



Molecular Dynamics: With Deterministic and Stochastic Numerical Methods (1st ed. 2015)

By Benedict Leimkuhler, Charles Matthews

Springer International Publishing AG. Hardback. Condition: new. BRAND NEW, Molecular Dynamics: With Deterministic and Stochastic Numerical Methods (1st ed. 2015), Benedict Leimkuhler, Charles Matthews, 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.



READ ONLINE
[1.28 MB]

Reviews

It is an awesome publication which i actually have ever read through. it had been writtern really properly and valuable. I found out this book from my i and dad recommended this pdf to discover.

-- Doyle Schmeler

This book is definitely not simple to begin on studying but quite fun to see. I actually have read and that i am sure that i will gonna read through yet again once again in the foreseeable future. It is extremely difficult to leave it before concluding, once you begin to read the book.

-- Brennan Koelpin