

1. Record Nr.	UNINA9910828065703321
Autore	Rapaport D. C.
Titolo	The art of molecular dynamics simulation // D.C. Rapaport [[electronic resource]]
Pubbl/distr/stampa	Cambridge : , : Cambridge University Press, , 2004
ISBN	1-107-14671-2 1-139-63703-7 0-511-64818-9 0-511-19374-2 0-511-56632-8 0-511-81658-8 0-511-19448-X
Edizione	[Second edition.]
Descrizione fisica	1 online resource (xiii, 549 pages) : digital, PDF file(s)
Disciplina	539/.6
Soggetti	Condensed matter - Computer simulation Molecular dynamics - Computer simulation
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Title from publisher's bibliographic system (viewed on 05 Oct 2015).
Nota di bibliografia	Includes bibliographical references (p. 519-531) and indexes.
Nota di contenuto	Cover; Half-title; Title; Copyright; Contents; Preface to the first edition; Preface to the second edition; About the software; 1 Introduction; 2 Basic molecular dynamics; 3 Simulating simple systems; 4 Equilibrium properties of simple fluids; 5 Dynamical properties of simple fluids; 6 Alternative ensembles; 7 Nonequilibrium dynamics; 8 Rigid molecules; 9 Flexible molecules; 10 Geometrically constrained molecules; 11 Internal coordinates; 12 Many-body interactions; 13 Long-range interactions; 14 Step potentials; 15 Time-dependent phenomena; 16 Granular dynamics 17 Algorithms for supercomputers 18 More about software; 19 The future; Appendix; References; Function index; Index; Colophon
Sommario/riassunto	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, first published in 2004, 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.
