

## Session TBD

Shantenu Jha- KEYNOTE

Associate Professor of Computer Engineering at Rutgers University

“Building Blocks for Adaptive Workflows”

Abstract

Next-generation exascale systems will fundamentally expand the reach of biomolecular simulations and the resulting scientific insight, enabling the simulation of larger biological systems (weak scaling), longer timescales (strong scaling), more complex molecular interactions, and robust uncertainty quantification (more accurate sampling). Solving biological problems that require longer timescales, involve more complex interactions and robust uncertainty quantification will require significant algorithmic improvements that incorporate high-level parallelism and leverage the statistical nature of molecular processes. Interestingly, many such simulation algorithms require adaptive workflows. We argue the need for workflow-systems using a building blocks approach to support adaptive workflows on extreme-scale heterogeneous and dynamic resources. We discuss RADICAL-Cybertools as an implementation of the building block concept, and discuss how RADICAL-Cybertools are being used to support adaptive workflows in biomolecular simulations and high-energy physics.

Bio

Shantenu Jha is an Associate Professor of Computer Engineering at Rutgers University. His research interests are at the intersection of high-performance distributed computing and computational science. Shantenu leads the the RADICAL-Cybertools project which are a suite of middleware building blocks used to support large-scale science and engineering applications. He collaborates extensively with scientists from multiple domains -- including but not limited to Molecular Sciences, Earth Sciences and High-Energy Physics. He was appointed a Rutgers Chancellor's Scholar (2015-2020) and was the recipient of the inaugural Chancellor's Excellence in Research (2016) for his cyberinfrastructure contributions to computational science. He is a recipient of the NSF CAREER Award (2013) and several prizes at SC'xy and ISC'xy. More details can be found at <http://radical.rutgers.edu/shantenu>

