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Nota di contenuto	Modeling and Simulation in Polymers; Contents; Preface; List of Contributors; 1 Computational Viscoelastic Fluid Mechanics and Numerical Studies of Turbulent Flows of Dilute Polymer Solutions; 1.1 Introduction and Historical Perspective; 1.2 Governing Equations and Polymer Modeling; 1.3 Numerical Methods for DNS; 1.3.1 Spectral Methods: Influence Matrix Formulation; 1.3.1.1 The Semi-Implicit/Explicit Scheme; 1.3.1.2 The Fully Implicit Scheme; 1.3.1.3 Typical Simulation Conditions; 1.3.2 The Positive Definiteness of the Conformation Tensor 1.4 Effects of Flow, Rheological, and Numerical Parameters on DNS of Turbulent Channel Flow of Dilute Polymer Solutions1.4.1 Drag Reduction Evaluation; 1.4.2 Effects of Flow and Rheological Parameters; 1.4.3 Effects of Numerical Parameters; 1.5 Conclusions and Thoughts on Future Work; References; 2 Modeling of Polymer Matrix Nanocomposites; 2.1 Introduction; 2.2 Polymer Clay Nanocomposites and Coarse-Grained Models; 2.2.1 Coarse-Grained Components; 2.2.2 Methods and Timescales; 2.2.2.1 Off-Lattice (Continuum) Approach; 2.2.2.2 Discrete Lattice Approach; 2.2.2.3 Hybrid Approach 2.2.3 Coarse-Grained Sheet2.2.3.1 Conformation and Dynamics of a

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4.2.4 Boundary Conditions

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Sommario/riassunto

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 f

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