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CCT Colloquium Series

The Statistical Temperature Molecular Dynamics (STMD) Enhanced Sampling Algorithm, and Applications**Tom Keyes, Boston University**

Professor

Johnston Hall 338
April 24, 2009 - 11:30 am**Abstract:**

Conventional simulation algorithms fail to sample all the significant states of systems where groups of configurations are separated by free energy barriers. Examples include proteins (2) and atomic clusters (3) with multiple energy funnels. STMD (1) uses forces scaled by the inverse of the statistical temperature, $T(U)$, where U is the potential energy, to obtain a flat-energy distribution, as opposed to the usual Boltzmann distribution. The result is an amazing ability to move rapidly over free energy barriers and attain ergodicity. STMD has been combined with CHARMM for realistic atomistic biomolecular simulations and a replica-exchange version is under development for the largest systems. The basic algorithm, applications so far, and future prospects will be discussed.

Speaker's Bio:

Tom Keyes attended Yale University, received a PhD with Daniel Kivelson at UCLA on the theory of light scattering from fluids, and worked on mode coupling theory as a postdoc with Irwin Oppenheim at MIT. He is currently Professor of Chemistry at Boston University, focusing on theory and simulation of biophysical and aqueous systems.

Refreshments will be served.**This lecture has a reception.**