

Monte Carlo simulations of the HP model (the “Ising model of protein folding”).

D. P. Landau, T. Wüst*, and Y.-W. Li
Center for Simulational Physics
The University of Georgia
Athens, GA 30602, U.S.A.

The HP model is a simple, prototypical lattice polymer model for protein folding. It consists of only two types of monomers, hydrophobic (H) and polar (P), in a sequence chosen so as to mimic a real protein [1]. Interactions are restricted to an attractive coupling between non-bonded hydrophobic monomers that occupy nearest-neighbor sites. Using Wang-Landau sampling with suitable Monte Carlo trial moves (pull and bond-rebridging moves combined) we have determined the density of states and thermodynamic properties for several characteristic sequences of H- and P-mers [2]. As the temperature is lowered these proteins first undergo a collapse “transition” to a globule state followed by a second “transition” into a native state. When placed in the proximity of an attractive surface, there is a competition between surface adsorption and folding that leads to an intriguing sequences of “transitions” that depend upon the relative interaction strengths and are largely inaccessible to “standard” Monte Carlo methods.

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* Current Address: Swiss Federal Research Institute WSL, CH-8903 Birmensdorf, Switzerland

References

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