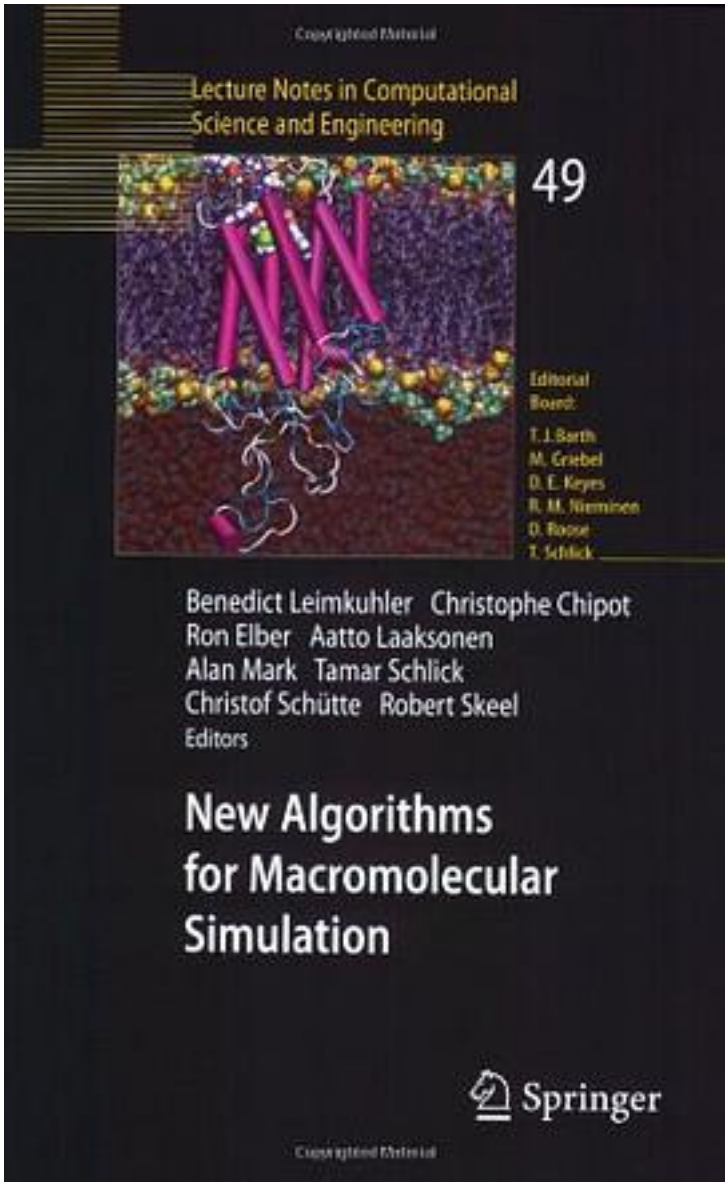
New Algorithms for Macromolecular Simulation



New Algorithms for Macromolecular Simulation_下载链接1_

著者:Leimkuhler, B. (EDT)/ Chipot, Christophe (EDT)/ Elber, Ron (EDT)/ Laaksonen, Aatto (EDT)/ Mark, Alan (EDT)/ Schlick, Tamar (EDT)/ Schutte, Christophe

出版者:Springer-Verlag New York Inc

出版时间:

装帧:Pap

isbn:9783540255420

Molecular simulation is a widely used tool in biology, chemistry, physics and engineering. This book contains a collection of articles by leading researchers who are developing new methods for molecular modelling and simulation. Topics addressed here include: multiscale formulations for biomolecular modelling, such as quantum-classical methods and advanced solvation techniques; protein folding methods and schemes for sampling complex landscapes; membrane simulations; free energy calculation; and techniques for improving ergodicity. The book is meant to be useful for practitioners in the simulation community and for those new to molecular simulation who require a broad introduction to the state of the art.

作者介绍:

目录:

标签

评论

New Algorithms for Macromolecular Simulation_下载链接1_

书评

New Algorithms for Macromolecular Simulation_下载链接1_