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Applications with MATLAB® provides expert insights into current and emerging methods, opportunities, and challenges associated with the computational techniques involved in nanoscale research. Written by, and for, those working in the interdisciplinary fields that comprise nanotechnology—including engineering, physics, chemistry, biology, and medicine—this book covers a broad spectrum of technical information, research ideas, and practical knowledge. It presents an introduction to computational methods in nanotechnology, including a closer look at the theory and modeling of two important

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nanoscale systems: molecular magnets and semiconductor quantum dots. Topics covered include: Modeling of nanoparticles and complex nano and MEMS systems Theory associated with micromagnetics Surface modeling of thin films Computational techniques used to validate hypotheses that may not be accessible through traditional experimentation Simulation methods for various nanotubes and modeling of carbon nanotube and silicon nanowire transistors In regard to applications of computational nanotechnology in biology, contributors describe tracking of nanoscale structures in

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cells, effects of various forces on cellular behavior, and use of protein-coated gold nanoparticles to better understand protein-associated nanomaterials. Emphasizing the importance of MATLAB for biological simulations in nanomedicine, this wide-ranging survey of computational nanotechnology concludes by discussing future directions in the field, highlighting the importance of the algorithms, modeling software, and computational tools in the development of efficient nanoscale systems.

The Finite Difference Time Domain (FDTD)

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method is an essential tool in modeling inhomogeneous, anisotropic, and dispersive media with random, multilayered, and periodic fundamental (or device) nanostructures due to its features of extreme flexibility and easy implementation. It has led to many new discoveries concerning guided modes in nanoplasmonic waveguides and continues to attract attention from researchers across the globe. Written in a manner that is easily digestible to beginners and useful to seasoned professionals, Computational Nanotechnology Using Finite Difference Time Domain describes the key concepts of the

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computational FDTD method used in nanotechnology. The book discusses the newest and most popular computational nanotechnologies using the FDTD method, considering their primary benefits. It also predicts future applications of nanotechnology in technical industry by examining the results of interdisciplinary research conducted by world-renowned experts. Complete with case studies, examples, supportive appendices, and FDTD codes accessible via a companion website, Computational Nanotechnology Using Finite Difference Time Domain not only delivers a

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practical introduction to the use of FDTD in nanotechnology but also serves as a valuable reference for academia and professionals working in the fields of physics, chemistry, biology, medicine, material science, quantum science, electrical and electronic engineering, electromagnetics, photonics, optical science, computer science, mechanical engineering, chemical engineering, and aerospace engineering.

Applications of nanotechnology continue to fuel significant innovations in areas ranging from electronics, microcomputing, and

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biotechnology to medicine, consumer supplies, aerospace, and energy production. As progress in nanoscale science and engineering leads to the continued development of advanced materials and new devices, improved methods of modeling and simulation are required to achieve a more robust quantitative understanding of matter at the nanoscale. Computational Nanotechnology: Modeling and Applications with MATLAB® provides expert insights into current and emerging methods, opportunities, and challenges associated with the computational techniques involved in nanoscale research. Written by, and for,

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those working in the interdisciplinary fields that comprise nanotechnology—including engineering, physics, chemistry, biology, and medicine—this book covers a broad spectrum of technical information, research ideas, and practical knowledge. It presents an introduction to computational methods in nanotechnology, including a closer look at the theory and modeling of two important nanoscale systems: molecular magnets and semiconductor quantum dots. Topics covered include: Modeling of nanoparticles and complex nano and MEMS systems Theory associated with micromagnetics Surface



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modeling of thin films Computational techniques used to validate hypotheses that may not be accessible through traditional experimentation Simulation methods for various nanotubes and modeling of carbon nanotube and silicon nanowire transistors In regard to applications of computational nanotechnology in biology, contributors describe tracking of nanoscale structures in cells, effects of various forces on cellular behavior, and use of protein-coated gold nanoparticles to better understand protein-associated nanomaterials. Emphasizing the importance of MATLAB for biological

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simulations in nanomedicine, this wide-ranging survey of computational nanotechnology concludes by discussing future directions in the field, highlighting the importance of the algorithms, modeling software, and computational tools in the development of efficient nanoscale systems.

Computational Finite Element Methods in Nanotechnology demonstrates the capabilities of finite element methods in nanotechnology for a range of fields. Bringing together contributions from researchers around the world, it covers key concepts as well as

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cutting-edge research and applications to inspire new developments and future interdisciplinary research. In particular, it emphasizes the importance of finite element methods (FEMs) for computational tools in the development of efficient nanoscale systems. The book explores a variety of topics, including: A novel FE-based thermo-electrical-mechanical-coupled model to study mechanical stress, temperature, and electric fields in nano- and microelectronics The integration of distributed element, lumped element, and system-level methods for the design, modeling, and simulation of nano- and micro-

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electromechanical systems (N/MEMS) Challenges in the simulation of nanorobotic systems and macro-dimensions The simulation of structures and processes such as dislocations, growth of epitaxial films, and precipitation Modeling of self-positioning nanostructures, nanocomposites, and carbon nanotubes and their composites Progress in using FEM to analyze the electric field formed in needleless electrospinning How molecular dynamic (MD) simulations can be integrated into the FEM Applications of finite element analysis in nanomaterials and systems used in medicine, dentistry, biotechnology, and other

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areas The book includes numerous examples and case studies, as well as recent applications of microscale and nanoscale modeling systems with FEMs using COMSOL Multiphysics® and MATLAB®. A one-stop reference for professionals, researchers, and students, this is also an accessible introduction to computational FEMs in nanotechnology for those new to the field.

This book provides a comprehensive overview of the computational physics for nanoscience and nanotechnology. Based on MATLAB and the C++ distributed computing paradigm, the book

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gives instructive explanations of the underlying physics for mesoscopic systems with many listed programs that readily compute physical properties into nanoscales. Many generated graphical pictures demonstrate not only the principles of physics, but also the methodology of computing.

Nanoscale science and computing is becoming a major research area as today's scientists try to understand the processes of natural and biomolecular computing. The field is concerned with the architectures and design of molecular self-assembly, nanostructures

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and molecular devices, and with understanding and exploiting the computational processes of biomolecules in nature. This book offers a unique and authoritative perspective on current research in nanoscale science, engineering and computing. Leading researchers cover the topics of DNA self-assembly in two-dimensional arrays and three-dimensional structures, molecular motors, DNA word design, molecular electronics, gene assembly, surface layer protein assembly, and membrane computing. The book is suitable for academic and industrial scientists and engineers working in nanoscale science, in

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particular researchers engaged with the idea of computing at a molecular level.

This textbook, aimed at advanced undergraduate and graduate students, introduces the basic knowledge required for nanomedicine and nanotechnology, and emphasizes how the combined use of chemistry and light with nanoparticles can serve as treatments and therapies for cancer. This includes nanodevices, nanophototherapies, nanodrug design, and laser heating of nanoparticles and cell organelles. In addition, the book covers the emerging fields



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of nanophotonics and nanoplasmonics, which deal with nanoscale confinement of radiation and optical interactions on a scale much smaller than the wavelength of the light. The applications of nanophotonics and nanoplasmonics to biomedical research discussed in the book range from optical biosensing to photodynamic therapies. Cutting-edge and reflective of the multidisciplinary nature of nanomedicine, this book effectively combines knowledge and modeling from nanoscience, medicine, biotechnology, physics, optics, engineering, and pharmacy in an easily digestible format. Among the topics

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covered in-depth are:

- The structure of cancer cells and their properties, as well as techniques for selective targeting of cancer and gene therapy.
- Nanoplasmonics: Lorentz-Mie simulations of optical properties of nanoparticles and the use of plasmonic nanoparticles in diagnosis and therapy.
- Nanophotonics: short and ultrashort laser pulse interactions with nanostructures, time and space simulations of thermal fields in and around the nanobioparticles, and nanoclusters heated by radiation.
- Modeling of soft and hard biological tissue ablation by activated nanoparticles, as well as

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optical, thermal, kinetic, and dynamic modeling. • Detection techniques, including the design and methods of activation of nanodrugs and plasmon resonance detection techniques. • Design and fabrication of nanorobots and nanoparticles. • Effective implementation of nanotherapy treatments. • Nanoheat transfer, particularly the heating and cooling kinetics of nanoparticles. • ...and more! Each chapter contains a set of lectures in the form of text for student readers and PowerPoints for use by instructors, as well as homework exercises. Selected chapters also contain computer

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practicums, including Maple codes and worked-out examples. This book helps readers become more knowledgeable and versant in nanomedicine and nanotechnology, inspires readers to work creatively and go beyond the ideas and topics presented within, and is sufficiently comprehensive to be of value to research scientists as well as students.

While its results normally complement the information obtained by chemical experiments, computer computations can in some cases predict unobserved chemical phenomena

Electronic-Structure Computational Methods

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for Large Systems gives readers a simple description of modern electronic-structure techniques. It shows what techniques are pertinent for particular problems in biotechnology and nanotechnology and provides a balanced treatment of topics that teach strengths and weaknesses, appropriate and inappropriate methods. It's a book that will enhance the your calculating confidence and improve your ability to predict new effects and solve new problems.

This book provides innovative chapters covering new methodologies and important

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applications in the fields of nanoscience and computational chemistry. The book offers scope for academics, researchers, and engineering professionals to present their research and development works that have potential for applications in several disciplines of nano and computational chemistry. Contributions range from new methods to novel applications of existing methods to help readers gain an understanding of the material and/or structural behavior of new and advanced systems. This book is a high quality tool for researchers, providing an overview of the field, explaining the basic

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underlying theory at a meaningful level, and giving numerous comparisons of different methods.

Trends in Computational Nanomechanics reviews recent advances in analytical and computational modeling frameworks to describe the mechanics of materials on scales ranging from the atomistic, through the microstructure or transitional, and up to the continuum. The book presents new approaches in the theory of nanosystems, recent developments in theoretical and computational methods for studying problems in which

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multiple length and/or time scales must be simultaneously resolved, as well as example applications in nanomechanics. This title will be a useful tool of reference for professionals, graduates and undergraduates interested in Computational Chemistry and Physics, Materials Science, Nanotechnology.

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