



WPI

DEPARTMENT OF MATHEMATICAL SCIENCES

Colloquium

Anastasios Matzavinos

Brown University

Data-driven modeling in systems biology

ABSTRACT: In this talk, we focus on the role of computationally intensive and data driven modeling in systems biology and biomedical engineering. Examples are drawn from (i) the investigation of soft matter in cell biology by means of molecular dynamics simulations and (ii) the challenges pertaining to detecting aneurysms and other arterial wall abnormalities via machine learning and Bayesian model selection. Thoughts on current and future paradigms in systems biology will also be provided.

In the first part of the talk, we consider the critical radius of pores in a lipid bilayer membrane. Recent experimental research demonstrated nucleated pores in a homopolymer film increasing or decreasing in size, contingent on whether they are larger or smaller than a critical size which scales linearly with film thickness. Using dissipative particle dynamics (DPD), a particle-based simulation method, we investigate the same scenario for a lipid bilayer membrane with a structure determined by lipid–water interactions. By altering key system parameters such as the number of particles per lipid and the periodicity, we identify conditions for pores of any initial size to seal or even remain stable, showing a fundamental difference in the behavior of lipid membranes from polymer films. As another example, we discuss DPD simulations of DNA polymers dispersed by a pressure-driven fluid flow across a periodic array of entropic barriers. We compare our simulations with nanofluidic experiments, which show polymers transitioning between various types of behaviors as pressure increases, and discuss physical insights afforded by the ability of the DPD method to model flows at the nanoscale.

In the second part of the talk, we discuss machine learning and Bayesian inference approaches to the patient-specific modeling of hemodynamics in arterial networks. We describe a Bayesian uncertainty quantification framework in the context of two major advances: an efficient parallel implementation, allowing parameter estimation for complex arterial network models, and a system for practical model selection, allowing evidence-based comparison between distinct models. We demonstrate the proposed methodology by generating simulated noisy flow velocity data from a branching arterial tree model in which a structural defect is introduced at an unknown location; our approach is shown to accurately locate the abnormality and estimate its physical properties even in the presence of significant observational and systemic error. Further applications to epidemiology and the data-driven selection of DNA methylation models may be addressed depending on the interests of the audience and time restrictions.

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