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Book Review: *Classical and Quantum Dynamics in Condensed Phase Simulations*

Classical and Quantum Dynamics in Condensed Phase Simulations. B. J. Berne, G. Ciccotti, and D. F. Coker, eds., World Scientific, New Jersey, 1998.

This volume is the proceedings of an international school of physics on computer simulation of rare events and the dynamics of classical and quantum condensed-phase systems held in July 1997. The book contains about thirty lectures delivered by leading specialists in the field, and is intended as a survey of recent advances in the art of computer simulation of condensed phase systems and of recent developments in the quantum dynamical treatment of such systems. The kinds of simulation methods discussed in the volume are (a) biased phase space sampling schemes, (b) multiple time-scale methods, and (c) static equilibrium methods for treating quantum systems. The contributions related to dynamics describe (d) methods for mixing quantum and (e) classical dynamics in condensed phase simulations and methods of treating all degrees of freedom quantum mechanically.

Each of the articles in this volume is written in a pedagogical manner with a long introduction to the subject together with an annotated bibliography. This makes the book valuable to beginners as well as those who wish to explore particular area in greater depth. I briefly describe the content of the book, which is divided into three parts:

I. An introduction to rare events, from barriers to electrons. This is meant to motivate the analysis that follows in the remainder of the book.

II. The art of simulation, which is devoted to simulation methods (a), (b) and (c) and related applications in various areas of condensed matter.

III. Quantum dynamics, which deals with methods (d) and (e) and related applications.

In Part I, David Chandler presents, in a series of three chapters, a broad overview of rare events in many body systems. He describes basic concepts associated with rare events and outlines different approaches for treating activated processes in both classical (e.g., isomerization reactions) and quantum (e.g., electron transfer reactions) systems and methods for finding transition pathways in phase space.

The second part of the book gives a detailed description of a number of simulation techniques, together with some representative physical applications. There are nine first chapters that deal with classical simulations methods. These include two lectures on Monte Carlo simulations by Valleau and Frenkel describing biased phase space sampling methods and two others, by Berne, and Ciccotti

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and Ferrario, describe methods for dealing with multiple time-scale problems and algorithms for dealing with constraints in molecular dynamics. Applications to problems in chemical physics are described for computing diffusive barrier crossing rate constraints (Ruiz-Montero). A number of more specialized chapters deal with applications to supercritical slowing down in Monte Carlo methods (Janke), molecular diffusion in glassy polymers (Theodorov), adsorption and diffusion of molecules in zeolites (Smit) and problems in sampling the phase space in the study of lattice models (Succi *et al.*). The following five chapters deal with the description and use of methods of incorporating static equilibrium quantum effects into molecular dynamics simulations for studying the kinetics of chemical reactions in solutions (Sprik). Other topics include a description of a computational approach based on path integral methods which is then applied to problems in quantum statistical mechanics (Tuckerman and Hughes, Marx, Jónsson *et al.*). More specialized applications are also described in this section. The last three chapters describe applications of the methods described earlier to the study of biological systems. This includes methods for studying the dynamics of peptides (Elber *et al.*), as well as applications to activated dynamics in ion channels (Roux and Crouzy, and Klein *et al.*).

The third part of the book describes methods useful in problems in quantum dynamics and in the physics of condensed phases. Techniques for mixing quantum and classical dynamics in molecular dynamics simulations are described in the four first chapters of this section (Tully, Rossky, Coker *et al*., and Kapral *et al.*). This is followed by the description of a semiclassical approach, which treats both electronic and nuclear degrees of freedom on the same footing by Miller. The following three chapters describe methods for treating all dynamical degrees of freedom quantum mechanically. A description of these are applied to tunneling and barrier crossing problems (Makri and Voth). This section also contains a discussion of an approach to simulations based on the Wigner representation as well as more specialized applications (Filinov *et al.*). Applications of these methods to electron transport (Laria *et al.*), Valance-bond models for proton transfer dynamic (Borgis and Vuilleumier), hydrogen transport in metals (Doll *et al.*), solvent effect in electronic transition (Procacci and Souaille) and surface diffusion and spectroscopy (Metiu) are given in the last six chapters.

In summary, this volume is a useful introduction to currently popular, and widely-used techniques in chemical and statistical physics. The authors are well-respected researchers in the field and the level is appropriate to graduate students and researchers.

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