

## Contents

**List of Contributors** XXI

**Preface** XXV

### **Part I: Probability** 1

|          |                                                             |
|----------|-------------------------------------------------------------|
| <b>1</b> | <b>Stochastic Processes</b> 3                               |
|          | <i>James R. Cruise, Ostap O. Hryniv, and Andrew R. Wade</i> |
| 1.1      | Introduction 3                                              |
| 1.2      | Generating Functions and Integral Transforms 4              |
| 1.2.1    | Generating Functions 4                                      |
| 1.2.2    | Example: Branching Processes 7                              |
| 1.2.3    | Other Transforms 9                                          |
| 1.2.3.1  | Moment Generating Functions 9                               |
| 1.2.3.2  | Laplace Transforms 10                                       |
| 1.2.3.3  | Characteristic Functions 10                                 |
| 1.3      | Markov Chains in Discrete Time 10                           |
| 1.3.1    | What is a Markov Chain? 10                                  |
| 1.3.2    | Some Examples 11                                            |
| 1.3.3    | Stationary Distribution 12                                  |
| 1.3.4    | The Strong Markov Property 12                               |
| 1.3.5    | The One-Step Method 13                                      |
| 1.3.6    | Further Computational Methods 14                            |
| 1.3.7    | Long-term Behavior; Irreducibility; Periodicity 15          |
| 1.3.8    | Recurrence and Transience 16                                |
| 1.3.9    | Remarks on General State Spaces 17                          |
| 1.3.10   | Example: Bak–Sneppen and Related Models 17                  |
| 1.4      | Random Walks 18                                             |
| 1.4.1    | Simple Symmetric Random Walk 18                             |
| 1.4.2    | Pólya's Recurrence Theorem 19                               |
| 1.4.3    | One-dimensional Case; Reflection Principle 19               |
| 1.4.4    | Large Deviations and Maxima of Random Walks 21              |
| 1.5      | Markov Chains in Continuous Time 22                         |

|          |                                                                         |           |
|----------|-------------------------------------------------------------------------|-----------|
| 1.5.1    | Markov Property, Transition Function, and Chapman – Kolmogorov Relation | 22        |
| 1.5.2    | Infinitesimal Rates and Q-matrices                                      | 23        |
| 1.5.3    | Kolmogorov Differential Equations                                       | 24        |
| 1.5.4    | Exponential Holding-Time Construction; “Gillespie’s Algorithm”          | 25        |
| 1.5.5    | Resolvent Computations                                                  | 26        |
| 1.5.6    | Example: A Model of Deposition, Diffusion, and Adsorption               | 27        |
| 1.5.6.1  | $N = 1$                                                                 | 28        |
| 1.5.6.2  | $N = 3$                                                                 | 28        |
| 1.6      | Gibbs and Markov Random Fields                                          | 29        |
| 1.6.1    | Gibbs Random Field                                                      | 29        |
| 1.6.2    | Markov Random Field                                                     | 30        |
| 1.6.3    | Connection Between Gibbs and Markov Random Fields                       | 31        |
| 1.6.4    | Simulation Using Markov Chain Monte Carlo                               | 31        |
| 1.7      | Percolation                                                             | 31        |
| 1.8      | Further Reading                                                         | 33        |
| 1.A      | Appendix: Some Results from Probability Theory                          | 33        |
| 1.A.1    | Set Theory Notation                                                     | 33        |
| 1.A.2    | Probability Spaces                                                      | 34        |
| 1.A.3    | Conditional Probability and Independence of Events                      | 35        |
| 1.A.4    | Random Variables and Expectation                                        | 35        |
| 1.A.5    | Conditional Expectation                                                 | 36        |
|          | References                                                              | 37        |
| <b>2</b> | <b>Monte-Carlo Methods</b>                                              | <b>39</b> |
|          | <i>Kurt Binder</i>                                                      |           |
| 2.1      | Introduction and Overview                                               | 39        |
| 2.2      | Random-Number Generation                                                | 40        |
| 2.2.1    | General Introduction                                                    | 40        |
| 2.2.2    | Properties That a Random-Number Generator (RNG) Should Have             | 40        |
| 2.2.3    | Comments about a Few Frequently Used Generators                         | 41        |
| 2.3      | Simple Sampling of Probability Distributions Using Random Numbers       | 42        |
| 2.3.1    | Numerical Estimation of Known Probability Distributions                 | 42        |
| 2.3.2    | “Importance Sampling” versus “Simple Sampling”                          | 42        |
| 2.3.3    | Monte-Carlo as a Method of Integration                                  | 43        |
| 2.3.4    | Infinite Integration Space                                              | 43        |
| 2.3.5    | Random Selection of Lattice Sites                                       | 44        |
| 2.3.6    | The Self-Avoiding Walk Problem                                          | 44        |
| 2.3.7    | Simple Sampling versus Biased Sampling: the Example of SAWs Continued   | 45        |
| 2.4      | Survey of Applications to Simulation of Transport Processes             | 46        |
| 2.4.1    | The “Shielding Problem”                                                 | 46        |
| 2.4.2    | Diffusion-Limited Aggregation (DLA)                                     | 46        |
| 2.5      | Monte-Carlo Methods in Statistical Thermodynamics: Importance Sampling  | 47        |

|          |                                                                                                           |           |
|----------|-----------------------------------------------------------------------------------------------------------|-----------|
| 2.5.1    | The General Idea of the Metropolis Importance-Sampling Method                                             | 47        |
| 2.5.2    | Comments on the Formulation of a Monte-Carlo Algorithm                                                    | 48        |
| 2.5.3    | The Dynamic Interpretation of the Monte-Carlo Method                                                      | 50        |
| 2.5.4    | Monte-Carlo Study of the Dynamics of Fluctuations Near Equilibrium and of the Approach toward Equilibrium | 51        |
| 2.5.5    | The Choice of Statistical Ensembles                                                                       | 52        |
| 2.6      | Accuracy Problems: Finite-Size Problems, Dynamic Correlation of Errors, Boundary Conditions               | 52        |
| 2.6.1    | Finite-Size–Induced Rounding and Shifting of Phase Transitions                                            | 52        |
| 2.6.2    | Different Boundary Conditions: Simulation of Surfaces and Interfaces                                      | 54        |
| 2.6.3    | Estimation of Statistical Errors                                                                          | 55        |
| 2.7      | Sampling of Free Energies and Free Energy Barriers                                                        | 56        |
| 2.7.1    | Bulk Free Energies                                                                                        | 56        |
| 2.7.2    | Interfacial Free Energies                                                                                 | 57        |
| 2.7.3    | Transition Path Sampling                                                                                  | 57        |
| 2.8      | Quantum Monte-Carlo Techniques                                                                            | 57        |
| 2.8.1    | General Remarks                                                                                           | 57        |
| 2.8.2    | Path-Integral Monte-Carlo Methods                                                                         | 58        |
| 2.8.3    | A Classical Application: the Momentum Distribution of Fluid $^4\text{He}$                                 | 59        |
| 2.8.4    | A Few Qualitative Comments on Fermion Problems                                                            | 59        |
| 2.9      | Lattice Gauge Theory                                                                                      | 61        |
| 2.9.1    | Some Basic Ideas of Lattice Gauge Theory                                                                  | 61        |
| 2.9.2    | A Famous Application                                                                                      | 62        |
| 2.10     | Selected Applications in Classical Statistical Mechanics of Condensed Matter                              | 62        |
| 2.10.1   | Metallurgy and Materials Science                                                                          | 63        |
| 2.10.2   | Polymer Science                                                                                           | 63        |
| 2.10.3   | Surface Physics                                                                                           | 67        |
| 2.11     | Concluding Remarks                                                                                        | 67        |
|          | Glossary                                                                                                  | 68        |
|          | References                                                                                                | 69        |
|          | Further Reading                                                                                           | 71        |
| <b>3</b> | <b>Stochastic Differential Equations</b>                                                                  | <b>73</b> |
|          | <i>Gabriel J. Lord</i>                                                                                    |           |
| 3.1      | Introduction                                                                                              | 73        |
| 3.2      | Brownian Motion / Wiener Process                                                                          | 75        |
| 3.2.1    | White and Colored Noise                                                                                   | 77        |
| 3.2.2    | Approximation of a Brownian Motion                                                                        | 80        |
| 3.3      | Stochastic Integrals                                                                                      | 80        |
| 3.3.1    | Itô Integral                                                                                              | 82        |
| 3.4      | Itô SDEs                                                                                                  | 84        |
| 3.4.1    | Itô Formula and Exact Solutions                                                                           | 86        |
| 3.5      | Stratonovich Integral and SDEs                                                                            | 90        |
| 3.6      | SDEs and Numerical Methods                                                                                | 92        |

|         |                                              |     |
|---------|----------------------------------------------|-----|
| 3.6.1   | Numerical Approximation of Itô SDEs          | 93  |
| 3.6.2   | Numerical Approximation of Stratonovich SDEs | 95  |
| 3.6.3   | Multilevel Monte Carlo                       | 97  |
| 3.7     | SDEs and PDEs                                | 98  |
| 3.7.1   | Fokker–Planck Equation                       | 99  |
| 3.7.2   | Backward Fokker–Planck Equation              | 102 |
| 3.7.2.1 | Sketch of Derivation.                        | 102 |
| 3.7.2.2 | Boundary Conditions                          | 103 |
| 3.7.3   | Filtering                                    | 103 |
|         | Further Reading                              | 104 |
|         | Glossary                                     | 104 |
|         | References                                   | 105 |

## Part II: Discrete Mathematics, Geometry, Topology 109

|          |                                                    |            |
|----------|----------------------------------------------------|------------|
| <b>4</b> | <b>Graph and Network Theory</b>                    | <b>111</b> |
|          | <i>Ernesto Estrada</i>                             |            |
| 4.1      | Introduction                                       | 111        |
| 4.2      | The Language of Graphs and Networks                | 112        |
| 4.2.1    | Graph Operators                                    | 113        |
| 4.2.2    | General Graph Concepts                             | 114        |
| 4.2.3    | Types of Graphs                                    | 115        |
| 4.3      | Graphs in Condensed Matter Physics                 | 115        |
| 4.3.1    | Tight-Binding Models                               | 115        |
| 4.3.1.1  | Nullity and Zero-Energy States                     | 117        |
| 4.3.2    | Hubbard Model                                      | 118        |
| 4.4      | Graphs in Statistical Physics                      | 120        |
| 4.5      | Feynman Graphs                                     | 124        |
| 4.5.1    | Symanzik Polynomials and Spanning Trees            | 125        |
| 4.5.2    | Symanzik Polynomials and the Laplacian Matrix      | 126        |
| 4.5.3    | Symanzik Polynomials and Edge Deletion/Contraction | 128        |
| 4.6      | Graphs and Electrical Networks                     | 129        |
| 4.7      | Graphs and Vibrations                              | 130        |
| 4.7.1    | Graph Vibrational Hamiltonians                     | 131        |
| 4.7.2    | Network of Classical Oscillators                   | 131        |
| 4.7.3    | Network of Quantum Oscillators                     | 133        |
| 4.8      | Random Graphs                                      | 134        |
| 4.9      | Introducing Complex Networks                       | 137        |
| 4.10     | Small-World Networks                               | 138        |
| 4.11     | Degree Distributions                               | 139        |
| 4.11.1   | “Scale-Free” Networks                              | 141        |
| 4.12     | Network Motifs                                     | 142        |
| 4.13     | Centrality Measures                                | 143        |
| 4.14     | Statistical Mechanics of Networks                  | 146        |
| 4.14.1   | Communicability in Networks                        | 147        |

|          |                                            |            |
|----------|--------------------------------------------|------------|
| 4.15     | Communities in Networks                    | 148        |
| 4.16     | Dynamical Processes on Networks            | 150        |
| 4.16.1   | Consensus                                  | 150        |
| 4.16.2   | Synchronization in Networks                | 151        |
| 4.16.3   | Epidemics on Networks                      | 153        |
|          | Glossary                                   | 154        |
|          | References                                 | 155        |
|          | Further Reading                            | 157        |
| <b>5</b> | <b>Group Theory</b>                        | <b>159</b> |
|          | <i>Robert Gilmore</i>                      |            |
| 5.1      | Introduction                               | 159        |
| 5.2      | Precursors to Group Theory                 | 160        |
| 5.2.1    | Classical Geometry                         | 161        |
| 5.2.2    | Dimensional Analysis                       | 161        |
| 5.2.3    | Scaling                                    | 162        |
| 5.2.4    | Dynamical Similarity                       | 163        |
| 5.3      | Groups: Definitions                        | 164        |
| 5.3.1    | Group Axioms                               | 165        |
| 5.3.2    | Isomorphisms and Homomorphisms             | 166        |
| 5.4      | Examples of Discrete Groups                | 166        |
| 5.4.1    | Finite Groups                              | 166        |
| 5.4.1.1  | The Two-Element Group $Z_2$                | 166        |
| 5.4.1.2  | Group of Equilateral Triangle $C_{3v}$     | 167        |
| 5.4.1.3  | Cyclic Groups $C_n$                        | 168        |
| 5.4.1.4  | Permutation Groups $S_n$                   | 168        |
| 5.4.1.5  | Generators and Relations                   | 169        |
| 5.4.2    | Infinite Discrete Groups                   | 169        |
| 5.4.2.1  | Translation Groups: One Dimension          | 169        |
| 5.4.2.2  | Translation Groups: Two Dimensions         | 170        |
| 5.4.2.3  | Space Groups                               | 170        |
| 5.5      | Examples of Matrix Groups                  | 170        |
| 5.5.1    | Translation Groups                         | 170        |
| 5.5.2    | Heisenberg Group $H_3$                     | 171        |
| 5.5.3    | Rotation Group $SO(3)$                     | 171        |
| 5.5.4    | Lorentz Group $SO(3, 1)$                   | 172        |
| 5.6      | Lie Groups                                 | 173        |
| 5.7      | Lie Algebras                               | 175        |
| 5.7.1    | Structure Constants                        | 175        |
| 5.7.2    | Constructing Lie Algebras by Linearization | 175        |
| 5.7.3    | Constructing Lie Groups by Exponentiation  | 177        |
| 5.7.4    | Cartan Metric                              | 178        |
| 5.7.5    | Operator Realizations of Lie Algebras      | 179        |
| 5.7.6    | Disentangling Results                      | 180        |
| 5.8      | Riemannian Symmetric Spaces                | 181        |

|          |                                                 |         |
|----------|-------------------------------------------------|---------|
| 5.9      | Applications in Classical Physics               | 182     |
| 5.9.1    | Principle of Relativity                         | 182     |
| 5.9.2    | Making Mechanics and Electrodynamics Compatible | 182     |
| 5.9.3    | Gravitation                                     | 184     |
| 5.9.4    | Reflections                                     | 185     |
| 5.10     | Linear Representations                          | 185     |
| 5.10.1   | Maps to Matrices                                | 185     |
| 5.10.2   | Group Element–Matrix Element Duality            | 186     |
| 5.10.3   | Classes and Characters                          | 187     |
| 5.10.4   | Fourier Analysis on Groups                      | 187     |
| 5.10.4.1 | Remark on Terminology                           | 188     |
| 5.10.5   | Irreps of $SU(2)$                               | 188     |
| 5.10.6   | Crystal Field Theory                            | 190     |
| 5.11     | Symmetry Groups                                 | 190     |
| 5.12     | Dynamical Groups                                | 194     |
| 5.12.1   | Conformal Symmetry                              | 194     |
| 5.12.2   | Atomic Shell Structure                          | 195     |
| 5.12.3   | Nuclear Shell Structure                         | 195     |
| 5.12.4   | Dynamical Models                                | 198     |
| 5.13     | Gauge Theory                                    | 199     |
| 5.14     | Group Theory and Special Functions              | 202     |
| 5.14.1   | Summary of Some Properties                      | 202     |
| 5.14.2   | Relation with Lie Groups                        | 202     |
| 5.14.3   | Spherical Harmonics and $SO(3)$                 | 203     |
| 5.14.4   | Differential and Recursion Relations            | 204     |
| 5.14.5   | Differential Equation                           | 205     |
| 5.14.6   | Addition Theorems                               | 206     |
| 5.14.7   | Generating Functions                            | 206     |
| 5.15     | Summary                                         | 207     |
|          | Glossary                                        | 208     |
|          | References                                      | 210     |
| <br>6    | <b>Algebraic Topology</b>                       | <br>211 |
|          | <i>Vanessa Robins</i>                           |         |
| 6.1      | Introduction                                    | 211     |
| 6.2      | Homotopy Theory                                 | 212     |
| 6.2.1    | Homotopy of Paths                               | 212     |
| 6.2.2    | The Fundamental Group                           | 213     |
| 6.2.3    | Homotopy of Spaces                              | 215     |
| 6.2.4    | Examples                                        | 215     |
| 6.2.5    | Covering Spaces                                 | 216     |
| 6.2.6    | Extensions and Applications                     | 217     |
| 6.3      | Homology                                        | 218     |
| 6.3.1    | Simplicial Complexes                            | 219     |
| 6.3.2    | Simplicial Homology Groups                      | 219     |

|        |                                               |     |
|--------|-----------------------------------------------|-----|
| 6.3.3  | Basic Properties of Homology Groups           | 221 |
| 6.3.4  | Homological Algebra                           | 222 |
| 6.3.5  | Other Homology Theories                       | 224 |
| 6.4    | Cohomology                                    | 224 |
| 6.4.1  | De Rham Cohomology                            | 226 |
| 6.5    | Morse Theory                                  | 226 |
| 6.5.1  | Basic Results                                 | 226 |
| 6.5.2  | Extensions and Applications                   | 228 |
| 6.5.3  | Forman's Discrete Morse Theory                | 229 |
| 6.6    | Computational Topology                        | 230 |
| 6.6.1  | The Fundamental Group of a Simplicial Complex | 230 |
| 6.6.2  | Smith Normal form for Homology                | 231 |
| 6.6.3  | Persistent Homology                           | 232 |
| 6.6.4  | Cell Complexes from Data                      | 234 |
|        | Further Reading                               | 236 |
|        | References                                    | 236 |
| 7      | <b>Special Functions</b>                      | 239 |
|        | <i>Chris Athorne</i>                          |     |
| 7.1    | Introduction                                  | 239 |
| 7.2    | Discrete Symmetry                             | 241 |
| 7.2.1  | Symmetries                                    | 241 |
| 7.2.2  | Coxeter Groups                                | 243 |
| 7.2.3  | Symmetric Functions                           | 244 |
| 7.2.4  | Invariants of Coxeter Groups                  | 246 |
| 7.2.5  | Fuchsian Equations                            | 247 |
| 7.3    | Continuous Symmetry                           | 250 |
| 7.3.1  | Lie Groups and Lie Algebras                   | 250 |
| 7.3.2  | Representations                               | 251 |
| 7.3.3  | The Laplace Operator                          | 253 |
| 7.3.4  | Spherical Harmonics                           | 255 |
| 7.3.5  | Separation of Variables                       | 256 |
| 7.3.6  | Bessel Functions                              | 256 |
| 7.3.7  | Addition Laws                                 | 258 |
| 7.3.8  | The Hypergeometric Equation                   | 258 |
| 7.3.9  | Orthogonality                                 | 260 |
| 7.3.10 | Orthogonal Polynomials                        | 260 |
| 7.4    | Factorization                                 | 261 |
| 7.4.1  | The Bessel Equation                           | 262 |
| 7.4.2  | Hermite                                       | 262 |
| 7.4.3  | Legendre                                      | 263 |
| 7.4.4  | "Factorization" of PDEs                       | 265 |
| 7.4.5  | Dunkl Operators                               | 267 |
| 7.5    | Special Functions Without Symmetry            | 268 |
| 7.5.1  | Airy Functions                                | 268 |

|          |                                        |            |
|----------|----------------------------------------|------------|
| 7.5.1.1  | Stokes Phenomenon                      | 269        |
| 7.5.2    | Liouville Theory                       | 269        |
| 7.5.3    | Differential Galois Theory             | 271        |
| 7.6      | Nonlinear Special Functions            | 272        |
| 7.6.1    | Weierstraß Elliptic Functions          | 272        |
| 7.6.1.1  | Lamé Equations                         | 277        |
| 7.6.2    | Jacobian Elliptic Functions            | 277        |
| 7.6.3    | Theta Functions                        | 278        |
| 7.6.4    | Painlevé Transcendents                 | 280        |
| 7.7      | Discrete Special Functions             | 283        |
| 7.7.1    | $\partial$ - $\delta$ Theory           | 283        |
| 7.7.2    | Quantum Groups                         | 283        |
| 7.7.3    | Difference Operators                   | 284        |
| 7.7.4    | $q$ -Hermite Polynomials               | 285        |
| 7.7.5    | Discrete Painlevé Equations            | 286        |
|          | References                             | 286        |
| <b>8</b> | <b>Computer Algebra</b>                | <b>291</b> |
|          | <i>James H. Davenport</i>              |            |
| 8.1      | Introduction                           | 291        |
| 8.2      | Computer Algebra Systems               | 292        |
| 8.3      | "Elementary" Algorithms                | 292        |
| 8.3.1    | Representation of Polynomials          | 292        |
| 8.3.2    | Greatest Common Divisors               | 294        |
| 8.3.2.1  | Intermediate Expression Swell          | 294        |
| 8.3.2.2  | Sparsity                               | 295        |
| 8.3.3    | Square-free Decomposition              | 295        |
| 8.3.4    | Extended Euclidean Algorithm           | 296        |
| 8.4      | Advanced Algorithms                    | 296        |
| 8.4.1    | Modular Algorithms—Integer             | 296        |
| 8.4.2    | Modular Algorithms—Polynomial          | 297        |
| 8.4.3    | The Challenge of Factorization         | 298        |
| 8.4.4    | $p$ -adic Algorithms—Integer           | 300        |
| 8.4.5    | $p$ -adic Algorithms—Polynomial        | 301        |
| 8.5      | Solving Polynomial Systems             | 301        |
| 8.5.1    | Solving One Polynomial                 | 301        |
| 8.5.2    | Real Roots                             | 303        |
| 8.5.3    | Linear Systems                         | 304        |
| 8.5.4    | Multivariate Systems                   | 304        |
| 8.5.5    | Gröbner Bases                          | 305        |
| 8.5.6    | Regular Chains                         | 308        |
| 8.6      | Integration                            | 308        |
| 8.6.1    | Rational Functions                     | 308        |
| 8.6.2    | More Complicated Functions             | 310        |
| 8.6.3    | Linear Ordinary Differential Equations | 311        |

|          |                                                    |            |
|----------|----------------------------------------------------|------------|
| 8.7      | Interpreting Formulae as Functions                 | 312        |
| 8.7.1    | Fundamental Theorem of Calculus Revisited          | 312        |
| 8.7.2    | Simplification of Functions                        | 313        |
| 8.7.3    | Real Problems                                      | 314        |
| 8.8      | Conclusion                                         | 315        |
|          | References                                         | 315        |
| <b>9</b> | <b>Differentiable Manifolds</b>                    | <b>319</b> |
|          | <i>Marcelo Epstein</i>                             |            |
| 9.1      | Introduction                                       | 319        |
| 9.2      | Topological Spaces                                 | 319        |
| 9.2.1    | Definition                                         | 319        |
| 9.2.2    | Continuity                                         | 320        |
| 9.2.3    | Further Topological Notions                        | 320        |
| 9.3      | Topological Manifolds                              | 320        |
| 9.3.1    | Motivation                                         | 320        |
| 9.3.2    | Definition                                         | 321        |
| 9.3.3    | Coordinate Charts                                  | 321        |
| 9.3.4    | Maps and Their Representations                     | 321        |
| 9.3.5    | A Physical Application                             | 322        |
| 9.3.6    | Topological Manifolds with Boundary                | 323        |
| 9.4      | Differentiable Manifolds                           | 323        |
| 9.4.1    | Motivation                                         | 323        |
| 9.4.2    | Definition                                         | 323        |
| 9.4.3    | Differentiable Maps                                | 324        |
| 9.4.4    | Tangent Vectors                                    | 324        |
| 9.4.5    | Brief Review of Vector Spaces                      | 325        |
| 9.4.5.1  | Definition                                         | 325        |
| 9.4.5.2  | Linear Independence and Dimension                  | 325        |
| 9.4.5.3  | The Dual Space                                     | 326        |
| 9.4.6    | Tangent and Cotangent Spaces                       | 326        |
| 9.4.7    | The Tangent and Cotangent Bundles                  | 327        |
| 9.4.8    | A Physical Interpretation                          | 328        |
| 9.4.9    | The Differential of a Map                          | 328        |
| 9.5      | Vector Fields and the Lie Bracket                  | 330        |
| 9.5.1    | Vector Fields                                      | 330        |
| 9.5.2    | The Lie Bracket                                    | 330        |
| 9.5.3    | A Physical Interpretation: Continuous Dislocations | 331        |
| 9.5.4    | Pushforwards                                       | 334        |
| 9.6      | Review of Tensor Algebra                           | 334        |
| 9.6.1    | Linear Operators and the Tensor Product            | 334        |
| 9.6.2    | Symmetry and Skew Symmetry                         | 337        |
| 9.6.3    | The Algebra of Tensors on a Vector Space           | 337        |
| 9.6.4    | Exterior Algebra                                   | 339        |
| 9.7      | Forms and General Tensor Fields                    | 341        |

|         |                                                            |     |
|---------|------------------------------------------------------------|-----|
| 9.7.1   | 1-Forms                                                    | 341 |
| 9.7.2   | Pullbacks                                                  | 341 |
| 9.7.3   | Tensor Bundles                                             | 342 |
| 9.7.4   | The Exterior Derivative                                    | 343 |
| 9.8     | Symplectic Geometry                                        | 345 |
| 9.8.1   | Symplectic Vector Spaces                                   | 345 |
| 9.8.2   | Symplectic Manifolds                                       | 345 |
| 9.8.3   | Hamiltonian Systems                                        | 346 |
| 9.9     | The Lie Derivative                                         | 347 |
| 9.9.1   | The Flow of a Vector Field                                 | 347 |
| 9.9.2   | One-parameter Groups of Transformations Generated by Flows | 348 |
| 9.9.3   | The Lie Derivative                                         | 348 |
| 9.9.3.1 | The Lie Derivative of a Scalar                             | 349 |
| 9.9.3.2 | The Lie Derivative of a Vector Field                       | 350 |
| 9.9.3.3 | The Lie Derivative of a 1-form                             | 350 |
| 9.9.3.4 | The Lie Derivative of Arbitrary Tensor Fields              | 350 |
| 9.9.3.5 | The Lie Derivative in Components                           | 351 |
|         | Further Reading                                            | 351 |
| 10      | Topics in Differential Geometry                            | 353 |
|         | <i>Marcelo Epstein</i>                                     |     |
| 10.1    | Integration                                                | 353 |
| 10.1.1  | Integration of $n$ -Forms in $\mathbb{R}^n$                | 353 |
| 10.1.2  | Integration of Forms on Oriented Manifolds                 | 354 |
| 10.1.3  | Stokes' Theorem                                            | 355 |
| 10.2    | Fluxes in Continuum Physics                                | 355 |
| 10.2.1  | Extensive-Property Densities                               | 355 |
| 10.2.2  | Balance Laws, Flux Densities, and Sources                  | 356 |
| 10.2.3  | Flux Forms and Cauchy's Formula                            | 356 |
| 10.2.4  | Differential Expression of the Balance Law                 | 357 |
| 10.3    | Lie Groups                                                 | 358 |
| 10.3.1  | Definition                                                 | 358 |
| 10.3.2  | Group Actions                                              | 358 |
| 10.3.3  | One-Parameter Subgroups                                    | 360 |
| 10.3.4  | Left- and Right-Invariant Vector Fields on a Lie Group     | 361 |
| 10.4    | Fiber Bundles                                              | 361 |
| 10.4.1  | Introduction                                               | 361 |
| 10.4.2  | Definition                                                 | 361 |
| 10.4.3  | Simultaneity in Classical Mechanics                        | 363 |
| 10.4.4  | Adapted Coordinate Systems                                 | 363 |
| 10.4.5  | The Bundle of Linear Frames                                | 363 |
| 10.4.6  | Bodies with Microstructure                                 | 364 |
| 10.4.7  | Principal Bundles                                          | 364 |
| 10.4.8  | Associated Bundles                                         | 365 |
| 10.5    | Connections                                                | 367 |

|         |                                                 |     |
|---------|-------------------------------------------------|-----|
| 10.5.1  | Introduction                                    | 367 |
| 10.5.2  | Ehresmann Connection                            | 368 |
| 10.5.3  | Parallel Transport along a Curve                | 368 |
| 10.5.4  | Connections in Principal Bundles                | 369 |
| 10.5.5  | Distributions and the Theorem of Frobenius      | 370 |
| 10.5.6  | Curvature                                       | 371 |
| 10.5.7  | Cartan's Structural Equation                    | 372 |
| 10.5.8  | Bianchi Identities                              | 372 |
| 10.5.9  | Linear Connections                              | 372 |
| 10.5.10 | The Canonical 1-Form                            | 373 |
| 10.5.11 | The Christoffel Symbols                         | 374 |
| 10.5.12 | Parallel Transport and the Covariant Derivative | 374 |
| 10.5.13 | Curvature and Torsion                           | 375 |
| 10.6    | Riemannian Manifolds                            | 377 |
| 10.6.1  | Inner-Product Spaces                            | 377 |
| 10.6.2  | Riemannian Manifolds                            | 379 |
| 10.6.3  | Riemannian Connections                          | 380 |
|         | Further Reading                                 | 380 |

### Part III: Analysis 383

|          |                                  |     |
|----------|----------------------------------|-----|
| 11       | <b>Dynamical Systems</b>         | 385 |
|          | <i>David A.W. Barton</i>         |     |
| 11.1     | Introduction                     | 385 |
| 11.1.1   | Definition of a Dynamical System | 385 |
| 11.1.2   | Invariant Sets                   | 386 |
| 11.2     | Equilibria                       | 386 |
| 11.2.1   | Definition and Calculation       | 386 |
| 11.2.2   | Stability                        | 387 |
| 11.2.3   | Linearization                    | 387 |
| 11.2.4   | Lyapunov Functions               | 388 |
| 11.2.5   | Topological Equivalence          | 389 |
| 11.2.6   | Manifolds                        | 390 |
| 11.2.7   | Local Bifurcations               | 391 |
| 11.2.8   | Saddle-Node Bifurcation          | 392 |
| 11.2.9   | Hopf Bifurcation                 | 393 |
| 11.2.10  | Pitchfork Bifurcation            | 396 |
| 11.2.11  | Center Manifolds                 | 398 |
| 11.3     | Limit Cycles                     | 399 |
| 11.3.1   | Definition and Calculation       | 399 |
| 11.3.1.1 | Harmonic Balance Method          | 399 |
| 11.3.1.2 | Numerical Shooting               | 400 |
| 11.3.1.3 | Collocation                      | 401 |
| 11.3.2   | Linearization                    | 402 |
| 11.3.3   | Topological Equivalence          | 403 |

|           |                                                         |            |
|-----------|---------------------------------------------------------|------------|
| 11.3.4    | Manifolds                                               | 403        |
| 11.3.5    | Local Bifurcations                                      | 404        |
| 11.3.6    | Period-Doubling Bifurcation                             | 404        |
| 11.4      | Numerical Continuation                                  | 405        |
| 11.4.1    | Natural Parameter Continuation                          | 405        |
| 11.4.2    | Pseudo-Arc-Length Continuation                          | 407        |
| 11.4.3    | Continuation of Bifurcations                            | 407        |
|           | References                                              | 408        |
| <b>12</b> | <b>Perturbation Methods</b>                             | <b>411</b> |
|           | <i>James Murdock</i>                                    |            |
| 12.1      | Introduction                                            | 411        |
| 12.2      | Basic Concepts                                          | 412        |
| 12.2.1    | Perturbation Methods versus Numerical Methods           | 412        |
| 12.2.2    | Perturbation Parameters                                 | 413        |
| 12.2.3    | Perturbation Series                                     | 415        |
| 12.2.4    | Uniformity                                              | 416        |
| 12.3      | Nonlinear Oscillations and Dynamical Systems            | 418        |
| 12.3.1    | Rest Points and Regular Perturbations                   | 418        |
| 12.3.2    | Simple Nonlinear Oscillators and Lindstedt's Method     | 419        |
| 12.3.3    | Averaging Method for Single-Frequency Systems           | 422        |
| 12.3.4    | Multifrequency Systems and Hamiltonian Systems          | 424        |
| 12.3.5    | Multiple-Scale Method                                   | 426        |
| 12.3.6    | Normal Forms                                            | 427        |
| 12.3.7    | Perturbation of Invariant Manifolds; Melnikov Functions | 429        |
| 12.4      | Initial and Boundary Layers                             | 429        |
| 12.4.1    | Multiple-Scale Method for Initial Layer Problems        | 429        |
| 12.4.2    | Matching for Initial Layer Problems                     | 431        |
| 12.4.3    | Slow-Fast Systems                                       | 432        |
| 12.4.4    | Boundary Layer Problems                                 | 433        |
| 12.4.5    | WKB Method                                              | 434        |
| 12.4.6    | Fluid Flow                                              | 434        |
| 12.5      | The "Renormalization Group" Method                      | 435        |
| 12.5.1    | Initial and Boundary Layer Problems                     | 436        |
| 12.5.2    | Nonlinear Oscillations                                  | 439        |
| 12.5.3    | WKB Problems                                            | 441        |
| 12.6      | Perturbations of Matrices and Spectra                   | 442        |
|           | Glossary                                                | 444        |
|           | References                                              | 446        |
|           | Further Reading                                         | 447        |
| <b>13</b> | <b>Functional Analysis</b>                              | <b>449</b> |
|           | <i>Pavel Exner</i>                                      |            |
| 13.1      | Banach Space and Operators on Them                      | 449        |
| 13.1.1    | Vector and Normed Spaces                                | 449        |

|           |                                           |            |
|-----------|-------------------------------------------|------------|
| 13.1.2    | Operators on Banach Spaces                | 450        |
| 13.1.3    | Spectra of Closed Operators               | 452        |
| 13.2      | Hilbert Spaces                            | 452        |
| 13.2.1    | Hilbert-Space Geometry                    | 452        |
| 13.2.2    | Direct Sums and Tensor Products           | 454        |
| 13.3      | Bounded Operators on Hilbert Spaces       | 454        |
| 13.3.1    | Hermitean Operators                       | 454        |
| 13.3.2    | Unitary Operators                         | 455        |
| 13.3.3    | Compact Operators                         | 456        |
| 13.3.4    | Schatten Classes                          | 456        |
| 13.4      | Unbounded Operators                       | 457        |
| 13.4.1    | Operator Adjoint and Closure              | 457        |
| 13.4.2    | Normal and Self-Adjoint Operators         | 458        |
| 13.4.3    | Tensor Products of Operators              | 460        |
| 13.4.4    | Self-Adjoint Extensions                   | 460        |
| 13.5      | Spectral Theory of Self-Adjoint Operators | 462        |
| 13.5.1    | Functional Calculus                       | 462        |
| 13.5.2    | Spectral Theorem                          | 463        |
| 13.5.3    | More about Spectral Properties            | 465        |
| 13.5.4    | Groups of Unitary Operators               | 467        |
| 13.6      | Some Applications in Quantum Mechanics    | 468        |
| 13.6.1    | Schrödinger Operators                     | 468        |
| 13.6.2    | Scattering Theory                         | 470        |
|           | Glossary                                  | 472        |
|           | References                                | 473        |
| <b>14</b> | <b>Numerical Analysis</b>                 | <b>475</b> |
|           | <i>Lyonell Boulton</i>                    |            |
| 14.1      | Introduction                              | 475        |
| 14.2      | Algebraic Equations                       | 476        |
| 14.2.1    | Nonlinear Scalar Equations                | 476        |
| 14.2.2    | Nonlinear Systems                         | 477        |
| 14.2.3    | Numerical Minimization                    | 479        |
| 14.3      | Finite-Dimensional Linear Systems         | 480        |
| 14.3.1    | Direct Methods and Matrix Factorization   | 480        |
| 14.3.2    | Iteration Methods for Linear Problems     | 482        |
| 14.3.3    | Computing Eigenvalues of Finite Matrices  | 485        |
| 14.4      | Approximation of Continuous Data          | 487        |
| 14.4.1    | Lagrange Interpolation                    | 487        |
| 14.4.2    | The Interpolation Error                   | 487        |
| 14.4.3    | Hermite Interpolation                     | 488        |
| 14.4.4    | Piecewise Polynomial Interpolation        | 489        |
| 14.5      | Initial Value Problems                    | 491        |
| 14.5.1    | One-Step Methods                          | 491        |
| 14.5.2    | Multistep Methods                         | 492        |

|           |                                                                                                        |            |
|-----------|--------------------------------------------------------------------------------------------------------|------------|
| 14.5.3    | Runge–Kutta Methods                                                                                    | 494        |
| 14.5.4    | Stability and Global Stability                                                                         | 495        |
| 14.6      | Spectral Problems                                                                                      | 496        |
| 14.6.1    | The Infinite-Dimensional min–max Principle                                                             | 497        |
| 14.6.2    | Systems Confined to a Box                                                                              | 498        |
| 14.6.3    | The Case of Unconfined Systems                                                                         | 499        |
|           | Further Reading                                                                                        | 499        |
|           | References                                                                                             | 500        |
| <b>15</b> | <b>Mathematical Transformations</b>                                                                    | <b>503</b> |
|           | <i>Des McGhee, Rainer Picard, Sascha Trostorf, and Marcus Waurick</i>                                  |            |
| 15.1      | What are Transformations and Why are They Useful?                                                      | 503        |
| 15.2      | The Fourier Series Transformations                                                                     | 506        |
| 15.2.1    | The Abstract Fourier Series                                                                            | 506        |
| 15.2.2    | The Classical Fourier Series                                                                           | 507        |
| 15.2.3    | The Fourier Series Transformation in $L^2(S_C(0, 1))$                                                  | 509        |
| 15.3      | The $z$ -Transformation                                                                                | 509        |
| 15.4      | The Fourier–Laplace Transformation                                                                     | 510        |
| 15.4.1    | Convolutions as Functions of $\partial_\rho$                                                           | 512        |
| 15.4.1.1  | Functions of $\partial_\rho$                                                                           | 512        |
| 15.4.1.2  | Convolutions                                                                                           | 513        |
| 15.4.2    | The Fourier–Plancherel Transformation                                                                  | 515        |
| 15.5      | The Fourier–Laplace Transformation and Distributions                                                   | 515        |
| 15.5.1    | Impulse Response                                                                                       | 517        |
| 15.5.2    | Shannon’s Sampling Theorem                                                                             | 517        |
| 15.6      | The Fourier-Sine and Fourier-Cosine Transformations                                                    | 518        |
| 15.7      | The Hartley Transformations $H_\pm$                                                                    | 519        |
| 15.8      | The Mellin Transformation                                                                              | 520        |
| 15.9      | Higher-Dimensional Transformations                                                                     | 521        |
| 15.10     | Some Other Important Transformations                                                                   | 522        |
| 15.10.1   | The Hadamard Transformation                                                                            | 522        |
| 15.10.2   | The Hankel Transformation                                                                              | 523        |
| 15.10.3   | The Radon Transformation                                                                               | 523        |
|           | References                                                                                             | 525        |
| <b>16</b> | <b>Partial Differential Equations</b>                                                                  | <b>527</b> |
|           | <i>Des McGhee, Rainer Picard, Sascha Trostorf, and Marcus Waurick</i>                                  |            |
| 16.1      | What are Partial Differential Equations?                                                               | 527        |
| 16.2      | Partial Differential Equations in $\mathbb{R}^{n+1}$ , $n \in \mathbb{N}$ , with Constant Coefficients | 529        |
| 16.2.1    | Evolutionarity                                                                                         | 530        |
| 16.2.2    | An Outline of Distribution Theory                                                                      | 531        |
| 16.2.3    | Integral Transformation Methods as a Solution Tool                                                     | 533        |
| 16.3      | Partial Differential Equations of Mathematical Physics                                                 | 537        |
| 16.4      | Initial-Boundary Value Problems of Mathematical Physics                                                | 540        |

|          |                                                                  |     |
|----------|------------------------------------------------------------------|-----|
| 16.4.1   | Maxwell's Equations                                              | 542 |
| 16.4.2   | Viscoelastic Solids                                              | 543 |
| 16.4.2.1 | The Kelvin–Voigt Model                                           | 543 |
| 16.4.2.2 | The Poynting–Thomson Model (The Linear Standard Model)           | 544 |
| 16.5     | Coupled Systems                                                  | 544 |
| 16.5.1   | Thermoelasticity                                                 | 545 |
| 16.5.2   | Piezoelectromagnetism                                            | 546 |
| 16.5.3   | The Extended Maxwell System and its Uses                         | 547 |
|          | References                                                       | 548 |
| <br>     |                                                                  |     |
| 17       | <b>Calculus of Variations</b>                                    | 551 |
|          | <i>Tomáš Roubíček</i>                                            |     |
| 17.1     | Introduction                                                     | 551 |
| 17.2     | Abstract Variational Problems                                    | 551 |
| 17.2.1   | Smooth (Differentiable) Case                                     | 552 |
| 17.2.2   | Nonsmooth Case                                                   | 554 |
| 17.2.3   | Constrained Problems                                             | 555 |
| 17.2.4   | Evolutionary Problems                                            | 556 |
| 17.2.4.1 | Variational Principles                                           | 556 |
| 17.2.4.2 | Evolution Variational Inequalities                               | 559 |
| 17.2.4.3 | Recursive Variational Problems Arising by Discretization in Time | 560 |
| 17.3     | Variational Problems on Specific Function Spaces                 | 562 |
| 17.3.1   | Sobolev Spaces                                                   | 562 |
| 17.3.2   | Steady-State Problems                                            | 563 |
| 17.3.2.1 | Second Order Systems of Equations                                | 564 |
| 17.3.2.2 | Fourth Order Systems                                             | 568 |
| 17.3.2.3 | Variational Inequalities                                         | 570 |
| 17.3.3   | Some Examples                                                    | 571 |
| 17.3.3.1 | Nonlinear Heat-Transfer Problem                                  | 571 |
| 17.3.3.2 | Elasticity at Large Strains                                      | 572 |
| 17.3.3.3 | Small-Strain Elasticity, Lamé System, Signorini Contact          | 573 |
| 17.3.3.4 | Sphere-Valued Harmonic Maps                                      | 574 |
| 17.3.3.5 | Saddle-Point-Type Problems                                       | 575 |
| 17.3.4   | Evolutionary Problems                                            | 575 |
| 17.4     | Miscellaneous                                                    | 576 |
| 17.4.1   | Numerical Approximation                                          | 576 |
| 17.4.2   | Extension of Variational Problems                                | 577 |
| 17.4.3   | $\Gamma$ -Convergence                                            | 581 |
|          | Glossary                                                         | 582 |
|          | Further Reading                                                  | 584 |
|          | References                                                       | 586 |
| <br>     |                                                                  |     |
|          | <b>Index</b>                                                     | 589 |