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MS6

Fast Reaction-Diffusion of Defects in Cadmium Telluride

In this talk, we discuss the asymptotic behavior of a reaction-diffusion system with extremely fast reactions. We use a perturbation method to derive a limiting equation for a simple reaction network and present numerical results for a more complicated model with a scheme derived from a bimolecular kinetic reaction model. Finally, we briefly discuss asymptotic preserving schemes for Cadmium Telluride Solar Cells. Cadmium Telluride is the leading silicon alternative for consumer solar cells. The behavior of the device can be modeled as a reaction-diffusion equation for charged carriers with a self-consistent coupled electric field. In the course of device production additional elements (such as Chlorine and Copper) are added to the device. These molecules enter the device as diffusing interstitial defects, but can react nearly instantaneously with the CdTe lattice. To better understand the fabrication of such devices, we must first understand this physical process.

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MS6

Electron Transport in Nanostructures: Physical Models and Numerical Methods

Research on electron devices scaling at the 5 nm gate-length has triggered a growing interest on two-dimensional (2D) materials, even beyond carbon-based electronics. Among them, transition metal dichalcogenides (TMDs), silicene, germanene, phosphorene, stanene, and topological insulators. Here we will focus on the use of pseudopotentials to treat the electronic structure of systems at the nanometer scale (2D crystals, nanowires, nanoribbons), their stability and properties, and to study electronic transport, both semiclassically (mobility, Monte Carlo) and from a quantum perspective (open systems). The former task requires fast matrix-free eigenvalue solvers and I will briefly show how our use of the Residual Minimization Method-Direct Iteration in Iterative Subspace (RMM-DIIS) and fast-Fourier transforms has been used to calculate the tunneling current between large graphene nanoribbons. Pseudopotential-based quantum transport, on the other hand, requires not only the implementation of sophisticated physical transport models, but also the solution of very large linear systems. We will present our formulation of the problem and results of the simulation of field-effect transistors with graphene nanoribbons and Si nanowires as active channels. Finally, we will discuss the mathematical formulation of a related problem, namely, the calculation of the dielectric response (or, simply put, of the position-dependent dielectric constant) of the nanostructures of interest.

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MS6

Modeling Spin-Dependent Phenomena for New Device Applications

To enhance performance and to reduce energy consumption, electron spin is investigated as replacement of electron charge for storage and computation in future electronic devices. In contrast to charge, spin is not conserved but relaxing to its equilibrium zero value. In the case of semiconductor films, technologies are needed to boost the spin lifetime to make the technology feasible. In silicon films the spin lifetime is determined by intervalley scattering. Applying stress appropriately decreases this undesired scattering effect, which should reduce the spin relaxation [Sverdlov and Selberherr, Phys. Rep. 585, 2015]. To confirm, we solve numerically the quantum mechanical description of the behavior of spin by calculating the wave functions and the scattering matrix elements via solving a kp Hamiltonian with spin-orbit interaction. For the computation of spin relaxation, the momentum dependence of the wave functions due to spin-orbit coupling responsible for spin admixture must be preserved, which significantly increases the demands for computational resources and requires extensive code parallelization. We predict a significant spin lifetime increase with appropriate viable stress. A universal behavior of the spin lifetime on the spin injection orientation is also obtained, with even a two times spin lifetime enhancement for relevant cases. These results confirm that electron spin can be used in electronic devices in a competitively to electron charge superior manner.

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MS6

Computational and Numerical Challenges in Semiconductor Process Simulation

Semiconductor process simulation enables to predict critical manufacturing steps of semiconductor devices and circuits. In particular, it allows for so-called structure prototyping used in the critical exploratory phases of new semiconductor technologies. The ever-ongoing reduction of feature sizes and the required move towards increasingly intricate device structures requires efficient methods to enable fast, accurate, and stable modeling solutions. This is particularly challenging for necessary three-dimensional modeling approaches due to the involved computational effort and the limited acceptable simulation run-times, dictated by the fast-pacing progress in electronics. In this talk, current challenges in semiconductor process simulation, with a focus on computational and numerical aspects, will be discussed along with suggested approaches to tackle those. Among the topics are high performance visibility computation for plasma etching, three-dimensional growth-rate modeling for silicon carbide oxidation, parallel level set redistancing for surface tracking, and efficient spatial discretizations for surface representations. The talk will also show the inter-disciplinary nature of the involved topics, enabling to introduce synergistic interfaces to other fields of research. The financial support by the Austrian Federal Ministry of Science, Research and Economy and the National Foundation for Research, Technology and Development is gratefully acknowledged.

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MS7

Walk-Based Centrality and Communicability Measures: Algorithms and Applications

In this talk I will review some network centrality and communicability measures based on walks. These measures can be given an elegant closed form in terms of functions of the adjacency matrix. I will introduce the notion of total communicability of a network as a measure of network connectivity and robustness and show that it can be computed very quickly even for large graphs. Finally, I will discuss efficient edge modification strategies (including edge removal, addition, and rewiring) that can be used to obtain networks with desirable communicability properties. The talk is based on recent work in collaboration with Christine Klymko (LLNL) and Francesca Arrigo (Strathclyde).

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MS7

Multilevel Model Reduction for Dynamic Power Grid Networks

An electric power grid system can be described by a system of differential-algebraic equations defined on a graph. A relevant task for the power grid community is to develop accurate model reduction for these systems, especially given the large size and stochasticity of the emerging grid. In this talk, we will look at multi-level approaches to constructing the reduced model. The basis of these approaches is the information contained in the weighted graph Laplacian generated by the admittance matrix of the grid. We describe this basis and examine some subtle challenges that these multi-level approaches face in order to achieve accurate simulation of dynamical power grid systems.

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MS7

Dynamic Processes Over Information Networks: Representation, Modeling, Learning and Inference

Large-scale and high resolution data from dynamic processes over networks are becoming increasing available nowadays from online social platforms, such as Twitter and Facebook. Such data provide great opportunities for understanding and modeling both macroscopic (network level) and microscopic (node-level) patterns in human dynamics. Such data have also fueled the increasing efforts on developing methods to address the challenges arising from understanding, predicting, controlling and distilling knowledge from these dynamic processes over networks, and answer query such as "who will do what and when?" To tackle these challenges, I will present a framework based on point processes for representing and modeling such data, and performing learning, inference and control over dynamic processes over networks.

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MS7

Influence Prediction for Continuous-Time Information Propagation on Networks Using Graph-Based Fokker-Planck Equation

We consider the problem of predicting influence, defined as