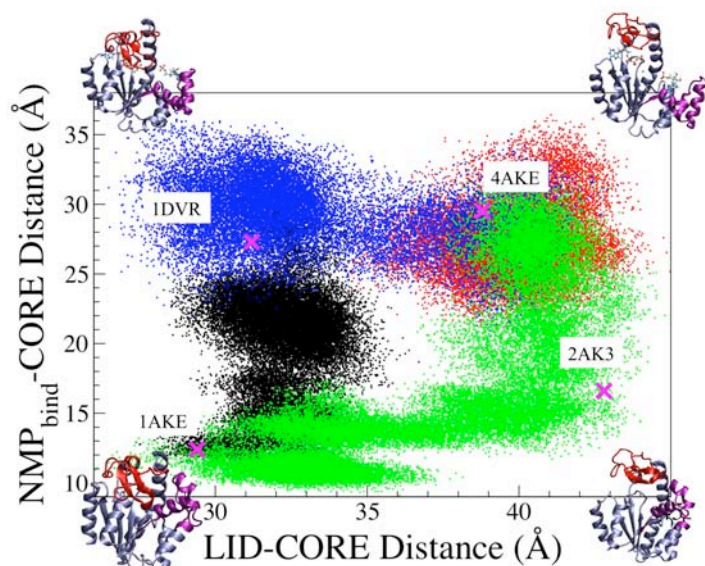
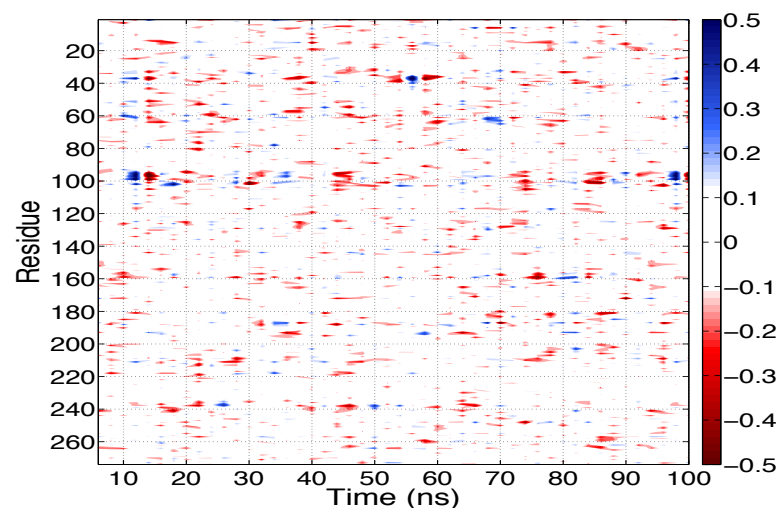


# Multiscale Simulation of Protein Conformational Changes and Intra-protein Communication



Domain-domain distances during conformational changes of adenylate kinase



Temporal changes (percentage) in residue mechanical coupling strength

- Two pathways connecting the open and closed states of adenylate kinase
- Local unfolding prevented opening from the closed conformation
- Mechanical coupling of residues changes during protein dynamics
- Mechanical coupling variation and conformational change are intermittent