Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Visualization of Topology through Simulation ANDREW MULDERIG, GREGORY BEAUCAGE, KARSTEN VOGTT, HANQIU JIANG, Univ of Cincinnati — Complex structures can be decomposed into their minimal topological description coupled with complications of tortuosity. We have found that a stick figure representation can account for the topological content of any structure and coupling with scaling measures of tortuosity we can reconstruct an object. This deconstruction is native to static small-angle scattering measurements where we can obtain quantitative measures of the tortuous structure and the minimal topological structure. For example, a crumpled sheet of paper is composed of a minimal sheet structure and parameters reflecting the extent of crumpling. This quantification yields information that can be used to calculate the hydrodynamic radius, radius of gyration, structural conductive pathway, modulus, and other properties of complex structures. The approach is general and has been applied to a wide range of nanostructures from crumpled graphene to branched polymers and unfolded proteins and RNA. In this poster we will demonstrate how simple structural simulations can be used to reconstruct from these parameters a 3d representation of the complex structure through a heuristic approach. Several examples will be given from nano-fractal aggregates.

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Date submitted: 11 Nov 2016 Electronic form version 1.4