
Contents

Preface	VII
1 Introduction	1
1.1 Why Deal with the Nanoscale?	1
1.2 Why Special Models for the Nanoscale?	3
1.3 How To Hone the Computational Tools	6
1.4 So What?	8
2 Finite-Difference Schemes	11
2.1 Introduction	11
2.2 A Primer on Time-Stepping Schemes.....	12
2.3 Exact Schemes	16
2.4 Some Classic Schemes for Initial Value Problems	18
2.4.1 The Runge–Kutta Methods	20
2.4.2 The Adams Methods	24
2.4.3 Stability of Linear Multistep Schemes	24
2.4.4 Methods for Stiff Systems	27
2.5 Schemes for Hamiltonian Systems	34
2.5.1 Introduction to Hamiltonian Dynamics	34
2.5.2 Symplectic Schemes for Hamiltonian Systems	37
2.6 Schemes for One-Dimensional Boundary Value Problems	39
2.6.1 The Taylor Derivation	39
2.6.2 Using Constraints to Derive Difference Schemes	40
2.6.3 Flux-Balance Schemes	42
2.6.4 Implementation of 1D Schemes for Boundary Value Problems	46
2.7 Schemes for Two-Dimensional Boundary Value Problems	47
2.7.1 Schemes Based on the Taylor Expansion	47
2.7.2 Flux-Balance Schemes	48
2.7.3 Implementation of 2D Schemes	50
2.7.4 The Collatz “Mehrstellen” Schemes in 2D	51

2.8	Schemes for Three-Dimensional Problems	55
2.8.1	An Overview	55
2.8.2	Schemes Based on the Taylor Expansion in 3D	55
2.8.3	Flux-Balance Schemes in 3D	56
2.8.4	Implementation of 3D Schemes	57
2.8.5	The Collatz “Mehrstellen” Schemes in 3D	58
2.9	Consistency and Convergence of Difference Schemes	59
2.10	Summary and Further Reading	64
3	The Finite Element Method	69
3.1	Everything is Variational	69
3.2	The Weak Formulation and the Galerkin Method	75
3.3	Variational Methods and Minimization	81
3.3.1	The Galerkin Solution Minimizes the Error	81
3.3.2	The Galerkin Solution and the Energy Functional	82
3.4	Essential and Natural Boundary Conditions	83
3.5	Mathematical Notes: Convergence, Lax–Milgram and Céa’s Theorems	86
3.6	Local Approximation in the Finite Element Method	89
3.7	The Finite Element Method in One Dimension	91
3.7.1	First-Order Elements	91
3.7.2	Higher-Order Elements	102
3.8	The Finite Element Method in Two Dimensions	105
3.8.1	First-Order Elements	105
3.8.2	Higher-Order Triangular Elements	120
3.9	The Finite Element Method in Three Dimensions	122
3.10	Approximation Accuracy in FEM	123
3.11	An Overview of System Solvers	129
3.12	Electromagnetic Problems and Edge Elements	139
3.12.1	Why Edge Elements?	139
3.12.2	The Definition and Properties of Whitney–Nédélec Elements	142
3.12.3	Implementation Issues	145
3.12.4	Historical Notes on Edge Elements	146
3.12.5	Appendix: Several Common Families of Tetrahedral Edge Elements	147
3.13	Adaptive Mesh Refinement and Multigrid Methods	148
3.13.1	Introduction	148
3.13.2	Hierarchical Bases and Local Refinement	149
3.13.3	<i>A Posteriori</i> Error Estimates	151
3.13.4	Multigrid Algorithms	154
3.14	Special Topic: Element Shape and Approximation Accuracy	158
3.14.1	Introduction	158
3.14.2	Algebraic Sources of Shape-Dependent Errors: Eigenvalue and Singular Value Conditions	160

3.14.3 Geometric Implications of the Singular Value Condition	171
3.14.4 Condition Number and Approximation	179
3.14.5 Discussion of Algebraic and Geometric <i>a priori</i> Estimates	180
3.15 Special Topic: Generalized FEM	181
3.15.1 Description of the Method	181
3.15.2 Trade-offs	183
3.16 Summary and Further Reading	184
3.17 Appendix: Generalized Curl and Divergence	186
4 Flexible Local Approximation MEthods (FLAME)	189
4.1 A Preview	189
4.2 Perspectives on Generalized FD Schemes	191
4.2.1 Perspective #1: Basis Functions Not Limited to Polynomials	191
4.2.2 Perspective #2: Approximating the <i>Solution</i> , Not the Equation	192
4.2.3 Perspective #3: Multivalued Approximation	193
4.2.4 Perspective #4: Conformity vs. Flexibility	193
4.2.5 Why Flexible Approximation?	195
4.2.6 A Preliminary Example: the 1D Laplace Equation	197
4.3 Trefftz Schemes with Flexible Local Approximation	198
4.3.1 Overlapping Patches	198
4.3.2 Construction of the Schemes	200
4.3.3 The Treatment of Boundary Conditions	202
4.3.4 Trefftz-FLAME Schemes for Inhomogeneous and Nonlinear Equations	203
4.3.5 Consistency and Convergence of the Schemes	205
4.4 Trefftz-FLAME Schemes: Case Studies	206
4.4.1 1D Laplace, Helmholtz and Convection-Diffusion Equations	206
4.4.2 The 1D Heat Equation with Variable Material Parameter	207
4.4.3 The 2D and 3D Laplace Equation	208
4.4.4 The Fourth Order 9-point Mehrstellen Scheme for the Laplace Equation in 2D	209
4.4.5 The Fourth Order 19-point Mehrstellen Scheme for the Laplace Equation in 3D	210
4.4.6 The 1D Schrödinger Equation. FLAME Schemes by Variation of Parameters	210
4.4.7 Super-high-order FLAME Schemes for the 1D Schrödinger Equation	212
4.4.8 A Singular Equation	213
4.4.9 A Polarized Elliptic Particle	215
4.4.10 A Line Charge Near a Slanted Boundary	216
4.4.11 Scattering from a Dielectric Cylinder	217

4.5	Existing Methods Featuring Flexible or Nonstandard Approximation	219
4.5.1	The Treatment of Singularities in Standard FEM	221
4.5.2	Generalized FEM by Partition of Unity	221
4.5.3	Homogenization Schemes Based on Variational Principles	222
4.5.4	Discontinuous Galerkin Methods	222
4.5.5	Homogenization Schemes in FDTD	223
4.5.6	Meshless Methods	224
4.5.7	Special Finite Element Methods	225
4.5.8	Domain Decomposition	226
4.5.9	Pseudospectral Methods	226
4.5.10	Special FD Schemes	227
4.6	Discussion	228
4.7	Appendix: Variational FLAME	231
4.7.1	References	231
4.7.2	The Model Problem	232
4.7.3	Construction of Variational FLAME	232
4.7.4	Summary of the Variational-Difference Setup	235
4.8	Appendix: Coefficients of the 9-Point Trefftz-FLAME Scheme for the Wave Equation in Free Space	236
4.9	Appendix: the Fréchet Derivative	237
5	Long-Range Interactions in Free Space	239
5.1	Long-Range Particle Interactions in a Homogeneous Medium	239
5.2	Real and Reciprocal Lattices	242
5.3	Introduction to Ewald Summation	243
5.3.1	A Boundary Value Problem for Charge Interactions	246
5.3.2	A Re-formulation with “Clouds” of Charge	248
5.3.3	The Potential of a Gaussian Cloud of Charge	249
5.3.4	The Field of a Periodic System of Clouds	251
5.3.5	The Ewald Formulas	252
5.3.6	The Role of Parameters	254
5.4	Grid-based Ewald Methods with FFT	256
5.4.1	The Computational Work	256
5.4.2	On Numerical Differentiation	262
5.4.3	Particle-Mesh Ewald	264
5.4.4	Smooth Particle-Mesh Ewald Methods	267
5.4.5	Particle-Particle Particle-Mesh Ewald Methods	269
5.4.6	The York-Yang Method	271
5.4.7	Methods Without Fourier Transforms	272
5.5	Summary and Further Reading	274
5.6	Appendix: The Fourier Transform of “Periodized” Functions	277
5.7	Appendix: An Infinite Sum of Complex Exponentials	278

6	Long-Range Interactions in Heterogeneous Systems	281
6.1	Introduction	281
6.2	FLAME Schemes for Static Fields of Polarized Particles in 2D	285
6.2.1	Computation of Fields and Forces for Cylindrical Particles	289
6.2.2	A Numerical Example: Well-Separated Particles	291
6.2.3	A Numerical Example: Small Separations	294
6.3	Static Fields of Spherical Particles in a Homogeneous Dielectric	303
6.3.1	FLAME Basis and the Scheme	303
6.3.2	A Basic Example: Spherical Particle in Uniform Field	306
6.4	Introduction to the Poisson–Boltzmann Model	309
6.5	Limitations of the PBE Model	313
6.6	Numerical Methods for 3D Electrostatic Fields of Colloidal Particles	314
6.7	3D FLAME Schemes for Particles in Solvent	315
6.8	The Numerical Treatment of Nonlinearity	319
6.9	The DLVO Expression for Electrostatic Energy and Forces	321
6.10	Notes on Other Types of Force	324
6.11	Thermodynamic Potential, Free Energy and Forces	328
6.12	Comparison of FLAME and DLVO Results	332
6.13	Summary and Further Reading	337
6.14	Appendix: Thermodynamic Potential for Electrostatics in Solvents	338
6.15	Appendix: Generalized Functions (Distributions)	343
7	Applications in Nano-Photonics	349
7.1	Introduction	349
7.2	Maxwell's Equations	349
7.3	One-Dimensional Problems of Wave Propagation	353
7.3.1	The Wave Equation and Plane Waves	353
7.3.2	Signal Velocity and Group Velocity	355
7.3.3	Group Velocity and Energy Velocity	358
7.4	Analysis of Periodic Structures in 1D	360
7.5	Band Structure by Fourier Analysis (Plane Wave Expansion) in 1D	375
7.6	Characteristics of Bloch Waves	379
7.6.1	Fourier Harmonics of Bloch Waves	379
7.6.2	Fourier Harmonics and the Poynting Vector	380
7.6.3	Bloch Waves and Group Velocity	380
7.6.4	Energy Velocity for Bloch Waves	382
7.7	Two-Dimensional Problems of Wave Propagation	384
7.8	Photonic Bandgap in Two Dimensions	386
7.9	Band Structure Computation: PWE, FEM and FLAME	389
7.9.1	Solution by Plane Wave Expansion	389
7.9.2	The Role of Polarization	390

7.9.3 Accuracy of the Fourier Expansion	391
7.9.4 FEM for Photonic Bandgap Problems in 2D	393
7.9.5 A Numerical Example: Band Structure Using FEM	397
7.9.6 Flexible Local Approximation Schemes for Waves in Photonic Crystals	401
7.9.7 Band Structure Computation Using FLAME	405
7.10 Photonic Bandgap Calculation in Three Dimensions: Comparison with the 2D Case.....	411
7.10.1 Formulation of the Vector Problem	411
7.10.2 FEM for Photonic Bandgap Problems in 3D	415
7.10.3 Historical Notes on the Photonic Bandgap Problem	416
7.11 Negative Permittivity and Plasmonic Effects	417
7.11.1 Electrostatic Resonances for Spherical Particles	419
7.11.2 Plasmon Resonances: Electrostatic Approximation	421
7.11.3 Wave Analysis of Plasmonic Systems.....	423
7.11.4 Some Common Methods for Plasmon Simulation	423
7.11.5 Trefftz-FLAME Simulation of Plasmonic Particles	426
7.11.6 Finite Element Simulation of Plasmonic Particles	429
7.12 Plasmonic Enhancement in Scanning Near-Field Optical Microscopy	433
7.12.1 Breaking the Diffraction Limit	434
7.12.2 Apertureless and Dark-Field Microscopy	439
7.12.3 Simulation Examples for Apertureless SNOM	441
7.13 Backward Waves, Negative Refraction and Superlensing	446
7.13.1 Introduction and Historical Notes	446
7.13.2 Negative Permittivity and the “Perfect Lens” Problem	451
7.13.3 Forward and Backward Plane Waves in a Homogeneous Isotropic Medium	456
7.13.4 Backward Waves in Mandelstam’s Chain of Oscillators.....	459
7.13.5 Backward Waves and Negative Refraction in Photonic Crystals	465
7.13.6 Are There Two Species of Negative Refraction?	471
7.14 Appendix: The Bloch Transform.....	477
7.15 Appendix: Eigenvalue Solvers	478
8 Conclusion: “Plenty of Room at the Bottom” for Computational Methods	487
References	489
Index	523