

# Kinetic Monte-Carlo simulations of radiation damage in structural materials



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The kinetic Monte-Carlo (KMC) method is a stochastic method intended to simulate the time evolution of some process. The treated system is advanced through time in an ordinary stochastic manner but with a timestep rigorously associated to each action. It is especially useful in studies of irradiation driven phenomena due to its power and flexibility. Although it was first developed in order to treat the diffusion of vacancies in a crystal lattice it has hence been developed in order to treat a vast range of phenomena. KMC is one of the few methods available to a nuclear scientist that can treat, on an atomistic level, spatial and temporal scales comparable to those in microstructural experiments.

This seminar will introduce you to the fundamentals of the kinetic Monte-Carlo method, starting from the physical motivations and justifications and working through the mathematical formalisms towards a comprehensive understanding. Different KMC flavours will be discussed as well as their ranges of applicability. Novel schemes, such as parallelisation and action filtering will be treated. Finally, we will discuss some practical applications with implications for structural materials of nuclear reactor systems.