Scientific Computing Seminar

A new Computational Paradigm in Multiscale Simulations: Application to Brain Blood Flow

Dr. Leopold Grinberg
Division of Applied Mathematics, Brown University

Abstract: Interfacing atomistic-based with continuum-based simulation codes is now required in many multiscale physical and biological systems. We present the computational advances that have enabled the first multiscale simulation on about 300K processors by coupling a high-order (spectral element) Navier-Stokes solver with a stochastic (coarse-grained) Molecular Dynamics solver based on Dissipative Particle Dynamics (DPD). We study blood flow in a patient specific cerebrovasculature with a brain aneurysm, and analyze the interaction of blood cells with the arterial walls causing thrombus formation and possibly aneurysm rupture. The blood flow patterns are resolved by Nektar - a spectral element solver (about 3 billion unknowns); the blood microrheology within the aneurysm is resolved by an in-house version of DPDLAMMPS (about 10 billions unknowns).

Biosketch of the speaker:
Leopold Grinberg obtained his PhD from Brown University in 2009. He is currently a Senior Research Associate at Brown University, Division of Applied Mathematics working with Prof. G.E. Karniadakis. His research interests encompass diverse topics in computational science, specifically High Performance Scientific Computing with applications in biomedical research. The major fields of Dr. Grinberg's research are:

Multi-scale simulations
Integration of available patient-specific data into numerical simulations
One- and three-dimensional modeling of a blood flow in large arterial networks
Developing scalable algorithms for solutions of tightly and loosely coupled systems
High-order methods
Multi-scale visualization

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