

Coarse-graining solvent structure using stochastic hard collision (SHC) dynamics

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The structure of coarse-grained particles is known to be recoverable from models with bounded potentials such as the penetrable sphere model or more complicated soft-interaction models. We have developed a stochastic hard collision model that allows one to effectively capture the structure arising from a corresponding soft-particle model while allowing for the computational efficiency arising from hard-particle models [*J. Chem. Phys.* **138**, 244901 (2013)]. We will report the extent to which this model provides correct dynamics at coarse-grained time-scales. The efficiency of the SHC model also provides an alternative to fine-grained solvent models for the characterization of the motion or reactions of finer-grained solutes.

This work has been partially funded by the National Science Foundation through grant number CHE 1700749.