Multi-scale Modeling from Multi-resolution Data: Unveiling Functional Motions of Macromolecular Machines

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Large-scale structural rearrangements in proteins and nucleic acids are important for a variety of functions including catalysis and regulation of activity. The recent developments in low-resolution experimental methods have revealed structures and structural transitions of large molecular assemblies at low-resolution. While most of the information on these dynamical transitions is based on experiment, computational methods must be employed to complement experimental observations. Methods that we have developed to extract high-resolution structural information from low-resolution data and applications to biological systems will be presented.

Bell Hall 143
Thursday, January 25, 2007, 11:00 AM