JCTC Journal of Chemical Theory and Computation

Introduction: Coarse-Graining in Molecular Modeling and Simulation

This partial special issue of the *Journal of Chemical Theory and Computation* is devoted to the topic of coarse-graining in molecular modeling and simulation. To my knowledge, it is the first time that coarse-graining concepts and techniques from the application areas of biomolecular, materials, and liquid-state systems have been published together in the same place. Not every current researcher working on this particular problem is represented in our partial special issue, but it contains an excellent cross-section of much of the important work being undertaken at the present time.

The impetus for coarse-grained molecular modeling and simulation primarily derives from the need to bridge the atomistic and mesoscopic scales. Typically speaking, there are 2−3 orders-of-magnitude in length and time separating these scales. At the mesoscopic scale, one sees the emergence of critically important phenomena (for example, complex self-assembly in biomolecular or materials systems). Modern molecular simulations, especially as they seek to make increasing contact with experimental results on complex systems, can and will play a crucial role in the exploration of mesoscopic phenomena and, in turn, the behavior of real biomolecular and materials systems. Coarse-graining promises to be a large step forward for the molecular simulation community overall, provided the many challenges faced by the technique can be overcome.

What then are the major challenges of coarse-graining? In many ways the answer to this question depends on the questions one wishes to ask. For example, one common and often legitimate approach is to develop reductionist or "toy" coarse-grained (CG) models that reveal the essential physics of a given class of systems. These models will of course not be quantitative, but they are usually very computationally efficient and informative. Another common approach is to develop CG models using experimental, thermodynamic, and/or average structural properties. A third approach is to bridge atomistic information upward in scale to the CG level in a "multiscale" fashion. All of these approaches have their strengths and weaknesses, and they are certainly complementary to each another.

An absolutely key question for all coarse-graining methodologies is the degree of transferability of the resulting CG models between various systems and from one set of thermodynamic conditions to another. By all rights, a CG model cannot be completely transferable because it is a reduced description of a complex system and some amount of information has been effectively averaged out in one way or another for the given conditions. On the other hand, some aspects of the CG model will certainly be transferable. The key goal is to understand what is and what is not transferable in the CG model and why it is that way. This is not merely a technical issue but instead a very deep problem rooted at the foundations of statistical mechanics. It is a problem that has not yet been solved, despite the many beautiful papers published in this issue and elsewhere. There is also the issue of CG dynamics (i.e., time-dependent behavior), which are not the same as real molecular dynamics. How different are the CG dynamics and why? Can a connection to real dynamics be made? Overall, how much are we to believe from these CG models anyway and how much can they be used to predict and explain unknown phenomena? As I am sure all of the authors in this partial special issue will agree, it is very exciting to be a part of this emerging conceptual challenge and to be able to make a contribution to finding the answer to these critical questions. A satisfactory solution will provide no less than a revolutionary step forward for the field of molecular modeling and simulation.

Gregory A. Voth
Guest Editor
Distinguished Professor of Chemistry
University of Utah

CT600124A

10.1021/ct600124a CCC: $33.50
Published on Web 04/15/2006