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THE DEPARTMENT OF ELECTRICAL ENGINEERING AND COMPUTER SCIENCE, CS DIVISION

## Presents the Spring 2012 EECS Distinguished Seminar Series

# Dr. Russell Schwartz

Carnegie Mellon University

# "Understanding Virus Capsid Assembly Through Stochastic Simulation"

Friday, March 16, 2012 • 11:00 a.m. • HEC 101

## Abstract

The formation of viruses has become a key model for understanding complex self-assembly in natural and artificial systems. Self-assembly, a process by which a set of components spontaneously forms some sort of structure or molecular machine under appropriate conditions, is ubiquitous in the biological world and has emerged as an important tool for nanotechnology and materials science. Viruses are a remarkable example of self-assembling machines that must build efficiently and reliably from a small number of components under a variety of adverse conditions. Yet many of the mechanisms by which they assemble and the reasons for which those mechanisms have evolved remain poorly understood. A major factor in this gap in our knowledge is that experimental methods for monitoring virus assembly can so far provide only limited, indirect measures of the actual assembly process. We have sought to better characterize the formation of viruses, and particularly pathways of assembly of viral protein coats (capsids), through the use of coarse-grained stochastic simulation models. Such models allow one to efficiently simulating long time scales and large ensembles of particles with limited prior assumptions about allowed pathways, making them an ideal tool for exploring implications of our theoretical models and conducting experiments *in silico* that we cannot conduct on real viral systems. These simulation models have revealed a surprising complexity of assembly mechanisms possible for even very simple viral models. We have further been developing numerical optimization methods to fit models to indirect measures of assembly progress for specific virus systems, which we demonstrate these methods through application to three viral systems: human papillomavirus (HPV), hepatitis B virus (HBV), and cowpea chloritic mottle virus (CCMV). These studies reveal some of the diversity of assembly mechanisms that may underlie virus assembly in nature and provide a platform for further computational experiments into the effects of environment on self-assembling systems.

## Biography

Russell Schwartz received the BS, MEng, and PhD degrees from the Department of Electrical Engineering and Computer Science at the Massachusetts Institute of Technology, the last in 2000. He later worked in the Informatics Research group at Celera Genomics on algorithms for genetic variation analysis. In 2002, he joined the faculty of Carnegie Mellon University where he is currently a Professor in Biological Sciences and the Lane Center for Computational Biology, as well as co-director of the Carnegie Mellon/University of Pittsburgh Joint Ph.D. Program in Computational Biology. His lab currently pursues a variety of projects in computational biology, including phylogenetics and population genetics, tumor evolution, and simulation methods for complex biophysical systems.

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