

1. Record Nr.	UNINA9910585771403321
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Titolo	Computational Multiscale Modeling of Fluids and Solids : Theory and Applications // by Martin Oliver Steinhauser
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2022
ISBN	9783030989545 9783030989538
Edizione	[3rd ed. 2022.]
Descrizione fisica	1 online resource (450 pages)
Collana	Graduate Texts in Physics, , 1868-4521
Disciplina	532 532.0015118
Soggetti	Mathematical physics Materials - Analysis Mathematics - Data processing Engineering mathematics Engineering - Data processing Geology Theoretical, Mathematical and Computational Physics Characterization and Analytical Technique Computational Mathematics and Numerical Analysis Mathematical and Computational Engineering Applications
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Introduction to Multiscale Modeling -- Multiscale Computational Materials Science -- Mathematical and Physical Prerequisites -- Fundamentals of Numerical Simulation -- Computational Methods on Electronic/Atomistic Scale.
Sommario/riassunto	The expanded 3rd edition of this established textbook offers an updated overview and review of the computational physics techniques used in materials modelling over different length and time scales. It describes in detail the theory and application of some of the most important methods used to simulate materials across the various levels of spatial and temporal resolution. Quantum mechanical methods such

as the Hartree-Fock approximation for solving the Schrödinger equation at the smallest spatial resolution are discussed as well as the Molecular Dynamics and Monte-Carlo methods on the micro- and meso-scale up to macroscopic methods used predominantly in the Engineering world such as Finite Elements (FE) or Smoothed Particle Hydrodynamics (SPH). Extensively updated throughout, this new edition includes additional sections on polymer theory, statistical physics and continuum theory, the latter being the basis of FE methods and SPH. Each chapter now first provides an overview of the key topics covered, with a new “key points” section at the end. The book is aimed at beginning or advanced graduate students who want to enter the field of computational science on multi-scales. It provides an in-depth overview of the basic physical, mathematical and numerical principles for modelling solids and fluids on the micro-, meso-, and macro-scale. With a set of exercises, selected solutions and several case studies, it is a suitable book for students in physics, engineering, and materials science, and a practical reference resource for those already using materials modelling and computational methods in their research.
