

Abstract Submitted  
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**First-passage Monte Carlo for simulations of alloy microstructure**<sup>1</sup> ALEKSANDAR DONEV, VASILY BULATOV, TOMAS OPPELSTRUP, MALVIN KALOS, GEORGE GILMER, BABAK SADIGH, Lawrence Livermore National Laboratory — We unveil a principally new Monte Carlo algorithm for simulations of multiple diffusing particles of finite dimensions that coalesce or annihilate on collisions. The algorithm is derived from the theory of first-passage processes and a time-dependent Green's function formalism. The new method circumvents the need for long and tedious diffusion hops by which the particles find each other in space. At the same time, the algorithm is exact and its computational efficiency is astonishing. The new algorithm is generally applicable in 1d, 2d, 3d, ... and to a wide variety of important physical situations, including nucleation, growth and coarsening of alloy particles, interstitial and vacancy clusters after quench or under irradiation. We will present simulation of multi-million particle ensembles covering over 10 decades of time of microstructural evolution.

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