

Kinetic Monte Carlo

From Phase Transitions and Crystal Growth to Econophysics

Lecturer

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Purpose

The aim of this school is to familiarize the students with the kinetic interpretation of the Monte Carlo method, to discuss the mathematical background of the master equation and when it will lead to physically reasonable kinetics and to present some selected applications from recent research. In condensed matter physics, the goal is to reproduce physical kinetics qualitatively and sometimes even quantitatively using a Monte Carlo method. In econophysics or finance, kinetic Monte Carlo simulations are used to model various stochastic aspects of market behavior, e.g., to synthesize time series of portfolios for risk analysis. Each of these areas will be exemplified by a 'hands-on' session where the applicants can try out what they have learned using simple programs on the computer.

Background and Motivation

The Monte Carlo method is still largely only perceived as a tool to study thermodynamic equilibrium properties, i.e., to solve high-dimensional integrals in configuration space. It does, however, in its most widely used form do so by generating a random walk in configuration space, described by the master equation

$$P_{n+1}(x) = P_n(x) + \sum_{x'} W(x' \rightarrow x) P_n(x') - \sum_x W(x \rightarrow x') P_n(x). \quad (1)$$

To ensure sampling of the configurations x according to their equilibrium statistical weight, the transition probabilities are generally taken to fulfil the detailed balance condition

$$W(x' \rightarrow x) P_n(x') = W(x \rightarrow x') P_n(x). \quad (2)$$

In this way there is a stochastic process connected with the Monte Carlo method and one can ask under which conditions 'n' can be interpreted as time. When does the Monte Carlo pseudo-kinetics correspond to the real kinetic properties of a physical system?

In simulations of the canonical ensemble the ratio of the transition probabilities is given by

$$\frac{W(x' \rightarrow x)}{W(x \rightarrow x')} = \frac{P_n(x)}{P_n(x')} = \exp\{-\beta(H(x) - H(x'))\} \quad (3)$$

where $\beta = 1/k_B T$. This fixes the thermal part of the transition probabilities to the ratio of the Boltzmann factors of the two states involved, but it does not tell which states x, x' are connected through transition probabilities and with which probability a certain channel $x \rightarrow x'$ leading away from a state x is selected (but we do know that the reverse move has to be suggested with equal probability).

It is the freedom of choosing the list of allowed moves $x \rightarrow x'$ that is the strength of the Monte Carlo method. Due to this freedom of choice, the method can be used to bridge between various levels of description in statistical mechanics. As far as the kinetics implied by these allowed moves is concerned, a range of scenarios is possible. In one limiting case, choosing a coarse level of description allows one to address collective phenomena on long time scales, but in this case the model kinetics matches the physical kinetics only in the very long time limit (for instance when the long time limit of the physical process is diffusive). In the other limit, one can attempt to reproduce the physical kinetics as closely as possible by a judicious choice of the types of moves and their respective rates. If sufficiently many different moves are included, and a microscopic theory is used to derive their rates, kinetic Monte Carlo simulations can come close to molecular dynamics simulation in terms of accuracy and microscopic detail, while allowing to access much larger length and time scales.

Besides these classical condensed matter and statistical physics problems collective phenomena in society and economics have recently become of interest to the physics community. When one deals with socio-economic questions the most basic level of kinetic modelling is a probabilistic one. With the introduction of computerized trading much empirical information, for instance, on the time evolution of stock prices and of the correlations between these evolutions for different stocks has been accumulated. Sophisticated mathematical models of these stochastic evolutions are available and can be explored using

kinetic Monte Carlo simulations to obtain a probabilistic prediction for the risk contained in an investment portfolio.

Schedule

- Monday, Oct. 14, 2002
 - Basics of the Monte Carlo method
 - Properties of the master equation and the generated stochastic process
 - When is Monte Carlo kinetics physically reasonable?
 - Diffusion processes
 - Diffusion in the double-well potential
 - From the double well potential to the egg-tray
 - Practical work: discussion in small groups; program a random walk
 - Poster session: Possibility for the participants to present their own work
- Tuesday, Oct. 15, 2002
 - One “classical” application: spinodal decomposition
 - Phase transformation kinetics (background)
 - The Ising model and its lattice gas interpretation
 - Glauber vs. Kawasaki kinetics
 - Practical work: Simulation of the 2d Ising model
- Wednesday, Oct. 16, 2002
 - What is meant by kinetic Monte Carlo
 - The n-fold way
 - Surface diffusion and ordering processes as an example
 - Contact to ab initio calculations of the relevant rates

- Practical work: perform some studies of surface diffusion and growth using ready program from FHI
- Thursday, Oct. 17, 2002
 - Introduction to financial markets and geometric Brownian motion
 - The Black-Scholes framework
 - Using MC simulations for the valuation of financial contracts
 - Measuring market risk, the Value-at-Risk (VaR) approach
 - Practical work: evaluation of complex derivative contracts and VaR-calculations