In Memory of Peter Smereka: Kinetic Monte Carlo---A Look Back and a Step Forward

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Abstract:

In this talk I will review some of the work Peter and I did together on Kinetic Monte Carlo (KMC). Much of this was focused on an approximate model for hetero-epitaxial growth with misfit between the film and substrate. I refer to this as weakly off-lattice KMC simulation. In the past couple of years I have worked with a student, Hamza Ruzayqat, to extend some of the work Peter and I did to improve the computational performance of these weakly off-lattice simulations to fully off-lattice KMC. The key idea is the use of approximate rates to build a rejection-based algorithm that allows one to achieve a computational boost by a factor that scales with the number of particles in the system. Off-lattice KMC is still quite expensive compared to the weakly off-lattice model, so we currently apply this method to nano-clusters containing around 100 particles rather than to thin films.