# Introducing the step Monte Carlo method for simulating dynamic properties

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The Monte Carlo (MC) approach is now an essential ingredient in many quantitative studies and branches of science including physics, finance-economics, biology, engineering, etc. In the field of condensed matter physics and materials science MC can be used to study, among many others, system of classical particles [1], classical spin systems [2], percolation and fractals problems. The MC algorithm is the natural choice for studying the static properties of a system, where dynamical effects are not required. Then, the advantages of Monte Carlo are the relative ease of implementation and the rapid convergence to steady state.

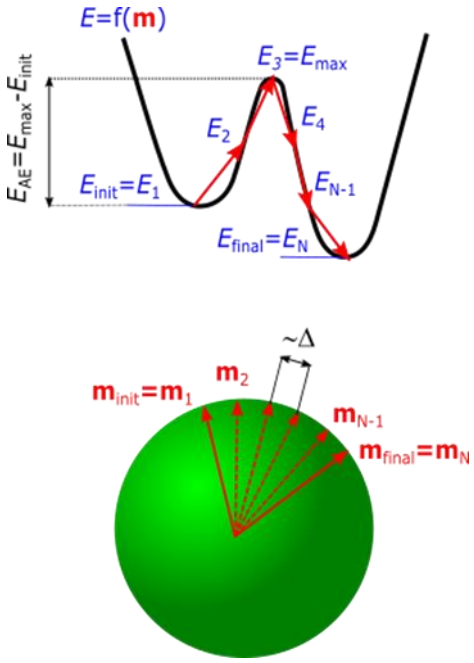


Fig. 1. Schematic illustration of the step Monte Carlo (sMC) method for the case of magnetization process (one Monte Carlo move). The magnetization direction $\mathbf{m}$ (bottom panels) can take any point on the unit sphere with energy $E = f(\mathbf{m})$ (top panels). $\mathbf{m}_{init}$ and $\mathbf{m}_{final}$ are initial and final (trial) direction of magnetic moment with energy $E_{init}$ and $E_{final}$ respectively. In the sMC approach the probability of accepting the final random state $\mathbf{m}_{final}$ depends on the activation energy $E_{AE} = E_{max} - E_{init}$, not on the relative energy $E_{final} - E_{init}$.

In the modified MC approach proposed here (similarly to the kinetic MC approach) the probability of accepting the final state depends on the activation energy, not on the relative energy between the final and initial state [3]. However, the barrier height is calculated on an ongoing basis, by generating intermediate states with a predefined step $\Delta$. Therefore, we name this method step Monte Carlo (sMC) [3]. Importantly, the sMC method correctly takes into account the presence of various local barriers and it obeys the detailed balance condition, even if the system is not in equilibrium. As a result, the appropriate dynamics of the tested system is simulated. The details of sMC algorithm are explained for the case of magnetization process. To test the correctness of sMC, we compare its results with those obtained by stochastic Landau-Lifshitz-Gilbert (sLLG) approach.

[1] D. Frenkel and B. Smit, "Understanding Molecular Simulation: From Algorithms to Applications", Academic Press, San Diego (2002).

[2] M. Sawicki, T. Devillers, S. Galeski, C. Simserides, S. Dobkowska, B. Faina, A. Grois, A. Navarro-Quezada, K. N. Trohidou, J. A. Majewski, T. Dietl, and A. Bonanni, *Phys. Rev. B*, **85**, 205204 (2012)

[3] D. Sztenkiel, "Introducing the step Monte Carlo method for simulating dynamic properties," arXiv:2209.08961 (2022).