Stochastic Modelling of Reaction–Diffusion Processes

RADEK ERBAN
University of Oxford

S. JONATHAN CHAPMAN
University of Oxford
# Contents

## Preface

Preface ix

## 1 Stochastic Simulation of Chemical Reactions

1.1 Stochastic Simulation of Degradation 1
1.2 Stochastic Simulation of Production and Degradation 8
1.3 Higher-Order Chemical Reactions 14
1.4 Stochastic Simulation of Dimerization 16
1.5 Gillespie Algorithm 25
Exercises 29

## 2 Deterministic versus Stochastic Modelling

2.1 Systems with Multiple Favourable States 34
2.2 Self-Induced Stochastic Resonance 37
2.3 Stochastic Focusing 42
2.4 Designing Stochastic Chemical Systems 49
Exercises 55

## 3 Stochastic Differential Equations

3.1 A Computational Definition of SDE 60
3.2 Examples of SDEs 62
3.3 Fokker–Planck Equation 66
3.4 Boundary Conditions on the Fokker–Planck Equation 72
3.5 Kolmogorov Backward Equation 75
3.6 SDEs with Multiple Favourable States 76
3.7 Chemical Fokker–Planck Equation 80
3.8 Analysis of Problem from Section 2.1 85
3.9 Analysis of Problem from Section 2.2 88
Exercises 92

## 4 Diffusion

4.1 Diffusion Modelled by SDEs 96
4.2 Compartment-Based Approach to Diffusion 100

© in this web service Cambridge University Press  www.cambridge.org
4.3 Diffusion and Velocity-Jump Processes 107
4.4 Diffusion to Adsorbing Surfaces 117
4.5 Reactive Boundary Conditions 125
4.6 Einstein–Smoluchowski Relation 130
Exercises 133

5 Efficient Stochastic Modelling of Chemical Reactions 137
5.1 A Simple Multiscale Problem 139
5.2 Multiscale SSA with Partial Equilibrium Assumption 142
5.3 Multiscale Modelling 148
5.4 First-Reaction SSA 151
5.5 Exact Efficient SSAs 152
Exercises 157

6 Stochastic Reaction–Diffusion Models 160
6.1 A Compartment-Based Reaction–Diffusion Algorithm 161
6.2 A Reaction–Diffusion SSA Based on the SDE Model of Diffusion 164
6.3 Compartment-Based SSA for Higher-Order Reactions 166
6.4 A Choice of Compartment Size h 169
6.5 Molecular-Based Approaches for Second-Order Reactions 174
6.6 Reaction Radius and Reaction Probability 177
6.7 Modelling Reversible Reactions 183
6.8 Biological Pattern Formation 186
Exercises 190

7 SSAs for Reaction–Diffusion–Advection Processes 192
7.1 SSAs for Diffusion–Advection Processes 193
7.2 Reaction–Diffusion–Advection SSAs 196
7.3 Bacterial Chemotaxis 199
7.4 Collective Behaviour of Locusts 206
7.5 Ions and Ion Channels 211
7.6 Metropolis–Hastings Algorithm 216
Exercises 222

8 Microscopic Models of Brownian Motion 226
8.1 One-Particle Solvent Model 227
8.2 Generalized Langevin Equation 233
8.3 Solvent as Harmonic Oscillators 242
8.4 Solvent as Points Colliding with the Diffusing Particle 246
8.5 Forces Between Atoms and Molecules 252
## Contents

8.6 Molecular Dynamics ........................................... vii
Exercises .................................................................. 257

9 **Multiscale and Multi-Resolution Methods** .......... 268
9.1 Coupling SDE-Based and Compartment-Based Models ....... 270
9.2 Coupling Molecular Dynamics with Langevin Dynamics .......... 278
9.3 Multi-Resolution Molecular and Brownian Dynamics .......... 285
Exercises .................................................................. 289

Appendix .................................................................. 293
*Appendix A* Deterministic Modelling of Chemical Reactions .... 293
*Appendix B* Discrete Probability Distributions .................. 295
*Appendix C* Continuous Probability Distributions .............. 296

References .................................................................. 297
Index ....................................................................... 305