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Composite Materials Engineering
19th International Conference, Faro, Portugal, June 12–14, 2019, Proceedings, Part IV
Multiscale Modeling and Simulation of Shock Wave-Induced Failure in Materials Science
Techniques and Applications
Multiscale Modeling of Additively Manufactured Metals
Multiscale Modelling of Polymer Properties
Computational Science – ICCS 2019
Computational Fluid Dynamics
Chemical Engineering in the Pharmaceutical Industry
Micromechanics of Composite Materials
Modeling, Analysis and Numerical Simulation

HOUSTON STONE

Modeling and Computational Analysis of Multiscale Phenomena in Fluid-Structure Interaction Problems John Wiley & Sons
Summary: A Generalized Multiscale Analysis Approach brings together comprehensive background information on the multiscale nature of the composite, constituent material behaviour, damage models and key techniques for multiscale modelling, as well as presenting the findings and methods, developed over a lifetime's research, of three leading experts in the field. The unified approach presented in the book for conducting multiscale analysis and design of conventional and smart composite materials is also applicable for structures with complete linear and nonlinear material behavior, with numerous applications provided to illustrate use. Modeling composite behaviour is a key challenge in research and industry; when done efficiently and reliably it can save money, decrease time to market with new innovations and prevent component failure.
New Computational Challenges in Materials, Structures, and Fluids CRC Press
Mechanical behaviors of materials are highly influenced by their architectures and/or microstructures. Hence, progress in material science involves understanding and modeling the link between the microstructure and the material behavior at different scales. This book gathers contributions from eminent researchers in the field of computational and experimental material modeling. It presents advanced experimental techniques to acquire the microstructure features together with dedicated numerical and analytical tools to take into account the randomness of the micro-structure.
Multiscale Modeling and Simulation in Science Springer
Modelling in polymer materials science has experienced a dramatic growth in the last two decades. Advances in modeling methodologies together with rapid growth in computational power have made it

possible to address increasingly complex questions both of a fundamental and of a more applied nature. Multiscale Modelling of Polymer Properties assembles research done on modeling of polymeric materials from a hierarchical point of view, in which several methods are combined in a multilevel approach to complex polymeric materials. Contributions from academic and industrial experts are organized in two parts: the first one addresses the methodological aspects while the second one focuses on specific applications. The book aims at comprehensively assessing the current state of the field, including the strengths and shortcomings of available modelling techniques, and at identifying future needs and trends. * Several levels of approximation to the field of polymer modelling; ranging from first-principles to purely macroscopic * Contributions from both academic and industrial experts with varying fields of expertise * Assesses current state of this emerging and rapidly growing field

MDPI

This book provides an overview of multiscale approaches and homogenization procedures as well as damage evaluation and crack initiation, and addresses recent advances in the analysis and discretization of heterogeneous materials. It also highlights the state of the art in this research area with respect to different computational methods, software development and applications to engineering structures. The first part focuses on defects in composite materials including their numerical and experimental investigations; elastic as well as elastoplastic constitutive models are considered, where the modeling has been performed at macro- and micro levels. The second part is devoted to novel computational schemes applied on different scales and discusses the validation of numerical results. The third part discusses gradient enhanced modeling, in particular quasi-brittle and ductile damage, using the gradient enhanced approach. The final part addresses thermoplasticity, solid-liquid mixtures and ferroelectric models. The contents are based on the international workshop “Multiscale Modeling of Heterogeneous Structures” (MUMO 2016), held in Dubrovnik, Croatia in September 2016.

Principles of Multiscale Modeling

Computational Multiscale Modeling of Fluids and SolidsTheory and Applications A systematic discussion of the fundamental principles, written by a leading contributor to the field.

Microflows and Nanoflows CRC Press

A guide to the important chemical engineering concepts for the development of new drugs, revised second edition The revised and updated second edition of Chemical Engineering in the Pharmaceutical Industry offers a guide to the experimental and computational methods related to drug product design and development. The second edition has been greatly expanded and covers a range of topics related to formulation design and process development of drug products. The authors review basic analytics for quantitation of drug product quality attributes, such as potency, purity, content uniformity, and dissolution, that are addressed with consideration of the applied statistics, process analytical technology, and process control. The 2nd Edition is divided into two separate books: 1) Active Pharmaceutical Ingredients (API’s) and 2) Drug Product Design, Development and Modeling. The contributors explore technology transfer and scale-up of batch processes that are exemplified experimentally and computationally. Written for engineers working in the field, the book examines in-silico process modeling tools that streamline experimental screening approaches. In addition, the authors discuss the emerging field of continuous drug product manufacturing. This revised second edition: Contains 21 new or revised chapters, including chapters on quality by design, computational approaches for drug product modeling, process design with PAT and process control, engineering challenges and solutions Covers chemistry and engineering activities related to dosage form design, and process development, and scale-up Offers analytical methods and applied statistics that highlight drug product quality attributes as design features Presents updated and new example calculations and associated solutions Includes contributions from leading experts in the field Written for pharmaceutical engineers, chemical engineers, undergraduate and graduation students, and professionals in the field of pharmaceutical sciences and manufacturing, Chemical Engineering in the Pharmaceutical Industry, Second Edition contains information designed to be of use from the engineer's perspective and spans information from solid to semi-solid to lyophilized drug products.

Multiscale Simulations and Mechanics of Biological Materials Springer

Multiscale Biomechanical Modeling of the Brain discusses the constitutive modeling of the brain at various length scales (nanoscale, microscale, mesoscale, macroscale and structural scale). In each scale, the book describes the state-of-the-experimental and computational tools used to quantify critical deformational information at each length scale. Then, at the structural scale, several user-based constitutive material models are presented, along with real-world boundary value problems. Lastly, design and optimization concepts are presented for use in occupant-centric design frameworks. This book is useful for both academia and industry applications that cover basic science aspects or applied research in head and brain protection. The multiscale approach to this topic is unique, and not found in other books. It includes meticulously selected materials that aim to connect the mechanistic analysis of the brain tissue at size scales ranging from subcellular to organ levels. Presents concepts in a theoretical and thermodynamic framework for each length scale Teaches readers not only how to use an existing multiscale model for each brain but also how to develop a new multiscale model Takes an integrated experimental-computational approach and gives structured multiscale coverage of the problems

Theory and Applications Springer

Most problems in science involve many scales in time and space. An example is turbulent ?ow where the important large scale quantities of lift and drag of a wing depend on the behavior of the small vortices in the boundarylayer. Another example is chemical reactions with concentrations of the species varying over seconds and hours while the time scale of the oscillations of the chemical bonds is of the order of femtoseconds. A third example from structural mechanics is the stress and strain in a solid beam which is well described by macroscopic equations but at the tip of a crack modeling details on a microscale are needed. A common dif?culty with the simulation of these problems and many others in physics, chemistry and biology is that an attempt to represent all scales will lead to an enormous computational problem with unacceptably long computation times and large memory requirements. On the other hand, if the discretization at a coarse level ignoresthe?nescale informationthenthesolutionwillnotbephysic allymeaningful. The in?uence of the ?ne scales must be incorporated into the model. This volume is the result of a Summer School on Multiscale Modeling and S- ulation in Science held at Boso ¤n, Lidingo ¤ outside Stockholm, Sweden, in June 2007. Sixty PhD students from applied mathematics, the sciences and engineering parti- pated in the summer

school.

A Unified Computational Fluid Dynamics Framework from Rarefied to Continuum Regimes ASM International

This book contains 23 papers presented at the ECCOMAS Multidisciplinary Jubilee Symposium - New Computational Challenges in Materials, Structures, and Fluids (EMJS08), in Vienna, February 18–20, 2008. The main intention of EMJS08 was to react adequately to the increasing need for interdisciplinary research activities allowing ef?cient solution of complex problems in engineering and in the applied sciences. The 15th anniversary of ECCOMAS (European Community on Computational Methods in Applied Sciences) provided a suitable frame for taking the afo- mentioned situation into account by inviting distinguished colleagues from d- ferent areas of engineering and the applied sciences, encouraging them to choose multidisciplinary topics for their lectures. The main themes of EMJS08 have a long tradition in engineering and in the applied sciences: materials, structures, and ?uids. The solution of scienti?c pr- lems involving ?uids together with solids and structures, not to forget the materials the structures are made of, is of paramount importance in a technical world of rapidly increasing sophistication, referred to as the Leonardo World by the eminent German philosopher Ju¨rgen Mittelstraß. More recently, the main themes of EMJS08 have gained considerable mom- tum, owing to signi?cant progress in nanotechnology. It enables resolution of a multitude of materials into their micro- and nanostructures. Covering aspects such as • Physical and chemical characterization • Multiscale modeling concepts, continuum micromechanics, and computational homogenization, as well as • Applications in various engineering ?elds the individual contributions to this book ?ow along different tracks of ?uids, materials, and structures.

Computational Multiscale Modeling of Fluids and Solids CRC Press

This book provides a compilation of innovative fabrication strategies and utilization methodologies that are frequently adopted in the advanced composite materials community. It addresses developing appropriate composites to efficiently utilize macro- and nanoscale features. It covers a selection of key aspects of composite materials, including history, reinforcements, matrix materials, mechanical properties, physical properties, theory, and applications. The volume reviews the research developments of a number of widely studied composite materials with different matrices. Key features of this book: Contains new coverage of nanocomposites Reflects the latest theoretical and engineering and industrial applications of composite materials Provides design methods with numerical information and technical formulations needed for researchers Presents a critical review of progress in research and development on composite materials Offers comments on future research direction and ideas for product development

Multiphysics and Multiscale Modeling Springer Science & Business Media

This book is the result of a careful selection of contributors in the field of CFD. It is divided into three sections according to the purpose and approaches used in the development of the contributions. The first section describes the "high-performance computing" (HPC) tools and their impact on CFD modeling. The second section is dedicated to "CFD models for local and large-scale industrial phenomena." Two types of approaches are basically contained here: one concerns the adaptation from global to local scale, - e.g., the applications of CFD to study the climate changes and the adaptations to local scale. The second approach, very challenging, is the multiscale analysis. The third section is devoted to "CFD in numerical modeling approach for experimental cases." Its chapters emphasize on the numerical approach of the mathematical models associated to few experimental (industrial) cases. Here, the impact and the importance of the mathematical modeling in CFD are focused on. It is expected that the collection of these chapters will enrich the state of the art in the CFD domain and its applications in a lot of fields. This collection proves that CFD is a highly interdisciplinary research area, which lies at the interface of physics, engineering, applied mathematics, and computer science.

Computational Multiscale Modeling of Multiphase Nanosystems Springer Science & Business Media

This document summarizes research done during the period June 14, 1989 through December 14, 1991 on a project aimed at the development of advanced computational methods for modeling multiscale fluid-structure interaction phenomena. The major thrust of the work reported is the development of the component parts of a new family of computational schemes that could be used to study large-scale problems in fluid-structure interaction. The overall theme of the project was the optimization of the computational process through the development of new adaptive techniques, data structures, a posteriori error estimates, and high-order solvers. The premise behind studying these types of high-order methods is that, with proper data structures, they could lead to exponential rates of convergence and thereby allow one to numerically solve very large problems, with features covering many different physical scales, using many fewer degrees of freedom than that required by conventional methods. In this spirit, the project was an ambitious one for it involved developing not only new adaptive algorithms for simulating the motion of elastic structures, but also techniques for fluid structure interaction and for modeling various regimes of incompressible viscous flows. Presumably, these methods could also be used to model the transition to turbulence and ultimately turbulent boundary layers on compliant surfaces.

Computational Methods for Solids and Fluids BoD – Books on Demand

The objectives of the master's thesis are to present, discuss and apply sequential multiscale modeling that combines analytical, numerical (finite element-based) and computational fluid dynamic (CFD) analysis to assist in the development of a radiantly driven macroscale solar thermal collector for energy harvesting. The solar thermal collector is a novel green energy system that converts solar energy to heat and utilizes dry air as a working heat transfer fluid (HTF). This energy system has important advantages over competitive technologies: it is self-contained (no energy sources are needed), there are no moving parts, no oil or supplementary fluids are needed and it is environmentally friendly since it is powered by solar radiation. This work focuses on the development of multi-physics and multiscale models for predicting the performance of the solar thermal collector. Model construction and validation is organized around three distinct and complementary levels.The first level involves an analytical analysis of the thermal transpiration phenomenon and models for predicting the associated mass flow pumping that occurs in an aerogel membrane in the presence of a large thermal gradient. Within the aerogel, a combination of convection, conduction and radiation occurs simultaneously in a domain where the pore size is comparable to the mean free path of the gas molecules. CFD modeling of thermal transpiration is not possible because all

the available commercial CFD codes solve the Navier Stokes equations only for continuum flow, which is based on the assumption that the net molecular mass diffusion is zero. However, thermal transpiration occurs in a flow regime where a non-zero net molecular mass diffusion exists. Thus these effects are modeled by using Sharipov's [2] analytical expression for gas flow characterized by high Knudsen number. The second level uses a detailed CFD model solving Navier Stokes equations for momentum, heat and mass transfer in the various components of the device. We have used state-of-the-art computational fluid dynamics (CFD) software, Flow3D (www. flow3d. com) to model the effects of multiple coupled physical processes including buoyancy driven flow from local temperature differences within the plenums, fluid-solid momentum and heat transfer, and coupled radiation exchange between the aerogel, top glazing and environment. In addition, the CFD models include both convection and radiation exchange between the top glazing and the environment. Transient and steady-state thermal models have been constructed using COMSOL Multiphysics.The third level consists of a lumped-element system model, which enables rapid parametric analysis and helps to develop an understanding of the system behavior; the mathematical models developed and multiple CFD simulations studies focus on simultaneous solution of heat, momentum, mass and gas volume fraction balances and succeed in accurate state variable distributions confirmed by experimental measurements.

Models, Databases and Simulation Tools Needed for Realization of Integrated Computational Mat. Eng. (ICME 2010) Elsevier

Environmental protection and sustainability are major concerns in today’s world, and a reduction in CO2 emission and the implementation of clean energy are inevitable challenges for scientists and engineers today. The development of electrochemical devices, such as fuel cells, Li-ion batteries, and artificial photosynthesis, is vital for solving environmental problems. A practical device requires designing of materials and operational systems; however, a multidisciplinary subject covering microscopic physics and chemistry as well as macroscopic device properties is absent. In this situation, multiscale simulations play an important role. This book compiles and details cutting-edge research and development of atomistic, nanoscale, microscale, and macroscale computational modeling for various electrochemical devices, including hydrogen storage, Li-ion batteries, fuel cells, and artificial photocatalysis. The authors have been involved in the development of energy materials and devices for many years. In each chapter, after reviewing the calculation methods commonly used in the field, the authors focus on a specific computational approach that is applied to a realistic problem crucial for device improvement. They introduce the simulation technique not only as an analysis tool to explain experimental results but also as a design tool in the scale of interest. At the end of each chapter, a future perspective is added as a guide for the extension of research. Therefore, this book is suitable as a textbook or a reference on multiscale simulations and will appeal to anyone interested in learning practical simulations and applying them to problems in the development of frontier and futuristic electrochemical devices.

Application to Laser Powder Bed Fusion Process Springer Science & Business Media

Multi-Scale Phenomena in Complex Fluids is a collection of lecture notes delivered during the ªrst two series of mini-courses from "Shanghai Summer School on Analysis and Numerics in Modern Sciences," which was held in 2004 and 2006 at Fudan University, Shanghai, China. This review volume of 5 chapters, covering various fields in complex fluids, places emphasis on multi-scale modeling, analyses and simulations. It will be of special interest to researchers and graduate students who want to work in the field of complex fluids.

Molecular Dynamics John Wiley & Sons

Multiscale mathematical modeling of flows containing particles is conducted in this study using computational fluid dynamics and molecular dynamics. The first study considered continuous media interaction of macro-scale fluid and micro-scale solid particles using computational fluid dynamics and rigid particle dynamics. This study investigates the potential enhancement of heat transfer properties of particulate fluid as well as the effect of injected particles on fluid profiles, and pressure on walls under different particle injection conditions. In the second part of this research, the molecular dynamics simulation was performed to simulate solid-liquid interaction at the molecular level (nanotechnology) to understand their behaviors. The results from two different scales were compared qualitatively.

Computational Fluid Dynamics (CFD) of Chemical Processes Springer Science & Business Media

In this Special Issue, one review paper highlights the necessity of multiscale CFD, coupling micro- and macro-scales, for exchanging information at the interface of the two scales. Four research papers investigate the hydrodynamics, heat transfer, and chemical reactions of various processes using Eulerian CFD modeling. CFD models are attractive for industrial applications. However, substantial efforts in physical modeling and numerical implementation are still required before their widespread implementation.

Computational Multiscale Modeling of Fluids and Solids Butterworth-Heinemann

Multiscale Modeling for Process Safety Applications is a new reference demonstrating the implementation of multiscale modeling techniques on process safety applications. It is a valuable resource for readers interested in theoretical simulations and/or computer simulations of hazardous scenarios. As multi-scale modeling is a computational technique for solving problems involving multiple scales, such as how a flammable vapor cloud might behave if ignited, this book provides information on the fundamental topics of toxic, fire, and air explosion modeling, as well as modeling jet and pool fires using computational fluid dynamics. The book goes on to cover nanomaterial toxicity, QPSR analysis on relation of chemical structure to flash point, molecular structure and burning velocity, first principle studies of reactive chemicals, water and air reactive chemicals, and dust explosions. Chemical and process safety professionals, as well as faculty and graduate researchers, will benefit from the detailed coverage provided in this book. Provides the only comprehensive source addressing the use of multiscale modeling in the context of process safety Bridges multiscale modeling with process safety, enabling the reader to understand mapping between problem detail and effective usage of resources Presents an overall picture of addressing safety problems in all levels of modeling and the latest approaches to each in the field Features worked out examples, case studies, and a question bank to aid understanding and involvement for the reader

Theory and Applications John Wiley & Sons

"Practical Aspects of Computational Chemistry" presents contributions on a range of aspects of Computational Chemistry applied to a variety of research fields. The chapters focus on recent theoretical developments which have been used to investigate structures and

properties of large systems with minimal computational resources. Studies include those in the gas phase, various solvents, various aspects of computational multiscale modeling, Monte Carlo simulations, chirality, the multiple minima problem for protein folding, the nature of binding in different species and dihydrogen bonds, carbon nanotubes and hydrogen storage, adsorption and decomposition of organophosphorus compounds, X-ray crystallography, proton transfer, structure-activity relationships, a description of the REACH programs of the European Union for chemical regulatory purposes, reactions of nucleic acid bases with endogenous and exogenous reactive oxygen species and different aspects of nucleic acid bases, base pairs and base tetrads.

Practical Aspects of Computational Chemistry Società Editrice Esculapio

The book presents select proceedings of Global meet on 'Computational Modelling and Simulation, Recent Innovations, Challenges and Perspectives, 2020. This book covers leading-edge technologies from different domains such as computation in optimization and control, multiscale and multiphysics modeling and computation analysis, environmental modeling, modeling approaches to enterprise systems and services, finite element analysis, dependability and security, high-performance computation/cloud computing applications, computational biology and chemistry and computational mechanics. The primary goal of this book is to strengthen pre-eminence in computational modeling and simulation by catalyzing the transformative use of innovative developments in a wide range of disciplines to achieve lasting societal impact. The book discusses on how to perform simulation of large complex dynamic systems in an efficient manner using advanced computational analysis. The inter-disciplinary nature of the book would be a valuable reference for academicians and research scientists, industrialists interested in modelling and simulation driven by computational technology.