

Contents

1	Introduction — 1
2	Random walk algorithms for solving integral equations — 8
2.1	Conventional Monte Carlo scheme — 8
2.2	Biased estimators — 14
2.3	Linear-fractional transformations and their relations to iterative processes — 16
2.4	Asymptotically unbiased estimators based on singular approximations — 23
2.5	Integral equation of the first kind — 30
3	Random walk-on-boundary algorithms for the Laplace equation — 35
3.1	Newton potentials and boundary integral equations of the electrostatics — 35
3.2	The interior Dirichlet problem and isotropic random walk-on-boundary process — 37
3.3	Solution of the Neumann problem — 43
3.4	Random estimators for the exterior Dirichlet problem — 50
3.5	Third BVP and alternative methods of solving the Dirichlet problem — 55
3.6	Inhomogeneous problems — 60
3.7	Continuity BVP — 62
3.7.1	Walk on boundary for the continuity problem — 64
3.8	Calculation of the solution derivatives near the boundary — 65
3.9	Normal derivative of a double-layer potential — 69
4	Walk-on-boundary algorithms for the heat equation — 72
4.1	Heat potentials and Volterra boundary integral equations — 72
4.2	Nonstationary walk-on-boundary process — 74
4.3	The Dirichlet problem — 77
4.4	The Neumann problem — 80
4.5	Third BVP — 81
4.6	Unbiasedness and variance of the walk-on-boundary algorithms — 85
4.7	The cost of the walk-on-boundary algorithms — 90
4.8	Inhomogeneous heat equation — 92
4.9	Calculation of derivatives on the boundary — 94

5	Spatial problems of elasticity — 99
5.1	Elastopotentials and systems of boundary integral equations of the elasticity theory — 99
5.2	First BVP and estimators for singular integrals — 102
5.3	Other BVPs for the Lamé equations and regular integral equations — 107
6	Variants of the random walk on boundary for solving stationary potential problems — 110
6.1	The Robin problem and the ergodic theorem — 110
6.1.1	Monte Carlo estimator for computing capacitance — 113
6.1.2	Computing charge density — 114
6.2	Stationary diffusion equation with absorption — 115
6.3	Multiply connected domains — 116
6.4	Stabilization method — 126
6.5	Nonlinear Poisson equation — 128
7	Splitting and survival probabilities in random walk methods and applications — 131
7.1	Introduction — 131
7.2	Survival probability for a sphere and an interval — 132
7.3	The reciprocity theorem for particle collection in the general case of Robin boundary conditions — 135
7.4	Splitting and survival probabilities — 138
7.4.1	Splitting probabilities for a finite interval and nanowire growth simulation — 138
7.4.2	Survival probability for a disc and the exterior of circular cylinder — 140
7.4.3	Splitting probabilities for concentric spheres and annulus — 141
7.5	Cathodoluminescence — 145
7.5.1	The random WOS and hemispheres algorithm — 147
7.6	Conclusion and discussion — 152
8	A random WOS-based KMC method for electron–hole recombinations — 153
8.1	Introduction — 153
8.2	The mean field equations — 155
8.3	Monte Carlo Algorithms — 157
8.3.1	Random WOS for the diffusion simulation — 157
8.3.2	Radiative and nonradiative recombination in the absence of diffusion — 160

8.3.3	General case of radiative and nonradiative recombination in the presence of diffusion —	161
8.4	Simulation results and comparison —	162
8.5	Summary and conclusion —	165
9	Monte Carlo methods for computing macromolecules properties and solving related problems —	166
9.1	Diffusion-limited reaction rate and other integral parameters —	167
9.1.1	Formulation of the problem —	167
9.1.2	Capacitance calculations —	170
9.2	Walk in subdomains and efficient simulation of Brownian motion exit points —	172
9.3	Monte Carlo algorithms for boundary-value conditions containing the normal derivative —	174
9.3.1	WOS algorithm for mixed boundary-value conditions —	174
9.3.2	Mean-value relation at a point on the boundary —	176
9.3.3	Construction of the algorithm and its convergence —	177
9.4	Continuity BVP —	179
9.4.1	Monte Carlo method —	180
9.4.2	Integral representation at a boundary point —	182
9.4.3	Estimate for the boundary value —	184
9.4.4	Construction of the algorithm and its convergence —	185
9.5	Computing macromolecule energy —	187
9.5.1	Mathematical model and computational results —	188

Bibliography —	193
-----------------------	------------