MATERIALS IN MAINZ SCIENCE

Technical Training: Theory

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Computer Simulation Methods in Condensed Matter Physics

Dates: August 28, September 4 and September 25, 2013
Time: 9-11am (c.t.)
Location: MAINZ Seminar Room, Staudinger Weg 9, 3rd floor, room number 03-122

Speaker: Prof. David Landau (University of Georgia; MAINZ Visiting Professor 2013)

August 28, 2013

Lecture 1: Introduction to Monte Carlo simulations in statistical physics

In all but the smallest systems of interacting atoms and molecules, the huge number of possible states render exact solution, or even enumeration of all the terms in the partition functions, impossible. Instead stochastic, or Monte Carlo, sampling, offers the best alternative. A variety of simple sampling and importance sampling Monte Carlo methods that are useful in statistical condensed matter physics will be introduced. Concepts of pseudo-random number production, correlation times, finite size scaling, and their implications for errors will be presented. Methods for extracting static and dynamic critical behavior near phase transitions will be considered.

September 4, 2013

Lecture 2: Introduction to spin dynamics and an application in magnetism

The deterministic equations of motion for interacting atomic-scale magnetic moments will be derived, and different algorithms that are useful for solving the resultant coupled equations of motion will be presented. The extraction of the dynamic structure factor from time-dedendent, space-dependent correlation functions will be presented, and an example will be given that will allow us to compare with experimental results from inelastic neutron scattering. Techniques for reduction of numerical errors will be discussed.

September 25, 2013

Lecture 3: Wang-Landau sampling at the interface between statistical physics and biochemistry: Systems with complex free energy landscapes.

A simple, but powerful, extended ensemble method known as Wang-Landau sampling will be introduced. We will see how “trapping” is avoided and thermodynamic properties at all temperatures (and/or other thermodynamic fields) may be calculated from a ***single*** simulation. Several examples of the application of Wang-Landau sampling, combined with innovative trial moves, to systems with complex free energy landscapes will be considered: We will move from spin glass models of materials science to lattice proteins models, to “real” protein models.