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Beyond anisotropy factors: physics-informed and data-driven analyses for scattering anisotropy in field-driven soft matter

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Abstract. *In situ* scattering measurements in flow and other fields have become a powerful experimental tool to characterize rheology and field-driven organization of complex fluids. Although anisotropic scattering in these experiments encodes in principle the molecular-scale deformation and orientational ordering of the material, analysis of anisotropic scattering has remained primitive, limited primarily to low-dimensional scalar measures that are often empirically correlated with material properties. Relating these measures of scattering to real-space structures and properties therefore requires *post hoc* physical models and assumptions whose applicability are material-specific, and may not prove accurate for a diverse range of materials and flows. This presentation summarizes our recent efforts to develop new models for diffuse anisotropic scattering; this includes both physics-informed approaches that incorporate known material symmetries and behavior, as well as data-driven approaches that leverage the ability to gather large data sets that represent many possible microstates of the same material to construct a microstructural model of the material. I will illustrate the utility of these methods for two relatively simple classes of complex fluids. The first involves suspensions of rodlike nanoparticles, where we hope to understand the combined effects of flow and particle-particle interactions on the development of orientational order and non-Newtonian rheology. The second involves solutions of flexible polymers, where we hope to understand how molecular deformations – particularly non-Gaussian stretching of both linear and nonlinear polymers – determines their rheology at extreme deformation rates. I will conclude with an outlook for how data-driven and physics-informed approaches can be combined with a new measurement and modeling framework, scattering-informed microstructure evolution during Lagrangian evolution (SIMPLE), to "learn" microconstitutive models of flowing complex fluids from large experimental data sets.

Bio. Matt Helgeson is currently the John W. Myers Founders Professor and Vice Chair for Graduate Studies in the Department of Chemical Engineering at UC Santa Barbara. He received his B.S. in Chemical Engineering at Carnegie Mellon University in 2004, and his Ph.D. in Chemical Engineering at the University of Delaware in 2009. He performed postdoctoral research at MIT before joining the faculty at UCSB. Helgeson's research focuses on design of complex fluids for materials processing, and the development of *in situ* measurement methods to support these efforts. His research has been recognized with a number of awards, including Early Career Awards from both the National Science Foundation (2013) and Department of Energy (2015), the Neutron Scattering Society of America Science Prize (2020), as well as the Victor K. LaMer Award (2011), Unilever Award (2016) and Outstanding Achievement in Nanoscience Award (2024) from the American Chemical Society.

Wednesday, August 20, 2025
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