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# Mathematical and Computational Models for Transport and Coupled Processes in Micro- and Nanotechnology

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As the range of applications of micro- and nanostructures continues to grow, the role of mathematical models and computational experiments in this field becomes increasingly important. Designing of and working with structures and devices on scales between a nanometer and a micron bring new fundamental challenges that can be addressed by combined efforts of researchers working in chemical kinetics, micro-scale fluid dynamics, heat-transfer, mathematical modeling, micro-scale solid mechanics and solid-state physics.

A number of talks along these directions were presented at the VII-th World Congress on Computational Mechanics in Los Angeles, in particular at the workshop on “Transport and Coupled Processes in Micro- and Nanotechnology” organized by the Guest Editors of this special issue. The workshop brought together engineers, mathematicians, and scientists working in this rapidly evolving field in order to discuss state-of-the-art models, procedures, and algorithms for the analysis of transport and coupled processes and phenomena encountered in micro- and nanotechnological applications. Such processes and phenomena are of increasing importance due to extreme sensitivity of nanomaterials and devices to mechanical, thermal and other effects that can lead to complete or partial failure. Several selected papers written by the authors who presented their talks in other sessions of WCCM-7 are also included in this special issue. We thank all our referees for their time and efforts in providing an important keystone for a high standard special issue.

The original contributions to this special issue covered a range of topics from micro-fluidics applications, thermo-fluids aspects of synthesis of macromolecules including carbon nanotubes to the analysis of semiconductor heterostructures, sensor and actuator control schemes on micro- and nano- levels, as well as biotechnological applications. Much of the discussion at the workshop was devoted to a hierarchical modeling approach as we welcomed contributions that discussed all aspects of modeling matter at the molecular/atomistic level and life at the cellular level, as well as contributions dealing with continuum mechanics methodologies in particular when the authors discussed the validity of these methods for micro- and nano- scale phenomena. Among other application areas, we would like to mention contributions in modeling of high-energy phenomena in a small scale range such as a short-pulse laser ablation as well as contributions in applications, stability and accuracy of combined atomistic and

continuum simulations. Many presentations discussed multi-scale modeling techniques in the context of transport and coupled phenomena and processes encountered in micro- and nanotechnology. The current issue includes 15 papers covering some of the above topics.

We hope that this special issue will become a useful reference for the researchers studying coupled and transport processes at micro- and nano- scale and will help strengthen interdisciplinary collaboration in this important field of nanoscience and nanotechnology.

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***Appendix:***

This special focus section included a review paper

- Computational Nanomechanics and Thermal Transport in Nanotubes and Nanowires

and 14 research papers covering the following areas and topics:

- Design of Spintronic Materials with Simple Structures
- Non-Equilibrium Molecular Dynamics Simulation of Nanojet Injection with Adaptive-Spatial
  Decomposition Parallel Algorithm
- A Numerical Algorithm for Magnetohydrodynamics of Ablated Materials
- Computational Models in Nano-Bioelectronics: Simulation of Ionic Transport in Voltage Operated Channels
- Efficient Numerical Schemes for Electronic States in Coupled Quantum Dots
- Enhanced Thermal Conductivity of Nanofluids Diagnosis by Molecular Dynamics Simulations
- Effects of Ampholyte Dissociation Constants on Protein Separation in On-Chip Isoelectric Focusing
- Quasicontinuum-Like Reduction of Density Functional Theory Calculations of Nanostructures
- Effect of Slip Boundary Condition on the Design of Nanoparticle Focusing Lenses
- A Penalty Method to Model Particle Interactions in DNA-Laden Flows
- An Atomistically Enriched Continuum Model for Nanoscale Contact Mechanics and Its
  Application to Contact Scaling
- Stiffness and Thickness of Boron-Nitride Nanotubes
- Kinetic Theory Analysis of Laser Ablation of Carbon
- Method of Submerged Stokeslets for Slip Flow About Ensembles of Particles