
Contents

1	Introduction	1
1.1	Why Simulation?	2
1.2	Purpose of the Book	5
1.3	Physical Processes in Semiconductors and Their Numerical Description	8
1.4	Simulation of Semiconductor Devices	10
1.5	An Example Simulation: The Game of Life	11
1.6	Organization of The Text	15
I	Basics	19
2	Fundamentals of Electromagnetism and its Numerical Analysis	21
2.1	Introduction to Numerical Differentiation	22
2.2	Vector Calculus	28
2.2.1	Plotting Vectors	29
2.2.2	Plotting Field Lines	29
2.3	Gradient of Scalar Functions	31
2.4	Divergence of Vectors	32
2.4.1	Calculation of the Divergence	34
2.5	Curl of Vectors	45
2.5.1	Derivation of Curl	49
2.5.2	The Importance of <i>Div</i> and <i>Curl</i>	54
2.6	Vector Operators in Curvilinear Coordinates	55
2.7	Electrostatics	56
2.7.1	The Electric Dipole	56
2.7.2	Solution of Laplace's Equation	58

2.8	Solution of PDEs on Irregular Meshes	59
2.8.1	The Functions <i>elen</i> and <i>ilen</i>	63
2.8.2	3D Meshes	72
2.9	Electromagnetism	76
2.9.1	Maxwell's Equations	77
2.9.2	Integral Form of Maxwell's Equations	77
2.9.3	Properties of Maxwell's Equations	79
2.10	Boundary Conditions on the Electromagnetic Fields	80
2.10.1	Divergence Equations	80
2.10.2	Curl Equations	81
2.11	Boundary Conditions on a Mesh	83
2.11.1	The Potential Mesh	83
2.11.2	The Field Mesh	84
2.11.3	Electromagnetic Waves and Boundary Conditions	84
2.12	Propagators in Electromagnetism	93
2.13	Solution of Problems in Electrostatics	96
2.13.1	Equations for Static Electric Fields	97
2.13.2	Boundary Conditions on a Perfect Conductor	98
2.13.3	Displacement Current	99
2.13.4	Solution of Laplace's Equation - Numerical Examples	100
2.13.5	Conductors in an Applied Electric Field	103
2.13.6	A Dielectric in an Electric Field	105
2.13.7	Use of Complex Geometries: a MEMS Example	108
2.14	Summary	114
3	Transport Phenomena and their Numerical Analysis	122
3.1	Conservation Equations	123
3.1.1	Boundary Conditions for Conservation Equations	124
3.2	Finite-Difference Solution of Transport Equations	125
3.2.1	Accuracy of Finite-Difference Schemes	128
3.2.2	Conservative Schemes	128
3.2.3	Diffusion of Dopants	129
3.2.4	Diffusion of Charged Particles in an Electric Field	138
3.2.5	Steady-State Diffusion	138
3.2.6	Steady-State Convection	139
3.3	Propagators in Transport Theory	143
3.3.1	Numerical Implementation of the Transport Propagator	145

3.3.2 Numerical Diffusion and Instability: a Comparison of the Propagator and an Explicit Scheme	153
3.4 Summary	159
II Semiconductor Simulation	165
4 The Semiconductor Equations	167
4.1 Introduction	167
4.2 Equilibrium Carrier Behavior in Semiconductors	167
4.3 Transport Equations for Semiconductors	173
4.3.1 Particle-Conservation Equations for Semiconductors	173
4.3.2 Heat-Conservation Equation	175
4.3.3 Boundary Conditions	177
4.3.4 Alternate Sets of Independent Variables	179
4.4 The Semiconductor Parameters	180
4.4.1 Permittivity	180
4.4.2 Carrier Mobilities	180
4.4.3 Carrier Velocity Saturation	184
4.4.4 Surface Scattering	185
4.4.5 Carrier Diffusion Coefficients	185
4.4.6 Recombination and Generation	185
4.4.7 Minority-Carrier Lifetimes	191
4.4.8 Degeneracy and Band-Gap Narrowing	193
4.4.9 Specific Mass Density and Specific Heat	195
4.4.10 Thermal Conductivity	195
4.4.11 Thermal Generation	195
4.4.12 Parameter Models for High-Field Transport	196
4.5 The Momentum Conservation Equation	196
4.6 Summary	197
4.7 Appendix	197
4.7.1 Solution of the Momentum Equation	197
4.7.2 Models for Ion Stopping	205
5 Numerical Solution of PDEs	210
5.1 Introduction	210
5.2 Numerical Techniques for Solving PDEs	211
5.2.1 Finite-Difference Methods	211

5.2.2	Substitution of Difference Operators for Differential Operators	212
5.2.3	Box Integration Method	214
5.2.4	Finite-Element Methods	221
5.2.5	Other Numerical Methods	221
5.3	Discretizing the Semiconductor Equations	222
5.3.1	Scaling the Semiconductor Equations	222
5.3.2	Discretization of Semiconductor Equations	224
5.3.3	The Scharfetter-Gummel Discretization	227
5.4	The Solution of Nonlinear Systems of Algebraic Equations	229
5.4.1	Fixed-Point Iterative Methods	230
5.4.2	Relaxation Methods	231
5.5	The Solution of Sparse Linear Systems of Algebraic Equations	231
5.5.1	Direct Methods	232
5.5.2	Indirect Methods	234
5.6	Review of Software for the Solution of PDEs	235
5.7	Validation of the Results of Simulations	236
5.8	Summary	239

6 The SGFramework 246

6.1	Introduction	246
6.2	An Overview of the SGFramework	248
6.3	The SGFramework Translator	250
6.3.1	The Scanner	252
6.3.2	The Parser	253
6.3.3	The SGFramework Grammar	255
6.3.4	The Parser's Finite-State Table	255
6.3.5	The Error Handler	256
6.3.6	The Symbol Table	256
6.3.7	The Math Expression Module	256
6.3.8	The Indices Module	260
6.3.9	The Statements Module	260
6.3.10	The Code Generator	261
6.4	The SGFramework Minimum-Degree Ordering Program	263
6.5	The SGFramework Mesh Generation Program	263
6.5.1	Mesh Specification File	264
6.5.2	Mesh Skeleton	264
6.5.3	Generating the Initial Mesh	266

6.5.4	Data Structures for Mesh Generation	266
6.5.5	Polygon Division into Rectangular Elements	269
6.5.6	Polygon Division into Triangular Elements	270
6.5.7	Summary	272
6.6	The SGFramework Mesh Refinement Program	273
6.6.1	Mesh Refinement	273
6.6.2	Refinement of Triangular and Rectangular Elements	275
6.6.3	Data Structures for Mesh Refinement	277
6.6.4	Summary	281
6.7	Interfacing the Mesh and Equation Specifications	281
6.7.1	Mesh Connectivity	281
6.7.2	Box-Integration Method	283
6.7.3	Finite-Difference Schemes and User-Defined Functions	285
6.7.4	Naming Scheme and Specification of PDEs	287
6.8	Specification of Boundary Conditions on Irregular 2D Meshes	290
6.9	SGFramework Build Script	293
6.10	SGFramework Visualization Tools	293
6.11	Summary	293
III	Semiconductor Devices	295
7	PN Junction Diodes	297
7.1	Electrostatic Description of a Simple Junction	298
7.1.1	One-Dimensional Semiconductor Device Electrostatics	299
7.1.2	PN Junctions — Analytic Treatment	300
7.1.3	Step Junction	300
7.1.4	The Built-In Potential	302
7.1.5	Linearly Graded Junction	303
7.1.6	Numerical Modeling of the PN Junction	304
7.2	(i, v) Characteristics	313
7.2.1	(i, v) Characteristics for Low Currents and Voltages	313
7.2.2	Numerical Evaluation of PN Junction (i, v) Characteristics	321
7.2.3	Reverse-Bias Breakdown and Avalanche	327
7.2.4	High-Current and High-Level Injection	342
7.3	Two-Dimensional Modeling of a Device	357
7.3.1	2D Input File	358
7.3.2	Review of Mesh Construction	365

7.3.3	Graphical Output	370
7.4	Small-Signal Analysis	372
7.4.1	Reverse-Bias Characteristics	372
7.4.2	Forward-Bias Characteristics	372
7.4.3	Numerical Modeling of Small-Signal Behavior	374
7.5	Transients in PN Junctions	380
7.5.1	Transient Behavior During Turn-Off	380
7.5.2	Transient Behavior During Turn-On	382
7.6	Photodiodes Based on PN and PIN Junctions	383
7.6.1	Light Absorption in a Semiconductor	383
7.6.2	Semiconductor Light Detectors	384
7.6.3	A Model of a PIN Diode Light Detector	384
7.7	Summary	386
8	Bipolar Junction Transistors	391
8.1	Static Characteristics	391
8.2	The Ebers-Moll Equations	394
8.3	BJT Time-Dependent Behavior	396
8.3.1	Small-Signal Analysis	396
8.3.2	Turn-On Transients in the BJT	398
8.3.3	Turn-Off Transients in the BJT	398
8.4	BJT Circuits	399
8.5	Numerical Model of the BJT	404
8.6	Summary	422
9	Junction Field-Effect Transistors	428
9.1	Static Characteristics	428
9.2	Small-Signal Analysis	431
9.3	Numerical Model of a JFET	431
9.4	Summary	440
10	Metal-Oxide-Semiconductor Structures	441
10.1	Electrostatics of the One-Dimensional MOS Structure	441
10.1.1	CV Characteristics of a MOS Capacitor	443
10.2	Metal-Oxide-Semiconductor Field Effect Transistors	448
10.2.1	(i, v) Characteristics of MOSFETs	448
10.2.2	Small-Signal Analysis of MOSFETs	452
10.3	Submicron Devices and VLSI	452

10.3.1 Scaling MOS Structures	452
10.4 MOSFET Mesh Specification File	457
10.5 MOSFET Equation Specification File	458
10.6 Results of the MOSFET Simulations	464
10.7 MOSFET Circuits	470
10.8 Summary	481
11 Power Semiconductor Devices	483
11.1 Introduction	483
11.2 Simulation of Breakdown in Semiconductors	484
11.2.1 Basic Semiconductor Equations with Impact-Ionization Model	485
11.2.2 Nonlinear Poisson Model	485
11.2.3 Derivation of the Nonlinear Poisson Model	485
11.2.4 Calculation of the Breakdown Voltage	486
11.2.5 Linear Poisson Model with Depletion-Region Logic	487
11.2.6 Justification of Linear Poisson Model with Depletion-Region Logic	487
11.2.7 Comparison of Breakdown Models	488
11.3 Power Diodes	490
11.3.1 Theory and Operation of PIN Diodes	491
11.3.2 Basic Structure and (i, v) Characteristics	491
11.3.3 Switching Characteristics	494
11.3.4 Breakdown Voltage	495
11.3.5 Conductivity Modulation	497
11.4 Optimization of a Semiconductor Device	499
11.4.1 Optimization of PIN Diodes with Field-Limiting Rings	499
11.4.2 Method of Optimization	502
11.5 Power MOSFETs	514
11.5.1 (i, v) Characteristics	518
11.5.2 Switching Characteristics	518
11.6 Thyristors	527
11.6.1 (i, v) Characteristics	530
11.6.2 Switching Characteristics	531
11.7 IGBTs	531
11.7.1 (i, v) Characteristics	533
11.8 Electrothermal Simulation of Power Devices	534
11.9 Summary	534

IV Advanced Topics	537
12 Mixed-Mode Simulations	539
12.1 Time-Dependent Circuits	539
12.2 Circuit Boundary Conditions for Device Models	549
12.2.1 A Diode Bridge Circuit	549
12.2.2 BJT with Inductive Load and Shunt Diode	558
12.3 Summary	569
13 Kinetic Transport Models	578
13.1 Kinetic Simulations	579
13.2 Monte Carlo Particle Simulation	581
13.3 Motion of Charged Particles in a Semiconductor	582
13.4 Integral Equation Methods in Kinetic Theory	583
13.5 Distribution Function Found from the Convected Scheme	584
13.5.1 The Ballistic Move	584
13.5.2 The Collision Operator	588
13.5.3 An Alternative Approach to Kinetic Calculations	588
13.5.4 Self-Consistent Calculations	589
13.5.5 Charged Particles in a Constant Electric Field	589
13.6 Kinetic Simulations Based on the Scattering Rates	591
13.6.1 Ion Motion Inside a Crystal	594
13.6.2 Ballistic Motion	596
13.6.3 Angular Distribution	600
13.6.4 Collisions of Injected Ions	601
13.6.5 Implementation of the Transition Matrix	601
13.7 Summary	601
14 Related Work	605
14.1 Dry Etching of Semiconductors	606
15 The SGFramework User's Manual	608
15.1 The Syntax and Grammar of the Equation Specification File	609
15.1.1 Comments	610
15.1.2 Numbers	610
15.1.3 Strings	611
15.1.4 Identifiers	612
15.1.5 Operators	614

15.1.6 Constants	615
15.1.7 Variables and Arrays	617
15.1.8 Functions	620
15.1.9 Constraint Equations	625
15.1.10 Procedures	628
15.1.11 Numerical Algorithm Parameters	637
15.2 The Syntax and Grammar of the Mesh Specification File	640
15.2.1 An Overview of the Mesh Specification File	640
15.2.2 Comments, Numbers, Identifiers and Constants	642
15.2.3 Coordinates	643
15.2.4 Points	643
15.2.5 Edges	644
15.2.6 Regions	644
15.2.7 Labels	645
15.2.8 Refinement Statements	645
15.2.9 Mesh Parameters	646
15.2.10 Element Refinement Criteria	647
15.3 Interfacing the Equation and the Mesh Specification Files	647
15.3.1 Importing an Irregular Mesh	648
15.3.2 Using Labels in Equation Specification Files	649
15.3.3 Mesh Connectivity Functions	650
15.3.4 Mesh Geometry Functions	651
15.3.5 Mesh Summation Functions	653
15.3.6 Precomputed Functions	654
15.4 SGFramework Executables	657
15.4.1 Build Script	657
15.4.2 Mesh Parser	659
15.4.3 Mesh Generator	661
15.4.4 Mesh Refiner	662
15.4.5 SGFramework Translator	663
15.4.6 Ordering Module	667
15.4.7 SGFramework Simulations	667
15.4.8 Extract Program	668
15.4.9 Group Program	669
15.4.10 Graphical Output	670