Bio

My name is Sukanya Sasmal. I am a fourth year Ph.D. student in Chemical Engineering.

Research Interests

My research interests are protein structure and dynamics, and computer simulations of proteins. I am currently working on understanding structural landscape of Amyloid-β peptide, which is the major molecular player in Alzheimer’s disease.

Personal Course Goals

My goal from this course is to be able to parallelize an in-house coarse-grain molecular dynamics code, which will help in better sampling of protein structural ensembles.

Replica-Exchange Molecular Dynamics (REMD)

REMD\cite{1} is a combined Monte-Carlo and molecular dynamics method used to facilitate a faster sampling of protein energy landscapes. In this technique, different copies of the same protein are simulated at different temperatures (known as replicas) and after some interval of time, the simulation is paused, and the position and velocities are swapped between neighboring replicas if a Monte-Carlo acceptance criterion is satisfied. During the course of the simulation, a certain configuration of protein gets heated up and cooled down repeatedly, because of the swapping of replicas. Protein dynamics is faster at higher temperatures, and the repeated heating and cooling process ensures a faster sampling of different protein structures and also a Boltzmann-weighted ensemble at each temperature.

Molecular dynamics simulations of real protein systems would not have been possible without parallelization. REMD adds more complexity to the process, because each replica is essentially one molecular dynamics simulation. All the replicas need to run in parallel, and also communicate with each other. These simulations if run on a single core, would take years to finish.

REMD is used commonly used for finding structural ensembles of proteins and polymers. It is implemented in standard molecular dynamics packages, like Amber\cite{2}, GROMACS\cite{3}, CHARMM, LAMMPS. Scaling of the speed of the simulations with the number of cores is not linear and depends on the system size and is an active area of research.

References: