Shortcuts to Parameter Sweep

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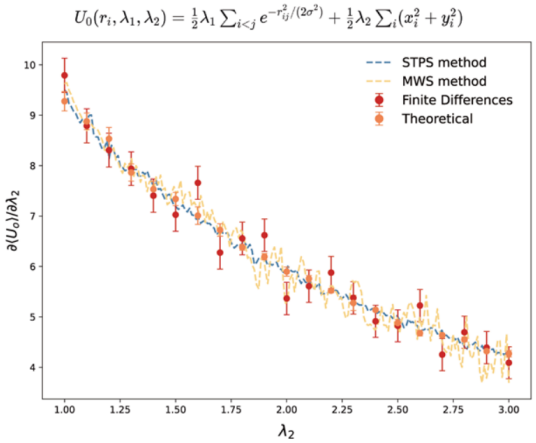

Computing equilibrium response functions, namely derivatives of observables with respect to control parameters, is a fundamental task in molecular simulation, with applications ranging from force-field optimization to material response prediction. Conventional approaches rely on finite-difference methods combined with parameter scanning, where equilibrium simulations are performed at multiple discrete parameter values and derivatives are approximated numerically. This strategy faces two critical limitations. For systems with slow relaxation dynamics, achieving equilibrium at each parameter point demands prohibitively long simulation times. Additionally, the finite-difference step size involves an inherent trade-off between truncation error and statistical noise, making it difficult to obtain accurate continuous response curves. Alternative methods based on Malliavin weights avoid finite-difference errors but suffer from auxiliary variables whose variance grows linearly with simulation time, limiting their reliability in long-duration or wide-range parameter scans [1].

In this work, we introduce a novel framework for computing continuous response functions built upon the shortcut-to-isothermality protocol [2], which we term the Shortcut to Parameter Sweep (STPS) method. The core idea is to drive the system through parameter space using an auxiliary potential that enforces the instantaneous equilibrium distribution at every moment of the finite-time nonequilibrium simulation. Under this protocol, we derive an analytical result showing that the response function at any instant during the driving process can be expressed exactly as a linear combination of static correlations evaluated under the instantaneous equilibrium distribution. This expression requires no finite-difference approximations and involves no auxiliary stochastic variables with diverging variance. Crucially, a single simulation suffices to recover the full continuous response curve over the entire parameter interval of interest.

We validate the STPS method across four representative model systems within the overdamped Langevin dynamics framework, including a harmonic oscillator with time-dependent stiffness, a harmonic oscillator with a linear dragging force, a linearly biased double-well potential, and a two-dimensional many-body system of Brownian particles with pairwise Gaussian kernel interactions. In all cases, results from the STPS method show excellent agreement with theoretical values obtained from direct numerical integration and with Malliavin weight sampling, while exhibiting markedly superior statistical stability under long-time driving.

We further discuss the natural extension of the framework to underdamped Langevin systems, where the auxiliary potential is constructed in full phase space and the response function retains an identical formal structure. The primary practical challenge lies in constructing the auxiliary potential for complex systems, and we outline promising future directions based on machine learning approaches to address this limitation. The STPS method offers a practical, broadly applicable, and statistically robust tool for sensitivity analysis in molecular and soft matter simulations.

References:

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