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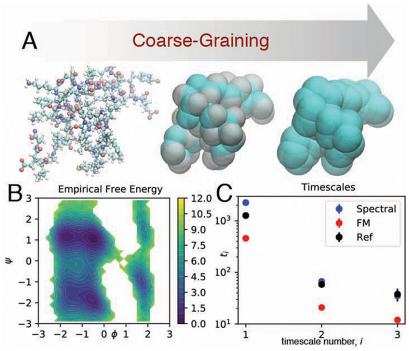
Spectral matching used to define effective coarse-grained models reproducing dynamics of a fine-grained system.



Typically used for molecular modeling of biomolecules, coarse-grained models mirror the behavior of complex systems and break them down into simpler components based on degree of granularity. Coarse-grained models have found practical applications in several areas, such as atmospheric science and molecular biophysics, but their definition still presents fundamental challenges. Although machine learning has been used to alleviate challenges to current coarse-graining methods that focus on reproducing thermodynamic properties, these techniques do not ensure that the kinetics and the timescales of the processes are also reproduced. In biomolecular systems research, reproducing kinetics is crucial to understanding biological mechanisms. Coarse-grained dynamics should retain the metastable processes of the original dynamics.

Clementi et al. used spectral matching to define coarse-grained models to reproduce the slowest dynamical processes and efficiently reproduce kinetic properties. They explored ways to preserve the kinetic properties of the system, using an approach appropriate for the design of general and transferable models that may be used to simulate not just one biomolecular system but a number of them. They also present an alternative approach effective for studying a specific system.

“The results presented in this article provide a proof of concept of the methodology by demonstrating it on simple toy systems. It is now important to use this approach on relevant biomolecular systems that cannot be studied by conventional simulation techniques at atomistic resolution,” Clementi said.

Spectral matching can be used in combination with current methods, such as force matching, to enforce kinetic consistency. The authors expect their methods will assist the research of biomolecular systems that are too large to simulate with conventional atomistic simulations. A particular long-term goal is the development of coarse-graining methods that reproduce slow dynamic mechanisms characterizing many biological processes.

Source: “Coarse-graining molecular systems by spectral matching,” by Feliks Nüske, Lorenzo Boninsegna, and Cecilia Clementi, *Journal of Chemical Physics* (2019). The article can be accessed at https://doi.org/10.1063/1.5100131.

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