Essay for the Special issue in Journal Macromolecular Theory and Simulations: Novel Simulation Approaches for Polymeric and Soft Matter Systems

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I. EDITORIAL

The last two decades have brought us a tremendous improvement in numerical methods, and the field of computer simulations has been established as the third pillar used to increase our knowledge of natural science. As such it is of equal importance as experiments and theory in sharpening our understanding of the complex real world phenomena. It is undeniable that the increase in computer power experienced in the last two decades has enormously contributed to boost simulations. One one hand, as the computer power increases so does the ambition of the researchers to describe even more complex systems which involve large differences in the spatial and time scales of their components. On the other hand, it is also clear that brute force alone will not pave the way to solving those issues. In the last decade the introduction of smart algorithms have been more profitable to science than the simple improvements in turn of pure CPU power. Therefore there is still an urgent and constant need for more efficient and clever algorithms, as well as for improved theoretical frameworks. Such achievements are of great interest for the scientific community as a whole, but here in this special issue we would like to highlight achievements and novel simulation approaches to certain areas of polymeric and soft matter systems.

Soft matter, also sometimes denoted as complex fluids, is inherently more difficult to deal with than simple, molecular fluids. Soft matter systems can consist of colloidal, polymeric systems, but also biological systems like blood, DNA, tissues, biological cells, or even bacterial colonies. Their structure shows more complex behavior, and the involved time and length scales are orders of magnitude larger that can even reach glassy behaviour. These systems therefore show a clear urge for efficient sampling techniques, or even the necessity to reduce the degrees of freedom by some coarse-graining strategy in order to reach the necessary length and time scales fort he problem under consideration. However, often it is not obvious to decide which degrees of freedom can be safely averaged over, and which ones one should keep. The choice of the correct coarse-graining strategy represents one of the most formidable challenges in this field due to the high dimensionality of the phase spaces one tries to reduce to a simpler form. Some books are available that cover simulation approaches in some depths [1–8] , however, as usual in active fields, the recent advances are quite scattered among different journals in different fields that makes it even harder for the interested researcher to be aware of the latest developments.

We felt it timely to invite some of the most prominent researchers in the field of soft matter to present their recent achievements within a special issue of the Journal of Macromolecular Theory and Simulations. However, the field is so vast, that it is impossible to cover it in depth. Thus we have been forced to focus on just a few of the many interesting developments in simulation approaches that are currently in the spot of soft matter researchers.

The first article by Ramakrishnan et al. [9] is a review that focuses on the current Monte Carlo techniques available to describe fluid membranes via the dynamically triangulated surface approach. In a subsequent feature article, Engin et al. [10] discuss the different approaches one can follow to coarse-grain peptides while highlighting the importance of *transferability* of the coarse-grained force field. In the following communication Balboa and Delgado-Buscalioni [11] analyze the tumbling dynamics of polymers subjected to shear flow, and discuss the different characteristic times that show up. The next paper by Rühle and Junghans [12] presents three hybrid schemes for systematic coarse-graining using as a test case a system of liquid Hexane molecules, and describe their VOTCA package that has implementations of these methods. Ellis et al. [13] describe another approach based on the use of integral equation theories to tackle the process of systematic coarse-graining of complex fluids. They use their generalized Yvon-Born-Green theory and apply it to liquid toluene, also investigating the issue of transferability of the coarse-grained force field. Next, Volkov et al. [14] study the very interesting case of how polyelectrolytes modify the interaction between membranes using the Wang-Landau algorithm. As for the case of hydrodynamic interactions, long-range Coulomb interactions are always a factor that complicates the modelling scenario. Next, Hsu et al. [15] examine carefully the scaling behaviour of bottle-brush polymers demonstrating the consequences of applying scaling arguments blindly without examining before the basic

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assumptions on which such scaling relations rely. They also discuss some important implications for interpreting experimental results properly. Next Kauzlarić et al. [16] provide us with insight about the basic formalism of the *friction matrix*. They discuss and compare critically three approaches of calculating the friction matrix. Afterwards, Praetorius and Voigt [17] present an approach aimed to capture advection phenomena of small particles in a solvent flow around various obstacles using a phase field crystal coupled to a flow field.

Within the realm of modeling complex flows, blood is perhaps one of the most daring quests. In an effort to improve our ability to describe blood systems, Melchiona [18] and Janoschek et al. [19] present us two different models for blood. In the first paper, Melchiona presents a model intended to be robust and suitable for being applied to large-scale arteries for which current models are not very well suited. In the following paper, Janoschek et al. also take a quite similar approach and study the applicability of a previously developed method to the case of confined blood flows. The final paper of this issue deals with bacterial colonies. Tao and Slater [20] refine a previously introduced cellular model intended to mimic biofilm colony growth by including the modeling of the extracellular polymeric substance with the goal of describing those complex collectivities which are doubtless one of the most challenging topics covered in this special issue.

We hope that the reader will find the articles in this issue not only interesting but also instructive. They might even serve as a source of inspiration to tackle new steps in the coarse-graining quest for a thorough understanding of soft matter systems. We feel that this field leaves still plenty of room for those willing to deal with nature in its full complexity!

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[10] O. Engin, A. Villa, C. Peter, M. Sayar, *A Challenge for Peptide Coarse Graining: Transferability of Fragment-Based Models*

[11] F. Balboa Usabiaga, R. Delgado-Buscalioni, *Characteristic times of a flexible polymer tumbling under shear flow*

[12] Victor Rühle, C. Junghans, *Hybrid approaches to coarse-graining using the VOTCA package: liquid hexane*

[13] C. R. Ellis, J. F. Rudzinski, W. G. Noid, *Applications of the generalized Yvon-Born-Green theory for coarse-graining molecular liquids*

[14] N. A. Volkov, P.N. Vorontsov-Velyaminov, A.P. Lyubartsev, *Two-dimensional Wang-Landau algorithm for osmotic pressure calculations in a polyelectrolyte-membrane system*

[15] H.-P. Hsu, W. Paul, K. Binder: *Understanding the multiple length scales describing the structure of bottle-brush polymers by Monte Carlo simulation methods*

[16] D. Kauzlaric,P. Espanol, A. Greiner S. Succi: *Three routes to the formulation of the formulation of the friction matrix in the coarse-grained description of atomic systems*

[17] S. Melchiona: *A model for red blood cells in simulations of large-scale blood flows*

[18] F. Janoschek, F. Toschi, J. Harting: *Simulations of Blood Flow in Plain Cylindrical and Constricted Vessels with Single Cell Resolution*

[19] S. Praetorius, A. Voigt: *A phase field crystal approach for particles in a flowing solvent*

[20] Y-G. Tao, G.W. Slater, *A simulation model of biofilms with autonomous cells: II. Explicit representation of the extracellular polymeric substance*