

The Fall 2006 Condensed Matter Seminar Series presents:

Dr. Edward Lyman (University of Pittsburgh)

*Measuring “Convergence” of  
Classical Molecular Simulations*

**Abstract:**

Classical equilibrium simulations of biomolecules struggle to sample a space of configurations that is globally sparse, yet locally very dense. Slow (in computer time) transitions between locally stable conformations exacerbate problems of initial state bias and statistical error that plague all simulations. I will discuss a new method to assess these types of errors, in which the sampled configurations are divided up to build a structural histogram. The statistical properties of the structural histogram then offer a unique view of the sampling of the simulation.

**11.08.06      4:00 P.M.      304 Robeson**