

Seminar

Non-Boltzmann Ensembles and Monte Carlo Simulation

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Boltzmann sampling based on Metropolis algorithm has been extensively used for simulating a canonical ensemble. An estimate of a mechanical property, like energy, of an equilibrium system can be made by averaging over a large number of microstates generated by Boltzmann Monte Carlo methods. However a thermal property like entropy is not easily accessible to these methods. The reason is simple. We can assign a numerical value for energy to each microstate. But we cannot carry out such an assignment for entropy. Entropy is not a property of a microstate. Entropy is a collective property of all the microstates of an equilibrium system. Toward calculating entropy and other thermal properties, a non-Boltzmann Monte Carlo technique called Umbrella sampling was proposed in the mid-seventies (of the last century). Umbrella sampling has since undergone several metamorphoses and we have now multi-canonical Monte Carlo method, entropic sampling, flat histogram methods, Wang-Landau algorithm etc. This class of methods generates non-Boltzmann ensembles which are un-physical. However, physical quantities can be calculated by un-weighting and re-weighting techniques. In this talk I shall tell you of a few non-Boltzmann Monte Carlo methods with emphasis on recent developments.

Wednesday, Mar 9th 2016

11:30 AM (Tea/Coffee at 11:15 AM)

Seminar Hall, TCIS