Equilibrium Maps: Characterizing the complex and stochastic behavior of nanosystems subjected to proportional loading

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Modeling nanosystems subjected to proportional loading, such as pulling nanotubes, poses significant challenges due to the comparable magnitudes of thermal fluctuations and applied stimuli at the nanoscale. The resulting stochastic evolution is influenced by the highly nonconvex potential energy surface (PES), which features multiple competing pathways. To address these challenges, we develop a novel simulation framework utilizing branch following and bifurcation techniques. This approach extends traditional concepts of the PES, equilibrium points, and transition networks to driven systems where the PES deforms under external loading. We introduce the concept of the Equilibrium Map (EM), a condensed representation capturing the evolving PES's equilibrium and kinetic characteristics, enabling the construction of system trajectories across diverse loading regimes and boundary conditions. Efficient parallel algorithms facilitate the scalable construction and management of EM data. Additionally, we address superbasins, clusters of stable states separated by low energy barriers, by implementing methods that accelerate dynamics within these regions, enabling long-timescale simulations. Application to a nanoslab under displacement-controlled loading demonstrates that the EM method qualitatively reproduces experimental observations, offering a powerful tool for nanoscale system modeling under proportional loading.