Modelling And Simulation Of Diffusive Processes Methods And Applications Simulation Foundations Methods And Applications

Organizations report that as much as 50% of investments in IS and IT solutions are judged to be outright failures or deemed highly unsatisfactory. Information Systems Innovation and Diffusion: Issues and Directions reports on innovation and diffusion research and presents theory-based guidelines that will increase the business value of IS/IT investments.

This book is a compilation of research accomplishments in the fields of modeling, simulation, and their applications, as presented at AsiaSim 2011 (Asia Simulation Conference 2011). The conference, held in Seoul, Korea, November 16–18, was organized by ASIASIM (Federation of Asian Simulation Societies), KSS (Korea Society for Simulation), CASS (Chinese Association for System Simulation), and JSST (Japan Society for Simulation Technology). AsiaSim 2011 provided a forum for scientists, academicians, and professionals from the Asia-Pacific region and other parts of the world to share their latest exciting research findings in modeling and simulation methodologies, techniques, and their tools and applications in military, communication network, industry, and general engineering problems.

Offers Both Standard and Novel Approaches for the Modeling of Systems Examines the Interesting Behavior of Particular Classes of Models Chaotic Modelling and Simulation: Analysis of Chaotic Models, Attractors and Forms presents the main models developed by pioneers of chaos theory, along with new extensions and variations of these models. Using more than 500 graphs and illustrations, the authors show how to design, estimate, and test an array of models. Requiring little prior knowledge of mathematics, the book focuses on classical forms and attractors as well as new simulation methods and techniques. Ideas clearly progress from the most elementary to the most advanced. The authors cover deterministic, stochastic, logistic, Gaussian, delay, Hénon, Holmes, Lorenz, Rössler, and rotation models. They also look at chaotic analysis as a tool to design forms that appear in physical systems; simulate complicated and chaotic orbits and paths in the solar system; explore the Hénon–Heiles, Contopoulos, and Hamiltonian systems; and provide a compilation of interesting systems and variations of systems, including the very intriguing Lotka–Volterra system. Making a complex topic accessible through a visual and geometric style, this book should inspire new developments in the field of chaotic models and encourage more readers to become involved in this rapidly advancing area.

Evaporation of solvent from a polymer solution has technological importance in technologies related to painting, coating, inkjet printing, manufacturing polymer films and production of electronic devices. Apart from the vast technological importance, it is one of the fundamental problems of soft condensed matter physics. A mathematical model in the framework of nonequilibrium

thermodynamics was developed to describe the evolution of concentration and temperature during evaporation of a solvent in a polymer solution. The governing equations derived from the fundamental equation of classical thermodynamics using the local equilibrium hypothesis, Prigogine's theorem and Onsager's reciprocity relations display more complex connection between heat and non-convective mass fluxes than what has been presented in the previous research works. The model developed herein describes evolution of concentration and temperature in an evaporating polymer solution in a thermodynamically consistent way and is able to capture the effect of thermal diffusion in polymer solutions. The derived governing equations which were formulated for a general 3D problem were solved numerically for a 1D solution casting problem using an explicit finite difference scheme. During the evaporation of solvent, the effect of thermal diffusion in polymer solutions manifests itself as an increase in local concentration of the solvent on the warm side of a temperature gradient. The results of the model also can qualitatively capture some experimental observations regarding the Soret effect in polymer solutions.

Numerical simulation and modelling of electric circuits and semiconductor devices are of primal interest in today's high technology industries. At the Oberwolfach Conference more than forty scientists from around the world, in cluding applied mathematicians and electrical engineers from industry and universities, presented new results in this area of growing importance. The contributions to this conference are presented in these proceedings. They include contributions on special topics of current interest in circuit and device simulation, as well as contributions that present an overview of the field. In the semiconductor area special lectures were given on mixed finite element methods and iterative procedures for the solution of large linear systems. For three dimensional models new discretization procedures including software packages were presented. Con nections between semiconductor equations and the Boltzmann equation were shown as well as relations to the quantum transport equation. Other issues discussed in this area include the design of simulation programs for semiconductors, vectorcomputers, and interface problems in several dimensions. Topics discussed in the area of circuit simulation include the index classification of differential-algebraic systems, connections with ill-posed problems, and regularization techniques. Split discretization procedures were given for the efficient calculation of periodic solutions of circuits taking into acount the latency. Homotopy methods and new numerical techniques for differential-algebraic systems were presented, and im provements of special numerical methods for standard software packages were sug gested. The editors VII Table of Contents Circuit Simulation Merten K.

ZEUS (Centres of European Supercomputing) is a network for information exchange and co-operation between European Supercomputer Centres. During the fall of 1994 the idea was put forward to start an annual workshop to stimulate the exchange of ideas and experience in parallel programming and computing between researchers and users from industry and

academia. The first workshop in this series, the ZEUS '95 Workshop on Parallel Programming and Computation, is organized at Linkoping University, where the Swedish ZEUS centre, NSC (National Supercomputer Centre) is located. This is open for all researchers and users in the field of parallel computing.

In this study an analytical and numerical modeling of the interaction between the process of diffusion and the mechanics of a solid are developed. It is then implemented on a fiber composite material, and several cases are simulated and analyzed. Starting with the a free energy as a function of the deformation and concentration, [Psi](F, C), a constitutive model is derived for the strain energy function & Psi_m(F), the coupled term of the free energy, & Psi_md(F, C), and the diffusion part of the free energy, & Psi_d(C). With these terms we define the stress, the coupling terms, and the diffusion flux respectively. These are then used in the balance of mass, the balance of linear momentum and the continuity equation. The equations are discretized using a finite difference scheme for the time variable, and a nonlinear finite element method for the spacial variables. The coupling is implemented using a staggering methodology. The staggering scheme allows for easy implementation and provides a convenient framework. Several phenomena are modeled, for example, strain-dependent diffusivity, concentration based saturation, diffuso-elasticity and nonuniform diffusion induced swelling. The simulations involve various parametric studies including using different elastic strain energy functions, such as Kirchhoff Saint Venant. Moreover, the simulations are conducted for both isotropic and orthotropic materials where we explore such effects as free swelling, and combined mechanical loading and diffusion boundary conditions.

This book constitutes the proceedings of the 6th International Conference on Functional Imaging and Modeling of the Heart, held in New York City, NY, USA in May 2011. The 24 revised full papers presented together with 29 revised poster papers were carefully reviewed and selected from about 120 initial submissions. The contributions feature current research and development efforts in the fields of cardiovascular modeling, physiology, and image-based analysis, at a range of scales and imaging methods. Topics addresses are such as imaging, signal and image processing, applied mathematics, biomedical engineering and computer science; biologically oriented fields such as cardiac physiology and biology; as well as clinical issues such as cardiology, radiology and surgery, with a common interest in the heart.

This practical introduction to stochastic reaction-diffusion modelling is based on courses taught at the University of Oxford. The authors discuss the essence of mathematical methods which appear (under different names) in a number of interdisciplinary scientific fields bridging mathematics and computations with biology and chemistry. The book can be used both for self-study and as a supporting text for advanced undergraduate or beginning graduate-level courses in applied mathematics. New mathematical approaches are explained using simple examples of biological models, which range in size from simulations of small biomolecules to groups of animals. The book starts with stochastic modelling of chemical reactions, introducing stochastic simulation algorithms and mathematical methods for analysis of stochastic models. Different stochastic spatio-temporal models are then studied, including models of diffusion and stochastic reaction-diffusion modelling. The methods covered include molecular dynamics, Brownian dynamics, velocity jump processes and compartment-based (lattice-based) models.

This book is the second edition of Numerical methods for diffusion phenomena in building physics: a practical introduction originally published by PUCPRESS (2016). It intends to stimulate research in simulation of diffusion problems in building physics, by providing an overview of mathematical models and numerical techniques such as the finite difference and finite-element methods traditionally used in building simulation tools. Nonconventional methods such as reduced order models, boundary integral approaches and spectral methods are presented, which might be considered in the next generation of building-energy-simulation tools. In this reviewed edition, an innovative way to simulate energy and hydrothermal

performance are presented, bringing some light on innovative approaches in the field.

The famous Black-Scholes model was the starting point of a new financial industry and has been a very important pillar of all options trading since. One of its core assumptions is that the volatility of the underlying asset is constant. It was realised early that one has to specify a dynamic on the volatility itself to get closer to market behaviour. There are mainly two aspects making this fact apparent. Considering historical evolution of volatility by analysing time series data one observes erratic behaviour over time. Secondly, backing out implied volatility from daily traded plain vanilla options, the volatility changes with strike. The most common realisations of this phenomenon are the implied volatility smile or skew. The natural question arises how to extend the Black-Scholes model appropriately. Within this book the concept of stochastic volatility is analysed and discussed with special regard to the numerical problems occurring either in calibrating the model to the market implied volatility surface or in the numerical simulation of the two-dimensional system of stochastic differential equations required to price non-vanilla financial derivatives. We introduce a new stochastic volatility model, the so-called Hyp-Hyp model, and use Watanabe's calculus to find an analytical approximation to the model implied volatility. Further, the class of affine diffusion models, such as Heston, is analysed in view of using the characteristic function and Fourier inversion techniques to value European derivatives.

Numerical Methods for Hyperbolic Equations is a collection of 49 articles presented at the International Conference on Numerical Methods for Hyperbolic Equations: Theory and Applications (Santiago de Compostela, Spain, 4-8 July 2011). The conference was organized to honour Professor Eleuterio Toro in the month of his 65th birthday. The topics covered include: • Recent advances in the numerical computation of environmental conservation laws with source terms • Multiphase flow and porous media • Numerical methods in astrophysics • Seismology and geophysics modelling • High order methods for hyperbolic conservation laws • Numerical methods for reactive flows • Finite volume and discontinous Galerkin schemes for stiff source term problems • Methods and models for biomedical problems • Numerical methods for reactive flows The research interest of Eleuterio Toro, born in Chile on 16th July 1946, is reflected in Numerical Methods for Hyperbolic Equations, and focuses on: numerical methods for partial differential equations, with particular emphasis on methods for hyperbolic equations; design and application of new algorithms; hyperbolic partial differential equations as mathematical models of various types of processes; mathematical modelling and simulation of physico/chemical processes that include wave propagation phenomena; modelling of multiphase flows; application of models and methods to real problems. Eleuterio Toro received several honours and distinctions, including the honorary title OBE from Queen Elizabeth II (Buckingham Palace, London 2000); Distinguished Citizen of the City of Carahue (Chile, 2001); Life Fellow, Claire Hall, University of Cambridge (UK, 2003); Fellow of the Indian Society for Shock Wave Research (Bangalore, 2005); Doctor Honoris Causa (Universidad de Santiago de Chile, 2008); William Penney Fellow, University of Cambridge (UK, 2010); Doctor Honoris Causa (Universidad de la Frontera, Chile, 2012). Professor Toro is author of two books, editor of two books and author of more than 260 research works. In the last ten years he has been invited and keynote speaker in more than 100 scientific events. Professor Toro has held many visiting appointments round the world, which include several

European countries, Japan, China and USA.

The book describes a computational model of the immune system reaction, C-ImmSim, built along the lines of the computer model known as the Celada-Seiden model (CS-model). The computational counterpart of the CS-model is called IMMSIM which stands for IMMune system SIMulator. IMMSIM was written in 1992 by the physicist Phil E. Seiden and the immunologist Franco Celada. This model was built around the idea of developing a computerized system to perform experiments similar in vivo experiments; a tool developed to help biologists testing theories and hypothesis about how the immune system works. C-ImmSim is best viewed as a collection of models in a single program. It incorporates the principal core facts of today's immunological knowledge, such as the diversity of specific elements, MHC restriction, clonal selection, thymic education of T cells, antigen processing and presentation (both the cytosolic and endocytic pathways are implemented), cell-cell cooperation, homeostasis of cells created by the bone marrow, hyper mutation of antibodies, maturation of the cellular and humoral response, and memory. Besides, an antigen can represent a bacterium, a virus, or an allergen or a tumor cell. C-ImmSim has been recently customized to simulate the HIV-1 infection. Moreover, it can simulate the immunotherapy for cancer. These features are all present in the code and people can choose to turn them on and off at compiling time. The book presents the basic model as well as the various customizations to implement the description of different diseases and the way they have been used in practice to produce new knowledge either from hypothesis or from lab-experiment data. In this respect, the book can be used as a practical guide to implement a computational model with which to study a specific disease and to try to address realistic clinical questions.

Operational Research (OR) deals with the use of advanced analytical methods to support better decision-making. It is multidisciplinary with strong links to management science, decision science, computer science and many application areas such as engineering, manufacturing, commerce and healthcare. In the study of emergent behaviour in complex adaptive systems, Agent-based Modelling & Simulation (ABMS) is being used in many different domains such as healthcare, energy, evacuation, commerce, manufacturing and defense. This collection of articles presents a convenient introduction to ABMS with papers ranging from contemporary views to representative case studies. The OR Essentials series presents a unique cross-section of high quality research work fundamental to understanding contemporary issues and research across a range of Operational Research (OR) topics. It brings together some of the best research papers from the esteemed Operational Research Society and its associated journals, also published by Palgrave Macmillan.

This volume presents a selection of survey and research articles based on invited lectures and contributed talks presented at the Workshop on Fluid Dynamics in Porous Media that was held in Coimbra, Portugal, in September 12-14, 2011. The contributions are devoted to mathematical modeling, numerical simulation and their applications, providing the readers a state-of-the-art overview on the latest findings and new challenges on the topic. The book includes research work of worldwide recognized leaders in their respective fields and presents advances in both theory and applications, making it appealing to a vast range of audience, in particular mathematicians, engineers and physicists.

This book addresses the problems involved in the modelling and simulation of shale gas reservoirs, and details recent advances in the field. It discusses various modelling and simulation challenges, such as the complexity of fracture networks, adsorption phenomena, non-Darcy flow, and natural fracture networks, presenting the latest findings in these areas. It also discusses the difficulties of developing shale gas models, and compares analytical modelling and numerical simulations of shale gas reservoirs with those of conventional reservoirs. Offering a comprehensive review of the state-of-the-art in developing shale gas models and simulators in the upstream oil industry, it allows readers to gain a better understanding of these reservoirs and encourages more systematic research on efficient exploitation of shale gas plays. It is a valuable resource for researchers interested in the modelling of unconventional reservoirs and graduate students studying reservoir engineering. It is also of interest to practising reservoir and production engineers.

The articles in this volume summarize the research results obtained in the former SFB 359 "Reactive Flow, Diffusion and Transport" which has been supported by the DFG over the period 1993-2004. The main subjects are physical-chemical processes sharing the difficulty of interacting diffusion, transport and reaction which cannot be considered separately. The modeling and simulation within this book is accompanied by experiments.

The first chapter provides an overview of the development of a novel agent-based simulation model of socio-environmental innovation diffusion. The second chapter shows the study about rendering of colours with three rendering engines. The third and fourth chapters are devoted to modelling clothes at different levels. The fifth chapter describes the modelling of computer simulation in the optimization of bioprocess technology. Chapters 6 and 7 formulate a physical model of deformation of steel and idea of constructing a scientific workshop focused on high-temperature processes. Chapter 8 formulates surrogate models. Chapter 9 shows computer simulation of high-frequency electromagnetic fields. Chapter 10 proposes the modelling of the task allocation problem by the use of Petri Nets. Chapter 11 presents various scenarios whose ranking is done according to defined criteria and weight coefficients.

This book addresses the key issues in the modeling and simulation of diffusive processes from a wide spectrum of different applications across a broad range of disciplines. Features: discusses diffusion and molecular transport in living cells and suspended sediment in open channels; examines the modeling of peristaltic transport of nanofluids, and isotachophoretic separation of ionic samples in microfluidics; reviews thermal characterization of non-homogeneous media and scale-dependent porous dispersion resulting from velocity fluctuations; describes the modeling of nitrogen fate and transport at the sediment-water interface and groundwater flow in unconfined aquifers; investigates two-dimensional solute transport from a varying pulse type point source and futile cycles in metabolic flux modeling; studies contaminant concentration prediction along unsteady groundwater flow and modeling synovial fluid flow in human joints; explores the modeling of soil organic carbon and crop growth simulation.

The book uses state-of-the-art theorizing about a topic that has attracted a lot of attention in the past five years or so. It provides a very useful review of the literature, and is very well written and on a novel topic. I especially liked the methodological rigour in the exposition of the model, yet at the same time the text remains accessible to a

wide readership. I highly recommend the book. Koen Frenken, Utrecht University, The Netherlands Modern economies are described as knowledge based . This book investigates the meaning of such a statement, assessing the relevance of knowledge and the channels through which knowledge is exchanged, both from a theoretical and an empirical perspective. Moving within the realm of complexity theory, the authors provide a methodological assessment of the knowledge diffusion debate as well as presenting theoretical and applied models of knowledge diffusion and innovation. They illustrate how geography plays a role in shaping innovative patterns and how dense networks generally result in more innovative environments. The book concludes that establishing the right connections within such dense networks appears to be more crucial than any other factor, thus highlighting the importance of linkages (or the effects of their absence) within innovation systems. Proposing a taxonomy of knowledge-sharing patterns, this book will be warmly welcomed by academics, researchers and postgraduate students in the areas of the economics of innovation, evolutionary economics and knowledge economics.

This volume on materials engineering comprises a collection of abstracts of recent scholarly papers and articles concerning a wide variety of topics related to the effects of structural defects and diffusion in many material areas, including thin-film manufacturing and facing metals.

This paper generates an organization-task interdependent network model based upon functional dependence between tasks and executive dependence between organizations and tasks in an complex product research and development (R&D) project. Then it develops and simulates the dynamic model of technical risk diffusion by analyzing the interaction between organizations and tasks when facing with technical risks. The results show that the technical risk diffusion caused by a few tasks can significantly turbulent the network in a short time; the diffusion process has three stages: slow stage, out of control stage, and relatively stable stage; the relationship between the organization network scale and the consequence of diffusion shows approximate “inverse U” shape; the more even executive dependence, the weaker the robustness of the network when fixes the number of organizations; there exists a best level of resource input which makes the impact of diffusion remain at the lowest level; there is no significant difference in the diffusion process under different attack strategies. This research riches the dynamic theory of risk diffusion, and has provided reference for optimization of complex product development project architecture and improving the risk resisting capacity of R&D projects.

Modelling and Simulation in the Science of Micro- and Meso-Porous Materials addresses significant developments in the field of micro- and meso-porous science. The book includes sections on Structure Modeling and Prediction, Synthesis, Nucleation and Growth, Sorption and Separation processes, Reactivity and Catalysis, and Fundamental Developments in Methodology to give a complete overview of the techniques currently utilized in this rapidly advancing field. It thoroughly addresses the major challenges in the field of microporous materials, including the crystallization mechanism of porous materials and

rational synthesis of porous materials with controllable porous structures and compositions. New applications in emerging areas are also covered, including biomass conversion, C1 chemistry, and CO2 capture. Authored and edited by experts in the field of micro- and meso-porous materials Includes introductory material and background both on the science of microporous materials and on the techniques employed in contemporary modeling studies Rigorous enough for scientists conducting related research, but also accessible to graduate students in chemistry, chemical engineering, and materials science