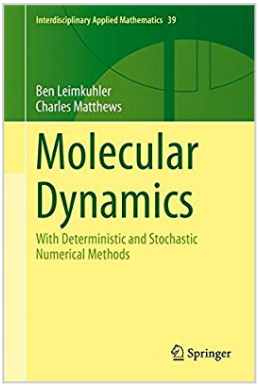

Molecular Dynamics: With Deterministic and Stochastic Numerical Methods (Interdisciplinary Applied Mathematics)

By Ben Leimkuhler, Charles Matthews

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This book describes the mathematical underpinnings of algorithms used for molecular dynamics simulation, including both deterministic and stochastic numerical methods. Molecular dynamics is one of the most versatile and powerful methods of modern computational science and engineering and is used widely in chemistry, physics, materials science and biology. Understanding the foundations of numerical methods means knowing how to select the best one for a given problem (from the wide range of techniques on offer) and how to create new, efficient methods to address particular challenges as they arise in complex applications.

Aimed at a broad audience, this book presents the basic theory of Hamiltonian mechanics and stochastic differential equations, as well as topics including symplectic numerical methods, the handling of constraints and rigid bodies, the efficient treatment of Langevin dynamics, thermostats to control the molecular ensemble, multiple time-stepping, and the dissipative particle dynamics method.

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Editorial Review

Review
“This book is strongly recommended both for individual study and as the basis of a graduate course in computational MD that covers current research topics; for an audience of mathematics students, who may feel uneasy with the rather pragmatic presentation that mixes analytical arguments, numerical demonstrations, and heuristics … . Researchers in the field ought to find the book to be worth occupying a spot in their bookshelves.” (Carsten Hartmann, SIAM Review, Vol. 57 (3), September, 2015)

From the Back Cover

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About the Author

Benedict Leimkuhler has worked extensively for more than two decades on the study of molecular dynamics algorithms. He is the author of research publications on constrained molecular dynamics, temperature controls, stochastic molecular dynamics methods, quantum methods, and advanced integration strategies (multiple time-stepping, adaptive methods). He currently holds the Chair of Applied Mathematics at the University of Edinburgh, is a Fellow of the Royal Society of Edinburgh and a Fellow of the Institute of Mathematics and Its Applications, and is on the editorial boards of four journals.

Charles Matthews obtained his PhD in applied mathematics from the University of Edinburgh, working in the area of numerical methods for stochastic differential equations. He has published research in both chemical physics and mathematics journals on discretization problems in molecular dynamics. He currently is a research staff member in the Department of Statistics at the University of Chicago, investigating sampling methodologies for molecular simulation and the modelling of power networks.

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