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Special Issue on "Monte Carlo Simulation of Soft Matter Systems" EDITORIAL

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Editorial on the Research Topic

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Since 1953 that it was introduced for the first time by Metropolis et al., the Monte Carlo method has developed to a powerful tool for addressing a variety of problems in a wide range of scientific, engineering and technological fields in Soft Matter. It has been used to equilibrate the dense phases of polymer systems through the design and implementation of ingenious moves and obtain reliable predictions of their thermodynamic, structural and conformational properties, to study self-assembly and chain self-organization, to predict complex phase diagrams and free energies, to test statistico-mechanical theories, and to model a variety of complex physico-chemical processes using the so called kinetic Monte Carlo method.

Recognizing the importance of the method over the years, in this Special Volume of Frontiers in Physics we invited contributions highlighting recent developments and new applications of the method in rapidly developing or newly emerging fields. Our Special Volume comprises in total seven (7) Articles:

In the first article, Sachin Shanbhag discusses temporal coarse-graining for blends of linear polymer chains based on an adaptive time step algorithm where the time step is determined by the shortest chains, but whose value increases as the simulation proceeds. The author compares the efficiency of the new algorithm against one using a constant-time step in test simulations of binary, ternary, and polydisperse blends, reporting speedups ranging from 50 to 1,500% for widely separated molecular weights of the blend components. The author also discusses future extensions of the idea to other polymer mixtures that are characterized by a wide disparity in their relaxation times such as star-linear and star-star blends, as well as mixtures containing H-polymers and combs.

In the second article, Piotr Polanowski and Andrzej Sikorski review recent advances in the study of cooperative motion in crowded Soft Matter systems, with emphasis on efficient dynamic Monte Carlo simulations of dense macromolecular systems where motion is strongly correlated, thereby leading to cooperative phenomena. They discuss, in particular, how cooperativity can be described in terms of the so called dynamic lattice liquid (DLL) model.

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In the third article, Nikolaos Cheimarios and collaborators review modern applications of Monte Carlo and kinetic Monte Carlo methods in deposition processes (PVD, CVD, ALD, electrodeposition), with emphasis on graphene growth, multi-scale modeling in CVD, deposition inside micro-structures, and implementation of surface reactions in kMC models. The authors further emphasize the opportunities offered by deep learning techniques to provide detailed input regarding realistic rate catalogs, thus minimizing the workload on the side of the user.

In the fourth article, Tobias Alexander Kampmann and collaborators discuss recent applications of the rejection-free event-chain Monte-Carlo algorithm to systems ranging from hard spheres to dense polymer melts, actin filaments and two-dimensional needles and colloidal disks. The latter can be thought of as a model system exhibiting anisotropic effective interactions. The authors also discuss possible future extensions of the method to elastic membranes and confined polymer networks, as well as to the investigation of the crumpling transition in biological systems.

In the fifth article, Montserrat Penaloza-Amion and collaborators discuss recent developments of SIMONA, a large-scale Monte Carlo algorithm for the efficient conformational sampling of different types of (macro) molecules. The authors discuss protocols for the Monte Carlo simulation of protein folding, polymer self-assembly, membrane peptides, and thin film formation by the deposition of molecules on a substrate. They also highlight on-going efforts for incorporating new features and capabilities in SIMONA to facilitate application to polymers.

In the sixth article, Vlasis Mavrantzas reviews recent progress in the design and implementation of powerful Monte Carlo moves for the efficient simulation of complex chain-like systems such as polymer nanocomposites, soft nanostructured materials, confined polymers, polymer rings and knots, hydrogels and networks, crystalline polymers, and many others. He highlights, in particular, extensions of the method to non-equilibrium systems (e.g., polymers under steady shear flow) guided by non-equilibrium thermodynamics, as well as hybrid simulation schemes where Monte Carlo moves are used in conjunction with self-consistent mean field theories.

In the seventh article, Werner Krauth reviews mathematical and algorithmic foundations of non-reversible Markov chains in the context of the event-chain Monte Carlo method. He discusses first some fundamental issues (transition matrices, balance equations, factorization, lifting, and thinning), and then he moves on to presenting results from application of the method to single particles on a path graph, to many particles in one dimension, and finally to statistico-mechanical models in more dimensions including several exactly solvable cases.

AUTHOR CONTRIBUTIONS

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