

LECTURE NOTES  
IN PHYSICS

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(Eds.)

# Novel Methods in Soft Matter Simulations



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# Novel Methods In Soft Matter Simulations Lecture Notes In Physics

**Mike Jess**

## Novel Methods In Soft Matter Simulations Lecture Notes In Physics:

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*New Algorithms for Macromolecular Simulation* Benedict Leimkuhler,Christophe Chipot,Ron Elber,Aatto Laaksonen,Alan Mark,Tamar Schlick,Christoph Schütte,Robert Skeel,2006-03-22 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

*Fluid Mechanics and the SPH Method* Damien Violeau,2012-05-03 This

book presents the SPH method for fluid modelling from a theoretical and applied viewpoint It explains the foundations of the method from physical principles and will help researchers students and engineers to understand how the method should be used and why it works well **Models for Polymeric and Anisotropic Liquids** Martin Kröger,2005-09-15 Models should be as simple as possible but no simpler For the physics of polymeric liquids whose relevant lengths and time scales are out of reach for first principles calculations this means that we have to choose a minimum set of sufficiently detailed descriptors such as architecture linear ring branched connectivity semiflexibility stretchability excluded volume and hydrodynamic interaction These universal fluids allow the prediction of material properties under external flow or electrodynamic fields the results being expressed in terms of reference units specific for any particular chosen material This book provides an introduction to the kinetic theory and computer simulation methods needed to handle these models and to interpret the results Also included are a number of sample applications and computer codes

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