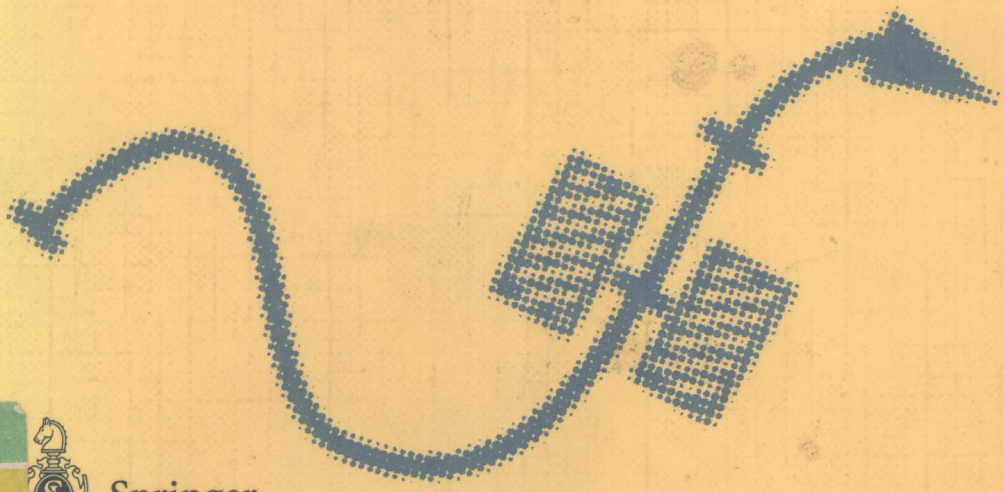
H. C. Öttinger

Stochastic Processes in Polymeric Fluids

Tools and Examples for Developing Simulation Algorithms



Springer

Hans Christian Öttinger

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Tools and Examples for Developing Simulation Algorithms

With 34 Figures and 3 Tables

Springer

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To Ricarda

Preface

> A SPECTER is haunting the scientific world—the specter of computers. All the powers of traditional science have entered into a holy alliance to exorcise this specter: puristic theoreticians and traditionalistic experimentalists, editors and referees of prestigious journals, philosophers of science and mathematicians. Where is a pioneering computer simulation that has not been decried as unreliable by its opponents in power?
>
> **The Computer Manifesto**

As a result of the enormous progress in computer technology made during the last few decades, computer simulations have become a very powerful and widely applicable tool in science and engineering. The main purpose of this book is a comprehensive description of the *background and possibilities* for the application of *computer simulation techniques in polymer fluid dynamics*. Modeling and understanding the flow behavior of polymeric liquids on the kinetic theory level is not merely a great intellectual challenge but rather a matter of immense practical importance, for example, in connection with plastics manufacture, processing of foods, and movement of biological fluids.

The classical computer simulation technique for static problems in statistical mechanics is the *Monte Carlo method* developed in the early 1950s. The name of this method underlines how unusual and strange the idea of using random numbers in the exact sciences is at first glance. However, the Monte Carlo method is a rigorous and efficient means for evaluating moments and static spatial correlation functions for given probability distributions. It is based on the theory of Markov chains. An ensemble of properly distributed configurations is created by Monte Carlo moves, where the transition probability from one configuration to another one involves only the ratio of the probabilities of these two configurations. In statistical mechanics, this method has been most successfully applied to calculating static equilibrium averages with the Boltzmann distribution. In particular, many static properties of polymer solutions and melts are most accurately and most reliably known from Monte Carlo simulations. Since, in this book, we are interested in the dynamics of polymeric liquids, the Monte Carlo method is here mentioned only for comparison with the stochastic simulation techniques suited for obtaining dynamic properties.

What Monte Carlo simulations are to the theory of static polymer properties, *Brownian dynamics simulations* and other simulations based on the *numerical integration of stochastic differential equations* are to the theory of polymer dynamics. Both simulation methods are unique tools to obtain exact results. By the term "exact" it is meant that the only error in the result of a computer simulation is a statistical error which, in principle, can be made arbitrarily small by running the corresponding computer program sufficiently long (of course, for a simulation technique to be useful for practical purposes, "acceptably" small statistical error bars should be obtained with a "reasonable" amount of computer time; the meaning of the rather vague terms in quotation marks clearly depends on the particular problem and on the computers available).

Why do *stochastic differential equations of motion*, which are the starting point for all the simulations considered in this book, occur very naturally in the theory of polymer dynamics? In view of the immense number of degrees of freedom and the wide range of time scales involved in polymer problems, the derivation of tractable kinetic theory models requires some coarse-grained or trace description of such problems (e.g., by mechanical bead-rod-spring rather than atomistic models). The effects of the rapidly fluctuating degrees of freedom associated with very short length scales are usually taken into account through random forces which perturb the time evolution of the slower degrees of freedom. For that reason, the basic equations for most kinetic theory models are stochastic in nature. From a more intuitive point of view, thermal noise turns the equations of motion into stochastic differential equations.

In computer simulations based on the numerical integration of stochastic differential equations, we construct stochastic trajectories. It is therefore crucial to give a precise meaning to these random objects, the trajectories of stochastic processes, and not only to introduce their probability distribution, as it is usually done in the applied sciences and engineering. This is particularly important for constructing sophisticated integration schemes, that is, for developing efficient simulation algorithms. The *art of designing efficient algorithms*, and the required mathematical background, are the main subjects of this book. Moreover, the investigation of stochastic differential equations of motion for the polymer configurations has additional advantages compared to the usual consideration of partial differential equations for the time-evolution of probability densities in configuration space: we obtain a more direct understanding of the polymer dynamics and a better feeling for the degree of complexity of various types of models.

Brownian dynamics simulations have been applied in the field of polymer dynamics since the late 1970s. However, the great progress made with numerical methods for stochastic differential equations has not really been exploited yet in simulating polymer dynamics. Brownian dynamics simulations are not only a nice toy, and they should not only be used in their most rudimentary form. If the state-of-the-art techniques discussed in this book are used (such as higher-order integration schemes, predictor-corrector schemes, Runge-Kutta ideas, implicit and semi-implicit methods, time-step extrapolation, non-

Gaussian random numbers, shifted random numbers, and variance reduction), one is now in a position to attack the most important and exciting problems in polymer dynamics, and some progress in this direction has already been made. On the one hand, one can work out the *universal dynamic properties* of long chain molecules. This expected universality, which is related to the famous self-similarity and scaling laws for high-molecular-weight polymers, may also serve as a justification of the simple mechanical models used in polymer kinetic theory. On the other hand, one can simulate extremely large ensembles of molecules and, in combination with the finite element method, one can then directly *solve complex flow problems* with kinetic theory models. The stresses required in the finite element calculation of the flow field are read off from the molecular configurations. These exciting perspectives are the motivation for attempting a systematic approach to stochastic simulation techniques in this book.

In order to motivate the development of the theory of stochastic processes we first sketch the background and framework for our later applications. The basic tasks and goals of polymer kinetic theory and its relation to polymer fluid mechanics are hence described in a brief general introduction (Chapter 1). Our stochastic approach to kinetic theory models is contrasted with the classical formulation. For developing efficient simulation techniques based on the numerical integration of the stochastic differential equations resulting from polymer kinetic theory, it is indispensable to have or acquire a sound understanding of mathematical stochastics, in particular of the subtleties of stochastic calculus. *Stochastic calculus is fundamentally, unavoidably and undeniably different from deterministic calculus*. The most important concepts of stochastics are explained in Part I of this book (Chapters 2 and 3). Although the development of stochastics is strictly confined to what is actually needed in this book, a great variety of concepts and methods of modern stochastics is introduced because it is found to be very helpful. Therefore, this book not only provides the background for designing simulation algorithms in polymer kinetic theory but also gives a multitude of concrete applications of abstract stochastic concepts, and it may hence also be used as a collection of nontrivial practical examples and as a challenge for mathematicians. Since the required stochastic concepts are rather natural and intuitive, an attempt is made to give simple definitions which are sufficiently precise for the purposes of polymer scientists, hopefully without too much provoking the mathematicians who are accustomed to even more rigor. As a stepping-stone to stochastic processes, Part I should be helpful in many branches of science and engineering. Part II of the book contains the application of the theory of stochastic processes to polymer kinetic theory. *The power of stochastic simulation techniques is illustrated* through many examples. By applying the theory of stochastic differential equations to dilute solution models, one is immediately led to Brownian dynamics simulations for the polymer dynamics (Chapter 4). We then discuss the treatment of models with constraints by Brownian dynamics simulations (Chapter 5). In the last chapter, the stochastic concepts are applied to develop stochastic simulation

algorithms for various reptation models for polymers in concentrated solutions and melts (Chapter 6).

For optimal benefitting from this book, some *mathematical background* and, perhaps even more important, the willingness for a certain mathematical abstraction are required. Indispensable is some familiarity with the most elementary ideas of set theory. Moreover, knowledge of the basic concepts of linear algebra (vector spaces, matrices, diagonalization, positive-definiteness) and of analysis (functions, convergence, calculus in $\mathbb{R}^d$, Fourier series and transforms, differential equations) is assumed. A background in differential geometry might simplify the reading and enhance the understanding of Sect. 5.1. Finally, some knowledge of measure theory, topology, symbolic computation, numerical mathematics, and computer science is not assumed, but it would be helpful for understanding certain details and examples. There are many exercises in which the reader is supposed to develop computer programs, where all the solutions are given in FORTRAN.

This book is based on several courses on polymer physics, kinetic theory and stochastic dynamical systems given over the last seven years to students of physics and material science. I owe an immeasurable debt of thanks to my teachers who introduced me in a very enlightening and fascinating manner to these and related fields: Josef Honerkamp, R. Byron Bird, and Joachim Meißner. A number of people have provided me with critical comments and suggestions for improving the manuscript: Jay D. Schieber, R. Byron Bird, Kathleen Feigl, Ludger Rüschendorf, Marshall Fixman, Manuel Laso, Martin Melchior, Ravi Prakash, Peter E. Kloeden, and many students. I wish to thank them all for their help. The assistance of Alain-Sol Sznitman and Hermann Rost in finding the mathematical background for processes with mean field interactions (Sect. 3.3.4) and Wesley P. Petersen's remarks on random number generators have been very helpful.

Zürich and Rafz, Switzerland Hans Christian Öttinger
September 1995

Symbols and Notation

Latin Symbols

A, B, C, A_j, B_j, A_ω	Events
$(A_t)_{t\in\mathbb{T}}$, $(B_t)_{t\in\mathbb{T}}$	Coefficients in the stochastic differential of a real-valued Itô-process [(3.37)]
$(\boldsymbol{A}_t)_{t\in\mathbb{T}}$, $(\mathbf{B}_t)_{t\in\mathbb{T}}$	Coefficients in the stochastic differential of a vector-valued Itô-process [(3.42)]
A, $\boldsymbol{A}$, $\boldsymbol{A}_\mu$	Drift term or drift vector in a stochastic differential equation (in general, a function of time and configuration)
$\overline{\boldsymbol{A}}$	Drift term including a spurious drift [(3.132)]
A^{R}_{jk}	Elements of the Rouse matrix [(4.6)]
A^{Z}_{jk}	Elements of the Zimm matrix [(4.74)]
$\mathcal{A}$, $\mathcal{A}'$, $\mathcal{A}''$, $\mathcal{A}_j$	σ-algebras
$\mathcal{A}(\mathcal{E})$	σ-algebra generated by a set of events $\mathcal{E}$ [Definition 2.5]
$\mathcal{A}^X$	σ-algebra induced by a measurable function X [p. 36]
$(\mathcal{A}_t)_{t\in\mathbb{T}}$	Increasing family of σ-algebras (e.g., induced by a stochastic process)
$\bar{\mathcal{A}}_t$	σ-algebra induced by the future of the Wiener process
$\mathcal{A}^*$	Completion of a σ-algebra $\mathcal{A}$
a, b	Limits of intervals, real constants (b also used for finite extensibility parameter)
a_{b}	Bead radius
a_{ev}	Range of the excluded-volume potential [(4.116)]
$\boldsymbol{a}(t)$, $\mathbf{A}(t)$	Contributions to the drift vector $\boldsymbol{A}$ for linear equations [(3.53)]
a^{R}_j	Eigenvalues of the Rouse matrix [(4.8)]
a^{Z}_j	Eigenvalues of the Zimm matrix [(4.75)]
B, $B_{\mu\nu}$, $\mathbf{B}$, $\mathbf{B}_{\mu\nu}$	Noise prefactor in the diffusion term of a stochastic differential equation (in general, a function of time and configuration)
$\mathbf{B}_j(t)$	Contribution to $\mathbf{B}$ for linear equations [(3.53)]
$\overline{\mathbf{B}}$	$\mathbf{B}$ in a predictor-corrector scheme [(4.111)]
$\mathcal{B}$ (or $\mathcal{B}^d$)	Borel σ-algebra on $\mathbb{R}$ (or on $\mathbb{R}^d$) [Example 2.7]
$\mathcal{B}^{\mathbb{T}}$	Borel σ-algebra on the set of functions $\mathbb{R}^{\mathbb{T}}$
b	Finite extensibility parameter [(4.118)]
$\overline{b}$	Shifted finite extensibility parameter [Exercise 4.32]
$\boldsymbol{b}_j$	Column vector of $\mathbf{B}$ (or of a contribution to $\mathbf{B}$ for linear equations)
C^{R}_{jk}	Elements of the Kramers matrix [(4.26)]
C^{Z}_{jk}	Elements of the modified Kramers matrix [Exercise 4.21]
$C^{\mathbb{T}}$	Set of continuous real functions on $\mathbb{T}$
$\mathbf{C}(t,t')$	Cauchy strain tensor [(4.17)]
c, c', c_g, c_j, c'_j	Real constants

$\boldsymbol{c}$	Column vector
D, D_c, D_h, D_r	Diffusion coefficients
$\mathbf{D}$	Diffusion matrix
d, d', d''	Dimensions
d_p	Distance between plates
d	Differential
$\mathbf{E}(t,t')$	Displacement gradient tensor [(4.14)]
$E(X\|\mathcal{A}')$	Conditional expectation of X given $\mathcal{A}'$ [Definition 2.51]
$E(X\|Y=y)$	Conditional expectation of X for given value y of Y [(2.56)]
$\mathcal{E}$, $\mathcal{E}_j$, $\mathcal{E}_t$	Generating systems for σ-algebras [Definition 2.5]
e	2.7182818...
F_t^B	Brownian force, random noise
$F_\mathrm{rel}^\mathrm{(m)}$	Effect of metric forces on the relative motion of two beads [Exercise 5.15]
$\boldsymbol{F}(\boldsymbol{r})$	Force field
$\boldsymbol{F}^\mathrm{c}$, $\boldsymbol{F}_k^\mathrm{c}$	Connector force (in spring k)
$\boldsymbol{F}_\mu$	Potential force on bead μ [(4.2)]
$\boldsymbol{F}_\mu^\mathrm{(e)}$	External force on bead μ
$\boldsymbol{F}_\mu^\mathrm{(m)}$	Metric force on bead μ [(5.62)]
$\overline{\boldsymbol{F}}_\mu^\mathrm{B}$	Smoothed Brownian force on bead μ [(4.66)]
$\mathcal{F}_k$	Generalized intramolecular forces [(5.24)]
$\mathcal{F}_k^\mathrm{(e)}$	Generalized external forces [(5.25)]
f	Relative frequency of the occurrence of an event
f_c, f_c'	Correction factors for the bias in variance reduced simulations [(4.36), (4.41)]
$G(t)$	Relaxation modulus [(1.15)]
g, $\widetilde{g}$, g_j, g_t, $g_t^{(n)}$	Generic names for functions with values in $\mathbb{R}$
$\boldsymbol{g}$, $\boldsymbol{g}_A$, $\boldsymbol{g}_B$, $\boldsymbol{g}_X$, $\boldsymbol{g}_Y$	Generic names for functions with values in $\mathbb{R}^d$ ($\boldsymbol{g}$ also used for gravitational field)
$\widetilde{\mathsf{g}}_{jk}$, g_{jk}, $\overline{\mathsf{g}}_{jk}$, $\hat{\mathsf{g}}_{jk}$	Elements of various modified metric matrices [(5.7), (5.9), (5.48), (5.49)]; the corresponding symbols without subscripts indicate determinants; the elements of the inverse matrices are denoted by capital letters, e.g. $\widetilde{\mathsf{G}}_{jk}$
H	Hookean spring constant
H_n	Hermite polynomials [(3.68)]
$H_{\mu\nu}$	Equilibrium-averaged hydrodynamic interactions between beads μ and ν [(4.69)]
$\mathbf{H}_{\mu\nu}$	Tensors associated with hydrodynamic interactions between beads μ and ν [(5.37)]
h^*, h	Hydrodynamic-interaction parameters [(4.70), p. 251]
$I(A)$	Set of indices of the elements contained in an event A [Example 2.13]
$I_t^{(n)}$, $\mathbf{I}_{t't}^{(2)}$	Iterated stochastic integrals [(3.65), (3.115)]

i	Imaginary unit
$\boldsymbol{J}$	Probability current [(3.83)]
j, k, l	Summation indices, integers
$\mathbf{K}$	Averaged structure tensor [Example 5.18]
k_B	Boltzmann's constant
L	Length of a rod
L_C	Contour length of a polymer chain [(6.20)]
$\mathcal{L}$, $\mathcal{L}_t$	Infinitesimal generator of a Markov process [(2.88)]
l_μ	Weight of bead μ in the center of resistance [(4.79)]
M, M_μ	Mass of a Brownian particle or bead μ
M_e	Molecular weight between entanglements [(6.15)]
M_p	Mass of a polymer chain
$\mathbf{M}$	Matrix
$\mathbf{M}_k$	Tensor describing the effect of a flow field on the generalized coordinate Q_k [(5.26)]
M_{jk}	Elements of a matrix with determinant M [Exercise 5.6]
m	Ratio of extensional rates [(1.17)]
N	Number of beads in bead-spring chains
N_C	Number of carbon atoms in the polymer backbone
N_p	Number of polymer chains in a system
N_T	Number of trajectories
N_t, N_y	Null sets labelled by t, y
n, n', n_j	Integers
n_p	Number density of polymers
n_A, n_B, n_{AB}	Number of occurrence of the events A, B, and $A \cap B$
$\boldsymbol{n}$	Unit normal vector
$o(\cdot)$	Term of lower order
P, P'	Probability measures
P_u	Probability for unobserved reflections [(6.18)]
P^X	Distribution of the random variable X [(2.27)]; $P(X \in \cdot) := P^X(\cdot)$
P^*	Completion of a probability measure
P_ω	Measure concentrated at a single point ω [Example 2.15]
$P(\cdot\|A)$	Conditional probability measure given the event A [(2.15)]
$P(X \in A\|Y = y)$	Conditional distribution of X for a given value y of Y [(2.54)]
$\overline{P}_{t_1 \ldots t_n}$	Family of finite-dimensional marginal distributions [(2.72)]
$\mathbf{P}$, $\mathbf{P}_{\mu\nu}$	Projection operators [Exercise 5.1, (5.41)]
$\mathcal{P}(\Omega)$	Set of all subsets of Ω
p, p_t	Probability densities
p^X	Probability density for P^X
p_ω	Probability density for P_ω (δ-function)

$p_{\alpha\Theta}$	Gaussian probability density with mean $\boldsymbol{\alpha}$ and covariance matrix $\boldsymbol{\Theta}$ [(2.21)]
p_{red}	Probability density in variance reduced simulations [Exercise 4.14]
$p(\cdot\|\cdot)$	Conditional probability density [(2.59)]
$p_{tt'}(x\|x')$	Transition probability density [(2.85)]
$\overline{p}_{t_1\ldots t_n}$	Family of finite-dimensional marginal probability densities
$\widetilde{p}$	Characteristic function [(2.13)]
p_j	Probabilities in discrete spaces
p_{h}	Hydrostatic pressure
Q, Q'	Length of $\boldsymbol{Q}$ [Example 4.13]
Q_j	Generalized coordinates
$\overline{\boldsymbol{Q}}$	Predicted value for $\boldsymbol{Q}$ in a predictor-corrector scheme [(4.33)]
$\widetilde{\boldsymbol{Q}}$	Biased random variables in variance reduced simulations
$\boldsymbol{Q}_j$, $\boldsymbol{Q}$	Connector vectors (or dummy variables) [Fig. 4.1]
$\boldsymbol{Q}'_k$	Normal modes associated with connector vectors
q, $\boldsymbol{q}$, $\boldsymbol{q}'$	Arguments of characteristic functions
R	Gas constant
$\overline{R}_{\text{g}}$	Root-mean-square radius of gyration
$\overline{R}_{\text{h}}$	Hydrodynamic radius [(4.91)]
R_F	Carlson's standard elliptic integral of the first kind [Example 4.17]
$\boldsymbol{R}_\mu$	Bead position vectors with respect to the center of mass [(5.1)]
r	Length of $\boldsymbol{r}$
$\boldsymbol{r}$, $\boldsymbol{r}'$	Position vectors
$\boldsymbol{r}_\mu$	Bead position vectors
$\boldsymbol{r}_{\text{c}}$	Center of mass position vector [Fig. 4.1, (5.1)]
$\boldsymbol{r}_{\text{h}}$	Center of resistance position vector [(4.78)]
$\widetilde{\boldsymbol{r}}_\mu$, $\overline{\boldsymbol{r}}_\mu$	Auxiliary bead positions in simulation algorithms for models with constraints
$S = (S_t)_{t\in\mathbb{T}}$, S', $\widehat{S}$	Wiener processes in the interval $[0, 1]$
$\widetilde{S}_j$, S', S''	Approximations for the process S at discrete times
S_V	Area of an oriented plane
s, s', s_0	Dummy variable in the probability density of S, S_0
T	Absolute temperature
T^{FP}	First passage time [(3.82)]
T_t^{LR}	Last reflection time [(3.93)]
$\mathbf{T}(\boldsymbol{x})$	Matrix of partial derivatives [Example 3.43]
$\mathcal{T}$	Time ordering [(3.56)]
t, t', t'', t_j, $t_j^{(n)}$	Time variables, labels
t_{block}	Time corresponding to a block of time steps
t_{max}	Maximum time argument

U_{RD}, $U_{\eta\lambda}$, $U_{\eta\mathrm{R}}$, $U_{\Psi\eta}$, $U_{\Psi\Psi}$	Universal ratios for long polymer chains [(4.92), (4.95), (4.97), (4.98), (4.99)]
$\boldsymbol{U} = (\boldsymbol{U}_t)_{t\in\mathbb{T}}$, $\boldsymbol{U}'$, $\widehat{\boldsymbol{U}}$	Stochastic process on the unit sphere
$\widetilde{\boldsymbol{U}}_j$	Approximations for the process $\boldsymbol{U}$ at discrete times
$\boldsymbol{u}$	Dummy variable in the probability density of $\boldsymbol{U}$
$\widehat{\boldsymbol{u}}$	Result of the deterministic time evolution of $\boldsymbol{u}$ [(6.6)]
V	Volume
$V^{(\mathrm{e})}$	External potential
V_{ev}	Excluded-volume potential [(4.116)]
$(V_t)_{t\in\mathbb{T}}$	Ornstein-Uhlenbeck velocity process
$\boldsymbol{V}$	Velocity
$\Delta\mathbf{V}$	Random matrix representing the antisymmetric part of the stochastic integral $\mathbf{I}^{(2)}_{t't}$ over a short time interval [(3.121)]
v_{ev}, U_{ev}	Strength of the excluded-volume potential [(4.116), (5.83)]
$\boldsymbol{v}(\boldsymbol{r}, t)$	Velocity field
$\boldsymbol{v}_0(t)$	Time dependent velocity vector
$\boldsymbol{v}_{\mathrm{rot}}(\boldsymbol{r})$	Rotational velocity field [Example 4.23]
$\Delta\boldsymbol{v}(\boldsymbol{r})$	Velocity perturbation
$W = (W_t)_{t\in\mathbb{T}}$	Wiener process [Example 2.79]
W^z, W^ϕ	Wiener processes
$(W^{(n)})_{n\in\mathbb{N}}$	Sequence of discretizations of the Wiener process
$\boldsymbol{W} = (\boldsymbol{W}_t)_{t\in\mathbb{T}}$	Wiener process in d dimensions [(2.83)]
$\boldsymbol{W}_\mu$	Wiener processes associated with bead positions
$\boldsymbol{W}'_\mu$	Wiener processes associated with normal modes [(4.10), (4.11)]
$\boldsymbol{W}_j$, $\boldsymbol{W}^{\mathrm{i}}$, W^{f}_j	Standard Gaussian random variables [Example 4.17]
X, X', Y, Y'	Real-valued random variables or stochastic processes, e.g. $X = (X_t)_{t\in\mathbb{T}}$ (whenever it is convenient, the time argument of a stochastic process is given in parentheses rather than as a subscript)
$\boldsymbol{X}$, $\boldsymbol{Y}$, $\boldsymbol{Y}^{\Delta t}$	Vector-valued random variables or stochastic processes
$\widetilde{X}_j$, $\widetilde{\boldsymbol{Y}}_j$, $\widetilde{W}_j$, $\widetilde{W}^{(n)}_j$	Random variables, stochastic processes at discrete times
$(X_n)_{n\in\mathbb{N}}$	Sequence of random variables
$(X^{(n)})_{n\in\mathbb{N}}$	Sequence of stochastic processes
x, x', x'', $\boldsymbol{x}$, y, $\boldsymbol{y}$	Dummy variables in functions or densities
$\overline{\boldsymbol{Y}}_j$	Predicted values in a predictor-corrector scheme [(3.133)]
$\Delta\widetilde{\boldsymbol{Y}}_j$	Auxiliary random variables [(4.115)]
$\mathbf{Z}$	Total effective friction tensor [(5.5)]
z	$\cos\theta$

Greek Symbols

α, $\boldsymbol{\alpha}$, α_t, $\boldsymbol{\alpha}_t$	Mean of a distribution
α_{B}	Strength of Brownian forces [(3.5)]
α_{s}	Exponent characterizing an α-stable distribution
β	Reduced shear rate [Fig. 4.15]
$\dot{\gamma}$, $\dot{\gamma}_0$	Shear rate [(1.4)]
γ_j	Lagrange multipliers
Δ	Correlation length parameter [(6.24)]
$\Delta \cdots$	Differences of variables
δ_{jk}	Kronecker's δ-symbol
$\delta(t)$	Dirac's δ-function
$\boldsymbol{\delta}$	Unit tensor or unit matrix (with components δ_{jk})
ϵ, $\bar{\epsilon}$, $\bar{\bar{\epsilon}}$	Dimensionless parameters in reptation models [(6.5), (6.30), (6.31)] (ϵ also used for small real numbers)
$\boldsymbol{\varepsilon}(t_j, t_{j+1}, t_n)$	Auxiliary tensor in variance reduced simulations [(4.52)]
$\dot{\epsilon}$	Extensional strain rate [(1.17)]
ζ	Friction coefficient
$\boldsymbol{\zeta}_\mu$	Bead friction tensors
$\boldsymbol{\zeta}_{\mu\nu}$	Effective friction tensors [(5.3)]
$\tilde{\boldsymbol{\zeta}}_{\mu\nu}$	Modified effective friction tensors [(5.4)]; $\tilde{\boldsymbol{\zeta}}_{\mu\nu} = \tilde{\zeta}_{\mu\nu}\,\boldsymbol{\delta}$ for isotropic tensors
η	Viscosity [(1.6)]
η_{p}	Polymer contribution to the viscosity
η_{s}	Solvent viscosity
$\bar{\eta}$	Trouton viscosity
$[\eta]_0$	Intrinsic viscosity [(4.96)]
Θ	Variance (special case of $\boldsymbol{\Theta}$)
Θ_{red}	Variance in variance reduced simulations
$\Theta_{\mathrm{f}}^{(j)}$	Eigenvalues of $\boldsymbol{\Theta}_{\mathrm{f}}$
$\boldsymbol{\Theta}$, $\boldsymbol{\Theta}'$, $\boldsymbol{\Theta}_{\mathrm{i}}$, $\boldsymbol{\Theta}_{\mathrm{f}}$, $\boldsymbol{\Theta}_t$	Covariance matrices
$\Theta_{tt'}$, $\boldsymbol{\Theta}_{tt'}$	Covariances of a Gaussian process
θ	Polar angle
κ	Elastic modulus of a rope
$\boldsymbol{\varkappa}$	Transposed velocity gradient tensor
$\overline{\boldsymbol{\varkappa}}$	Perturbed velocity gradient tensor
λ, λ_H, λ_h, λ_j, λ^{rd}	Time constants
λ_η	Characteristic time scale associated with the intrinsic viscosity [(4.94)]
$\boldsymbol{\lambda}_\mu$	Weight tensors [(5.6)]
μ_1, μ_2	Extensional viscosities [(1.19), (1.20)]
μ, μ', ν	Summation indices
$\overline{\mu}$	First passage time distribution for the Wiener process in $[0, 1]$ [(3.91)]
$\overline{\nu}$	Memory function in reptation models [(6.33)]

ν_{ev}	Exponent characterizing the chain length dependence of the polymer size in the presence of excluded volume
π	3.1415926...
$\overline{\pi}$	Conditional distribution of first passage times for the Wiener process in $[0,1]$ [(3.92)]
ρ	Mass density
ρ_{p}	Polymer mass density
σ	Width of a one-dimensional distribution [(2.12)]
$\overline{\sigma}$	Width of a one-dimensional distribution with infinite variance
σ_{B}	Contribution to σ_{F} caused by Brownian forces
σ_{F}	Rope tension in the reptating-rope model [(6.20)]
σ_{sf}	Empirical steric factor [(4.119)]
$\boldsymbol{\sigma}$	Generalization of σ to d dimensions (a matrix with elements σ_{jk})
$\boldsymbol{\tau}$	Stress tensor [(1.2)]
$\boldsymbol{\tau}^{\mathrm{p}}$	Polymer contribution to the stress tensor [(4.18)]
$\boldsymbol{\tau}^{\mathrm{rv}}$	Random variable associated with the polymer contribution to the stress tensor [(4.29)]
$\widehat{\boldsymbol{\tau}}$, $\widehat{\boldsymbol{\tau}}^n$	Auxiliary tensors in a reptation model [(6.38)]
υ	Order of convergence [(3.111), (3.118)]
$\boldsymbol{\Upsilon}_j^n$, $\overline{\boldsymbol{\Upsilon}}_j^n$	Supporting values [(3.127), (3.129)]
$\boldsymbol{\Phi}_t$	Fundamental matrix of a system of homogeneous linear differential equations [(3.56), (3.62)]
$\boldsymbol{\Phi}_{\mathrm{app}}(t_{j+1}, t_n)$	Auxiliary tensor in variance reduced simulations [(4.52)]
ϕ	Polar angle
$(\phi_t)_{t\in\mathbb{T}}$	Increasing process [(3.88)]
χ_A	Indicator function of a set A
Ψ_1, Ψ_2	Normal stress coefficients [(1.7), (1.8)]
Ω, Ω', Ω'', Ω_j	Sure event, set of all possible outcomes
Ω_t	Time-dependent domain of a stochastic process
Ω_{jk}^{R}, Ω_{jk}^{Z}	Elements of orthogonal matrices [(4.7), (4.75)]
$(\Omega, \mathcal{A})$	Measurable space
$(\Omega, \mathcal{A}, P)$	Probability space
$\boldsymbol{\Omega}_{\Theta_{\mathrm{f}}}$	Orthogonal matrix diagonalizing $\boldsymbol{\Theta}_{\mathrm{f}}$
$\boldsymbol{\Omega}(\boldsymbol{r})$	Hydrodynamic-interaction tensor [(4.62), (4.67)]; $\boldsymbol{\Omega}_{\mu\nu} := \boldsymbol{\Omega}(\boldsymbol{r}_\mu - \boldsymbol{r}_\nu)$
ω_0	Frequency
ω, ω_j	Possible outcome in a random experiment, $\omega \in \Omega$

Subscripts

app	Approximate quantity (probability density, transition probability density, or expectation evaluated with an approximate probability density)