THE JOURNAL OF PHYSICAL CHEMISTRY B

 VOLUME 108, NUMBER 21, MAY 27, 2004

Tribute to Hans C. Andersen

This issue of *The Journal of Physical Chemistry B* is dedicated to our friend and co-worker, Hans Andersen. His groundbreaking research has qualitatively and quantitatively extended the range of questions that can be addressed with statistical mechanics by analytic theory and computer simulations. He has created and solved elegant and useful analytical models of complex dynamical systems. He has made important advances in the fundamental theory of computer simulations and its applications to realistic chemical and physical problems. He has formulated and successfully answered questions dealing with the nature of structure and dynamics in liquids, membranes, glasses, and crystals. We are proud to know him and proud to have had the opportunity to work with him.

Hans' two most cited works are "Role of Repulsive Forces in Determining the Structure of Simple Liquids"[1] and "Molecular Dynamics Simulations at Constant Pressure and/or Temperature".[2] These two publications are referred to thousands of times. The first was the cornerstone for each of our careers. It provided both a powerful physical perspective on the role of entropy and repulsive forces in determining the intermolecular structure of liquids and a set of extremely useful calculational techniques. It is extensively discussed in basic texts on statistical

10.1021/jp0402129 CCC: $27.50
Published on Web 05/20/2004

mechanics and liquid-state theory and is generally regarded as the standard equilibrium theory of simple liquids.

The second of these papers is Hans' far-reaching and influential generalization of the molecular dynamics technique to different ensembles. In that work, Hans established a general conceptual framework with which to attack the wide class of problems that arise when dealing with external constraints different from those implied by the standard (microcanonical) molecular dynamics approach. His introduction of auxiliary fields and an effective Lagrangian for their dynamics coupled to that of the system of interest revolutionized the methodology of computer simulations. It is to molecular dynamics what Gibbs ensembles are to Boltzmann's principles of statistical mechanics.

Hans used these ideas to facilitate what remains a most significant simulation study of glass formation. Soon after, Aneesur Rahman and Michele Parrinello recognized the power of this approach and used it in the first successful simulation studies of solid−solid phase transitions. Michael Klein then adopted the concept in extensive studies of molecular solid phase transitions. Moreover, Hans' Lagrangian is a central feature of the Carr−Parinello method for quantum molecular dynamics simulations. Indeed, such is the importance and ubiquity of this idea; it is difficult to imagine the current state of computer simulations without Andersen's seminal contribution.

While carrying out his own landmark studies on phase transitions and dynamics in supercooled liquids, Hans has also given us an assortment of other techniques and ideas for performing computer simulations and modeling complex systems: the often-used velocity Verlet and RATTLE algorithms; a method for calculating equilibrium constants for the formation of physical clusters in the gas phase; a method for calculating the solubility of solutes; a method for calculating diffusion constants of adsorbates on surfaces; a method for calculating equilibrium concentrations of vacancies in solids; a method for employing Hartree−Fock theory in conjunction with molecular dynamics; kinetically constrained dynamics for modeling structural glasses; and analytical treatments of excitation transport in random materials. This incomplete listing demonstrates the remarkable breadth of Hans Andersen's research contributions, which have been rightfully recognized in an assortment of awards, including election to the National Academy of Sciences in 1992.

Less well known but just as remarkable is Hans Andersen's activities as a professor and mentor. Hans is a brilliant lecturer and a meticulous teacher. In nearly every course he teaches, Hans produces a volume of lecture notes worthy of publication as a textbook. Hans is also a generous research advisor, spending endless hours in discussions and doing calculations himself to be sure his students are on the right track. During our collaboration with him in the early 1970s, Hans was a young assistant professor. He was our friend and contemporary and not an advisor in any official capacity. Yet he did provide ample advice both directly and through his actions, showing us how to think about, explain, and do science in the clearest possible way. We place ourselves in that lucky group of students and postdocs who have directly experienced the excitement of working with and learning from Hans Andersen. The impact he had on us was strong and continues to this day. This volume of research articles illustrates the impact Hans Andersen has had on workers throughout the world in almost every area of physical chemistry.

David Chandler
John D. Weeks

References and Notes

(1) Weeks, J. D.; Chandler, D.; Andersen, H. C. *J. Chem. Phys.* **1971**, *54*, 5237.
(2) Andersen, H. C. *J. Chem. Phys.* **1980**, *72*, 2384.