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The extremely powerful technique of molecular dynamics simulation involves solving the classical many-body problem in contexts relevant to the study of matter at the atomistic level. Since there is no alternative approach capable of handling this extremely broad range of problems at the required level of detail, molecular dynamics methods have proved themselves indispensable in both pure and applied research. This book is a blend of tutorial and recipe collection, providing both an introduction to the subject for beginners and a reference manual for the more experienced practitioner. It is organized as a series of case studies that take the reader through each of the steps from formulating the problem, developing the necessary software, and then using the programs to make actual measurements. The second edition of the book includes a substantial amount of new material as well as completely rewritten software.