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What Must We Know to Gain Useful Knowledge from a Complex Surface?¹

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Complex potential surfaces can be analyzed, in principle, to yield virtually any desired information about their topographies. However for a system of more than about 20 particles, the surfaces are so complex that the only feasible ways to work with them involve the extraction of some minimal set of data that can provide the information we most want. Molecular dynamics and Monte Carlo searches, especially with long-range exploration algorithms or coarse-graining, are two well-studied approaches. Kinetic methods based on master equations provide another with the power to reach long time scales. Their largest difficulty is finding a way to construct a master equation based on a suitably small subset of the information that will yield, with reliability, the important rates we need, specifically the rates of the slow but attainable processes. We review several approaches that we have been pursuing: reduction of the kinetics to interbasin passage, reduction of the number of coordinates to just the most important, by principal component analysis, and sampling of pathways on the surface.

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