Computer simulations for multiscale systems can be faster, better, more reliable

September 20 2012

University of Oregon scientists have found a way to correctly reproduce not only the structure but also important thermodynamic quantities such as pressure and compressibility of a large, multiscale system at variable levels of molecular coarse-graining.

The method is a mathematically driven predictive modeling of a real system, built on liquid state theory, and utilizing powerful computing resources. The team's theory appears in the Sept. 21 issue of the journal Physical Review Letters.

Understanding multiscale systems is of vital importance in biology and material engineering. Because physical properties of multiscale systems develop on an extended range of times and lengths—with changes involving many orders of magnitude—computer simulations at the atomic resolution can exceed even the most advanced computational capabilities.

In recent years theoretical coarse-graining methods have gained attention in the scientific community because they provide an efficient alternative to traditional simulations, which represent explicitly every atom of the molecular system. In course graining, atomistic-level information is removed to make computations at long time- and large length-scales possible. The key issue is how to develop reliable and controllable coarse-graining procedures. Most coarse-graining methods correctly predict the structure of a liquid, but they fall short in predicting thermodynamic properties such as pressure or compressibility.

The new theory has the capability to ensure both structural and thermodynamic consistency, said Marina G. Guenza, professor of theoretical physical chemistry and project leader.

Last year, in the journal Physical Review E, Guenza and doctoral student Ivan Lyubimov, a co-author of the new paper, documented a procedure to reconstruct the realistic dynamics of multiscale systems from the motion measured in dynamic simulations of coarse-grained macromolecules. In this newly published article, the same coarse-graining formalism is shown to reproduce correctly the pressure and compressibility of the system, providing a reliable method to simulate complex macromolecular systems in an extended range of length and timescales.

Thermodynamic properties are important in the mixing of liquid materials used in making plastics, said Anthony J. Clark, a UO doctoral student in physics and lead author of the new paper. "Pressure has been a high-level issue in coarse-graining," he said. "It is important to be able to reproduce the distribution of molecules in a system, and pressure is a hard physical quantity to predict. Our theory now will provide the interaction potentials of coarse-grained molecules, which correctly predict both the structure and the thermodynamics of the sample."

The improvements to the formula for the computational simulation mean that manufacturers soon may be able to use a computer code and input information for the materials they plan to mix and quickly determine the behavior of a finished product, said Guenza, a member of the UO's Institute of Theoretical Science, Materials Science Institute and Institute of Molecular Biology.

A problem in working with polymers, for example, is that they often don't blend easily. Controlling for thermodynamic components is vital.

"These molecules are very complex," said co-author Jay McCarty, a doctoral student in chemistry who derived the equations that prove the thermodynamic consistency of Clark's potential and ran the atomistic simulations the test the theory. "They move at different timescales and cover many lengthscales. Our goal is to bridge phenomena that happen at different scales at the molecular level."

Many manufacturing processes rely on often costly, time-consuming and wasteful trial-and-error procedures. While the scientific program is still under development to be extended to a larger number of systems, Guenza said, the recent developments have addressed major stumbling blocks.

On the horizon, she said, is a web-based computer program at the UO, which manufacturers and researchers will be able to access to run predictive coarse-graining simulations that will facilitate the study of polymeric systems and improve the efficiency of working with these samples.

"Dr. Guenza's work to improve our understanding of multi-scale systems has the potential to create new efficiencies in research and manufacturing," said Kimberly Andrews Espy, vice president for research and innovation, and dean of the graduate school. "It reflects the University of Oregon's commitment to re-engineering the science, manufacturing and business processes related to critical products with the aim of fostering a more sustainable future for our planet and its people."

Provided by University of Oregon

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