Record Nr. UNINA9911009142503321 Autore Bottoni Maurizio Titolo Molecular Dynamics - Theory and Applications / / by Maurizio Bottoni, Simone Mantovani, Gaetano Zanghirati Cham:,: Springer Nature Switzerland:,: Imprint: Springer,, 2025 Pubbl/distr/stampa **ISBN** 3-031-84567-6 Edizione [1st ed. 2025.] Descrizione fisica 1 online resource (487 pages) Collana Mechanical Engineering Series, , 2192-063X Altri autori (Persone) MantovaniSimone ZanghiratiGaetano Disciplina 541.394 Soggetti Fluid mechanics Mechanics, Applied Molecular dynamics Atmospheric science Nuclear engineering **Engineering Fluid Dynamics Engineering Mechanics** Molecular Dynamics Atmospheric Science **Nuclear Energy** Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Nota di contenuto Chapter 1. Basic concepts of molecular dynamics -- Chapter 2. Examples of applications -- Chapter 3. Special applications of the discrete random deviation -- Chapter 4. Kaburaki, Nambu and the Japanese school -- Chapter 5. Aerosols and Atmospheric Physics --Chapter 6. Thermal Confinement -- Chapter 7. Look into the future. Sommario/riassunto This book originated from seminars given at the Institute of Nuclear Energy Technology (INET) of Tsinghua University, China, by the author in 1999. The courses gave graduate students a basic understanding of numerical techniques that would enable them to deal with problems of Computational Fluid Dynamics (CFD) and of molecular dynamics at research level. In subsequent years the lecture notes have been re-

organized and implemented for students of atmospheric sciences of

the Physics Department of the University of Ferrara, Italy. The lecture notes are divided into eight chapters, where some chapters are characterized by a scholastic approach. Specifically, Chapter 1 describes the theoretical basis of molecular dynamics, Chapter 2 gives examples of applications, like the Bénard problem; and Chapter 3 presents a summary of applications of DLA (Diffusion Limited Aggregation). The remainder of the book follows a less conventional approach, mainly informed by the author's experience in the development of computer programs and in teaching. Chapter 4 is dedicated to a comparison of traditional and advanced methods of analysing nuclear safety problems in thermal and fast reactors, Chapter 5 concerns simulation of thermophoresis and aerosol displacement in atmospheric physics, and Chapter 6 discusses thermal confinement of cosmic particles due to thermophoretic forces in space domain. Addressing the recognized difficulty of proceeding from the theoretical formulations found in textbooks to properly working computer programs, and the typically large gap between the theoretical foundation and the final result, Molecular Dynamics - Theory and Applications is ideal for graduate level researchers and practitioners working in the development of codes for simulating physical problems. Describes a method to analysis of sodium vapor flow in the safety analysis of sodium cooled fast breeder reactors Gives a summary and examples of applications of several variants of Diffusion Limited Accreation Explains how to construct computer programs for simulation of thermophoresis and thermal confinement of particles.