Transition Path Sampling in Small Polymers

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Computer simulations can provide detailed information about the structure and dynamics of complex molecular systems such as polymers and proteins. Processes such as the folding of proteins involve the exploration of a rugged energy landscape to give a compact structure that is, according to one of the principal tenets of biology, closely linked to the protein's function. The discovery of such structures by computer is a hot topic of study. Even more fascinating is the study of proteins that retain some configurational freedom and flexibility, which is also presumably a key factor in the way they work. Here, the process of transition between one state and another is of great interest[1].

Recently we have studied the dynamics of polymer folding and unfolding, using a technique called forward flux sampling[2]. This mini-project will go further, and examine the pathways of reorganisation for a relatively short polymer chain: a simple model that is known to form right-handed and left-handed helical forms[3], that may interconvert. The system is interesting because the molecule itself is achiral; the formation of mirror-image low-energy forms depends sensitively on the length of the chain and the chain stiffness. The aim is to use Transition Path Sampling (TPS[4]) to study the interconversion pathways, and estimate the rate of interconversion. This approach simulates the dynamics of paths that belong to a particular ensemble: those that start in one state and end in the other. It is also hoped to explore the usefulness of combining TPS with the Wang-Landau method (WL-TPS[5]) to improve the efficiency of the simulations. This method examines the system at a wide range of energies, in the course of a single simulation[6].

This project would suit a student with an interest in computer programming, and some knowledge of statistical mechanics and thermodynamics. No knowledge of biology is required, as the models are very simple. The project would be a suitable introduction to a PhD studying more complex models of intrinsically disordered proteins, in collaboration with colleagues in the department of Chemistry.

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