Special Guest Lectures

Many Big Jobs: Computing in the eXtreme Digital Era

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Johnston Hall 338
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Abstract:
Powerful computing resources like IBM Blue waters, D E Shaw's Anton, and heterogeneous GPU/CPU machines will soon become available as part of NSF's TeraGrid eXtreme Digital (XD) resources. To take full advantage of the power of these resources, researchers are rethinking their computing strategies. There is now increased demand for workflow tools to efficiently manage the computations and data associated with XD resources. Here we present two case studies of ongoing projects utilizing the ManyJobs and BigJobs workflow tools developed in collaboration with Loni Institute Researchers and the LSU Center for Computation & Technology. In one case ManyJobs is used to manage simulations of the deformation of an alveolar-airway model distributed across five different LONI supercomputing sites. Each task is a parallel code using MPI and PetSc. In the other case, BigJobs is utilized to conduct a large number of all atom molecular dynamics simulations on TeraGrid resources. Each simulation is itself a high performance computing task. Access Grid viewing is in 338 Johnston Hall. Live presentation at 101 Stanley Thomas Hall, Tulane University.

Speaker's Bio:
Tom Bishop is a Research Associate Professor at the Center for Computational Science at Tulane University, New Orleans, Louisiana. He is an Adjunct Associate Professor in the Biochemistry Department. Member of the New Orleans Protein Folding Intergroup, Center for Bioenvironmental Research, Louisiana Optical Network Initiative, and Ascona B-DNA Consortium.

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