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Multiscale Modeling and Uncertainty Quantification of Materials and Structures-Manolis Papadrakakis 2014-07-02 This book contains the proceedings of the IUTAM Symposium on Multiscale Modeling and Uncertainty Quantification of Materials and Structures that was held at Santorini, Greece, September 9 – 11, 2013. It consists of 20 chapters which are divided in five thematic topics: Damage and fracture, homogenization, inverse problems–identification, multiscale stochastic mechanics and stochastic dynamics. Over the last few years, the intense research activity at micro scale and nano scale reflected the need to account for disparate levels of uncertainty from various sources and across scales. As even over-refined deterministic approaches are not able to account for this issue, an efficient blending of stochastic and multiscale methodologies is required to provide a rational framework for the analysis and design of materials and structures. The purpose of this IUTAM Symposium was to promote achievements in uncertainty quantification combined with multiscale modeling and to encourage research and development in this growing field with the aim of improving the safety and reliability of engineered materials and structures. Special emphasis was placed on multiscale material modeling and simulation as well as on the multiscale analysis and uncertainty quantification of fracture mechanics of heterogeneous media. The homogenization of two-phase random media was also thoroughly examined in several presentations. Various topics of multiscale stochastic mechanics, such as identification of material models, scale coupling, modeling of random microstructures, analysis of CNT-reinforced composites and stochastic finite elements, have been analyzed and discussed. A large number of papers were finally devoted to innovative methods in stochastic dynamics.

Uncertainty Quantification in Multiscale Materials Modeling-Yan Wang 2020-03-12 Uncertainty Quantification in Multiscale Materials Modeling provides a complete overview of uncertainty quantification (UQ) in computational materials science. It provides practical tools and methods

along with examples of their application to problems in materials modeling. UQ methods are applied to various multiscale models ranging from the nanoscale to macroscale. This book presents a thorough synthesis of the state-of-the-art in UQ methods for materials modeling, including Bayesian inference, surrogate modeling, random fields, interval analysis, and sensitivity analysis, providing insight into the unique characteristics of models framed at each scale, as well as common issues in modeling across scales.

Numerical Methods for Porous Media Flow-Bradley W. McCaskill 2018 The way in which we manage subsurface resources is directly determined by the availability and quality of information we have about the dynamical systems that govern them. Typically this information is obtained by solving mathematical models that are posed on the domain of interest. Unfortunately, both the construction and process of solving these models can be a nontrivial task. In this dissertation we explore solutions to several problems related to modeling fluid flow through porous media. One aspect of this dissertation is the development of a nonstandard multiscale finite element method for solving elliptic boundary value problems. The so-called multiscale Robin method can be viewed as a merger of traditional domain decomposition methods with the framework of multiscale finite element methods. The novelty of this method is that its efficiency and accuracy are governed by a geometric enrichment of the solution space. An application of the multiscale Robin method to uncertainty quantification through the use of a stochastic representation method is considered. To this end, the multiscale Robin methodology is adapted to the framework of coupled elliptic boundary value problems. A computationally cheap and efficient method for the simulation of two-phase flow through poroelastic media is also proposed. Specifically, through the use of a artificial stabilization term and an element based post processing reasonable estimates of solutions to the associated geomechanic subsystem can be obtained. Finally, we adapt a continuous data assimilation algorithm to a model for miscible flow through porous media. The existence of weak solutions and convergence properties of the resulting model solution are studied. In all chapters a variety of numerical examples are used to evaluate the performance of each proposed solution methodology.

Uncertainty Quantification of Multiscale Models-Anna Nikishova 2020

Multiscale Modeling and Uncertainty Quantification for Nuclear Fuel Performance- 2017 In this project, we will address the challenges associated with constructing high fidelity multiscale models of nuclear fuel performance. We (*) propose a novel approach for coupling mesoscale and macroscale models, (*) devise efficient numerical methods for simulating the coupled system, and (*) devise and analyze effective numerical approaches for error and uncertainty quantification for the coupled multiscale system. As an integral part of the project, we will carry out analysis of the effects of upscaling and downscaling, investigate efficient methods for stochastic sensitivity analysis of the individual macroscale and mesoscale models, and carry out a posteriori error analysis for computed results. We will pursue development and implementation of solutions in software used at Idaho National Laboratories on models of interest to the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program.

Workshop on Uncertainty Quantification and Multiscale Materials Modeling- 2011

Stochastic Uncertainty Quantification for Multiscale Modeling of Polymeric Nanocomposites-Nam Vu-Bac 2015

Uncertainty Quantification-Christian Soize 2017-04-24 This book presents the fundamental notions and advanced mathematical tools in the stochastic modeling of uncertainties and their quantification for large-scale computational models in sciences and engineering. In particular, it focuses in parametric uncertainties, and non-parametric uncertainties with applications from the structural dynamics and vibroacoustics of complex mechanical systems, from micromechanics and multiscale mechanics of heterogeneous materials. Resulting from a course developed by the author, the book begins with a description of the fundamental mathematical tools of

probability and statistics that are directly useful for uncertainty quantification. It proceeds with a well carried out description of some basic and advanced methods for constructing stochastic models of uncertainties, paying particular attention to the problem of calibrating and identifying a stochastic model of uncertainty when experimental data is available. This book is intended to be a graduate-level textbook for students as well as professionals interested in the theory, computation, and applications of risk and prediction in science and engineering fields.

Uncertainty Quantification in Multiscale Stochastic Models of Catalytic Reactions-Marcel Nunez 2018 Multiscale modeling, a key tool in probing the fundamentals of catalytic reactions, has seen increased usage enabled by advances in computational hardware. Within the multiscale modeling paradigm, kinetic Monte Carlo (KMC) is employed to simulate chemical reaction networks, as mean-eld models often fail to provide a meaningful description of the complex phenomena involved. Due to KMC's high computational cost and stochastic noise, quantifying uncertainty for the purposes of rening the model and assessing predictive reliability is dicult. Uncertainty arises from errors in input parameters (parametric uncertainty) and assumptions made about the physical system (model form uncertainty). □ In this thesis, we develop tools to quantify errors from each of the aforementioned sources and make recommendations for model renement. We address parametric uncertainty by developing ecient sensitivity analysis techniques, which identify the most influential parameters. Likelihood ratio sensitivity analysis (LRSA) computes all sensitivities without the need for additional runs, as required by nite dierence methods, but encounters tremendous variance in systems with disparate time scales. To overcome this limitation of LRSA, we derive mathematical theory that enables its use in well-mixed multiscale KMC and implement the method in original software. The new multiscale technique accurately computes sensitivities in a model system for which the traditional LRSA performs poorly. To address spatial KMC, we develop acceleration techniques and statistical criteria that ensure sucient sampling for LRSA. As a result, LRSA can be applied to real chemistry. We apply our methodology to the water-gas shift reaction on Pt, an important component of hydrogen production from biomass. We address model form uncertainty by revisiting two common assumptions: the structure of the catalyst surface is uniform and the identity of the active site is known. □ A framework for optimizing catalyst structure based on local descriptors is developed, allowing for atom-by-atom design of defected surfaces and consequent improvements in activity. In order to restrict our search to physically relevant structures, surface energy is also computed. Activity is maximized and surface energy is minimized simultaneously using multi-objective simulated annealing. A set of Pareto optimal structures is found, oering targets for synthesis. We apply our approach to oxygen reduction on Pt, the key reaction in automotive fuel cells. Our approach resolves discrepancy between experiment and theory regarding the extent to which defects can improve activity. We extend the approach to chemistries involving coupled active sites, for which KMC simulation is needed. KMC simulation data from many dierent structures is used to train a neural network for use as a surrogate model in the optimization. The neural network is updated as the optimization progresses in an online machine learning approach. In doing so, geometric eects such as diusion limitations and bifunctional site coupling are accurately captured within the structure optimization. The impact on the optimal structure is analyzed, yielding new insights into catalyst structure/activity relationships.

Model Validation and Uncertainty Quantification, Volume 3-H. Sezer Atamturktur 2014-04-11 This third volume of eight from the IMAC - XXXII Conference, brings together contributions to this important area of research and engineering. The collection presents early findings and case studies on fundamental and applied aspects of Structural Dynamics, including papers on: Linear Systems Substructure Modelling Adaptive Structures Experimental Techniques Analytical Methods Damage Detection Damping of Materials & Members Modal Parameter Identification Modal Testing Methods System Identification Active Control Modal Parameter Estimation Processing Modal Data

Data-Driven Modeling for Additive Manufacturing of Metals-National Academies of Sciences, Engineering, and Medicine 2019-11-09 Additive manufacturing (AM) is the process in which a three-dimensional object is built by adding subsequent layers of materials. AM enables novel material compositions and shapes, often without the need for specialized tooling.

This technology has the potential to revolutionize how mechanical parts are created, tested, and certified. However, successful real-time AM design requires the integration of complex systems and often necessitates expertise across domains. Simulation-based design approaches, such as those applied in engineering product design and material design, have the potential to improve AM predictive modeling capabilities, particularly when combined with existing knowledge of the underlying mechanics. These predictive models have the potential to reduce the cost of and time for concept-to-final-product development and can be used to supplement experimental tests. The National Academies convened a workshop on October 24-26, 2018 to discuss the frontiers of mechanistic data-driven modeling for AM of metals. Topics of discussion included measuring and modeling process monitoring and control, developing models to represent microstructure evolution, alloy design, and part suitability, modeling phases of process and machine design, and accelerating product and process qualification and certification. These topics then led to the assessment of short-, immediate-, and long-term challenges in AM. This publication summarizes the presentations and discussions from the workshop.

Biological Applications of Uncertainty Quantification, Including Multiscale Daphnia Magna Population Modeling-Kaska Adoteye 2016

Uncertainty Quantification in Multiscale Atomistic-Continuum Models- 2011

Trails in Kinetic Theory-Giacomo Albi 2021 In recent decades, kinetic theory - originally developed as a field of mathematical physics - has emerged as one of the most prominent fields of modern mathematics. In recent years, there has been an explosion of applications of kinetic theory to other areas of research, such as biology and social sciences. This book collects lecture notes and recent advances in the field of kinetic theory of lecturers and speakers of the School Trails in Kinetic Theory: Foundational Aspects and Numerical Methods hosted at Hausdorff Institute for Mathematics (HIM) of Bonn, Germany, 2019, during the Junior Trimester Program Kinetic Theory. Focusing on fundamental questions in both theoretical and numerical aspects, it also presents a broad view of related problems in socioeconomic sciences, pedestrian dynamics and traffic flow management.

Computational Science – ICCS 2019-João M. F. Rodrigues 2019-06-07 The five-volume set LNCS 11536, 11537, 11538, 11539 and 11540 constitutes the proceedings of the 19th International Conference on Computational Science, ICCS 2019, held in Faro, Portugal, in June 2019. The total of 65 full papers and 168 workshop papers presented in this book set were carefully reviewed and selected from 573 submissions (228 submissions to the main track and 345 submissions to the workshops). The papers were organized in topical sections named: Part I: ICCS Main Track Part II: ICCS Main Track; Track of Advances in High-Performance Computational Earth Sciences: Applications and Frameworks; Track of Agent-Based Simulations, Adaptive Algorithms and Solvers; Track of Applications of Matrix Methods in Artificial Intelligence and Machine Learning; Track of Architecture, Languages, Compilation and Hardware Support for Emerging and Heterogeneous Systems Part III: Track of Biomedical and Bioinformatics Challenges for Computer Science; Track of Classifier Learning from Difficult Data; Track of Computational Finance and Business Intelligence; Track of Computational Optimization, Modelling and Simulation; Track of Computational Science in IoT and Smart Systems Part IV: Track of Data-Driven Computational Sciences; Track of Machine Learning and Data Assimilation for Dynamical Systems; Track of Marine Computing in the Interconnected World for the Benefit of the Society; Track of Multiscale Modelling and Simulation; Track of Simulations of Flow and Transport: Modeling, Algorithms and Computation Part V: Track of Smart Systems: Computer Vision, Sensor Networks and Machine Learning; Track of Solving Problems with Uncertainties; Track of Teaching Computational Science; Poster Track ICCS 2019 Chapter “Comparing Domain-decomposition Methods for the Parallelization of Distributed Land Surface Models” is available open access under a Creative Commons Attribution 4.0 International License via link.springer.com.

Multiscale Methods-Jacob Fish 2010 Small scale features and processes

occurring at nanometer and femtosecond scales have a profound impact on what happens at a larger scale and over an extensive period of time. The primary objective of this volume is to reflect the state-of-the-art in multiscale mathematics, modeling, and simulations and to address the following barriers: What is the information that needs to be transferred from one model or scale to another and what physical principles must be satisfied during thetransfer of information? What are the optimal ways to achieve such transfer of information? How can variability of physical parameters at multiple scales be quantified and how can it be accounted for to ensure design robustness?The multiscale approaches in space and time presented in this volume are grouped into two main categories: information-passing and concurrent. In the concurrent approaches various scales are simultaneously resolved, whereas in the information-passing methods the fine scale is modeled and its gross response is infused into the continuum scale. The issue of reliability of multiscale modeling and simulation tools which focus on a hierarchy of multiscale models and an a posteriori model of errorestimation including uncertainty quantification, is discussed in several chapters. Component software that can be effectively combined to address a wide range of multiscale simulations is also described. Applications range from advanced materials to nanoelectromechanical systems (NEMS), biologicalsystems, and nanoporous catalysts where physical phenomena operates across 12 orders of magnitude in time scales and 10 orders of magnitude in spatial scales.This volume is a valuable reference book for scientists, engineers and graduate students practicing in traditional engineering and science disciplines as well as in emerging fields of nanotechnology, biotechnology, microelectronics and energy.

Structural Health Monitoring 2013: A Roadmap to Intelligent Structures-Fu-Kuo Chang 2013-09-26 Original research on SHM sensors, quantification strategies, system integration and control for a wide range of engineered materials New applications in robotics, machinery, as well as military aircraft, railroads, highways, bridges, pipelines, stadiums, tunnels, space exploration and energy production Continuing a critical book series on structural health monitoring (SHM), this two-volume set (with full-text searchable CD-ROM) offers, as its subtitle implies, a guide to greater integration and control of SHM systems. Specifically, the volumes contain new research that will enable readers to more efficiently link sensor detection, diagnostics/quantification, overall system functionality, and automated, e.g., robotic, control, thus further closing the loop from inherent signal-based damage detection to responsive real-time maintenance and repair. SHM performance is demonstrated in monitoring the behavior of composites, metals, concrete, polymers and selected nanomaterials in a wide array of surroundings, including harsh environments, under extreme (e.g., seismic) loading and in space. New information on smart sensors and network optimization is enhanced by novel statistical and model-based methods for signal processing and data quantification. A special feature of the book is its explanation of emerging control technologies. Research in these volumes was initially presented in September 2013 at the 9th International Workshop on Structural Health Monitoring (IWSHM), held at Stanford University and sponsored by the Air Force Office of Scientific Research, the Army Research Laboratory, and the Office of Naval Research.

Multiscale Materials Modeling for Nanomechanics-Christopher R. Weinberger 2016-08-30 This book presents a unique combination of chapters that together provide a practical introduction to multiscale modeling applied to nanoscale materials mechanics. The goal of this book is to present a balanced treatment of both the theory of the methodology, as well as some practical aspects of conducting the simulations and models. The first half of the book covers some fundamental modeling and simulation techniques ranging from ab-inito methods to the continuum scale. Included in this set of methods are several different concurrent multiscale methods for bridging time and length scales applicable to mechanics at the nanoscale regime. The second half of the book presents a range of case studies from a varied selection of research groups focusing either on a the application of multiscale modeling to a specific nanomaterial, or novel analysis techniques aimed at exploring nanomechanics. Readers are also directed to helpful sites and other resources throughout the book where the simulation codes and methodologies discussed herein can be accessed. Emphasis on the practicality of the detailed techniques is especially felt in the latter half of the book, which is dedicated to specific examples to study nanomechanics and multiscale materials behavior. An instructive avenue for learning how to effectively apply these simulation tools to solve nanomechanics problems is to study previous endeavors. Therefore, each chapter is written by a unique team of experts who have used multiscale

materials modeling to solve a practical nanomechanics problem. These chapters provide an extensive picture of the multiscale materials landscape from problem statement through the final results and outlook, providing readers with a roadmap for incorporating these techniques into their own research.

Computational Science - ICCS 2020-Valeria V. Krzhizhanovskaya 2020 The seven-volume set LNCS 12137, 12138, 12139, 12140, 12141, 12142, and 12143 constitutes the proceedings of the 20th International Conference on Computational Science, ICCS 2020, held in Amsterdam, The Netherlands, in June 2020.* The total of 101 papers and 248 workshop papers presented in this book set were carefully reviewed and selected from 719 submissions (230 submissions to the main track and 489 submissions to the workshops). The papers were organized in topical sections named: Part I: ICCS Main Track Part II: ICCS Main Track Part III: Advances in High-Performance Computational Earth Sciences: Applications and Frameworks; Agent-Based Simulations, Adaptive Algorithms and Solvers; Applications of Computational Methods in Artificial Intelligence and Machine Learning; Biomedical and Bioinformatics Challenges for Computer Science Part IV: Classifier Learning from Difficult Data; Complex Social Systems through the Lens of Computational Science; Computational Health; Computational Methods for Emerging Problems in (Dis-)Information Analysis Part V: Computational Optimization, Modelling and Simulation; Computational Science in IoT and Smart Systems; Computer Graphics, Image Processing and Artificial Intelligence Part VI: Data Driven Computational Sciences; Machine Learning and Data Assimilation for Dynamical Systems; Meshfree Methods in Computational Sciences; Multiscale Modelling and Simulation; Quantum Computing Workshop Part VII: Simulations of Flow and Transport: Modeling, Algorithms and Computation; Smart Systems: Bringing Together Computer Vision, Sensor Networks and Machine Learning; Software Engineering for Computational Science; Solving Problems with Uncertainties; Teaching Computational Science; UNcErtainty QUantIficatiOn for ComputationAl modeLs *The conference was canceled due to the COVID-19 pandemic.

Uncertainty Quantification and Model Calibration-Jan Peter Hessling 2017-07-05 Uncertainty quantification may appear daunting for practitioners due to its inherent complexity but can be intriguing and rewarding for anyone with mathematical ambitions and genuine concern for modeling quality. Uncertainty quantification is what remains to be done when too much credibility has been invested in deterministic analyses and unwarranted assumptions. Model calibration describes the inverse operation targeting optimal prediction and refers to inference of best uncertain model estimates from experimental calibration data. The limited applicability of most state-of-the-art approaches to many of the large and complex calculations made today makes uncertainty quantification and model calibration major topics open for debate, with rapidly growing interest from both science and technology, addressing subtle questions such as credible predictions of climate heating.

Mesoscale Models-Sinisa Mesarovic 2018-11-19 The book helps to answer the following questions: How far have the understanding and mesoscale modeling advanced in recent decades, what are the key open questions that require further research and what are the mathematical and physical requirements for a mesoscale model intended to provide either insight or a predictive engineering tool? It is addressed to young researchers including doctoral students, postdocs and early career faculty,

Uncertainty Quantification for Hyperbolic and Kinetic Equations-Shi Jin 2018-03-20 This book explores recent advances in uncertainty quantification for hyperbolic, kinetic, and related problems. The contributions address a range of different aspects, including: polynomial chaos expansions, perturbation methods, multi-level Monte Carlo methods, importance sampling, and moment methods. The interest in these topics is rapidly growing, as their applications have now expanded to many areas in engineering, physics, biology and the social sciences. Accordingly, the book provides the scientific community with a topical overview of the latest research efforts.

Uncertainty Quantification and Management for Multi-scale Nuclear

Materials Modeling- 2015 Understanding and improving microstructural mechanical stability in metals and alloys is central to the development of high strength and high ductility materials for cladding and cores structures in advanced fast reactors. Design and enhancement of radiation-induced damage tolerant alloys are facilitated by better understanding the connection of various unit processes to collective responses in a multiscale model chain, including: dislocation nucleation, absorption and desorption at interfaces; vacancy production, radiation-induced segregation of Cr and Ni at defect clusters (point defect sinks) in BCC Fe-Cr ferritic/martensitic steels; investigation of interaction of interstitials and vacancies with impurities (V, Nb, Ta, Mo, W, Al, Si, P, S); time evolution of swelling (cluster growth) phenomena of irradiated materials; and energetics and kinetics of dislocation bypass of defects formed by interstitial clustering and formation of prismatic loops, informing statistical models of continuum character with regard to processes of dislocation glide, vacancy agglomeration and swelling, climb and cross slip.

Transdisciplinary Multispectral Modeling and Cooperation for the Preservation of Cultural Heritage-Antonia Moropoulou 2019-02-20 This two-volume set CCIS 961 and 962 constitutes the refereed post-conference proceedings of the First International Conference on Transdisciplinary Multispectral Modeling and Cooperation for the Preservation of Cultural Heritage, TMM_CH 2018, held in Athens, Greece, in October 2018. 73 revised full papers of 237 submissions are included in these volumes. The papers of the first volume are organized in the following topical sections: the project of the rehabilitation of Holy Sepulchre's Holy Aedicule as a pilot multispectral, multidimensional, novel approach through transdisciplinary and cooperation in the protection of monuments; digital heritage; novel educational approach for the preservation of monuments; resilience to climate change and natural hazards; conserving sustainably the materiality of structures and architectural authenticity; and interdisciplinary preservation and management of cultural heritage. And the papers of the second volume are organized in the following topical sections: sustainable preservation and management lessons learnt on emblematic monuments; cross-discipline earthquake protection and structural assessment of monuments; cultural heritage and pilgrimage tourism; reuse, circular economy and social participation as a leverage for the sustainable preservation and management of historic cities; inception – inclusive cultural heritage in Europe through 3D semantic modelling; heritage at risk; and advanced and non-destructive techniques for diagnosis, design and monitoring.

Reviews in Computational Chemistry-Abby L. Parrill 2018-11-06 The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered on molecular modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 31 include: Lattice-Boltzmann Modeling of Multicomponent Systems: An Introduction Modeling Mechanochemistry from First Principles Mapping Energy Transport Networks in Proteins The Role of Computations in Catalysis The Construction of Ab Initio Based Potential Energy Surfaces Uncertainty Quantification for Molecular Dynamics

Multiscale Methods in Computational Mechanics-René de Borst 2010-10-09 This work gives a modern, up-to-date account of recent developments in computational multiscale mechanics. Both upscaling and concurrent computing methodologies will be addressed for a range of application areas in computational solid and fluid mechanics: Scale transitions in materials, turbulence in fluid-structure interaction problems, multiscale/multilevel optimization, multiscale poromechanics. A Dutch-German research group that consists of qualified and well-known researchers in the field has worked for six years on the topic of computational multiscale mechanics. This text provides a unique opportunity to consolidate and disseminate the knowledge gained in this project. The addition of chapters written by experts outside this working group provides a broad and multifaceted view of this rapidly evolving field.

Applied Spectroscopy and the Science of Nanomaterials-Prabhakar Misra 2014-10-21 This book focuses on several areas of intense topical interest related to applied spectroscopy and the science of nanomaterials. The eleven chapters in the book cover the following areas of interest relating to applied spectroscopy and nanoscience: · Raman spectroscopic characterization, modeling and simulation studies of carbon nanotubes, · Characterization of plasma discharges using laser optogalvanic spectroscopy, · Fluorescence anisotropy in understanding protein conformational disorder and aggregation, · Nuclear magnetic resonance spectroscopy in nanomedicine, · Calculation of Van der Waals interactions at the nanoscale, · Theory and simulation associated with adsorption of gases in nanomaterials, · Atom-precise metal nanoclusters, · Plasmonic properties of metallic nanostructures, two-dimensional materials, and their composites, · Applications of graphene in optoelectronic devices and transistors, · Role of graphene in organic photovoltaic device technology, · Applications of nanomaterials in nanomedicine.

Stochastic Multiscale Modeling of Polycrystalline Materials-Bin Wen 2013 Mechanical properties of engineering materials are sensitive to the underlying random microstructure. Quantification of mechanical property variability induced by microstructure variation is essential for the prediction of extreme properties and microstructure-sensitive design of materials. Recent advances in high throughput characterization of polycrystalline microstructures have resulted in huge data sets of microstructural descriptors and image snapshots. To utilize these large scale experimental data for computing the resulting variability of macroscopic properties, appropriate mathematical representation of microstructures is needed. By exploring the space containing all admissible microstructures that are statistically similar to the available data, one can estimate the distribution/envelope of possible properties by employing efficient stochastic simulation methodologies along with robust physics-based deterministic simulators. The focus of this thesis is on the construction of lowdimensional representations of random microstructures and the development of efficient physics-based simulators for polycrystalline materials. By adopting appropriate stochastic methods, such as Monte Carlo and Adaptive Sparse Grid Collocation methods, the variability of microstructure-sensitive properties of polycrystalline materials is investigated. The primary outcomes of this thesis include: - Development of data-driven reduced-order representations of microstruc- ture variations to construct the admissible space of random polycrystalline microstructures. - Development of accurate and efficient physics-based simulators for the estimation of material properties based on mesoscale microstructures. - Investigating property variability of polycrystalline materials using efficient stochastic simulation methods in combination with the above two developments. The uncertainty quantification framework developed in this work integrates information science and materials science, and provides a new outlook to multiscale materials modeling accounting for microstructure and process uncertainties. Predictive materials modeling will accelerate the development of new materials and processes for critical applications in industry.

Computational Modelling and Uncertainty Quantification of Blood Flow in the Coronary Arteries-Justin Sheldon Tran 2018 Atherosclerotic coronary artery disease continues to negatively impact the lives of millions worldwide. Computational fluid dynamics modeling of coronary blood flow has the potential to help improve clinical outcomes and aid in treatment planning. Significant advancements in coronary blood flow modeling in recent years have opened a wide range of applications such as assessing risk for disease progression or providing a platform for virtual surgery and treatment planning. To encourage the growth of this field and promote adoption of computational results in the clinic, it is crucial that these tools be made as automated as possible so they can be applied to large patient cohorts. In addition, the variability of computational results with respect to uncertainties in the inputs and model must be better understood and systematically quantified. Addressing these concerns is the subject of this thesis. In the first part, a framework for automatically tuning the lumped parameter boundary conditions in simulations of coronary blood flow is developed and demonstrated. Specifying boundary conditions in complex computational models is not a trivial task, especially when the dimensionality of the input space is high and multiple constraints on the outputs need to be satisfied simultaneously. Specifically in the context of patient-specific coronary simulations, clinical data such as the blood pressure, cardiac output, and coronary flow waveforms must be simultaneously satisfied with a large set of input parameters that include

lumped resistances, capacitances, and heart model parameters. A typical user can eventually gain expertise to modify the input parameters to satisfy targets, but this manual tuning is time-consuming and not easily reproduced. We thus formulate the automated tuning process as a Bayesian inverse problem in which the model parameters are treated as random variables, and optimal parameters are determined by finding the maximum of the posterior distribution of input parameters. We also perform sensitivity analysis on the input parameters to determine a subset of thirteen parameters that most influence the clinical targets. In the second part, we perform uncertainty quantification on patient-specific simulations of coronary artery bypass graft hemodynamics. Vein graft failure in patients with coronary bypass continues to be a major clinical issue with relatively little knowledge about the mechanisms for failure. Simulations have shown that predicted quantities such as wall shear stress or wall strain can be useful in predicting vein graft failure, but adoption of such results in clinical practice is hindered due to the fact simulations can only produce deterministic results with no range of confidence. Uncertainty quantification provides a framework for quantifying the uncertainty in computational results, and we applied it to assess the variability in computed predictions of time-average wall shear stress and wall strain under uncertainty in the lumped parameter boundary conditions and vessel wall material properties. To achieve this aim efficiently, we develop a novel submodeling strategy for reducing the computational cost of the analysis. We also, for the first time, consider spatial variability in the graft wall material properties by using a random field description. We finally propagate these uncertainties forward using a newly developed multi-resolution approach. The results show that the time-averaged wall shear stress is relatively well estimated with confidence intervals about 35\% of the mean value, but the wall strain exhibited significantly more variability due to the large uncertainty in the material properties. In the third part, we perform a comparison of methods for modeling wall deformability in vascular blood flow simulations. Though sometimes neglected, wall deformability can have significant impacts on the computational results, affecting predictions of wall shear stress and precluding calculation of stresses and strains in the vessel wall. There are several methods proposed in the literature for modeling wall deformability, two of the most popular being the Arbitrary Lagrangian Eularian (ALE) and Couple Momentum Methods (CMM). Although both methods capture the essential characteristics of wall deformability, they can produce different results and computational performance. This provides a rigorous comparison which will aid in the choice of deformable wall model. Additionally, we consider the concept of prestress. Because the geometry for a patient-specific simulation is extracted from medical image data of the \textit{in vivo} cardiovascular system, the vessel walls carry an internal stress which holds the geometry in equilibrium with hemodynamic pressures and viscous stresses. We implement prestress in both ALE and CMM contexts and confirm that it is necessary to avoid over-inflation of the anatomic domain. Although studied mostly within the context of coronary flow simulations, the methods and approaches outlined in this thesis are designed to be generally applicable across other domains in computational modeling, fluid dynamics, and biomechanics. Automated tuning is a general framework for assimilating multiple sources of target data to inform optimal input parameter values, and can broadly be applied in multiscale modeling. The methods for uncertainty quantification can be adapted to assess variability of simulations in other computational fluid mechanics and biomechanics contexts. The results from the wall deformability comparison can also be extended to apply to other contexts including other cardiovascular diseases, respiratory flow, and medical devices. In addition to providing insights into coronary flow simulations, this thesis aims to motivate the importance of tuning, uncertainty quantification, and model comparisons for other cardiovascular simulations and multiscale biological modeling more broadly.

Modeling and Experimental Characterization of Nanocomposite Materials-Homayoun Hadavinia 2020-04-15 This Special Issue gathers research from different branches of science and engineering disciplines working on experiments and modelling of nanocomposites into one volume. The Guest Editor welcomes papers dedicated to experimental, computational, and theoretical aspects dealing with many important state-of-the-art technologies and methodologies regarding the synthesis, fabrication, characterization, properties, design, and applications, and both finite element analysis and molecular dynamic simulations, of nanocomposite materials and structures. Full papers covering novel topics, extending the frontiers of the science and technology of nanoreinforced composites are encouraged. Reviews covering topics of major interest will be also considered.

Machine Learning and Data Mining in Materials Science-Norbert Huber 2020-04-22

Proceedings of the International Conference on Advances in Computational Mechanics 2017-Hung Nguyen-Xuan 2018-02-20 This book provides an overview of state-of-the-art methods in computational engineering for modeling and simulation. This proceedings volume includes a selection of refereed papers presented at the International Conference on Advances in Computational Mechanics (ACOME) 2017, which took place on Phu Quoc Island, Vietnam on August 2-4, 2017. The contributions highlight recent advances in and innovative applications of computational mechanics. Subjects covered include: biological systems; damage, fracture and failure; flow problems; multiscale multiphysics problems; composites and hybrid structures; optimization and inverse problems; lightweight structures; computational mechatronics; computational dynamics; numerical methods; and high-performance computing. The book is intended for academics, including graduate students and experienced researchers interested in state-of-the-art computational methods for solving challenging problems in engineering.

Integrated Design of Multiscale, Multifunctional Materials and Products-David L. McDowell 2009-09-30 Integrated Design of Multiscale, Multifunctional Materials and Products is the first of its type to consider not only design of materials, but concurrent design of materials and products. In other words, materials are not just selected on the basis of properties, but the composition and/or microstructure iw designed to satisfy specific ranged sets of performance requirements. This book presents the motivation for pursuing concurrent design of materials and products, thoroughly discussing the details of multiscale modeling and multilevel robust design and provides details of the design methods/strategies along with selected examples of designing material attributes for specified system performance. It is intended as a monograph to serve as a foundational reference for instructors of courses at the senior and introductory graduate level in departments of materials science and engineering, mechanical engineering, aerospace engineering and civil engineering who are interested in next generation systems-based design of materials. First of its kind to consider not only design of materials, but concurrent design of materials and products Treatment of uncertainty via robust design of materials Integrates the "materials by design approach" of Olson/Ques Tek LLC with the "materials selection" approach of Ashby/Granta Distinquishes the processes of concurrent design of materials and products as an overall systems design problem from the field of multiscale modeling Systematic mathematical algorithms and methods are introduced for robust design of materials, rather than ad hoc heuristics--it is oriented towards a true systems approach to design of materials and products

Molecular Dynamics and Machine Learning in Drug Discovery-Sergio Decherchi 2021-06-08 Dr. Sergio Decherchi and Dr. Andrea Cavalli are co-founders of BiKi Technologies s.r.l. - a company that commercializes a Molecular Dynamics-based software suite for drug discovery. All other Topic Editors declare no competing interests with regards to the Research Topic subject.

Computational Science – ICCS 2018-Yong Shi 2018-06-11 The three-volume set LNCS 10860, 10861 and 10862 constitutes the proceedings of the 18th International Conference on Computational Science, ICCS 2018, held in Wuxi, China, in June 2018. The total of 155 full and 66 short papers presented in this book set was carefully reviewed and selected from 404 submissions. The papers were organized in topical sections named: Part I: ICCS Main Track Part II: Track of Advances in High-Performance Computational Earth Sciences: Applications and Frameworks; Track of Agent-Based Simulations, Adaptive Algorithms and Solvers; Track of Applications of Matrix Methods in Artificial Intelligence and Machine Learning; Track of Architecture, Languages, Compilation and Hardware Support for Emerging ManYcore Systems; Track of Biomedical and Bioinformatics Challenges for Computer Science; Track of Computational Finance and Business Intelligence; Track of Computational Optimization, Modelling and Simulation; Track of Data, Modeling, and Computation in IoT and Smart Systems; Track of Data-Driven Computational Sciences; Track of

Mathematical-Methods-and-Algorithms for Extreme Scale; Track of Multiscale Modelling and Simulation Part III: Track of Simulations of Flow and Transport: Modeling, Algorithms and Computation; Track of Solving Problems with Uncertainties; Track of Teaching Computational Science; Poster Papers

Uncertainty Quantification in Computational Fluid Dynamics-Hester Bijl 2013-09-20 Fluid flows are characterized by uncertain inputs such as random initial data, material and flux coefficients, and boundary conditions. The current volume addresses the pertinent issue of efficiently computing the flow uncertainty, given this initial randomness. It collects seven original review articles that cover improved versions of the Monte Carlo method (the so-called multi-level Monte Carlo method (MLMC)), moment-based stochastic Galerkin methods and modified versions of the stochastic collocation methods that use adaptive stencil selection of the ENO-WENO type in both physical and stochastic space. The methods are also complemented by concrete applications such as flows around aerofoils and rockets, problems of aeroelasticity (fluid-structure interactions), and shallow water flows for propagating water waves. The wealth of numerical examples provide evidence on the suitability of each proposed method as well as comparisons of different approaches.

TMS 2016 145th Annual Meeting & Exhibition, Annual Meeting Supplemental Proceedings-The Minerals, Metals & Materials Society (TMS) 2016-12-01

Predictive Theoretical and Computational Approaches for Additive Manufacturing-National Academies of Sciences, Engineering, and Medicine 2016-12-21 Additive manufacturing (AM) methods have great potential for promoting transformative research in many fields across the vast spectrum of engineering and materials science. AM is one of the leading forms of advanced manufacturing which enables direct computer-aided design (CAD) to part production without part-specific tooling. In October 2015 the National Academies of Sciences, Engineering, and Medicine convened a workshop of experts from diverse communities to examine predictive theoretical and computational approaches for various AM technologies. While experimental workshops in AM have been held in the past, this workshop uniquely focused on theoretical and computational approaches and involved areas such as simulation-based engineering and science, integrated computational materials engineering, mechanics, materials science, manufacturing processes, and other specialized areas. This publication summarizes the presentations and discussions from the workshop.

Integrated Design of Multiscale, Multifunctional Materials and Products-Jitesh Panchal 2010 Integrated Design of Multiscale, Multifunctional Materials and Products is the first of its type to consider not only design of materials, but concurrent design of materials and products. In other words, materials are not just selected on the basis of properties, but the composition and/or microstructure iw designed to satisfy specific ranged sets of performance requirements. This book presents the motivation for pursuing concurrent design of materials and products, thoroughly discussing the details of multiscale modeling and multilevel robust design and provides details of the design methods/strategies along with selected examples of designing material attributes for specified system performance. It is intended as a monograph to serve as a foundational reference for instructors of courses at the senior and introductory graduate level in departments of materials science and engineering, mechanical engineering, aerospace engineering and civil engineering who are interested in next generation systems-based design of materials. Key Features: * First of its kind to consider not only design of materials, but concurrent design of materials and products. * Treatment of uncertainty via robust design of materials * Integrates the "materials by design approach" of Olson/Ques Tek LLC with the "materials selection" approach of Ashby/Granta * Distinquishes the processes of concurrent design of materials and products as an overall systems design problem from the field of multiscale modeling * Systematic mathematical algorithms and methods are introduced for robust design of materials, rather than ad hoc heuristics--it is oriented towards a true systems approach to design of materials and products

Computational Science – ICCS 2020-Valeria V. Krzhizhanovskaya