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Visual-Analytics Tools for Analyzing Polymer Conformational Dynamics SIDHARTH THAKUR, Renaissance Computing Institute, NC State Univ, SYAMAL TALLURY, MELISSA PASQUINELLI, Fiber & Polymer Sci, NC State Univ — The goal of this work is to supplement existing methods for analyzing spatial-temporal dynamics of polymer conformations derived from molecular dynamics simulations by adapting standard visual-analytics tools. We intend to use these tools to quantify conformational dynamics and chemical characteristics at interfacial domains, and correlate this information to the macroscopic properties of a material. Our approach employs numerical measures of similarities and provides matrix- and graph-based representations of the similarity relationships for the polymer structures. We will discuss some numerical measures that encapsulate geometric and spatial attributes of polymer molecular configurations. These methods supply information on global and local relationships between polymer conformations, which can be used to inspect important characteristics of stable and persistent polymer conformations in specific environments. Initially, we have applied these tools to investigate the interface in polymer nanocomposites between a polymer matrix and carbon nanotube reinforcements and to correlate this information to the macroscopic properties of the material. The results indicate that our visual-analytic approach can be used to compare spatial dynamics of rigid and non-rigid polymers and properties of families of related polymers.

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