

**BHE-025**

**Understanding Molecular, Cellular, and Physiological Interactions through  
Computation Biology and Nanotechnology for Disease Therapeutics and Diagnostics**

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**Abstract**

The combination of an improved understanding of the nanoscience in molecular systems, methods for mathematical modeling and simulation, and complementary experimental techniques is generating great promise for predictive models of increasingly complex cellular biological systems. Understanding the inherent molecular interactions in these spatiotemporal environments is critical with many diseases including cancer and diabetic nephropathy. Cellular environments are generally small, densely-packed, and irregularly structured that are subject to large local concentration differences. These factors are likely to be lacking from both the classic systems biology models and in the *in vitro* experiments generally used to parameterize them.

The goals for this project are to develop modeling methods that can account for challenging spatial constraints, characterize their performance relative to space-blind differential equation models, and develop experimental techniques to determine the conditions under which spatial considerations are necessary to reliably capture self-assembly dynamics that affect disease diagnosis and treatment.