1106-VL-2100 **Kyle Golenbiewski*** (kyle@math.utk.edu), **Tim P. Schulze** and **Peter Smereka**. *Analysis of an energy localization method used in Kinetic Monte Carlo simulations of heteroepitaxial growth.* Preliminary report.

Heteroepitaxial growth consists of slowly depositing one material onto a crystalline substrate formed from a second material. An important feature of this process is that the natural lattice spacing of the deposited material may differ from that of the substrate's, resulting in elastic strain. Simulation of such growth using Kinetic Monte Carlo is often based on rates determined by differences in elastic energy between two configurations. This, however, is computationally challenging due to the long range nature of elastic interactions. Adopting an atomistic approach, we consider a method in which the elastic field is updated using highly accurate local approximations, though the energies themselves are far less accurate. Namely, we approximate the elastic energy barrier by constraining the displacement field with an atom removed to agree with the displacement field when the atom is present outside some local region. In order to gain insight into this energy localization method, we appeal to a continuum analogue of the discrete mechanical system. For the scenario of an isolated island sitting on an unbounded and otherwise flat film on a flat substrate, we extend earlier results for a 2D system to 3D. (Received September 15, 2014)