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Multi-scale simulations of soft matter: from block copolymers to biomolecular condensates

Polymers are ubiquitous in both synthetic and biological materials and underlie technologies as diverse as surfactants, adhesives, proteins and DNA. One of the defining features of all polymeric materials is that they are characterized by a wide range of length scales, often involving phenomena that span nanometers to microns. This hierarchy of length scales presents significant challenges for polymeric simulations. Existing models that can resolve phenomena at monomeric length scales (e.g. Atomistic simulations) are far too expensive to access mesoscopic processes, whereas coarse-grained models that can access these large length scales must necessarily omit chemical details, which often enter calculations through phenomenological parameters. As such, there is a significant need for new computational techniques that can accurately and efficiently predict how chemical changes at the smallest length scales will propagate up to the largest length scales in a material.

In this talk, I describe recent efforts by my group to develop multi-scale simulations of polymeric materials that can link monomeric to mesoscopic length scales. In the first part of the talk, I describe a new "multi-representation" simulation method where particle-based and field-theoretic simulations are linked together into a unified framework. This approach can accelerate polymer simulations by several orders of magnitude and can rapidly equilibrate mesoscopic length scales while preserving monomer-scale details and dynamics. Notably, this multi-representation approach leverages the formal equivalence between particle and field-based models and involves no approximation. The utility of this approach is illustrated by examining the self-assembly of complex sphere phases in block copolymer melts. In the second part of the talk, I demonstrate how these multi-representation simulations can be extended to explain the phase separation of biomolecular condensates. Our approach can recapitulate recent experimental data on prion-like domains and can resolve how subtle modifications to the amino acid sequence can modulate their phase behavior. Taken together, this work demonstrates that multi-resolution simulations that combine particle and field-theoretic simulations can unlock new insights into the multi-scale physics that characterize synthetic and biological polymers.

Short Bio

Joshua Lequieu is an Assistant Professor of Chemical and Biological Engineering at Drexel University. He received a B.S. in Chemical Engineering from Cornell University, and a Ph.D. in Molecular Engineering from the University of Chicago under the guidance of Juan J. de Pablo. Following a postdoc in the Materials Research Lab at the University of California, Santa Barbara with Glenn H. Fredrickson, he joined Drexel University in 2020. He is the recipient of the 2019 Edward J. Kramer Prize in Materials, the 2021 Charles E. Kaufman Foundation New Investigator Award, and the 2021 Outstanding Teaching Award from Drexel University.