Polymerization of fibrinogen into fibrin fibers and ultimately a stable fibrin network is one of the most widely studied research areas in the field of thrombosis. In the past, researchers have performed extensive studies to unveil the mechanisms of fibrin polymerization. However, mechanisms of fiber branching and cross-linking of the long fiber strands is still an elusive phenomenon, and is quite difficult to simulate. Computational modeling of fibrin polymerization and the underlying mechanisms are not well developed and only a few studies have been conducted in this area. In this context, we propose a new type of dissipative particle dynamics (DPD) to simulate the polymerization of fibrinogen into a fibrin network. First, a coarse grain (CG) model of the fibrinogen molecule was developed using an Iterative Boltzmann Inversion (IBI) method in conjunction with artificial neural networks (ANNs). The CG model was coupled with DPD water models and the force fields were characterized to match the self-diffusion coefficient from experiments. Using distance-based rules through attractive potentials, we simulated the biochemical reaction that occurs when a fibrin network is formed. Our results correlate with SEM experimental results of fibrin clots, such as bilateral, trilateral branching, thick fibers, and continuous strand formation. This methodology encompasses a new class of DPD simulations that is applicable to other polymerization models and large biomolecular simulations. The impact of the present work is multidisciplinary and the final goal is to understand the evolving mechanics underlying venous thrombosis to develop better treatments and thrombolytic strategies.

Figure 1: Using our Reactive DPD (R-DPD) method, we simulated fibrin clot polymerization and network formation.

* Corresponding author:
Dr. Rodney D. Averett
597 D W Brooks Dr., Athens, GA 30602
School of Chemical, Materials and Biomedical Engineering
University of Georgia.
Phone: (706)-542-0863
Email: raverett@uga.edu

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