

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

Arthur James Wells

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Modeling and Simulation in Polymers Purushottam D. Gujrati,Arkady I. Leonov,2010-03-30 Filling a gap in the literature and all set to become the standard in this field this monograph begins with a look at computational viscoelastic fluid mechanics and studies of turbulent flows of dilute polymer solutions It then goes on discuss simulations of nanocomposites polymerization kinetics computational approaches for polymers and modeling polyelectrolytes Further sections deal with tire optimization irreversible phenomena in polymers the hydrodynamics of artificial and bacterial flagella as well as modeling and simulation in liquid crystals The result is invaluable reading for polymer and theoretical chemists chemists in industry materials scientists and plastics technologists

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

Jamming, Yielding, and Irreversible Deformation in Condensed Matter Carmen Miguel,Miguel Rubi,2006-02-21 This collection of ten tutorial reviews by leading researchers in the field introduces and renews recent advances on irreversible deformation phenomena in solid state and soft condensed matter physics The focus in applications is on amorphous materials crystalline solids under stress and more generally elastic manifolds driven by external processes This book addresses in particular nonspecialists and graduate students wishing to enter the field

Multiscale Modelling of Soft Matter ,2010 *Complex Systems* Michio Tokuyama,Irwin Oppenheim,Hideya Nishiyama,2008-03-10 Sendai Japan 25 28 September 2007

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Computational Modeling of Materials and Processing Joseph Habib Simmons,1997 The proceedings of the May 1995 symposium contain 32 papers representing myriad disciplines and size scales and reflecting interactions between theoretical computational and experimental research Modeling at the atomistic and molecular level includes calculations of glass and crystalline struct

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