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Milestoning: A rigorous coarse graining method for simulating properties of biological molecules[1]

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Milestoning is a method for calculating kinetics and thermodynamics of long time processes typically not accessible for straightforward Molecular Dynamics (MD) simulation. In the Milestoning approach, the system of interest is partitioned into cells by dividing hypersurfaces (Milestones) and transitions are computed between nearby hypersurfaces. Kinetics and thermodynamics are derived from the statistics of these local transitions. We describe an extension to the original Milestoning that we called Directional Milestoning. It avoids the use of a reaction coordinate, provides exact first hitting distribution at the interfaces, and supports sufficiently long relaxation time between the interfaces for better accuracy. I will describe the adjusted theory and algorithm, and will present results on a model system alanine dipeptide and for the folding of the helical peptide WAAAH. Interestingly the kinetic of folding of WAAAH shows significant co-operativity and is close to an all or none transition. The calculations are consistent with experimental measurements of kinetic, thermodynamic, and structure of this peptide.

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