Simulating Fiber Aggregation in Shear Flow with Dissipative Particle Dynamics JUSTIN STIMATZE, DAVID EGOLF, JEFFREY URBACH, Department of Physics, Georgetown University — We have developed a mesoscale simulation of fiber aggregation using LAMMPS and its implementation of dissipative particle dynamics. Fiber-fiber interactions are approximated by combinations of standard pairwise forces, allowing exploration of multiple interaction-influenced fiber behaviors such as aggregation and bundling. We determine viscosity, stresses, fluid velocity field, and fiber forces while simulating the evolution of a model fiber system in shear flow. Preliminary simulations supported by AFOSR HPC resources have demonstrated several aggregate types dependent on system parameters. Explorations of fiber interaction mechanisms and parameters may enable greater insight into processes such as nanocomposite material manufacturing and silk fibrillation.

Justin Stimatze
Department of Physics, Georgetown University

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