

Index

a

- acceptance probability
 - in a rejection method with combination of variables 75
 - in rejection methods 84, 85–87, 89–90, 93
 - – exercises 95–96
 - in rejection with repetition methods
 - – simple case 97, 99–100
 - – relation with correlation function 102
 - – influence in the error 102–103
 - – low average acceptance 103–104
 - – dynamical methods 104–107
 - – – Glauber 108
 - – – Metropolis et al. 107–108
 - – – Gaussian distribution 108–110
 - – – – Poisson 111–112
 - – – – multidimensional distributions 112–116
 - – – Heat-bath method 116
 - – – exercises 121–123
 - in applications to statistical mechanics 128–130
 - – interacting particles 132, 133
 - – Ising model 138, 140, 143, 146
 - – lattice Φ^4 154
 - – at the critical region 162
 - – exercises 164
 - in hybrid Monte Carlo 280–283
 - in collective algorithms 355–356
- Adams-Bashford-Moulton method 229
 - with integration of linear terms 229
 - for partial differential equations 308–309
 - for stochastic partial differential equations 315–316
 - warming 229, 309
 - exercises 323–325
- additive noise 173, 196
 - in the decay from an unstable state 233
 - transformation to - 224–225
- advection 293
 - equation 296–297
 - exercises 321
- agent 235
- aliasing 302, 369
 - error 316–321, 371
 - in FFT 375
- alloy separation 134, *see* Kawasaki interpretation of the Ising Model
- α addition property 69–70
- annihilation, *see* self-annihilation
- archer 32–33
- area-preserving algorithms 278–285
- arrival time 1, 16
- asymptotic
 - distribution 105, 116, 125, 285, 344
 - – exercises 345
 - behavior near a critical point 157–163
- autocorrelation
 - time 101–102, 128
 - – near a critical point 160–162
 - function 102, 128
 - , *see also* correlation
- average
 - values 6, *see also* mean, variance, moments, central moments
 - – of jointly Gaussian variables, *see* Wick theorem
 - – exercises 29–30, 62–63, 95–96
 - acceptance, *see* acceptance probability
 - local - 143
 - of functions 120, 127, 131–132, 136–137
 - , *see* ensemble, magnetization,
 - over trajectories 218, 221, exercises 230–233
 - over time, exercises 231
- Avogadro number 61, 125

b

backward

– Euler method 208

– rate, exercise 259

balance, *see* detailed balance

barrier 224

– exercises 189, 233, 258

bath, *see* heat-bath algorithm

Bayes theorem 25–26

– in rejection methods 74–75

Berg approach for multicanonical simulations 364

Bernoulli distribution 6–7, 34

– generation 44–45

– use to generate a binomial distribution 70

– use in rejection methods 75, 85, 99

– acceptance in Metropolis algorithm 108

Bessel functions 54–56, 74, 344

 β decay 1, 2, 4, 11–12, 16, 235, 244–245

Bhanot approach in multicanonical simulations 363

bifurcation

– pitchfork, exercises 188

– Hopf, exercises 188

bilingual 235–235

bin size 358

binary

– experiment 6–8, 170

– variable 34, 149

– alloy, *see* alloy

binomial distribution 7–8

– limit of many repetitions 10–11

– limit to a Gaussian distribution 13–14

– approximation 14

– in hit-and-miss methods 32–33

– generation 49–50, 70–71

– to describe random walk 174

– to describe a two-state particle 239–240

– to describe disintegration processes 245

– in the generating function method 253

– exercises 95, 257–258

birth-and-death process 245–246, 251–254

– exercises 259, 273

bistable exercises 188–189, 233

Boltzmann

– distribution 2, 125, 148

– – in hybrid Monte Carlo 284

– factor 125, 136, 151, 154, 163

– – in hybrid Monte Carlo 283–285

– – in multicanonical simulations 361

– constant 125, 169

– description of the Brownian motion 167, 186

Boltzmann-Gibbs factor 140

boundary condition

– in continuity equation for probability 182

– in passage time problems 223–224

– for partial differential equations 287, 292

– for stationary probability distribution 185–186

– – exercises 188

– periodic

– – for a sum 90, exercise 95

– – in multidimensional distributions 113, 115

– – in Ising model 139

– – in lattice ϕ^4 model 150

– – for partial differential equations 292, 294

– – for pseudospectral algorithms 300–301, 311, 316

– – in the generation of n-dimensional correlated Gaussian variables 338, 340–343

– – in the calculation of correlations 348

boundary value problems 235

Bortz-Kalos-Lebowitz 145, *see* residence time algorithmbounding 249, 246, 267–268, *see also* chemical reaction

Box-Mueller-Wiener algorithm 40, 68, 88

– exercises 94

broadcasting, fluctuations in radio 173

Brownian motion 167–170, 186

– Einstein's description 167–169, 181

– Langevin's description 169–170, 173

– timescales 180

– Master equation description 243

Bruce implementation of Monte Carlo for lattice ϕ^4 model, exercise 164

Buffon problem, exercise 29

c

cancer, statistical incidence exercise 29

candidate sites 352–354

canonical distribution 276, 279, 361–362, 363–364

Cardano's formula 54

Cauchy distribution 39

– generation 39

– use in rejection methods 93–94

– exercises 95

cdf, *see* cumulative distribution function

cell

– lattice 150

– in coarse graining 289–291

– in finite difference methods 291–293

centered space

– derivatives 291–292

- – exercises 322–323
- forward time - 295–297
- central-limit theorem 12
- central moments 6
- certainty 1, 11
- chain, *see* Markov chain
- change
 - in probability 247
 - of variables 6, 37,
 - – use to generate random variables 67–72
 - – use for multidimensional distributions 79–81
 - – in Stratonovich interpretation 179
 - – to integrate exactly the linear terms 225
 - – – in partial differential equations 306
 - – – in stochastic partial differential equations 313
 - – – exercises 233
 - – to generate n-dimensional correlated Gaussian variables 337–339
 - proposed - 114, 116
 - – configuration - 128, 132–133,
 - – – in Metropolis algorithm 137–138
 - – – in Kawasaki interpretation of Ising algorithm 143
 - – – in heat-bath algorithm 146
 - – – in Monte Carlo methods 153
 - – energy - 129–130, 132–133
 - – – in Glauber proposal, exercise 122–123
 - – – in Metropolis algorithm 140
 - – – in Kawasaki interpretation of Ising algorithm 144
 - – – in Monte Carlo methods 153, 155
 - – of a single particle position 132–133
 - – of many variables 132, 163, 281, 351–356, *see also* collective update
 - – exercises 122–123, 163–165, 286
- chaos, *see* Nikolaevskii equation
- Chapman-Kolmogorov equations 238–239
- characteristic configuration 128–129
- Chebyshev's theorem 20
 - use of - 21–22, 33, 35, 100
- chemical
 - potential 143
 - reaction 235, 241, 246–248, 267–268
 - – exercises 273
 - turbulence, *see* Nikolaevskii equation
- Chi and Chi-square distributions 14–16
- choice
 - optimal in importance sampling 51–53
 - in rejection methods 85, 87, 92–93
 - – exercises 95
 - in collective algorithms 355–356
 - in multicanonical simulations 362, 364
- Glauber - 129, 138
- – exercises 121–122
- Metropolis - 108, 138, 280, 285
- – exercises 121–122
- van Beijeren and Schulman - exercises 122
- to generate Poisson distribution 110–111
- to generate multidimensional distributions 115
- cluster 351–356
- coalescence of droplets 154
- coarsening 146
- coarse-grained description of Brownian motion 167
- coarse-graining 289–292
- coin tossing 1–2, 170, 174
- collective
 - algorithms for spin systems 351–356
 - update 130, 132, 163, 351–356, *see also* hybrid Monte Carlo
 - state 265
- colored noise 181, *see also* Ornstein-Uhlenbeck process
 - exercises 187, 231
- combination of variables for random number generation 72–74
- compressibility 126
- conditional probability 23–26
 - in Markov chains 27
 - in multidimensional distributions 76
 - in rejection methods 85–86
 - in heat-bath algorithm 117, 146
 - in equilibrium statistical mechanics 128, *see also* detailed balance
 - in stochastic processes 171
 - in Master equations 236, 238, 239
 - – exercises 257
 - in the residence-time algorithm 269
- confidence 21
 - limits 23, 35, *see also* Chebyshev's theorem
- configuration
 - microscopic 125
 - – Ising model 134
 - probability of a - 126–127, 137
 - change of -, *see* change/proposed/configuration
 - characteristic, *see* characteristic configuration
 - generation, *see* change/proposed/configuration
- congruential generator 329
 - mixed - 330
 - multiplicative - 330
 - examples 331
 - test 332

- congruential generator (*contd.*)
 - exercises 335
- connectivity
 - full 134, 137
 - nearest neighbor 139
 - mapping in collective algorithms, *see* Fortuin and Kasteleyn mapping, Niedermayer algorithm, Wolf algorithm
- conservation
 - of probability 182–183, 243, *see also* Liouville equation
 - of energy 276, 279, 284
 - – exercises 286
- conserved order parameter 284
- constant of motion 273
 - exercises 274
- contact area between two metals 145
- contagious disease 241
 - exercises 259, 273
- continuity equation 168, 182, 185
- convergence
 - to a stationary solution 28,
 - in mean square limit, *see* mean square convergence
 - of trajectories 198
 - of moments 198
 - of Berg recursive procedure 364
 - of Wang and Landau approach 364
- corrector, *see* predictor-corrector methods
- correlation
 - coefficient 17
 - matrix of joint Gaussian variables 18–19, 82
 - function 101–102, 117–118
 - – nonlinear 120
 - – of a series 347–350
 - – exercises 121–123
 - time 101–102, 110, 112, 114, 117–119
 - – nonlinear 120
 - – exercises 121–123
 - in configurations 128, 140, 143
 - – exercises 163–164, 286
 - in stochastic process 173
 - – random walk 174
 - – Wiener process 175
 - – white noise 175–177
 - – Ornstein-Uhlenbeck process 180
 - – – numerical realization 202
 - – – process g_n 204
 - – – correlation time vs time step 209–212
 - – colored noise - 181
 - – exercises 187–188, 231–232
 - in stochastic partial differential equations
 - – space-time white noise 288
 - – coarse graining 289–291
 - – in Fourier space 312–313
 - – exercises 324
 - prey-predator - 255
 - spurious - in random number generation 332–335
 - – exercises 336
 - , *see also* generation correlated Gaussian variables
- Courant-Friedrichs-Levy criterium 295–299
 - exercises 322–323
- covariance 17
- Crank-Nicolson method 299
 - exercises 322
- critical
 - temperature 135, 137, 143, 146, 152, 158–160
 - exponent 152, 157–160, 162–163
 - region 155–163
 - slowing-down 156, 161–163
 - point 157–162
 - fluctuations 160–161
 - opalescence 161
 - exercises 163–165
- cumulant 160–161
 - exercises 164
- cumulative distribution function, cdf 4
 - Bernoulli - 7
 - uniform - 8–9
 - Gaussian - 12–13
 - Gamma 65
 - joint - 16
 - multidimensional - 76
 - max of two random variables 70
 - piecewise approximation 91–94
 - inverse - method 37
 - – approximate 40–41
 - – Bernoulli 44–45
 - – Cauchy 39
 - – discrete random variables 43–44
 - – exponential 38
 - – Gamma 41–43
 - – Gaussian 40–41
 - – geometric 45–46
 - – Poisson 47–49
 - – power-law 39–40
 - – Rayleigh 40
 - – using Newton-Raphson 42–43, 54–55
 - – using piecewise linear interpolation 65–66
 - exercises 94–95
- Curie temperature 142

- cyclic loops
- in Markov chains 28
- in random number generators 328–329

d

- de Moivre-Laplace theorem, 13, 174
- decay
 - from an unstable state 222–224
 - – exercises 232
 - radioactive, *see* β decay
- decimated series 118–119
- density of states 361
- deposition of particles 288
- detailed balance
 - in Markov chains 27–28, 86
 - in dynamical methods 106–107
 - in Metropolis algorithm 108
 - in multidimensional distributions 116
 - in heat-bath method 116, 146
 - Glauber 129
 - for interacting particles 132
 - in lattice ϕ^4 model 155
 - in Master equations 237–238, 241–242
 - in hybrid Monte Carlo 280
 - in collective algorithms 355–356
 - exercises 30, 164
- diagrammatic representation of Wick's theorem 19
- diffusion
 - coefficient 168–170
 - Einstein's - law 170
 - equation 168
 - – finite difference methods 295–296, 299
 - – – exercises 322
 - of a Brownian particle, *see* Brownian motion
 - process in an alloy 143
 - term 173
- dynamical methods, *see* rejection methods
 - with repetition
- Dirac delta 4–5
- discrete Fourier transform, *see* Fourier transform, discrete
- discretization
 - time
 - – in stochastic differential equations 194
 - – in partial differential equations 293–300
 - space 307
 - – for stochastic partial differential equations, *see* coarse graining
 - spatial derivatives
 - – centered 291
 - – upstream 293
 - exercises 321–323
- disintegration, *see* β decay

- distribution
 - probability -, *see* probability distribution
 - cumulative probability -, *see* cumulative probability distribution
 - first passage time -, *see* first passage time
 - canonical -, *see* canonical distribution
 - multicanonical -, *see* multicanonical distribution
 - energy -, *see* energy distribution
- divergence
 - at the critical point 157–162, 351, 360
 - moments - in linear equation with multiplicative noise 219–220
 - numerical - 294, 296–297
- double-well potential 234
- drift term 173

e

- effective
 - potential, exercise 188–189
 - inverse temperature 363
- efficiency
 - finite differences vs
 - in collective algorithms 351–356
 - in generating n Gaussian random variables, exercise 345
 - in importance sampling 53
 - – exercises 62–63
 - in random number generation 339
 - of an integration method 60–61
 - of a rejection method 86–87, 93
 - – exercises 94–95
 - Adams–Bashford–Moulton vs Heun pseudospectral methods, exercise 323
 - first reaction method vs residence time algorithm, exercise 273
 - hybrid Monte Carlo vs rejection, exercise 286
- Einstein's
 - fluctuation-dissipation relations 136, 359, 362
 - description of Brownian motion 167–169
- electron
 - emission, *see* β decay
 - spin 1, 3
- Energy
 - barrier, *see* Michaelis-Menten reaction
 - change, *see* change/proposed/energy
 - conservation 279
 - – exercise 286
 - distribution 2, 359–360, 361–366
 - equipartition, *see* equipartition theorem
 - fluctuations 136
 - Helmholtz free -, *see* Helmholtz free energy

- Energy (*contd.*)
 - in Ising model 137
 - histogram 359–360, 361–366
 - interaction - in Ising model 134
 - internal 126–127
 - in Ising model 129
 - in lattice Φ^4 model
 - kinetic -, *see* residence time algorithm
 - average value 131, 276
 - of a Brownian particle 169
 - fake 279
 - potential - 131, 132
- ensemble
 - average 136
 - of Brownian particles 167–168
 - of trajectories 181–182
 - of particles 265, 267
 - microcanonical -, *see* microcanonical ensemble
 - multicanonical -, *see* multicanonical simulations
- enthalpy 134
- entropy 126–127, 128
 - in multicanonical simulations 361–366
- enzymatic reaction, *see* Michaelis-Menten reaction
- epidemic spreading 235, *see* contagious disease
- equilibrium 127–129
 - thermal 125
 - of a Brownian particle 169
 - sampling with molecular dynamics 276
 - in hybrid Monte Carlo 281–282
 - , *see also* thermalization
- equipartition theorem 131
- ergodic
 - Markov chain 28
 - algorithm 109–110, 116, 119
- error
 - function 12
 - complementary 130
 - inverse 41, 68
 - approximations 41, exercise 94
 - in pseudospectral methods 316–321, *see also* aliasing
 - integration
 - Euler-Maruyama algorithm 197
 - Milshtein algorithm 197–199
 - in the linear equation with multiplicative noise 218
 - in hybrid Monte Carlo 277, 283–284
 - , *see also* order/algorithm
 - spatial discretization 291, 293
 - statistical 3, 20–22
 - for the sum of random variables 23
 - in hit-and-miss 32–33
 - in uniform sampling 35
 - in general sampling 36
 - in importance sampling 51–52
 - in Monte Carlo importance sampling for sums 59
 - in determining the efficiency of integration methods 60
 - in rejection methods 89
 - in rejection with repetition 100–103
 - in Metropolis algorithm 110
 - increase with correlation time 114
 - in equilibrium statistical mechanics 132, 156
 - near the critical region 156, 160–162
 - in hybrid Monte Carlo 276
 - minimization
 - in importance sampling 51–53, 56
 - exercises 63
 - in dynamical methods 110, 117–119
 - exercises 122–123
 - in multicanonical simulations 364
 - exercises 62–63, 121
 - systematic
 - in piecewise linear inversion of cdf 94
 - in dynamical methods 120
 - in integrating Hamilton's equations 276, 283–284
- escape rate 244, 269–270
- estimator 4,
 - radioactive decay rate, 11
 - mean 21–22
 - standard deviation 21–22
 - unbiased 32, 35, 54
 - optimal - 52
 - efficiency 60–61
 - exercises 62–63
 - in dynamical methods 102
 - for the correlation time 118
 - of a stochastic process 197–199
 - correlation function 347–349
 - magnetization, *see* magnetization
 - entropy 361, 364
 - density of states 362
 - error, *see* error/statistical
- Euler algorithm
 - backward 208
 - deterministic 209
 - explicit 208
 - forward 208
 - implicit 208
 - semi-implicit 208
 - for molecular dynamics 276–277
 - for partial differential equations 295

- Euler-Maruyama algorithm 197–198
- comparison with leap-frog for hybrid Monte-Carlo 283–284
- event 1–2
- Poisson 10–11, 71
- exponential 11–12
- conditional 23–25
- rare 216–220
- in radioactive decay, *see* β decay
- expectation, a priori 2
- expected
 - value 6, *see* mean, variance, moments, central moments
 - frequency 2–3, 11
- experiment, probabilistic 1–4, 6–8, 12, 16–17, 20–22, 32–33, 36, 170, 172
- exponential distribution 11–12
- relation with Poisson distribution 11–12, 71
- generation 38
- use in integral evaluation 56
- use to generate the Γ distribution 69
- use to generate Poisson distribution 71–72
- use to generate other distributions 76–77
- first jump time 242, 261, *see also* first reaction method
- exponent, *see* critical exponent
- external field, *see* magnetic field
- extrapolation
 - integration step 198
 - polynomial, *see* Adams-Bashford-Moulton method
 - Histogram, *see* Histogram extrapolation
 - Ferrenberg–Swendsen, *see* Ferrenberg–Swendsen extrapolation
- f**
- factor
 - acceptance, *see* acceptance probability
 - Boltzmann, *see* Boltzmann, factor
 - Boltzmann-Gibbs, *see* Boltzmann-Gibbs factor
 - normalization, *see* normalization
 - structure 342–344
- factorization, probability 16, 56, 333
- fast Fourier transform 373–375
- storage of Fourier modes 304–305
- use in pseudospectral methods 300
- – Heun 306–307
- – midpoint Runge-Kutta 307–308
- – predictor-corrector 308–309
- – fourth-order Runge-Kutta 310–311
- use in stochastic pseudospectral methods
- – Heun 314–315
- – predictor-corrector 315–316
- – exercises 323–325
- use to generate n-dimensional correlated Gaussian variables 337
- – free model 338–340
- – translational invariance 340–344
- – exercises 344–345
- feedback shift register generator 333
- Ferrenberg-Swendsen extrapolation 357–360, 362
- ferromagnetism 126, 134–136, 143
- TW exerciseI 323
- Fibonacci generator 334–335
- field
 - coarse-grained, *see* coarse-graining
 - description in terms of partial differential equations 287–288
 - external, *see* magnetic field
 - Gaultois 333
 - local, *see* local field
 - magnetic, *see* magnetic field
 - mean, *see* mean-field
 - modal decomposition 300
 - model 149–150
 - stochastic 288
- finite differences method 287–300
- evaluation of spatial derivatives 291, 293
- for diffusion equation 295
- for Fokker-Planck equation with constant coefficients 297
- for KPZ equation 292, 297–300
- stability, *see* von Neumann stability analysis
- exercises 321–323
- finite-size
 - effects 156–160
 - scaling 160–161
 - – exercises 164
- First passage time 221–224
- distribution 221
- mean 221
- numerical evaluation 223–224
- variance 221
- exercises 232–233
- first reaction method 261–268
- fluctuating force, *see* Brownian motion
- fluctuation
 - of the order parameter 136
 - energy 136
 - microscopic 136
 - magnetization, *see* magnetization fluctuations, magnetic susceptibility
 - near a critical point, *see* critical fluctuations
 - in a Brownian particle, *see* Brownian motion

- fluctuation (*contd.*)
 - large 219, 220, *see also* critical fluctuations
 - at a unstable point 222–223, exercise 232
 - anomalous exercise 233
- fluctuation-dissipation, *see* Einstein's fluctuation-dissipation relation
- flux
 - particle 182
 - probability 185
 - , *see also* advection
- Fokker-Planck equation 181–184
 - multivariate 184–185
 - numerical integration with finite differences 296–297
 - stationary solution 185–186
 - – exercises 188–189
 - to approximate Master equations 256–257
 - – exercises 259
- Fortuin and Kasteleyn mapping 351
- forward
 - Euler, *see* Euler algorithm forward
 - time centered space 295
 - – for the diffusion equation 295
 - – for Fokker-Planck equation with constant coefficients 297
 - – for advection equation 296
- Fourier
 - acceleration 285
 - operator 301
 - – inverse 301
 - transform 301, 367
 - – use in pseudospectral methods 300–303
 - – discrete 368–372
 - – – in pseudospectral methods
 - – – to generate n-dimensional correlated Gaussian variables 337–344
 - – fast, *see* fast Fourier transform
 - – in von Neumann ansatz 294
 - space 302–304
 - – spatial derivatives 373
 - – nonlinear terms 302–304
 - – white noise 312–313
 - mode 300–303, 318–320, 367–372
 - series 367–368
 - filtering method 364
- fractal
 - Ising model structure 143–144
 - Wiener process 185
- free
 - Lagrangian 90, 338
 - – exercises 286, 344–345
 - energy, *see* Helmholtz free energy
 - Gaussian - model 126, 338–340
- FSR, *see* Feedback shift register generator
- g**
- Galerkin method 337–338
- Gamma distribution 13–14
 - cumulative function 65
 - numerical generation 41–43, 69
 - use in importance sampling 51–54
 - use in combination of variables 74
 - exercises 286
- Gaulois field 333
- Gaussian
 - distribution 12–13
 - – cutoff - 84–87, 104
 - – joint - 18–20
 - – statistical errors 21, 23
 - – exercises 29–30
 - – approximation for entropy 365–366
 - – approximation to changes in energy 129–130
 - – approximation to a binomial distribution 33, 174
 - – momentum distribution 131, 284, 285
 - – generation
 - – – using approximate inverse cdf 40–41, exercise 94
 - – – using Box-Mueller-Wiener algorithm 67–69, exercise 94
 - – – using interpolation for inverse cdf, exercise 94
 - – – using Metropolis algorithm 108–110, 117–118, exercises 122
 - – – n-dimensional uncorrelated 81–84
 - – – n-dimensional correlated 337–344, exercises 344–345
 - – product of - 81
 - – use to implement Φ^4 model, exercise 164
 - – use in hybrid Monte Carlo 279–280, 282
 - stochastic process 172, *see* white noise, Wiener process, Ornstein-Uhlenbeck process
 - free model, *see* free/Gaussian
- generalized
 - hybrid-Monte Carlo, *see* Hybrid Monte-Carlo/generalized
 - sampling method, *see* sampling/generalized
- generating function 251
 - method for Master equations 251–254
 - – exercises 257–258, 273
- generation of random numbers, *see* random number generation

- geometric distribution 8
 - generation 45
 - modified 46
 - use to evaluate sums with Monte Carlo 58–59
 - use in rejection methods 91
 - – exercises 95
- Gibbs factor, *see* Boltzmann-Gibbs factor
- Gillespie algorithm, *see* residence time algorithm
- Glauber acceptance probabilities 108
 - exercises 121–123
 - in statistical mechanics 129
 - in the Ising model 138, 142
 - in lattice Φ^4 model 155
- h**
- Hamiltonian 125, 127, 131
 - Ising - 134–135
 - Heisenberg - 148
 - Lattice ϕ^4 - 150
 - Numerical methods preserving - properties 277–279
 - fake - 279
 - average error in - 283
- Hamilton's equations 125, 275
- hard-core repulsion 133
- hard-spheres model 133, 163, 355
- heat-bath algorithm 116–117, 146–148, 153–154, 164
 - - type 316, 320
- heat, specific 126–127, 151, 359–360, 361–362
 - per particle 136, 360
 - scaling relations 159
- Heisenberg model 148–149
- Helmholtz free energy 126, 129, 137
- herding behavior, exercise 274
- Heun method
 - deterministic 206–209
 - stochastic white noise 207–208
 - stochastic Ornstein-Uhlenbeck noise 208–209
 - numerical implementation 209–211
 - multidimensional 213–215
 - for first passage time 223–224
 - with exact integration of linear part 226–227
- hit-and-miss method 31–33, 60–61
 - exercises 62–63
- homogeneous
 - Markov chain, *see* Markov chain, homogeneous
 - Fokker-Planck 195
- Hopf bifurcation 188 (exercise)
- Hybrid Monte Carlo 275–281
 - tuning of parameters 281–283
 - relation to Langevin dynamics 283–284
 - generalized 284–285
 - exercises 288
- i**
- importance sampling, *see* sampling, importance
- infection process 241
 - exercises 259
- instability
 - of a fixed point 217–218
 - – threshold 218
 - of finite difference methods, *see* von Neumann stability analysis
 - – condition, *see* Courant-Friedrichs-Lewy criterion
- integral calculation
 - with hit-and-miss, *see* hit-and-miss method
 - with uniform sampling, *see* sampling, uniform
 - with general sampling, *see* sampling, general
 - with importance sampling, *see* sampling, importance
 - N-dimensional 56–57
 - exercises 62–63, 121
 - with rejection with repetition, *see* rejection with repetition
- integral
 - Riemann, *see* Riemann integral
 - stochastic, *see* stochastic integral
- interaction
 - magnetic 127, *see* Ising model
 - interacting particles 130–134
 - potential 131–134
 - exercises 164
 - leading to annihilation, *see* self-annihilation
- interfacial growth, *see* KPZ equation
- internal energy 126–127
 - per particle 136
 - in lattice ϕ^4 model 151–153
- inversion of the cumulative distribution function, *see* cumulative distribution function/inverse
- irreducibility condition 28
 - exercises 30
- Ising model 127, 134–137
 - Metropolis algorithm for the - 137–143
 - Kawasaki interpretation 143–146
 - Heat-Bath Algorithm for the - 146–148
 - Data analysis around the critical point 155–157

Ising model (*contd.*)

- Finite-size effects 157–160
- Critical slowing down 161–163
- exercises 163–165
- to test random numbers 334
- collective algorithms 351
- histogram extrapolation 357–359
- density of states in the 3D - 363
- isothermal compressibility, 126
- Itô
- calculus 178–179
- interpretation 178–179
- exercises 187
- Euler-Maruyama algorithm 197

j

- Jacobian 18, 68–69, 278, 280, 337
- Jayne’s principle, 2
- Jensen’s inequality 129, exercise 30
- Joint pdf 16,
 - Gaussian 18–20
 - exercises 30
 - change of variables 67
- jump
 - in Brownian motion, *see* Brownian motion
 - in Master equations, *see* Master equations

k

- Kardar-Parisi-Zhang equation, *see* KPZ equation
- Kawasaki interpretation of the Ising model 143–147
- kinetic Monte Carlo, *see* residence time algorithm
- Kirman’s model for herding behavior 274
- KPZ equation 288–289
 - discretization 292
 - finite differences Milshstein method 297
 - – von Neumann stability analysis 297–298
 - – numerical implementation 299
 - finite differences Heun method 299
 - – numerical implementation 300
 - stochastic pseudospectral algorithms 311–315
 - exercises 322–325
- Kramer’s law exercises 234

l

- lagged Fibonacci generator, *see* Fibonacci generator
- Lagrange multipliers 52
- Lagrangian (free) 90, 338,
 - exercises 286, 344–345
- Lambert function, exercises 258

- Landau mean-field approximation, *see* mean-field
 - Wang and - method, *see* Wang-Landau method
 - Langevin
 - description of Brownian motion 169–170
 - random force 170
 - equation, *see* Stochastic differential equations
 - dynamics related to hybrid Monte Carlo, *see* hybrid Monte Carlo
 - language dynamics 235–236
 - lattice
 - regular -, Ising model 134–135, 334
 - – programing for 2D - 138–143
 - square -, 134–135, 144, 148, 156–158
 - – programing 138–143
 - – exercises 163–164
 - triangular -, 134–135
 - linear -, 134–135
 - cubic, exercises 164
 - torus topology 139
 - fully connected 137
 - division in sublattices 142
 - - Φ^4 model 149–152
 - discretization for PDEs 287, 289
 - , *see also* Heisenberg model, Potts model, collective algorithms, coarse graining
 - leap-frog algorithm 277–281
 - comparison with Langevin dynamics 283–284
 - for hybrid Monte Carlo 284–285
 - exercises 286
 - Lennard-Jones potential 132–133
 - likeness 1–2
 - linear combination of Gaussian variables 86
 - linear chain 135
 - linear equation with multiplicative noise 216–221
 - linear terms, exact integration 224–230., *see also* pseudospectral algorithms
 - Liouville equation 182–183
 - theorem 278
 - local
 - average 143
 - field 149
 - Lotka-Volterra model 249–251
 - mean field 255–256
 - residence time algorithm 270–273
 - exercises 258, 273
- ## m
- macroscopic order 135
 - magnetic moment 127, 134

- interaction 127–128
- field
 - - in Ising model 135–136, 140, 143
 - - in Heisenberg model 148–150
- susceptibility 136, 151, 157–158, 160, 162
- magnetism 127, *see also* Ising model
- magnetization 136, 140, 145, 151–153, 156, 158–160, 357, 361
- spontaneous - 136–137, 151–152, 156–157
- fluctuations 140, 151, *see also* magnetic susceptibility
- correlation time 162
- exercises 163–164
- marginal probability 20, 24
- Markov
 - chain 26–28, 86, 100–102, 105–107, 119–120, 162
 - - exercises 29–30, 121
 - - not homogeneous 115–116
 - - multiple - Monte Carlo 361
 - process 28, 171–172, *see also* Wiener process and Ornstein-Uhlenbeck process
 - - Master equation for - 235–238
- Marsaglia
 - theorem 332
 - planes 332
 - - exercises 335
- mass action law 248
- Master equation 235–257
 - two state system 235–236
 - for particles, *see* particle point of view method
 - for occupation numbers, *see* occupation numbers point of view method
 - general case 242–244
 - radioactive decay 244–245
 - birth and death process 245–246
 - AB chemical reaction 246–248
 - self-annihilation 248–249
 - , *see also* Lotka-Volterra, Generating function method, mean field, Fokker-Planck equation,
 - exercises 257–259
 - numerical simulations 261–273
 - - first reaction method 261–268
 - - residence time algorithm 268–273
 - - exercises 273–274
- mean
 - first passage time 121
 - - exercises 232
 - square convergence 179, 198
 - square displacement 173
 - value 6
 - - Bernoulli distribution 7
 - - binomial distribution 8
 - - geometric distribution 8
 - - uniform distribution 9
 - - Poisson distribution 10
 - - Exponential distribution 11
 - - Gaussian distribution 12
 - - Gamma distribution 14
 - - Chi distribution 16
 - - sum of random variables 17
 - - - independent 22
 - - statistical error 20–22
 - - sample - 22, 35–37, 54, 56, 60, 97, 100
 - - Wiener process 175
 - - white noise 177
 - - Ornstein-Uhlenbeck process 180
- mean-field
 - Ising model 134, 152
 - Master equation 254–255, 268, 272–273
 - exercises 258–259, 274
- metal alloy 134, 143–146
- Metropolis et al. algorithm 107–112
 - generalization 112–116
 - tuning 118
 - exercises 121–122
 - in statistical mechanics 128–129, 132, 137–143
 - lattice Φ^4 model 152–155
 - comparison with exact solution 156
 - results for magnetic susceptibility 158
 - in critical slowing down 162–163
 - exercises 163–164
 - in Hybrid Monte Carlo 275, 279–281, 285
 - comparison with collective algorithms 351, 355
- Michaelis-Menten reaction exercises 258, 273
- microcanonical ensemble 276, 363
- microscopic configuration 125–127, 134
- microscopic fluctuations 144
- midpoint Runge-Kutta 227–229
 - for stochastic partial differential equations 307–308
- Mil'shtein algorithm 196–197
 - integration error 197–198
 - numerical implementation 199–200
 - for several variables 213
 - for finite difference methods in stochastic partial differential equations 292, 295–297
 - for KPZ equation, 297–300
 - exercises 230–233

- mixed congruential generator 330–332
 - molecular dynamics 275–277
 - moment 6,
 - of the Hamiltonian 127
 - of the magnetization 160
 - convergence 198
 - numerical evaluation in stochastic differential equations 200
 - for the linear equation with multiplicative noise 218–220
 - of the first passage time 221, 224
 - in processes described by a Master Equation 252
 - in the context of mean-field theory for Master Equations 254–256
 - to check random number generators 328
 - exercises 230–231, 258, 274
 - , *see also* central moment, magnetic moment, mean
 - Monte Carlo
 - integration 33–62
 - – advantages 56–57
 - – efficiency 60–61
 - , *see* hit-and-miss, sampling methods
 - – exercises 62–63
 - simulation
 - – step (MCS) 115, 140, 162
 - – tuning 117–121
 - – applications to statistical mechanics 125–163
 - , *see* Metropolis et al. algorithm, heat-bath algorithm
 - – exercises 121–123, 163–165
 - kinetic -, *see* residence time algorithm
 - dynamic -, *see* residence time algorithm
 - hybrid -, *see* hybrid Monte Carlo
 - exchange - 361
 - multiple Markov chain - 361
 - transition matrix - 361
 - multicanonical simulation 363–366
 - Moore neighborhood 164
 - multicanonical simulations 361–366
 - multidimensional distribution 76–81, 112–116
 - Gaussian 82–84, 337
 - multiplier, *see* Lagrange multiplier
 - multiplicative noise 173, 197, *see also* Milshtein method, Heun method
 - linear - 217–220
 - single point - 291
 - multiple point - 292
 - multiplicative congruential generator, *see* congruential generator multiplicative
- n**
- nearest neighbors 134–135, 137–139
 - with different spin as measure of contact area 145
 - in lattice Φ^4 model 150–151
 - exercises 164
 - neighbor
 - nearest, *see* nearest neighbors
 - array 139–140
 - division in sublattices 142–143
 - in collective algorithms 351–356
 - Newton’s binomial theorem 253
 - Newton–Raphson method 42
 - to invert the cumulative distribution 42, 54, 65–66, 79
 - n-fold way, *see* residence time algorithm
 - Nikolaevskii equation 301
 - in Fourier space 302
 - pseudospectral methods
 - – exact integration of linear terms 305
 - – Heun 306–307
 - – midpoint Runge-Kutta 307–308
 - – predictor-corrector 308–309
 - – fourth-order Runge-Kutta 310–311
 - – exercises 323–324
 - Niedermayer algorithm 351–352, 356
 - noise 173
 - term 173
 - additive 173
 - multiplicative 173
 - white, *see* white noise
 - colored, *see* colored noise
 - nonlinear correlation
 - function 120
 - time 120
 - exercises 122–123
 - normalization
 - probability density function 3
 - cumulative probability function 4
 - correlation 17
 - Novikov’s theorem 183
 - exercises 30
- o**
- occupation number 239–240
 - point of view method 239–242
 - – in radioactive decay 244–245
 - – in birth and death process 245–246
 - – in a chemical reaction 246–248
 - – in self-annihilation 248–248
 - – in Lotka-Volterra model 248–251
 - – in first reaction method 265–268
 - – in residence time algorithm 270–273

- Onsager solution of the Ising model 145, 164, 157
 - opalescence, critical 169
 - opinion formation 135–136
 - optimal
 - estimator, *see* estimator/optimal
 - choice in importance sampling 52–54
 - – exercises 63
 - acceptance 109
 - algorithm parameters 117–119
 - – in hybrid Monte Carlo 279
 - – in collective algorithms 356
 - – exercises 121–123, 164, 286
 - sampling in multicanonical simulations 362–363
 - order-disorder transition 135, 143, *see also* order parameter
 - order
 - algorithm
 - – Milshtein 196–199
 - – Euler-Maruyama 196–197
 - – Euler for ordinary differential equations
 - – – explicit 208, 276–277
 - – – implicit 208
 - – – semi-implicit 208
 - – Heun for ordinary differential equations 208
 - – stochastic Heun 208
 - – Midpoint Runge-Kutta 227, 229–230
 - – Adams-Bashford-Moulton 229–230
 - – leap-frog 277
 - spatial discretization
 - – centered space 291
 - – upwind 293
 - parameter 136, 152, 157–158, 161, 285, *see also* magnetization
 - – exercises 164
 - Ornstein-Uhlenbeck process 180
 - correlation time 180
 - as example of colored noise 181
 - exact generation of trajectories 201–202
 - numerical integration of stochastic differential equations driven by - 202–204
 - – exact generation of $g_{h(t)}$ 204–206
 - – Heun method 208–211
 - outcome, *see* experiment, probabilistic
- p**
- parallel tempering 361
 - parameter tuning
 - in dynamical methods 112, 117–121
 - near the critical region 162–163
 - in hybrid Monte Carlo 279, 281–283
 - particle
 - number 126
 - noninteracting 126
 - interacting, *see* interacting particles
 - Brownian, *see* Brownian motion
 - conservation, *see* conservation of particles
 - point of view method in Master equations 236–239
 - – in first reaction method 261–265
 - – in residence time algorithm 268–270
 - deposition 288
 - partition function 126–127, 129
 - in lattice Φ^4 model
 - passage time, *see* first passage time
 - paramagnetic
 - phase 135–136
 - to ferromagnetic transition 134
 - Pawula’s theorem 256–257
 - pdf, *see* probability density function
 - percolation 351
 - phase
 - separation 134, 146–147
 - transition 135–136
 - – precursor 143
 - – lattice Φ^4 model 150–152
 - – , *see also* critical region
 - ferromagnetic - 135
 - paramagnetic - 135
 - Poisson distribution 10–11
 - relation with exponential distribution 11–12
 - Gaussian limit 13
 - comparison with Gamma distribution 14
 - exercises 29
 - generation
 - – from cumulative distribution function 47–49
 - – using change of variables 71–72
 - – using rejection methods 93–94
 - – using Metropolis algorithm 110–112
 - – exercises 95, 122
 - use to generate a Bessel distribution
 - in birth and death process 254, exercises 259
 - population dynamics, *see* Lotka-Volterra model
 - potential
 - thermodynamic 126, 137, 364
 - energy 131
 - interaction 131–134
 - Lennard-Jones 132–133
 - chemical 143
 - lattice Φ^4 model 150, 152
 - exercises 163–165
 - effective, exercises 188–189

- Potts model, exercise 164
 - Fortuin and Kasteleyn mapping onto percolation model 351
 - Power-law
 - distribution
 - in bounded domain 39
 - in infinite domain 39–40
 - singularity 158, 351
 - growth of Monte Carlo correlation time near critical point 162
 - exercise 163–164
 - ad hoc correlation 342–344
 - exercise 345
 - precursor, *see* phase transition precursor
 - predictor-corrector method 191–192, *see* Adams-Bashford-Moulton
 - prey-predator, *see* Lotka-Volterra model
 - probability
 - acceptance, *see* acceptance probability
 - concept 1–2
 - assignation 2–3
 - conditional, *see* conditional probability
 - of a microscopic configuration 125
 - density function (pdf) 3
 - for a continuous variable 3
 - for a discrete variable 5
 - of a sum of random variables 22–23, 69
 - of the maximum of two variables 70
 - combination of variables 72
 - in polar coordinates 67–68, 79
 - in spherical coordinates 79–80
 - joint - 16–18
 - factorization 16
 - Gaussian variables 18–20
 - correlated 337
 - , *see also* Markov chain, multidimensional distribution
 - in hit-and-miss method 31
 - in change of variables method 67
 - in rejection methods 85, 90
 - of a stochastic process 170–172
 - exercises 29–30
 - marginal - 20, 24
 - conditional, *see* conditional probability
 - stationary stationary probability distribution
 - transition, *see* transition rates
 - change of variables 67
 - distribution
 - Bernoulli, *see* Bernoulli distribution
 - Boltzmann, *see* Boltzmann distribution
 - canonical, *see* canonical distribution
 - binomial, *see* binomial distribution
 - Cauchy, *see* Cauchy distribution
 - Chi and Chi-square, *see* Chi distribution
 - energy, *see* energy distribution
 - exponential, *see* exponential distribution
 - first passage time, *see* first passage time
 - Gamma, *see* Gamma distribution
 - Gaussian, *see* Gaussian distribution
 - geometric, *see* geometric distribution
 - multicanonical, *see* multicanonical distribution
 - Poisson, *see* Poisson distribution
 - power-law, *see* power-law distribution
 - Raleigh, *see* Raleigh distribution
 - uniform, *see* uniform distribution
 - current 185–186, 237, 243
 - exercises 188–189
 - process, *see* stochastic process
 - pseudorandom number 328, *see also* random number
 - pseudospectral methods
 - comparison with finite differences 303, 305
 - for partial differential equations 300–305
 - with exact integration of linear terms 306
 - Heun 306–307
 - midpoint Runge-Kutta 307–308
 - predictor-corrector 308–309
 - fourth-order Runge-Kutta 310–311
 - for stochastic partial differential equations 311–313
 - with exact integration of linear terms 313–314
 - Heun 314–315
 - predictor-corrector 315–316
 - integration error 316–321
 - exercises 323–325
- r**
- radio broadcasting fluctuations 173
 - radioactive decay, *see* β decay
 - random
 - number generation
 - Bernoulli distribution 44–45
 - binomial
 - inverse cdf 49–50
 - change of variables 70–71
 - Cauchy distribution 39
 - exponential distribution 38
 - Gamma distribution
 - Newton-Raphson to invert the cdf 41–43
 - change of variables 69
 - Gaussian distribution
 - approximate inverse cdf 40–41, exercise 94

- Box-Mueller-Wiener algorithm 67–69, exercise 94
 - interpolation for inverse cdf, exercise 94
 - Metropolis algorithm 108–110, 117–118, exercises 122
 - n-dimensional uncorrelated 81–84
 - n-dimensional correlated 337–344, exercises 344–345
 - geometric distribution 45
 - Poisson distribution
 - inversion of discrete cdf 47–49
 - change of variables 71–72
 - rejection methods 93–94
 - Metropolis algorithm 110–112
 - exercises 95, 122
 - power law distribution in bounded domain 39
 - power law distribution in infinite domain 39–40
 - Raleigh distribution 40
 - uniform
 - von Neumann method 328–329
 - congruential generators 329–330
 - feedback shift register generators 333–334
 - RCARRY and lagged Fibonacci generators 335
 - , *see also* rejection methods, cumulative distribution function/inverse
 - variable 2–5, *see* probability
 - update 115
 - walk 109, 170–171
 - limit to Wiener process 174–175
 - rare events 216–221
 - Rayleigh distribution 40
 - generation 40
 - use in Box-Mueller-Wiener algorithm 68–69
 - RCARRY generator 335
 - realization
 - Markov chain 105
 - Langevin random force 169
 - Wiener process 175
 - stochastic process 177, 191–192, 198, *see also* stochastic process/trajectory
 - rejection
 - methods 84–94
 - with combination of variables 74–75
 - exercises 94–96
 - with repetition methods 97
 - simple case 97–100
 - statistical error 100–103
 - dynamical methods 103–107, *see also* Metropolis et al. algorithm, heat-bath algorithm
 - tuning the algorithms 117–121
 - replica exchange 361
 - residence time algorithm 268–270
 - for Lotka-Volterra model 270–273
 - exercises 273–274
 - response function 136, 161
 - reversibility 277–278, 284–286, exercises 286
 - Riemann
 - integral 31, 36
 - zeta function, exercise 345
 - Runge-Kutta methods 191–192
 - Heun, *see* Heun method
 - midpoint, *see* midpoint Runge-Kutta
 - fourth-order 310–311
 - exercises 324
- s**
- sampling methods
 - uniform 34–36
 - generalized 36–37
 - importance 50–56
 - for sums 57–60
 - efficiency 60–61
 - exercises 62–63
 - scaling 159–161
 - exercises 164
 - self-annihilation
 - segregation 134
 - sequential update 115–116, 142
 - simulated tempering 361
 - SIR model, exercises 259, 273
 - specific heat, *see* heat, specific
 - spin 1, 3
 - variable 127
 - dynamics, *see* Ising model
 - collective algorithms 351–356
 - spinodal decomposition 154
 - spontaneous magnetization, *see* magnetization/spontaneous
 - square lattice, *see* lattice/square
 - stability
 - of a fixed point 217–218
 - of finite difference methods, *see* von Neumann stability analysis
 - condition, *see* Courant-Friedrichs-Lewy criterion
 - standard deviation 6, 20, 21, 23, 32, 35, 37, 60, 349
 - exercises 62

- stationary probability distribution
 - Markov chain 27–28
 - exercises 30
 - dynamical methods 106, 116–117, 119–121, 128
 - exercises 121–122
 - Fokker-Planck equation 185–186
 - exercises 187
 - stochastic process
 - exercises 230–233
 - also, *see* Ornstein-Uhlenbeck process
 - Master equations 237–238, 253–254, *see also* detailed balance
 - exercises 259
 - hybrid Monte Carlo 283, 285
 - statistical error
 - minimization 51–53, 56
 - exercises 63
 - stiff equations 305
 - Stirling approximation 10, 11, 93
 - stochastic
 - differential equation 172–173
 - driven by white noise 174–177
 - interpretation, *see* stochastic integral
 - for the Ornstein-Uhlenbeck process 180
 - colored noise 181
 - numerical simulation 191–192
 - Milshtein algorithm 192–197
 - integration error 197–198
 - numerical implementation 199–200
 - multidimensional 212–213
 - Euler-Maruyama algorithm 197–198
 - Exact generation of Ornstein-Uhlenbeck trajectories 201–202
 - Exact generation of process $g_{h(t)}$ 205–206
 - Euler algorithm for Ornstein-Uhlenbeck noise 203–204
 - Heun method
 - white noise 207–208
 - Ornstein-Uhlenbeck noise 208–209
 - numerical implementation 207–211
 - multidimensional 213–216
 - exact integration of linear terms 224–225
 - Heun method 226–227
 - midpoint Runge-Kutta 227–229
 - predictor-corrector 228–229
 - integration error 229–230
 - exercises 230–233
 - integral 177–179
 - Ito interpretation 177
 - Stratonovich interpretation 179
 - exercises 187
 - partial differential equation 287–288
 - coarse graining 289–291
 - finite difference methods 291–293
 - Milshtein 297
 - stability analysis 298
 - numerical implementation 299–300
 - Heun 299
 - stability analysis 299
 - numerical implementation 300
 - pseudospectral methods 311–312
 - coarse graining in Fourier space 312–313
 - exact integration of the linear terms 313
 - Heun 314
 - numerical implementation 314–315
 - predictor-corrector 315–316
 - numerical implementation 316
 - exercises 322–323
 - process 167, 170
 - Langevin approach 169–170, 173, *see* stochastic differential equation
 - Einstein’s approach 167–169, 181, *see* Fokker-Planck equation
 - characterization 170–172
 - , *see also* Brownian motion, white noise, colored noise, Wiener process, Ornstein-Uhlenbeck process
 - exercises 187–189
 - resonance, exercise 245
 - Stokes law 169
 - storage
 - of nodes in a square lattice 138
 - of Fourier modes 304–305
 - Stratonovich
 - calculus 178–179
 - interpretation 178–179
 - structure factor 342–344
 - successions of random variables 16–18, *see also* Markov chain
 - generalization 171, *see* stochastic process
 - surface growth 288
 - susceptibility, *see* magnetic susceptibility
 - Swendsen and Wang algorithm 351
 - symmetry breaking 135
 - symplectic algorithms 278, *see also* leap-frog algorithm
 - systematic
 - error, *see* error/systematic
 - correction 365

t

- tempering
 - simulated 361
 - parallel 361
- thermalization
 - dynamical methods 99–100, 119–120
 - Ising model 140–141
 - critical region 156, 163
- thermodynamic
 - limit 157, 255
 - potential 126, 137, 364
- trajectory
 - in phase space 167
 - of a Brownian particle, *see* Brownian motion
 - stochastic 170–171
 - – random walk 171
 - – Wiener process 174–175
 - – averages 173
 - – numerical generation 191–192, *see* stochastic differential equation/numerical generation
 - – exercises 230–233
 - deterministic 181
- transient anomalous fluctuations, exercise 233
- transition rates
 - in Markov chains 27
 - – exercises 30
 - in dynamical methods 100, 105–106
 - – Metropolis 108
 - – Glauber 108
 - – van Beijeren and Schulman 108
 - – multidimensional 115–116
 - – heat-bath 116
 - in Master equations 235, 236, 243
 - – exercises 257–259
 - in multicanonical simulations 365
- translational invariance 340–344
- trial 85–86
 - repeated 97–98, 104, 116, 145
 - – exercises 163
- tuning parameters, *see* parameter tuning
- turbulence, *see* Nikolaevskii equation

u

- unbiased estimator, *see* estimator/unbiased
- uniform
 - distribution 8–9
 - – generation
 - – – effect of finite precision 327
 - – – requirements 329
 - – – residual correlations 332
 - – generators
 - – – von Neumann method 328–329

- – – congruential 329–330
- – – feedback shift register 333–334
- – – RCARRY and lagged Fibonacci 335
- sampling methods, *see* sampling methods
- uniform
 - universality class 152
- update
 - random 115
 - sequential 115–116, 142
 - collective 130, 132, 163, 275, 351–356
 - exercises 163
- upstream space derivatives 293
 - use in the advection equation 297
 - – exercises 321–322

v

- van Beijeren and Schulman transition
 - probability 108
- variance, 2
 - Bernoulli distribution 7
 - binomial distribution 8
 - Chi distribution 16
 - exponential distribution 11
 - first passage time 221
 - – exercises 232
 - Gamma distribution 14
 - Gaussian distribution 12
 - geometric distribution 8
 - interpretation 20–22
 - minimum
 - – in importance sampling 51–53, 56
 - – – exercises 63
 - – in dynamical methods 119
 - Poisson distribution 10
 - sample - 22, 35–37, 51, 56, 58, 60, 97, 100, 102
 - sum of random variables 17
 - – independent 22
 - uniform distribution 9
 - exercises 29
- Verlet algorithm, *see* leap-frog algorithm
- von Neumann
 - algorithm for random number generation
 - 328–329
 - – exercises 335
 - ansatz 294
 - stability analysis 293–294
 - – advection equation 296–297
 - – diffusion equation 295–296
 - – Fokker-Planck equation with constant coefficients 296
 - – KPZ equation 297–299
 - – exercises 321–322

W

- Wang-Landau method 364
- weight function 390
- white noise
 - characterization 174–177
 - in space and time 288
 - – discretization, *see* coarse graining
 - – in Fourier space 312–313
 - Itô interpretation, *see* Itô
 - Stratonovich interpretation, *see* Stratonovich
 - time discretization, *see* stochastic differential equation/integration
 - exercises 187–189
- Wick's theorem 18–20
- Wiener process 174
 - correlation 175
 - derivative 175–177
 - in the numerical integration of sde with white noise 193–196
 - in the solution of the linear equation with multiplicative noise 219
 - mean 175
- Wolf algorithm 351–356

Z

- ziggurat rejection method 94