Course Announcement: Bernd A. Berg – Markov Chain Monte Carlo Simulations

Thursday, 11:00 – 12:30, GrHosSR

With the emergence of high performance computing Markov Chain Monte Carlo (MCMC) simulations have become a major enabling technique in applied sciences (biology, chemistry, physics, applied mathematics and also social sciences). The goal of this course is to provide a self-contained presentation. This includes not only MCMC methods themselves, but also its statistical foundations and the statistics needed to analyze MCMC data. The course is addressed to scientists and students, who need ready to work recipes and running computer code will be provided. Illustrative examples will cover applications in statistical physics, particle physics and bio-chemistry. According to the wishes of the participants the emphasize between different topics can be shifted and applications in social sciences may be added. The course language can be either German or English. Textbook: *Markov Chain Monte Carlo Simulations and Their Statistical Analysis* by Bernd A. Berg, World Scientific, 2004.

1. Sampling, statistics and computer code
   - probability distributions, sampling and random numbers
   - organization of the computer code
   - Gaussian distribution, confidence intervals, order statistics and heapsort
   - functions and expectation values of random variables
   - sums of independent random variables and characteristic functions
   - linear transformation of random variables
   - the central limit theorem and binning
2. Error analysis for independent random variables
   - Gaussian confidence intervals and error bars
   - estimators of the variance and bias, statistical error bar routines
   - the Gaussian difference test
   - Gaussian error analysis for small samples (χ^2 and student distribution)
   - the error of the error bar and the variance ratio test (F-test)
   - The jackknife approach
   - determination of parameters (linear and Levenberg-Marquardt fitting)
3. Markov Chain Monte Carlo
   - preliminaries: The canonical ensemble and the two-dimensional Ising model
   - lattice labeling
   - sampling, re-weighting and importance sampling
   - the Metropolis algorithm
   - the heath bath algorithm
   - illustrations of Monte Carlo simulations I : discrete systems
   - illustrations of Monte Carlo simulations II: continuous systems
4. Error analysis for Markov chain data
   - autocorrelations, integrated autocorrelation time and binning
   - self-consistent versus reasonable error analysis and large scale simulations
   - analysis of MCMC data (examples)
   - comparison of MCMC algorithms
   - fitting of MCMC data
5. Advanced Topics
   - simulations of generalized ensembles
   - free energy and entropy calculations
   - event driven simulations
   - cluster algorithms
   - parallel computing (replica exchange method, checkerboard algorithm)
   - applications in particle physics (lattice gauge theory)
   - MCMC simulations of biomolecules