) and \( x_3 = z \). The divergence of a tensor is necessary to describe the kinetic force density from optical radiation pressure.

**Dyadic products** of two equal-size tensors represent their outer product,

\[ \mathbf{T}^2 = \mathbf{T} \mathbf{T} = \mathbf{T} \cdot \mathbf{T} = [\mathbf{T}]^\intercal [\mathbf{T}], \quad (A.6) \]

where \( ^\intercal \) represents a transpose operation, that swaps columns and rows of a tensor. The same operation can be applied to equal-size vectors or matrices.

**Scalar products** of two equal-size tensors represent their inner product,

\[ \mathbf{T} \cdot \mathbf{T} = [\mathbf{T}]^\intercal [\mathbf{T}], \quad (A.7) \]

where \( ^\intercal \) represents a transpose operation, that swaps the columns and rows of a tensor. The same operation can be applied to equal-size vectors or matrices.

**The Kronecker-Delta** or unit matrix can be represented as a square diagonal matrix with each diagonal element equal to one,

\[ \delta_{\alpha\beta} = \begin{cases} 1, & \alpha = \beta, \\ 0, & \alpha \neq \beta, \end{cases} \quad [\mathbf{I}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (A.8) \]

The unity matrix may also be referred to as the identity matrix.
A.3. Polynomials and functions

The Levi-Civita matrix maps elements representing the sign for the permutation of dimensional indices, such that they have total antisymmetry. Given two dimensional indices, $\alpha$ and $\beta$,

$$\varepsilon_{\alpha\beta} = \begin{cases} +1, & \{\alpha, \beta\} = \{1, 2\}, \\ -1, & \{\alpha, \beta\} = \{2, 1\}, \\ 0, & \alpha = \beta, \end{cases} \quad (A.9)$$

while given three dimensional indices, $\alpha$, $\beta$, and $\gamma$,

$$\varepsilon_{\alpha\beta\gamma} = \begin{cases} +1, & \{\alpha, \beta, \gamma\} = \{1, 2, 3\}, \{2, 3, 1\}, \{3, 1, 2\}, \\ -1, & \{\alpha, \beta, \gamma\} = \{3, 2, 1\}, \{1, 3, 2\}, \{2, 1, 3\}, \\ 0, & \alpha = \beta, \beta = \gamma, \gamma = \alpha. \end{cases} \quad (A.10)$$

The Levi-Civita matrices in two and three dimensions,

$$[\Upsilon_{2D}] = \begin{bmatrix} 0 & +1 \\ -1 & 0 \end{bmatrix} \quad \text{and} \quad [\Upsilon_{3D}] = \begin{bmatrix} 0 & +1 & -1 \\ -1 & 0 & +1 \\ +1 & -1 & 0 \end{bmatrix}, \quad (A.11)$$

resemble the co-factor matrices used in the expansion of a determinant. Therefore, the Levi-Civita symbol or matrix is useful for mapping the cross-product between multiple vectors represented within tensors, such as the electrodynamic lattice-Boltzmann method.

A.3 Polynomials and functions

Approximations of functions can be represented using Taylor series polynomials and Hermite polynomials as detailed in this section. Lyapunov functions are also defined.

Taylor series polynomials represent the sum of a function’s derivatives at a point, which converges to the function itself for an infinite number of terms,

$$f(x) = \sum_{m=0}^{\infty} \frac{f^{(m)}(a)}{m!} (x - a)^m. \quad (A.12)$$

Taylor series having a finite number of terms may be used to derive central difference equations. Given a finite number of elements, $N_m$, a Taylor
A.3. Polynomials and functions

series is a polynomial representation of a real function having an order of accuracy proportional to the number of its terms, \( O((x - a)^{N_m+1}) \),

\[
f(x) = \sum_{m=0}^{N_m} \frac{f^{(m)}(a)}{m!}(x - a)^m + O((x - a)^{N_m+1}).
\]  

(A.13)

**Hermite polynomials** approximate Gaussian distribution functions. The sequence of Hermite polynomials are described by

\[
H^{(n)}(x) = (-1)^n \frac{1}{w(x)} \frac{d^n}{dx^n} w(x), \quad w(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}
\]  

(A.14)

The first six Hermite polynomials are listed in Table A.1.

<table>
<thead>
<tr>
<th>Even</th>
<th>Odd</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H^{(0)}(x) = 1)</td>
<td>(H^{(1)}(x) = x)</td>
</tr>
<tr>
<td>(H^{(2)}(x) = x^2 - 1)</td>
<td>(H^{(3)}(x) = x^3 - 3x)</td>
</tr>
<tr>
<td>(H^{(4)}(x) = x^4 - 6x^2 + 3)</td>
<td>(H^{(5)}(x) = x^5 - 10x^3 + 15x)</td>
</tr>
</tbody>
</table>

Hermite polynomials can also be extended to \( d \) spatial dimensions,

\[
H^{(n)}(\mathbf{x}) = (-1)^n \frac{1}{w(\mathbf{x})} \nabla^{(n)} w(\mathbf{x}), \quad w(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} e^{-\frac{\mathbf{x}^2}{2}}
\]  

(A.15)

wherein each Hermite polynomial is orthogonal with respect to \( w(\mathbf{x}) \). Multi-dimensional Hermite polynomials are used to derive the second-order discrete Maxwell-Boltzmann distribution function representing the equilibrium condition of an ideal gas, in addition to the electric field amplitude profile for a three-dimensional Gaussian beam [79].

**Lyapunov functions** are scalar functions used to prove the stable equilibrium of an ordinary differential equation. The existence of Lyapunov functions can be a necessary and adequate condition for stability. The Lyapunov function for an autonomous dynamical system is

\[
g: \mathbb{R}^n \to \mathbb{R}^n, \quad \frac{dx}{dt} = g(x),
\]  

(A.16)

with an equilibrium point at \( x = 0 \). Lyapunov functions were used to derive a stable electrodynamic lattice-Boltzmann method, and are sufficient to demonstrate its stability [39].
Appendix B

Momentum flux density tensors expanded

In this section, the common electrodynamic momentum flux density tensors are expanded into a single matrix form. This is required to derive their divergence, and program their central differences.

B.1 Abraham’s momentum flux density tensor

\[
\begin{pmatrix}
-E_x D_x + D_y E_y + D_z E_z \\
-H_x B_x + H_y B_y + H_z B_z \\
-D_y E_x - B_y H_x - E_y D_x + H_y B_x \\
-D_z E_x - B_z H_x - E_z D_x - H_z B_x \\
-E_x D_y + B_x H_y - E_x D_y - H_x B_y \\
-D_x E_y - B_x H_y - E_x D_y - H_x B_y \\
-E_x D_z + B_x H_z - E_x D_z - H_x B_z \\
-D_x E_z - B_x H_z - E_x D_z - H_x B_z \\
\end{pmatrix}
\]

B.2 Minkowski’s momentum flux density tensor

\[
\begin{pmatrix}
-\frac{1}{2} D_x E_x + \frac{1}{2} D_y E_y + \frac{1}{2} D_z E_z \\
-\frac{1}{2} H_x B_x + \frac{1}{2} B_y H_y + \frac{1}{2} B_z H_z \\
-D_y E_x - B_y H_x \\
-\frac{1}{2} D_z H_z \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
-\frac{1}{2} D_x E_x - \frac{1}{2} D_y E_y + \frac{1}{2} D_z E_z \\
-\frac{1}{2} D_y H_y + \frac{1}{2} B_z H_z \\
-D_y E_x - B_y H_x \\
-\frac{1}{2} D_z H_z \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
-\frac{1}{2} D_x E_x + \frac{1}{2} D_y E_y - \frac{1}{2} D_z E_z \\
-\frac{1}{2} D_y H_y - \frac{1}{2} B_z H_z \\
-D_y E_x - B_y H_x \\
-\frac{1}{2} D_z H_z \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
-\frac{1}{2} D_x E_x - \frac{1}{2} D_y E_y - \frac{1}{2} D_z E_z \\
-\frac{1}{2} D_y H_y - \frac{1}{2} B_z H_z \\
-D_y E_x - B_y H_x \\
-\frac{1}{2} D_z H_z \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
1 D_x E_x + \frac{1}{2} D_y E_y - \frac{1}{2} D_z E_z \\
1 B_x H_x + \frac{1}{2} B_y H_y - \frac{1}{2} B_z H_z \\
1 D_x E_x + \frac{1}{2} D_y E_y - \frac{1}{2} D_z E_z \\
1 B_x H_x + \frac{1}{2} B_y H_y - \frac{1}{2} B_z H_z \\
\end{pmatrix}
\]

113
B.3 Einstein & Laub's momentum flux density tensor

\[ \mathbf{T} = \begin{pmatrix}
\frac{\mu_0}{2} (E_x^2 + E_y^2 + E_z^2) & -D_x E_y - B_z H_y & -D_x E_z - B_z H_z \\
\frac{\mu_0}{2} (H_x^2 + H_y^2 + H_z^2) & -D_y E_x - B_y H_x & -D_y E_z - B_y H_z \\
-D_x E_x - B_x H_x & -D_y E_y - B_y H_y & \frac{\mu_0}{2} (E_x^2 + E_y^2 + E_z^2) \\
\end{pmatrix} \]

B.4 Chu's momentum flux density tensor

\[ \mathbf{T} = \begin{pmatrix}
\frac{\epsilon_0}{2} (E_x^2 + E_y^2 + E_z^2) & -\epsilon_0 E_x E_y - \mu_0 H_x H_y & -\epsilon_0 E_x E_z - \mu_0 H_x H_z \\
\frac{\mu_0}{2} (H_x^2 + H_y^2 + H_z^2) & -\epsilon_0 E_y E_x - \mu_0 H_y H_x & -\epsilon_0 E_y E_z - \mu_0 H_y H_z \\
-\epsilon_0 E_z E_x - \mu_0 H_z H_x & -\epsilon_0 E_z E_y - \mu_0 H_z H_y & \frac{\epsilon_0}{2} (E_x^2 + E_y^2 + E_z^2) \\
\end{pmatrix} \]

B.5 Ampere's momentum flux density tensor

\[ \mathbf{T} = \begin{pmatrix}
\frac{\epsilon_0}{2} (E_x^2 + E_y^2 + E_z^2) & -\epsilon_0 E_x E_y - \frac{1}{\mu_0} B_z B_y & -\epsilon_0 E_x E_z - \frac{1}{\mu_0} B_z B_z \\
\frac{1}{2\mu_0} (B_x^2 + B_y^2 + B_z^2) & -\epsilon_0 E_y E_x - \frac{1}{\mu_0} B_y B_x & -\epsilon_0 E_y E_z - \frac{1}{\mu_0} B_y B_z \\
-\epsilon_0 E_z E_x - \frac{1}{\mu_0} B_z B_x & -\epsilon_0 E_z E_y - \frac{1}{\mu_0} B_z B_y & \frac{\epsilon_0}{2} (E_x^2 + E_y^2 + E_z^2) \\
\end{pmatrix} \]
B.6 Helmholtz momentum flux density tensor

\[
\mathbf{T} = \begin{bmatrix}
\epsilon_{CM}(E_x^2 + E_y^2 + E_z^2) - \epsilon E_x^2 \\
+ \mu_{CM}(H_x^2 + H_y^2 + H_z^2) - \mu H_x^2 \\
- \epsilon E_y H_x - \mu H_y H_x \\
- \epsilon E_z H_x - \mu H_z H_x
\end{bmatrix}
\]

where \(\epsilon_{CM}\) and \(\mu_{CM}\) are the permittivity and the permeability for a Clausius-Mossotti medium, while \(\epsilon\) and \(\mu\) are the standard permittivity and permeability. Each are given by

\[\epsilon_{CM} = \epsilon_0 \frac{2 + 2\epsilon_r - \epsilon_r^2}{6}, \quad \epsilon = \epsilon_0 \epsilon_r, \quad (B.1)\]

\[\mu_{CM} = \mu_0 \frac{2 + 2\mu_r - \mu_r^2}{6}, \quad \mu = \mu_0 \mu_r. \quad (B.2)\]

B.7 Divergence of a stress-tensor

The divergence of a stress-tensor is used to calculate the force density on a medium. The row and column indices are represented using \(\alpha = \{1, 2, 3\}\) and \(\beta = \{1, 2, 3\}\). Substituting \(\alpha = \{x, y, z\}\) and \(\beta = \{x, y, z\}\) is a common practice for representing the row and column indices, such that the stress-tensor is represented as,

\[
T_{\alpha\beta} \in \mathbf{T}, \quad [\mathbf{T}] = \begin{bmatrix}
T_{11} & T_{12} & T_{13} \\
T_{21} & T_{22} & T_{23} \\
T_{31} & T_{32} & T_{33}
\end{bmatrix} = \begin{bmatrix}
T_{xx} & T_{xy} & T_{xz} \\
T_{yx} & T_{yy} & T_{yz} \\
T_{zx} & T_{zy} & T_{zz}
\end{bmatrix}.
\]

Divergence of this stress-tensor can then be represented as

\[
\nabla \cdot \mathbf{T} = \frac{\partial}{\partial x_{\alpha}} T_{\alpha\beta} e_{\beta} = \begin{bmatrix}
\frac{\partial}{\partial x} T_{xx} + \frac{\partial}{\partial y} T_{xy} + \frac{\partial}{\partial z} T_{xz} \\
\frac{\partial}{\partial y} T_{yx} + \frac{\partial}{\partial y} T_{yy} + \frac{\partial}{\partial z} T_{yz} \\
\frac{\partial}{\partial z} T_{zx} + \frac{\partial}{\partial z} T_{zy} + \frac{\partial}{\partial z} T_{zz}
\end{bmatrix}.
\]

The divergence operator applies to all dimensions in which there is spatial variation of the electric and magnetic fields. In the case of a two-dimensional \(xy\)-plane simulation, spatial variation only occurs in the \(xy\)-plane, such that the terms \(\frac{\partial}{\partial z} T_{xx} = 0, \frac{\partial}{\partial z} T_{xy} = 0, \frac{\partial}{\partial z} T_{xz} = 0, \frac{\partial}{\partial y} T_{xz} = 0\) and \(\frac{\partial}{\partial z} T_{zz} = 0\). Therefore, the divergence of the stress-tensor may be represented as
B.7. Divergence of a stress-tensor

\[ \nabla \cdot \mathbf{T} = \begin{bmatrix} \frac{\partial}{\partial x} T_{xx} + \frac{\partial}{\partial y} T_{xy} + 0 \\ \frac{\partial}{\partial x} T_{yx} + \frac{\partial}{\partial y} T_{yy} + 0 \\ 0 + 0 + 0 \end{bmatrix}, \quad (B.5) \]

which demonstrates zero variation along the \( z \)-coordinate. The three-dimensional vector with no information contained in one of its dimensions may be represented as a two-dimensional vector,

\[(\nabla \cdot \mathbf{T})_{xy} = \begin{bmatrix} \frac{\partial}{\partial x} T_{xx} + \frac{\partial}{\partial y} T_{xy} \\ \frac{\partial}{\partial x} T_{yx} + \frac{\partial}{\partial y} T_{yy} \end{bmatrix} = \begin{bmatrix} \Delta T_x \\ \Delta T_y \end{bmatrix}. \quad (B.6)\]

Two examples of the divergence are provided below for the Minkowski and Chu formalisms. These two formalisms are chosen for their opposing interpretation of light-matter interactions.

B.7.1 Two-dimensional Minkowski stress-tensor divergence

\[ \nabla \cdot \mathbf{T} = \frac{1}{2} \begin{bmatrix} \frac{\partial}{\partial x} (-D_x E_x + D_y E_y + B_z H_z) + \frac{\partial}{\partial y} (-2D_x E_y) \\ \frac{\partial}{\partial x} (-2D_y E_x) + \frac{\partial}{\partial y} (D_x E_x - D_y E_y + B_z H_z) \end{bmatrix}. \quad (B.7) \]

B.7.2 Two-dimensional Chu stress-tensor divergence

\[ \nabla \cdot \mathbf{T} = \frac{1}{2} \begin{bmatrix} \frac{\partial}{\partial x} \left( \frac{\varepsilon_0}{2} (-E_x^2 + E_y^2) + \frac{\mu_0}{2} H_z^2 \right) + \frac{\partial}{\partial y} (-\varepsilon_0 E_x E_y) \\ \frac{\partial}{\partial x} (-\varepsilon_0 E_y E_x) + \frac{\partial}{\partial y} \left( \frac{\varepsilon_0}{2} (E_x^2 - E_y^2) + \frac{\mu_0}{2} H_z^2 \right) \end{bmatrix}. \quad (B.8) \]
Appendix C

Dimensional Conversions

Tab. C.1 provides a full list of the dimensional conversions used in both the electrodynamic and kinetic sub-systems.

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Dimensionless ($x, t$)</th>
<th>Dimensional ($x', t'$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time ($e$)</td>
<td>$t_e$</td>
<td>$t'_e = t_e \Delta t/2$</td>
</tr>
<tr>
<td>Time ($k$)</td>
<td>$t_k$</td>
<td>$t'_k = t_k \Delta t$</td>
</tr>
<tr>
<td>Position vector</td>
<td>$x$</td>
<td>$x = x \Delta x$</td>
</tr>
<tr>
<td>Velocity</td>
<td>$u$</td>
<td>$u = u(\Delta x/\Delta t)$</td>
</tr>
<tr>
<td>Mass density</td>
<td>$\rho$</td>
<td>$\rho' = \rho \rho_c$</td>
</tr>
<tr>
<td>Electric field intensity</td>
<td>$E$</td>
<td>$E' = E$</td>
</tr>
<tr>
<td>Magnetic field intensity</td>
<td>$H$</td>
<td>$H' = H/\eta_0$</td>
</tr>
<tr>
<td>Energy density</td>
<td>$W_e$</td>
<td>$W'_e = W_e \epsilon_0$</td>
</tr>
<tr>
<td>Poynting’s vector</td>
<td>$S_e$</td>
<td>$S'_e = S_e/\eta_0$</td>
</tr>
<tr>
<td>Momentum density ($e$)</td>
<td>$G_e$</td>
<td>$G'_e = G_e/(c^2 \eta_0)$</td>
</tr>
<tr>
<td>Momentum density ($k$)</td>
<td>$G_k$</td>
<td>$G'_k = G_k(\rho_c \Delta x/\Delta t)$</td>
</tr>
<tr>
<td>Momentum-flux tensor</td>
<td>$T_e$</td>
<td>$T'_e = T_e \epsilon_0$</td>
</tr>
<tr>
<td>Force density</td>
<td>$f_k$</td>
<td>$f'_k = f_k[\rho_c \Delta x/(\Delta t)^2]$</td>
</tr>
</tbody>
</table>
Appendix D

Program Implementations

This section contains several program implementations of various MATLAB functions used in the ELBM and PLBM representing electrodynamic and kinetic sub-systems. Note that the functions are provided for the case of a two-dimensional simulation.

D.1 Electrodynamic lattice-Boltzmann method

force density

The following script is an excerpt of the electrodynamic lattice-Boltzmann method’s force density using simple central difference formulas. It is more convenient to write in an expanded form.

```matlab
function [F,G] = force(model,nx,ny,er,ur,dtp,E,H,Gp,NE,dxp)
e0=8.8541878128e-12; %free space permittivity
u0=1.25663706e-6; %free space permeability
c=299792458; %speed of light
eta0=sqrt(u0/e0); %free space impedance
H=H/(2*eta0); %dimensional conversion
E=E/2; %dimensional conversion

% Initialize arrays according to the electric field polarization
if NE>1
    F=zeros(size(E)); G=zeros(size(E));
else
    F=zeros(size(H)); G=zeros(size(H));
end
ii=4:nx-4;
jj=4:ny-4;

% Momentum density
if NE>1
    G(jj,ii,1)=E(jj,ii,1).*H(jj,ii,1)/(c^2);
end
```

118
D.1. Electrodynamic lattice-Boltzmann method force density

\[
G(jj, ii, 2) = -E(jj, ii, 2) \cdot H(jj, ii, 1)/(c^2);
\]

\[
G(jj, ii, 1) = -E(jj, ii, 1) \cdot H(jj, ii, 1)/(c^2);
\]

\[
G(jj, ii, 2) = E(jj, ii, 1) \cdot H(jj, ii, 2)/(c^2);
\]

end

\[
F = \text{zeros(size}(G));
\]

\% Abraham force density, polarization dependent
if strcmp(model, 'AB') == 1
  \% for a TM mode
  if NE > 1
    t11 = (1/2) \cdot (e0 \cdot er \cdot (\text{sum}(E.\cdot2,3) - 2 \cdot E(:,:,2).^2) + u0 \cdot ur \cdot (\text{sum}(H.\cdot2,3)));
    t22 = (1/2) \cdot (e0 \cdot er \cdot (\text{sum}(E.\cdot2,3) - 2 \cdot E(:,:,1).^2) + u0 \cdot ur \cdot (\text{sum}(H.\cdot2,3)));
    t12 = e0 \cdot (-er \cdot E(:,:,1) \cdot E(:,:,2)); t21 = t12;
  else
    t11 = (1/2) \cdot (e0 \cdot er \cdot (\text{sum}(E.\cdot2,3)) + u0 \cdot ur \cdot (\text{sum}(H.\cdot2,3) - 2 \cdot H(:,:,2).^2));
    t22 = (1/2) \cdot (e0 \cdot er \cdot (\text{sum}(E.\cdot2,3)) + u0 \cdot ur \cdot (\text{sum}(H.\cdot2,3) - 2 \cdot H(:,:,1).^2));
    t12 = u0 \cdot (-ur \cdot H(:,:,1). \cdot H(:,:,2)); t21 = t12;
  end

\% Einstein & Laub force density, polarization dependent
elseif strcmp(model, 'EL') == 1
  if NE > 1
    t11 = (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot \text{sum}(H.\cdot2,3)) - e0 \cdot er \cdot E(:,:,2).^2;
    t12 = (-e0 \cdot er \cdot E(:,:,1) \cdot E(:,:,2)); t21 = t12;
    t22 = (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot \text{sum}(H.\cdot2,3)) - e0 \cdot er \cdot E(:,:,1).^2;
  else
    t11 = (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot \text{sum}(H.\cdot2,3)) - u0 \cdot ur \cdot H(:,:,1).^2;
    t12 = (-u0 \cdot ur \cdot H(:,:,1) \cdot H(:,:,2)); t21 = t12;
    t22 = (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot \text{sum}(H.\cdot2,3)) - u0 \cdot ur \cdot H(:,:,1).^2;
  end

\% Chu force density, polarization dependent
elseif strcmp(model, 'CHU') == 1
  \% for a TM mode
  if NE > 1
    t11 = e0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) - 2 \cdot E(:,:,2).^2) + u0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(H.\cdot2,3));
    t12 = e0 \cdot (-er \cdot E(:,:,1) \cdot E(:,:,2)); t21 = t12;
    t22 = e0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) - 2 \cdot E(:,:,1).^2) + u0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(H.\cdot2,3));
  else
    t11 = e0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(H.\cdot2,3)) - 2 \cdot H(:,:,2).^2);
    t12 = -u0 \cdot H(:,:,1) \cdot H(:,:,2)); t21 = t12;
    t22 = e0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(E.\cdot2,3) + u0 \cdot (1/2) \cdot (e0 \cdot \text{sum}(H.\cdot2,3)) - 2 \cdot H(:,:,1).^2);
  end

\% Helmholtz force density, polarization dependent
elseif strcmp(model, 'HLM') == 1
  ecm = (2 + 2 \cdot er \cdot er - er^2)/6;
  ucm = (2 + 2 \cdot ur - ur^2)/6;
  if NE > 1
    t11 = e0 \cdot ecm \cdot \text{sum}(E.\cdot2,3) - 2 \cdot e0 \cdot er \cdot E(:,:,2)^2 + u0 \cdot ucm \cdot H(:,:,1).^2;
    t12 = e0 \cdot (-er \cdot E(:,:,1) \cdot E(:,:,2)); t21 = t12;
    t22 = e0 \cdot ecm \cdot \text{sum}(E.\cdot2,3) - 2 \cdot e0 \cdot er \cdot E(:,:,1)^2 + u0 \cdot ucm \cdot H(:,:,1).^2;
  else
    t11 = u0 \cdot ucm \cdot \text{sum}(H.\cdot2,3) - u0 \cdot ur \cdot H(:,:,2)^2 + 2 \cdot e0 \cdot ecm \cdot (E(:,:,1).^2);
    t12 = u0 \cdot (-ur \cdot H(:,:,1) \cdot H(:,:,2)); t21 = t12;
    t22 = u0 \cdot ucm \cdot \text{sum}(H.\cdot2,3) - u0 \cdot ur \cdot H(:,:,1)^2 + 2 \cdot e0 \cdot ecm \cdot (E(:,:,1).^2);
  end
D.2 Shan-Chen force density with applicable equation of state

Modulation operators are used to distribute the velocity vectors across periodic boundaries. This enables the definition of the gradient operator in the Shan-Chen force density throughout all lattice nodes in the simulation domain. However, the implementation for a multi-range lattice would have greater implementation complexity.

% Shan-Chen force density
function [fx, fy] = force(nx, ny, cx, cy, rho, w, G, fx, fy)

% Equation of state parameters: \( \rho_0 / \rho_1 = 1180 \)
a = 1; b = 4; R = 1;
Tc = 0.3773*a/(b*R); T = 0.531*Tc;
for j = 1:ny
for i = 1:nx
fxs = 0.0;
fys = 0.0;
for k = 1:8
newx = 1 + mod(i-1 + cx(k), nx) + nx;
newy = 1 + mod(j-1 + cy(k), ny);
r = rho(newx, newy);
p = [(r^R*Tc+(b*r/4)^2-(b*r/4)^3))/((1-b*r/4)^2)-a*r^2;
pp = 2*(p-r^3)/(G^3);
psi = sqrt(sign(pp)*pp);
fxs = fxs - G*w(k)*psi*cx(k);
fys = fys - G*w(k)*psi*cy(k);
end
end
end
end
end
D.3. Periodic boundary conditions

Periodic boundary conditions are implemented over each boundary lattice node, avoiding any redundancies. This requires that only discrete velocities leaving the domain are considered for re-initialization on the opposite side of the domain, and that only one periodic boundary exists for each cell.

\[
\begin{align*}
    r &= \rho(i,j); \\
p &= \left( r + 8 \times \left( 1 + \left( b \times r/4 \right) + \left( b \times r/4 \right)^2 - \left( b \times r/4 \right)^3 \right)/\left( 1 - b \times r/4 \right)^3 \right) - a \times r^2; \\
    pp &= 2 \times (p - r/3)/(G/3); \\
    psi &= \sqrt{\text{sign}(pp) \times pp}; \\
    fx(i,j) &= psi \times fxs; \\
    fy(i,j) &= psi \times fys;
\end{align*}
\]

D.4 Collision operation

The single-relaxation collision operation for a Shan-Chen forcing scheme is represented in two-dimensions and three-dimensions.

\[
\begin{align*}
    \% Periodic boundary condition \\
    \% left boundary \\
    n(1,:,1) &= n(nx,:,1); \\
    n(1,:,5) &= n(nx,:,5); \\
    n(1,:,8) &= n(nx,:,8); \\
    \% right hand boundary \\
    n(nx,:,3) &= n(1,:,3); \\
    n(nx,:,7) &= n(1,:,7); \\
    n(nx,:,6) &= n(1,:,6); \\
    \% bottom boundary \\
    n(:,1,2) &= n(:,ny,2); \\
    n(:,1,5) &= n(:,ny,5); \\
    n(:,1,6) &= n(:,ny,6); \\
    \% top boundary \\
    for i=2:nx-1 \\
        n(i,ny,4) &= n(i,1,4); \\
        n(i,ny,8) &= n(i,1,8); \\
        n(i,ny,7) &= n(i,1,7);
    end
\end{align*}
\]
D.4. Collision operation

\[
uxf = \frac{1}{\omega} forc_x ./ rho + ux; \quad \text{velocity with imparted momentum: } x \rightarrow
\]
\[
uyf = \frac{1}{\omega} forc_y ./ rho + uy; \quad \text{velocity with imparted momentum: } y \rightarrow
\]

for \( j = 1:ny \)
  
  for \( i = 1: nx \)
    
    \[
t_1 = uxf(i,j) \times uxf(i,j) + uyg(i,j) \times uyf(i,j); \quad \text{norm of velocity squared}
    \]
  
  for \( m = 1:9 \)
    
    \[
t_2 = uxf(i,j) \times vx(m) + uyf(i,j) \times vy(m);
    \quad \text{equilibrium condition}
    \]
    
    \[
    neq(i,j,m) = rho(i,j) \times w(m) \times (1.0 + 3.0 \times t_2 + 4.5 \times t_2^2 - 1.5 \times t_1);
    \quad \text{collision operation}
    \]
    
    \[
n(i,j,m) = (1 - \omega) \times n(i,j,m) + \omega \times neq(i,j,m);
    \]
  
  end

end

end

Multi-relaxation time collision operators require conversion between the moment space and the velocity space. Such conversion is accomplished using a transformation matrix.

\[
\text{function } [n] = collision(nx,ny,ux,uy,n,rho,M,Minv,Deltam,forc_x,forc_y)
\]

I = eye(size(M));

% Calculate the equilibrium condition in moment space

\[
nmeq(:,:,1) = rho \times (-2 + 3 \times (ux \times ux + uy \times uy));
\]
\[
nmeq(:,:,2) = rho \times (1 - 3 \times (ux \times ux + uy \times uy));
\]
\[
nmeq(:,:,3) = rho \times ux;
\]
\[
nmeq(:,:,4) = -rho \times ux;
\]
\[
nmeq(:,:,5) = rho \times uy;
\]
\[
nmeq(:,:,6) = -rho \times uy;
\]
\[
nmeq(:,:,7) = rho \times (ux \times ux - uy \times uy);
\]
\[
nmeq(:,:,8) = rho \times ux \times uy;
\]
\[
nmeq(:,:,9) = rho;
\]

%transform \( 'n' \) into moment space as \( 'nmom' \)

for \( i = 1: nx \)
  
  for \( j = 1: ny \)
    
    \[
    smf = 0.0;
    \]
    
    for \( m = 1:9 \)
      
      \[
      smf = smf + M(q,m) \times n(i,j,m);
      \]
    
    end

    nmom(i,j,q) = smf;
  
  end

end

% collision of \( 'nmom' \) in momentum space with forcing term added.

for \( j = 1: ny \)
D.5  Propagation operation

for i=1:nx
for q=1:9
    ssmb=0.0;
    for m=1:9
        ssmb=ssmb-Deltam(q,m)\((\text{nmom}(i,j,m)-\text{nmeq}(i,j,m))+(I(q,m)-(1/2)Deltam(q,m))smeq(i,j,m))\);% with force added
    end
    nmom(i,j,q)=ssmb;
end
end

% transform 'nmom' back into velocity space as 'n'
for i=1:nx
    for j=1:ny
        for q=1:9
            smf=0.0;
            for m=1:9
                smf=smf+Minv(q,m)\*nmom(i,j,m);
            end
            n(i,j,q)=n(i,j,q)+smf;
        end
    end
end

D.5  Propagation operation

The propagation/streaming operation is identical in each method, and is greatly simplified by circularly shifting of the discrete outcomes of \(n_m(x,t)\). In this manner, the propagation/streaming operation program can be generalized to represent any discrete velocity set.

% Propagation/streaming:
function [n]=stream(n,vx,vy)
    for m=1:8
        n(:, :, m)=circshift(squeeze(n(:, :, m)), [vx(m), vy(m)]);
    end
end