

# Electrical & Computer Engineering Seminar Series

## Computer Engineering

---

### *The Power of Many: Abstractions Adaptivity and Applications*



**Shantenu Jha**  
Associate Professor  
Rutgers University

**Wednesday, March 20, 2019**  
11:15am - 12:05 pm  
204 Evans Hall

---

An important class of HPC applications are naturally expressed as ensembles, where a set of many, distinct computational tasks execute in a coordinated manner to produce a collective outcome. It is also often the case that scientific problems that have traditionally been expressed as a single computational task can also be reformulated using ensembles. The ensemble computational model is highly relevant with the end of Dennard scaling and has the ability to overcome limitations of single task applications to achieve significant performance gains on large-scale parallel machines. Not surprisingly, the concept of running ensembles on large-scale HPC systems is thus gaining in importance.

Using biomolecular simulations as a case study, we trace developments in ensemble-based applications over the past 15 years. In doing so, we discuss the abstractions (pilot-systems) and software systems (RADICAL-Cybertools) we have developed. We will discuss scientific advances across multiple domains engendered by RADICAL-Cybertools, and how RADICAL-Cybertools along with advances in statistical adaptive algorithms have enabled ensemble-based applications to overcome traditional limitations of single task applications. However, in spite of several orders of magnitude improvement in efficiency, much greater improvements are needed. We will close with recent investigations of novel application architectures motivated by the RADICAL, if not subversive idea of further improving and providing greater power to the many!

**Shantenu Jha** is an Associate Professor of Computer Engineering at Rutgers University and the Chair of the Department (Center) for Data Driven Discovery at Brookhaven National Laboratory. He was appointed a Rutgers Chancellor's Scholar in 2015. He has held visiting positions at the University of Edinburgh and UCL. Shantenu's research interests are at the intersection of high-performance distributed computing and computational & data-driven science. He is the PI of RADICAL Lab and the lead investigator of RADICAL-Cybertools project which are a suite of middleware building blocks used to support large-scale science and engineering applications. He is proud to play a part in the upcoming revolution at the interface of computing and health-science — global health and “personalized” medicine. He collaborates extensively with scientists from multiple domains – including but not limited to Molecular Sciences, Earth Sciences and High-Energy Physics. Shantenu was the recipient of the inaugural Chancellor's Excellence in Research (2016) for his cyberinfrastructure contributions to computational science. He was also awarded a Rutgers Board of Trustees Fellowship for Scholarly Excellence (2014). He is a recipient of the NSF CAREER Award (2013) and several best paper prizes at SC'xy and ISC'xy. His current research has been funded by multiple NSF awards and US Department of Energy (DoE); his work has also been funded by US National Institute for Health (NIH), and the UK EPSRC.