Advanced Computer Simulation Approaches for Soft Matter Sciences III

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Preface

"Soft matter" is nowadays used to describe an increasingly important class of materials that encompasses polymers, liquid crystals, molecular assemblies building hierarchical structures, organic-inorganic hybrids, and the whole area of colloidal science. Common to all is that fluctuations, and thus the thermal energy k_BT and entropy, play an important role. "Soft" then means that these materials are in a state of matter that is neither a simple liquid nor a hard solid of the type studied in hard condensed matter, hence sometimes many types of soft matter are also named "complex fluids."

Soft matter, either of synthetic or biological origin, has been a subject of physical and chemical research since the early finding of Staudinger that long chain molecules exist. From then on, synthetic chemistry as well as physical characterization underwent an enormous development. One of the outcomes is the abundant presence of polymeric materials in our everyday life. Nowadays, methods developed for synthetic polymers are being more and more applied to biological soft matter. The link between modern biophysics and soft matter physics is quite close in many respects. This also means that the focus of research has moved from simple homopolymers to more complex structures, such as branched objects, heteropolymers (random copolymers, proteins), polyelectrolytes, amphiphiles and so on. While basic questions concerning morphology, dynamics, and rheology are still a matter of intense research, additional, more advanced topics are also being tackled, for example the link between structure and function or non-equilibrium aspects.

For many years there have been attempts to understand these systems thoroughly using theoretical concepts. Beginning with the early work of Flory, simplified models were studied, which were able to explain certain generic/universal aspects but failed to provide a solid theoretical basis for this universal behavior. It was then up to the seminal works of de Gennes and Edwards to provide a link between the statistical mechanics of phase transitions (critical phenomena) and polymer chain conformations. This link to the modern concepts of theoretical physics provided huge momentum for the field, which shaped many theoretical schools and formed the basis for modern soft matter physics. Despite all these developments, soft matter theory is still an active and growing research field. Due to the high degree

of complexity of the problems it is not surprising that analytical theory can only treat highly idealized and simplified models. Consequently, with the availability of computers, problems in polymer science were among the first to be tackled by simulations. Even now, the problem of an isolated self-avoiding walk cannot be solved exactly in three dimensions. As early as 1954, Hammersley and Morton, and Rosenbluth and Rosenbluth tried to overcome the related attrition problem in growing self-avoiding walks by introducing "inversely restricted sampling." In addition, basic multichain features (such as the noncrossability of chains) are hard to deal with analytically and can only be included properly by a simulation approach. Thus, with the rising availability of computing power, simulation methods began to play an increasingly important role in soft matter research. Computing power is, however, only one aspect. Even more important has been the development of advanced numerical methods and highly optimized programs. Very different areas, ranging from quantum chemistry studying molecules on the sub-Ångstrøm level all the way to macroscopic fluid dynamics, have to come together and offer a unique set of research opportunities. Over the years, the role of computer simulations has gone beyond the traditional aspect of checking approximative solutions of analytical models and bridging the gap between experiments and theory. They are now an independent, in some cases even predictive, tool in materials research, for example for complex molecular assemblies or specific rheological problems.

It is the purpose of this small series of volumes in *Advances in Polymer Sciences* to provide an overview of the latest developments in the field. For this, internationally renowned experts review recent work in the general area of soft matter simulations. The third volume contains three contributions. The first two chapters review several coarse-grained methods to include the effects of hydrodynamics in mesoscopic particle simulations that use an implicit solvent, whereas the last chapter deals with advanced sampling methods to study rare events.

The first two contributions deal with methods or systems where hydrodynamic interactions play a dominant role. Studying coarse-grained mesoscopic systems, hydrodynamic interactions are unimportant for static properties in equilibrium. However, the inclusion of hydrodynamic effects becomes indispensable for all problems of dynamics of solutions in bulk or under confinement, especially when it comes to flow-induced structure formation. This would automatically be achieved by a standard molecular dynamics simulation, which takes full account of the solvent molecules. This, however, is only feasible in some very exceptional cases, even for the upcoming computer generation, and is still applicable to only very small systems. Because of that, solvent-free methods play a very important role and have been improved significantly over the last few years. In the first contribution G. Gompper, T. Ihle, D.M. Kroll, and R.G. Winkler focus on an algorithm that was initially proposed by Malevanets and Kapral in 1999, and is now called multiparticle collision dynamics (MPC) or stochastic rotation dynamics (SRD). The method consists of alternating streaming and collision steps in an ensemble of point particles that locally conserve mass, momentum, and energy. The second contribution by B. Dünweg and A.J.C. Ladd reviews in depth the standard D3Q19 lattice-Boltzmann model and extensions thereof. Here the Boltzmann equation is solved on a grid, where the fluid

velocities are stored, employing mass and momentum conservation. The authors discuss in depth the "fluctuating" lattice-Boltzmann algorithm, followed by a detailed discussion of complementary methods for the coupling of solvent and solute. Both presented methods consistently couple full hydrodynamic interactions and thermal fluctuations and, since they deal with complementary methods, give an excellent comprehensive overview over the field. Both contributions also conclude with examples in which the methods are applied to soft matter systems such as colloidal suspensions and polymer solutions.

In the third contribution, C. Dellago and P. Bolhuis review several recently developed methods for studying rare-event transitions, which are important in understanding molecular processes such as nucleation events, chemical reactions transport phenomena in liquids and solids, or slow processes such as protein folding. Such transition events are rare because the stable basins are separated from each other by high free-energy barriers of either potential energy, entropic, or combined origin. Several methods have been proposed to speed up the sampling of these transitions, like metadynamics, the finite temperature string method, forward flux sampling, and others. The authors cover in depth the transition path sampling methodology to which they have both added important contributions.

We are confident that this collection of reviews will be a very useful guide to interested scientists and advanced students, and it also provides detailed background information for experienced researchers in the field.

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