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Exact kinetic Monte Carlo approach for diffusion without the lattice hops VASILY BULATOV, TOMAS OPPELSTRUP[1], GEORGE GILMER, MALVIN KALOS, BABAK SADIGH, Lawrence Livermore National Laboratory, WEI CAI, Mechanical Engineering Department, Stanford University — We present a new algorithm for kinetic Monte Carlo simulations applicable to a wide range of physical situations where multiple Brownian particles of finite dimensions diffuse, collide and react with each other. In its spirit, the new approach is reminiscent of the so-called event-based Monte Carlo algorithm (*JERK*) developed over the years in SACLAY (France). Similar to *JERK*, the algorithm alleviates the need to simulate every single diffusional hop but focuses on more significant changes in the system's configuration. Yet, unlike *JERK*, the new algorithm is approximation-free and its accuracy is limited only by the quality of the diffusion and reaction rate coefficients. The new approach is based on the exact Green's function solutions obtainable in the time-dependent theory of first-passage processes. Applications of the new approach will be discussed, including Oswald ripening, semiconductor processing, defect microstructure evolution in fusion and fission reactor materials, and diffusion-controlled reactions in confined geometries.

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