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Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications

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Preface

Due to the vastness, novelty, and complexity of the interface between mathematical modeling and nanoscience and nanotechnology, many important areas in these disciplines remain barely explored. In progressing further, multidisciplinary research communities have come to a clear understanding that, along with experimental techniques, mathematical modeling and analysis have become crucial in the study, development, and applications of systems at the nanoscale. This volume puts together selected contributions from the participants in the Banff International Research Station (BIRS) workshop *Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications*. The contributors are experts working on different aspects of the analysis, modeling, and applications of nanoscale systems, with particular focus on low-dimensional nanostructures and coupled mathematical models for their description. The development of such models requires concerted efforts from mathematicians, physicists (both theoreticians and experimentalists), and computational scientists, including those working on biological nanostructures. The contributions may serve as up-to-date introductions to different topics in nano- and biosystems, identification of important challenges, evaluation of current methodologies, and exploration of promising approaches.

Topics treated in the book belong to three categories:

Part I: Charge and Spin Transport in Low-Dimensional Structures.
Part II: Modeling Biological Phenomena from Nano- to Macro-scales.
Part III: Mathematics for 2D Materials and Properties of Confined Nanostructures.

In Part I and Part II, Birnir describes different models of nonlinear transport in semiconductor quantum wells and superlattice structures. This chapter reviews the obtention of envelope function and Hartree approximation for quantum wells from the Schrödinger equation, and a dynamical system and bifurcation study for the corresponding time-dependent Liouville–von Neumann matrix density under a laser field. Possible applications are listed. On a different vein, Birnir describes time-dependent electron transport using the sequential tunneling model of a weakly

coupled superlattice, i.e., a certain number of identical quantum wells separated by thick barriers. A weakly coupled semiconductor superlattice is a nonlinear dynamical system whose nonlinearity is due to sequential resonant tunneling between adjacent quantum wells and to the Poisson equation between electron density and potential at the wells. For different *dc* voltage and parameter values, there are stable stationary states, time-periodic solutions, and period doubling routes to chaos. Birnir also discusses the effects of noise and imperfections on the attractors with applications to true random number generators and other devices.

H. T. Grahn et al. review experiments on weakly coupled semiconductor superlattices including recent observations of spontaneous chaotic and quasi-periodic self-oscillations in doped GaAs/AlGaAs superlattices at room temperature. Based on them, an all-electronic true random number generator has been demonstrated at room temperature with achievable bit rates of up to 80 Gbit/s. This is about two orders of magnitude larger than typical bit rates for currently available all-electronic true random number generators. The paper also reports synchronization of chaos, which is useful for secure communications and possible applications to advanced secure multiuser communication methods using large networks of coupled superlattices.

R. Sanchez discusses models of electron or heat transport in mesoscopic conductors when detailed balance is locally broken and indicates several possible realizations. Kaupusz and Melnik discuss non-perturbative approaches in nanoscience with possible applications to charge transport and optical phenomena. They focus on finite-size effects in spin systems near the critical point, based on Monte Carlo (MC) method and some analytical arguments. They report Monte Carlo simulations of the three-dimensional Ising model for small and large linear lattice sizes, providing numerical evidence that the asymptotic decay of corrections to finite-size scaling is remarkably slower than expected before. M. Willatzen discusses a continuum model for coupled acousto-optical phonons in piezoelectric materials.

In Part II, Bonilla et al. review stochastic models of tumor-induced growth of blood vessels (angiogenesis). In this complex multiscale process, diffusing vessel endothelial growth factors induce sprouting of blood vessels that carry oxygen and nutrients to hypoxic tissue. They study a model of stochastic differential equations for blood vessels coupled to reaction–diffusion equations for biochemical field densities and derive coupled integro-differential equations for the mean densities. The density of active blood vessel tips solves these equations and it approaches a soliton-like wave before the vessel tips arrive at the tumor. The authors also include a review of other approaches ranking from reinforced random walks to cellular Potts models.

Carpio et al. study formation of bacterial biofilms both inside flows and on solid surfaces. To analyze this multiscale system, they use elastic rod and plate models that incorporate information from the biomass production and differentiation process at the microscale, such as growth rates, growth tensors or inner stresses, as well as constraints imposed by the interaction with the environment.

Plata and Prados analyze the unfolding pathway of biomolecules comprising several independent modules in pulling experiments with atomic force microscopes. The unfolding pathway is the order in which modules of a biomolecule fixed to platform and tip of the microscope open when pulled with a specific velocity. The authors study a simple mechanical model of the biomolecule under pulling and predict a critical pulling velocity: Below it, the weakest module opens first, whereas, above it, the module at the pulled end opens first. They also discuss the robustness of critical velocity and its dependence on the model parameters and propose an experiment to test the theoretical predictions.

Neu et al. present a heuristic derivation of a geometric minimum action method that can be used to determine most-probable transition paths in noise-driven dynamical systems. The latter are ubiquitous in applications to physics and biology. In traditional descriptions that employ Fokker–Planck equations for the probability density, detailed balance ensures that there is a globally stable equilibrium density. The authors pay particular attention to systems that violate detailed balance and emphasize the role of the stochastic vorticity tensor in ascertaining fulfillment or violation thereof. The authors explore the general method through a detailed study of a two-dimensional quadratic shear flow which exhibits bifurcating most-probable transition pathways.

In Part III, Yatsyhin and collaborators describe classical density functional theory (DFT) and apply it to simple equilibrium models. Classical DFT is an ab initio theoretical–computational framework with a firm foundation in statistical physics. It systematically accounts for fluid spatial inhomogeneity, as well as for the non-localities of intermolecular fluid–fluid and fluid–substrate interactions. The theory expresses the grand canonical free energy of a system as a functional of its one-body density, thus generating a hierarchy of N-body correlation functions. Unconstrained minimization of a properly approximated free-energy functional with respect to the one-body density then yields the basic DFT equation. The authors review recent progress in the understanding of planar prewetting and interface unbending on planar substrates and compute substrate–fluid interfaces and wetting isotherms. Guo et al. explain how to model metastability in CdTe solar cells due to Cu migration.

Urata and Li discuss how to couple multiscale molecular dynamics with the finite element method.

Carr et al. present a general method for the electronic characterization of aperiodic 2D materials using ab-initio tight-binding models. They study the subclass of twisted, stacked heterostructures, but their formalism can be implemented for any 2D system without long-range interactions. Their method provides a multiscale approach for dealing with the ab-initio calculation of electronic transport properties in stacked nanomaterials, allowing for fast and efficient simulation of multilayered stacks in the presence of twist angles, magnetic field, and defects. Tuszynski et al. discuss molecular dynamics and related computational methods with applications to drug discovery. Hoiles and Krishnamurthy describe mesoscopic and macroscopic models for the bioelectronic interface of engineered artificial membranes.

This volume will be useful to researchers interested in coupled mathematical models, and their analysis for physical and biological nanoscale systems impacts applications in biotechnology and medicine, quantum information processing, and optoelectronics. Potential audience of the book includes researchers in applied mathematics, physicists, and biologists.

Lastly, we would like to express our gratitude to the Banff International Research Station for making the workshop possible through their hospitality and financial and logistic support. We thank Ruth Allewelt, from Springer, for help, patience, and competence in completing this book.

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