UNIVERSITY OF HOUSTON
ITES - Nonlinear Dynamics Seminar

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A New Multi-scale, Multi-layer and Top-down Approach for Protein Structure Prediction

Abstract

We have developed a new Monte Carlo protocol, which combines coarse-grained normal modes and a Hamiltonian at a different scale, to enhance sampling. Our approach has been demonstrated to be very effect in determining the overall topology of proteins, and molecular envelope as well. We hope that eventually we will be able to computationally bridge a gap between the x-ray crystallography, which requires crystal, and cryo-EM, that can only work with large complexes.

September 18, 2006

3:00 pm in S & R Building 1 (SR1), Room 634

Persons with disabilities, who desire accommodations, should contact the Math Department at telephone: 713-743-3500.