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The simulation of physical systems requires a simplified, hierarchical approach which models each level from the atomistic to the macroscopic scale. From quantum mechanics to fluid dynamics, this book systematically treats the broad scope of computer modeling and simulations, describing the fundamental theory behind each level of approximation. Berendsen evaluates each stage in relation to its applications giving the reader insight into the possibilities and limitations of the models. Practical guidance for applications and sample programs in Python are provided. With a strong emphasis on molecular models in chemistry and biochemistry, this book will be suitable for advanced undergraduate and graduate courses on molecular modeling and simulation within physics, biophysics, physical chemistry and materials science.