1056-76-285 Holly N. Clark* (hclark@math.utk.edu) and Tim P. Schulze. Multistep Kinetic Monte Carlo. Preliminary report.

In general, Monte Carlo refers to a class of algorithms that solve problems using random numbers. Kinetic Monte Carlo (KMC) can be used to simulate the time evolution of processes with well-defined rates. We analyze a multi-step KMC algorithm aimed at speeding up the single-step procedure and apply the algorithm to study a model for the growth of a surface dendrite. The growth of the dendrite is initiated when atoms diffusing on a substrate cluster due to lower hopping rates for highly coordinated atoms. The boundary of the cluster is morphologically unstable when the flux of new atoms is supplied in the far field, a scenario that could be generated by masking a portion of a substrate that is subject to some kind of deposition process. We allow atoms far from the growing dendrite to take large hops while atoms near the dendrite follow a usual single-step KMC algorithm. We study how coarse-graining affects the distribution of waiting times for hops, and how to accurately couple the multi-step and single-step regions. (Received August 25, 2009)