Scilight

NEWS | NOVEMBER 08 2019

Inverse Henderson problem generalization fills gap for numerical simulations of soft matter FREE

Mara Johnson-Groh

Scilight 2019, 450002 (2019)
https://doi.org/10.1063/1.5134789

Scilight

7 November 2019

Inverse Henderson problem generalization fills gap for numerical simulations of soft matter

Mara Johnson-Groh

A new generalization of the inverse Henderson problem fills a gap that previously existed in the theoretical foundation for many bottom-up coarse-graining techniques employed in soft matter simulations.

Numerical simulations of soft matter require multi-scale techniques to properly account for all major particle interactions. One common technique known as bottom-up coarse graining simulates soft matter systems using particles with reduced degrees of freedom, with finer details only considered when necessary. To effectively employ these techniques requires overcoming the inverse Henderson problem, which involves the computation of the potential between pairs of particles.

In 1974, Henderson proved that the pair potentials in a system are uniquely determined in the canonical ensemble and claimed the same result for systems in the thermodynamic limit. Henderson's proof used a version of the Gibbs variational principle that is only valid in a finite volume box. According to Frommer et al, this makes his attempt to extend his conclusion to include the thermodynamical limit incomplete, leaving a gap in the proof, which the authors sought to clear up in their theoretical paper.

To bridge this gap, the authors introduced a specific variant of the Gibbs variational principle known as the Georgii's variant, and showed that a rigorous proof of Henderson's theorem is indeed possible in the thermodynamic limit. This was used to show that when certain parameters of two different systems coincide, they can be assumed to be the same. The result remains true if the chemical potential is given instead of the density. This new proof also holds true for certain classes of pair potentials including the most relevant ones for applications.

The researchers plan to continue refining the model to eventually prove convergence of iterative solutions, which would improve numerical simulation efforts in chemistry and physics.

Source: "A note on the uniqueness result for the inverse Henderson problem," by F. Frommer, M. Hanke, and S. Jansen, *Journal of Mathematical Physics* (2019). The article can be accessed at https://doi.org/10.1063/1.5112137.