Challenges for canonical multiscale MD simulation

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Multiple timestepping [1] and reversible averaging [2] are examples of schemes designed to simulate conservative systems evolving on disparate timescales. These methods can exhibit linear or nonlinear resonances which lead to instabilities in constant energy simulation. On the other hand, introduction of resonant augmenting dynamics is exactly the point of thermostatting schemes such as Nose dynamics [3] and generalizations [4]. In this talk, I will discuss these two types of resonances and their interplay, and consider the implications for construction of canonical multiscale methods.

References

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