Chez Pierre

Presents ...

Monday, May 4, 2009
12:00pm
MIT Room 4-331

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"CSAW: Simulation of Protein Folding"

CSAW (conditioned self-avoiding walk) is a computer simulation that treats a protein in solution as a molecular chain in 3D Brownian motion. The unfolded chain is modeled by SAW (self-avoiding walk). To describe folding in water, we impose conditions that represent interactions, including the hydrophobic interactions and hydrogen bonding. In this talk, I will not assume previous knowledge of protein, and supply the necessary background. I will illustrate the capabilities of the model as a theoretical laboratory. These include the energy landscape, and time evolution of the dynamical structure function, showing the emergence of phonon modes. I will present preliminary results that show a first-order phase transition dividing two stages of the folding, leading from a "collapsed" phase to the "molten globule".