CPP 24: French-German Session: Simulation Methods and Modeling of Soft Matter IV

Time: Tuesday 11:30–12:45 Location: ZEU/0255

CPP 24.1 Tue 11:30 ZEU/0255

Systematic coarse-graining with density dependent potential: Application to small organic molecules, multicomponent mixtures and polymers — •Sayan Dutta[1,2,3], Maria C. Lesniewski[4], W. G. Noid[4], Denis Andrienko[5], and Arash Nikoubashman[2,3] — [1]Leibniz-Institut für Polymerforschung — [2]Technische Universität Dresden — [3]Johannes Gutenberg-Universität Mainz — [4]Pennsylvania State University, University Park, PA, USA — [5]Max-Planck Institut für Polymerforschung Mainz

Conventional coarse-graining (CG) approaches approximate the underlying many body interactions through effective pair potentials. Although this strategy works well for reproducing structural and thermodynamic properties in bulk systems, it often fails in heterogeneous systems, such as droplets or films, due to the inherently strong density fluctuations in those systems. To address this issue, we incorporated local-density-dependent potentials (LDPs) that treat these many-body contributions explicitly within a mean-field formalism. We develop a CG force-field framework that integrates LDPs, enabling accurate simulation of conjugated organic molecules, organic liquid mixtures, and polymeric systems. This approach provides a more accurate description of thermodynamic and interfacial properties of these systems. Further, it facilitates the establishment of structure-function description that helps in rational designing of functional materials.

CPP 24.2 Tue 11:45 ZEU/0255

A data-driven decoupled multiscale scheme for anisotropic finite strain magneto-elasticity — •Heinrich T. Roth, Philipp Gebhart, Karl A. Kalina, Thomas Wallmersperger, and Markus Kästner — TU Dresden, Dresden, Germany

Structured magnetorheological elastomers (MREs) are composite materials exhibiting magneto-mechanical coupling effects, such as the magnetostrictive and magnetorheological effect. They consist of magnetizable particles arranged in chain-like structures within a soft elastomer matrix. As explicitly resolving their microstructure in real-world samples is infeasible, a multiscale modeling approach is required.

In this work, we present a framework for the macroscale modeling of structured MREs using physics-augmented neural networks (PANNs) [1,2]. The framework begins with data generation, where a representative volume element (RVE) undergoes macroscopic magneto-mechanical loadings in Finite Element (FE) simulations. The resulting homogenized microscale variables form a macroscale dataset for the training and testing of the PANN macromodel, which satisfies key physical principles [1]. Finally, the trained PANN model is used in a decoupled multiscale scheme as the material model for a macroscale FE simulation to examine the magnetostriction of a spherical sample.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] H.T. Roth et al., arXiv:2510.24197, 2025. [2] K.A. Kalina et al., CMAME 421, 2024.

CPP 24.3 Tue 12:00 ZEU/0255

In Silico Self-Assembly of Magnetic Colloidal Polymers with Magnetization Dynamics — •Deniz Mostarac[1], Sofia Kantorovich[2], and Philip J. Camp[1] — [1]School of Chemistry, University of Edingburgh, EH9 3FJ Edinburgh , United Kingdom — [2]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria

Polymer-like mesostructures formed by crosslinked magnetic nanoparticles (MNPs) have created a new class of stimuli-responsive materials magnetic colloidal polymers (MCPs) that show enhanced optical, thermal, mechanical, rheological, and adsorption properties compared to conventional magnetic fluids. The interplay between magnetic interactions and solvophilic/solvophobic forces produces complex, field-tunable self-assembly. In our previous work, we investigated isolated MCPs and showed that solvophobicity drives compact, magnetically frustrated conformations, with structural features determined by crosslink type and MNP properties. These distinctions strongly affect MCP dynamics under shear and external fields. In this contribution we study the self-assembly of solvophobic MCPs while explicitly modeling MNP magnetodynamics with finite anisotropy. Our simulations capture internal magnetization dynamics over long times and at system sizes sufficient for bulk behavior. We show that coupling between Brownian and Néel relaxation, together with nonlinear magnetization, yields distinct structural, magnetic, and dynamical features in MCP suspensions governed by solvophobicity and intrinsic NP magnetism.

CPP 24.4 Tue 12:15 ZEU/0255

Pulling knotted polymer rings and concatenated knotted polymer rings in order to understand the effects of entanglement on the mechanical properties of polymers materials — •Franco Ferrari[1], Neda Abbasi Taklimi[1], Marcin Piatek[1], and Luca Tubiana[2] — [1]CASA* and Institute of Physics, University of Szczecin, Szczecin, Poland — [2]Physics Department, University of Trento, Via Sommarive 14, Trento I-38123, Italy

The topological structure of polymers is expected to produce relevant effects on the mechanical properties of polymer systems. However, to assess the contribution of topology by experiment is difficult, mainly due to technical obstacles in controlling the entanglement during the synthesis process, in particular the formation of knots and concatenations. In this contribution presented are the results of numerical simulations focusing on the mechanical properties of topologically entangled polymer systems. First, the case of single knotted polymers pulled by an external force are discussed. Next, the stress-strain curves of a few concatenated knots with forces applied at different locations are shown. To check the validity of our simulations based on the Wang-Landau algorythm, two different methods are employed and their consistency is verified. The final goal of this research is to understand the mechanical properties of more complex polymer materials characterized by an uniform distribution of knots or concatenated knots of a given topological type.

CPP 24.5 Tue 12:30 ZEU/0255

Prediction of Ultra-Long Time-Scale Dynamics from Picoseconds to Seconds: Integral of First-Passage Times — •Qiyun Tang — School of Physics, Southeast University, Nanjing, China

The dynamics of non-equilibrium nanostructure formation span over 13 orders of magnitude in time, from molecular vibrations at picoseconds to macroscopic processes at seconds or longer. Predicting such ultra-long time-scale dynamics poses significant challenges for conventional molecular simulation methods. We recently proposed a new approach-Integral of first-passage times (IFS)-to predict the evolution of non-equilibrium nanostructures, and the resulting structural distributions align well with experimental observations [1]. Furthermore, we have verified that the dynamics predicted by IFS are consistent with direct simulations in cases of low free energy barriers, while under high free energy barriers, the ultra-long time-scale dynamics predicted by IFS agree with experimental measurements [2]. Utilizing this method, we have also systematically investigated the relationship between polymer adsorption dynamics and surface curvature [3,4]. The IFS method bridges microscopic picosecond-scale dynamics with macroscopic growth kinetics of nanostructures, offering an effective approach for designing and controlling non-equilibrium nanostructures.

[1]Q.Tang, C. Rossner, P. Vana, M. Müller, Biomacromolecules 2020, 21: 5008. [2]Q. Tang, Y. Huang, M. Müller, Phys. Rev. E 2024, 110: 044502. [3]J. Zhang, Q. Tang, Phys. Rev. Mater. 2024, 8: 105602. [4]Y. Huang, C. Tang, Q. Tang,*Nanoscale 2024, 16: 19806.