Venkataramani, V.; **Sureshkumar, R.**; **Khomami, B.**

A computationally efficient approach for Hi fidelity fine graining from bead-spring models to bead-rod models. (English) Zbl 1391.76802

J. Non-Newton. Fluid Mech. 149, No. 1-3, 20-27 (2008).

Summary: The Random Walk Spring (RWS) [P.T. Underhill, P.S. Doyle, On the coarse-graining of polymers into bead-spring chains, J. Non-Newtonian Fluid Mech. 122 (2004) 3-31; P.T. Underhill, P.S. Doyle, Development of bead-spring models using the constant extension ensemble, J. Rheol. 49 (5) (2005) 963-987] model is used to examine the influence of successive fine graining on the macroscopic stress predictions of bead-spring models to ascertain if quantitative agreement with bead-rod models can be achieved at much reduced CPU times. Specifically, the predictions for macroscopic stresses in homogeneous flows, namely, steady and transient shear and uniaxial elongation at several degrees of fine graining have been presented. In turn, the appropriate level of fine graining for modeling bead-rod predictions over a broad range of flow strengths is proposed. Finally, CPU time analysis of the various fine grained bead-spring models is reported to illustrate the significant advantages of using these models in comparison to bead-rod models.

MSC:

76T25 Granular flows

Keywords:

Brownian dynamics; coarse-graining; bead-spring model; bead-rod model; successive fine graining

Full Text: DOI

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