Future Objectives: The computational methods I have been developing are general and can be extended to many other molecular systems. There are always new issues that arise when shifting to different problems. Over time, the biophysical models related to the DCM will be extended to predict physicochemical properties of small molecules, nucleic acids, supramolecules and condense phases of aqueous solutions. I have already developed hybrid methods that provide very fast algorithms to explore conformations and simulate long-time dynamics in proteins to help understand their biological function. From applications point of view, the problems related to rational design of proteins and polypeptides require high-throughput bioinformatics research. The *FAST* software will provide a core platform for which many different applications (a partial list given below) can be tackled. As the methods are currently in alpha-phase testing, more pharmacological chemistry applications will be considered.

Applications

1. Exploring native state conformational ensembles
2. Exploring conformational pathways, protein unfolding and partial unfolding
3. Structure/function studies
4. Rational protein design
5. Prediction of protein-substrate binding sites and binding affinities
6. Prediction of functional allosteric effects
7. Build more accurate homology models and structural alignment tools
8. Develop faster ensemble-based electrostatic calculation methods for pKa predictions
9. Protein folding predictions including thermodynamic & mechanical properties of the transition state
10. Prediction of protein oligomerization states that accurately describe protein-protein interactions
11. Prediction of aggregation
12. Prediction of formulations for stabilizing therapeutic proteins

See my research summary for on-going projects.

Application software will be made available as soon as testing and benchmarking is complete.