



Numerical Methods for Polymeric Systems

By -

Springer. Hardcover. Condition: New. 223 pages. Dimensions: 9.3in. x 6.3in. x 0.8in. Polymers occur in many different states and their physical properties are strongly correlated with their conformations. The theoretical investigation of the conformational properties of polymers is a difficult task and numerical methods play an important role in this field. This book contains contributions from a workshop on numerical methods for polymeric systems, held at the IMA in May 1996, which brought together chemists, physicists, mathematicians, computer scientists and statisticians with a common interest in numerical methods. The two major approaches used in the field are molecular dynamics and Monte Carlo methods, and the book includes reviews of both approaches as well as applications to particular polymeric systems. The molecular dynamics approach solves the Newtonian equations of motion of the polymer, giving direct information about the polymer dynamics as well as about static properties. The Monte Carlo approaches discussed in this book all involve sampling along a Markov chain defined on the configuration space of the system. An important feature of the book is the treatment of Monte Carlo methods, including umbrella sampling and multiple Markov chain methods, which are useful for strongly interacting systems such as polymers at low...



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