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**Non-Uniqueness in Energy Minimization of Atomistic and Multiscale Problems: A Branch-Following and Bifurcation Investigation<sup>1</sup>**

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Static multiscale and atomistic simulations aim to obtain an equilibrium configuration (local energy minimum) of a body composed of discrete atoms subject to applied loads and/or displacements. Often a system of “proportional loading” is considered and the evolution of the body’s equilibrium configuration is determined in an incremental fashion as the scalar “loading parameter” is varied. At each step, a minimization procedure, such as the conjugate gradient method, is employed using the previous relaxed configuration as an initial guess. A practical problem with such simulations is that due to the highly nonlinear nature of such problems, many equilibrium configurations should be expected. Therefore, the real possibility of multiple competing physical processes is encountered. Unfortunately, the simulation procedure described above provides only one of the possible equilibrium evolutions. Even more troubling is the fact that this one equilibrium evolution will, generally, depend on the numerical energy minimization method employed and the particular values used for its parameters. This work takes a different approach to the exploration of the equilibrium behavior of atomistic and multiscale systems. It performs a *Branch-Following and Bifurcation* (BFB) investigation in order to map out a large number of equilibrium configurations over a wide range of the problem’s loading parameter. Once a reasonably complete picture of the system’s *possible behaviors* is in hand, it is then possible to interpret these results to draw conclusions about the most likely behavior of the system. To illustrate this novel application of BFB methods to atomistic multiscale problems, some representative problems will be presented including the results for a small “simple” atomic slab subjected to axially compressive displacements. The set of possible equilibrium states found is much more complex than first expected and is a vivid illustration of the complex behavior these systems are capable of. These results will be described and some suggestions for “new” simulation/interpretation procedures will be discussed.

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