Exploring global energy landscape of lattice protein models via Monte Carlo methods

Efficient exploration of the configuration space of a protein is essential for its structure prediction. In this talk we will consider two recent Monte Carlo developments for such a task: (i) equi-energy (EE) sampler and (ii) fragment regrowth via energy-guided sequential sampling (FRESS). The EE sampler provides accurate estimation of the density of states of the energy landscape, which then allows detailed study of the thermodynamics of lattice protein folding. The FRESS algorithm provides an efficient means to sequentially simulate a protein structure. As an illustration we will consider 2D and 3D HP models. For the benchmark sequences, we not only found new lower energies for all the 3D sequences longer than 80 residues with little computing effort, but also were able to accurately estimate the density of states that characterizes the global energy landscape.