Thesis Defense in Chemistry

Monday, October 14, 2019 at 1:15pm
Room 329 Pupin

The Critical Assessment of Protein Dynamics using Molecular Dynamics (MD) Simulations and Nuclear Magnetic Resonance (NMR) Spectroscopy Experimentation

Presented by Andrew Hsu, Friesner and Palmer Groups

The biological functions of proteins often rely on structural changes and the rates at which these conformational changes occur. The flexibility of particular regions of a protein can be identified by NMR spin relaxation through the measurement of order parameters. While NMR can characterize the extent and time scales of these conformational fluctuations, NMR cannot produce explicit complex atomistic-level mechanisms needed for the full understanding of such processes.

MD simulations can provide such detailed studies of the coupling interactions among specific residues and protein regions. However, care and consideration must be taken to ensure that the simulation and its subsequent analyses correctly mimics experimental reality.

In this thesis talk, I will discuss strategies for improving results generated by NMR, through (i) improving analytical techniques of measured NMR data; and through (ii) supporting experimental results with atomistically-detailed MD simulations that can elucidate specific motions of the protein. Applications of this work is exemplified through the proteins *E. coli* ribonuclease HI and the bZip transcription factor domain of the *S. cerevisiae* protein GCN4.

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