

1. Record Nr.	UNINA9910739404303321
Autore	Battimelli Giovanni
Titolo	Computer Meets Theoretical Physics : The New Frontier of Molecular Simulation / / by Giovanni Battimelli, Giovanni Ciccotti, Pietro Greco
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2020
ISBN	3-030-39399-2
Edizione	[1st ed. 2020.]
Descrizione fisica	1 online resource (214 pages)
Collana	The Frontiers Collection, , 1612-3018
Disciplina	530
Soggetti	Physics Chemistry, Physical and theoretical Computer simulation Sociophysics Econophysics Numerical and Computational Physics, Simulation History and Philosophical Foundations of Physics Theoretical and Computational Chemistry Popular Science in Physics Simulation and Modeling Data-driven Science, Modeling and Theory Building
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	A new science -- The origins of simulation -- The growth of molecular dynamics -- Molecular simulation lands in Europe -- CECAM and the development of molecular simulation -- Simulation comes of age -- Quantum systems and critical phenomena -- A first finishing line and some provisional conclusions.
Sommario/riassunto	This book provides a vivid account of the early history of molecular simulation, a new frontier for our understanding of matter that was opened when the demands of theoretical physicists were met by the availability of the modern computers. Since their inception, electronic computers have enormously increased their performance, thus making possible the unprecedented technological revolution that characterizes

our present times. This obvious technological advancement has brought with it a silent scientific revolution in the practice of theoretical physics. In particular, in the physics of matter it has opened up a direct route from the microscopic physical laws to observable phenomena. One can now study the time evolution of systems composed of millions of molecules, and simulate the behaviour of macroscopic materials and actually predict their properties. Molecular simulation has provided a new theoretical and conceptual tool that physicists could only dream of when the foundations of statistical mechanics were laid. Molecular simulation has undergone impressive development, both in the size of the scientific community involved and in the range and scope of its applications. It has become the ubiquitous workhorse for investigating the nature of complex condensed matter systems in physics, chemistry, materials and the life sciences. Yet these developments remain largely unknown outside the inner circles of practitioners, and they have so far never been described for a wider public. The main objective of this book is therefore to offer a reasonably comprehensive reconstruction of the early history of molecular simulation addressed to an audience of both scientists and interested non-scientists, describing the scientific and personal trajectories of the main protagonists and discussing the deep conceptual innovations that their work produced.
