

**STATISTICAL CONSIDERATIONS OF REWEIGHTING BASED SIMULATION METHODS FOR IMPROVED SAMPLING.** Donald Hamelberg, Department of Chemistry, Georgia State University, P. O. Box 4098, Atlanta, Georgia 30302-4098

Application of simulation-based methods to calculating thermodynamic properties of biomolecular systems is fast becoming indispensable in the field of biochemistry and biophysics. One persistent theme is to find a fast, yet accurate, sampling scheme to achieve the desired results. Various advanced simulation techniques rely heavily on successfully reweighting the sampled configurations. The sampled points of a system on a modified potential energy landscape, for example, are reused with different statistical weights to evaluate the desired properties on the original potential. We provide a quantitative method to estimate the number of sampled points required in the crucial step of reweighting the distribution. Proper execution of these types of analyses could provide a quick guesstimate of how long a simulation should be run.