PH550: Monte Carlo techniques in Statistical Physics

Course Content/ Syllabus:

Introduction: simulation methods, necessity of simulation, physical problems.
Probability and distribution functions: an overview, special Probability Distributions, Binomial, Poisson, Normal and their relations in the limiting conditions, Uniform distribution, central limit theorem. Over view of thermodynamics and statistical mechanics: thermodynamic potentials, parameters, response functions, statistical ensembles, averages, partition functions, free energy, thermodynamic quantities.

Markov process: Markov chain, transition matrix, probability of a state, equilibrium probability distribution. Steady state, global balance, discrete and continuous representation of time, master equation, condition of steady state and steady state distributions.

Random number generator: Congruential method, frequency test, correlation test, parking lot test, random numbers of a given distribution. Monte Carlo simulation: Physical problems, MC estimates of statistical average. simple sampling and importance sampling techniques.
Simple sampling MC: radioactive decay, boundary value problems, random walks, self-avoiding walks and percolation.
Overview of phase transition and Ising model: Features of first and second order transitions, Phase diagrams, Features of critical phenomena, order parameter, critical phenomena in different systems, response, correlation and fluctuation, critical opalescence. Ising model, ground state, Ferro-para magnetic transition.

Importance sampling MC: Ergodicity and detailed balance, Metropolis algorithm, application to Ising model in two dimension, Metropolis importance sampling scheme for Ising model, equilibrium, determination of critical temperature and critical behaviour of thermodynamic quantities, error analysis, finite size effect, correlation, critical slowing down.
Cluster flipping algorithms: Fortuin-Kasteleyn theorem, Swendsen-Wang method, Wolf method. Finite size scaling: direct measurement of critical exponents, finite-size scaling methods, application to Ising model and percolation. MC simulation of non-equilibrium systems: self-organized criticality and sandpile, dynamic phase transition and kinetic Ising model.

References:

1. D. P. Landau and K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, Cambridge (2000).
2. 2. M. E. J. Newman and G. T. Barkema, Monte Carlo Methods in Statistical Physics, Clarendon (1999).
3. 3. K. Binder and D. W. Heermann, Monte Carlo Simulations in Statistical Physics, Springer (1992).
4. 4. J. M. Yeomans, Statistical Mechanics of Phase transitions, (Clarendon press, Oxford, 1992).
5. 5. W. H. Press, S. A. Teu kolsky, W. T. Vellerling, B. P. Flannery, Numerical Recipes, (Cambridge university Press, Cambridge, 1998).