T_CSUH Bi-Weekly Seminar

Texas Center for Superconductivity at the University of Houston

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Mesoscopic Modeling of Biomolecules

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Room 102, University of Houston Science Center
12:00 Noon – 1:00 p.m.

Abstract

Reconstruction algorithms from coarse-grained models to fine-grained (all-atomistic) models of biomolecules are essential in implementing multi-scale simulations. We developed an innovative algorithm for reconstruction that results in high precision all-atom structures (SCAAL). Our method is validated by the computation of structural differences in reconstructed conformations and Protein Data Bank structures for 67 proteins. Significant improvements are observed while we consider a special relevance between the side chain and the backbone of a protein into our modeling method.

Bio

Professor Margaret Cheung joined University of Houston as a junior faculty member in 2006. Research projects include development of physics principles and application of high-performance computing methods for studying various topics in theoretical biophysics, soft condensed matter, and nano-scale materials.

Professor Cheung received her B.S. in Chemistry from National Taiwan University and her Ph.D. in Physics from the University of California, San Diego. She was a Sloan Postdoctoral Fellow in Computational Biology at the University of Maryland.

Persons with disabilities who require special accommodations in attending this lecture should call (713) 743-8210 as soon as possible.

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