Monte Carlo methods

Objetives :

Monte Carlo methods are extensively used in numerous scientific fields : applied mathematics (optimization, integration, networks simulations…), physics (statistical mechanics, out-of-equilibrium thermodynamics, electronic structures…), materials science (microstructures, ageing, grain growth…), biology (protein conformation, morphogenesis…), economy (economic models, financial markets…). The objective of the course is to acquire the fundamentals that are common to all Monte Carlo applications (justification, principles, numerical implementation). The method is illustrated through various examples that are developed during practical sessions.

Plan :

1. The Monte Carlo method : what is it for ?
2. Monte Carlo methods for numerical integration.
3. Random numbers and their generation.
4. Statistical Physics: a quick reminder.
    a. Boltzmann and the fundamental hypothesis of statistical mechanics;
    b. How to demonstrate the Gibbs distribution in three slides.
5. The Monte Carlo method:
    a. Macroscopic quantities: the necessity of importance sampling;
    b. Markov chain and the Master equation;
    c. Ergodicity and convergence;
    d. Metropolis (and other…) algorithms.
6. Application 1 : Equilibrium thermodynamics of order-disorder transitions.
7. Application 2 : Kinetics in alloys (diffusion through vacancies, resident time algorithm).
8. Application 3 : Grain growth and recrystallization.
9. Application 4 : Diffusion-limited aggregation.