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First-passage Monte Carlo for materials under irradiation[1] ALEKSANDAR DONEV, VASILY BULATOV, Lawrence Livermore National Labs — The key challenge in simulations of irradiated materials is that of time scale. Typically, atomistic simulations extend to less than one nanosecond whereas kinetic Monte Carlo (kMC) simulations struggle to reach hours of simulated irradiation. Based on a time-dependent Green's function formalism, our new kMC algorithm extends the simulated time horizon from minutes to tens and hundreds of years while retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes.

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