Multiscale polymeric fluid simulations using massively parallel computers

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ABSTRACT

We present a computationally efficient approach to allow for multiscale simulations of non-Newtonian polymeric fluids in three-dimensional square-square contraction geometries. This work extends previous results with a FENE dumbbell model [1] to more general bead-spring chain models with up to five FENE spring segments.

Multiscale approaches for polymeric fluids involve model equations of high dimensionality. In the case of five spring segments, the configuration space of the polymer model is fifteen-dimensional. Due to the enormous computational complexity of the problem, massively parallel computations are essential for our simulations. Our parallel implementation can be ideally combined with a dimension-adaptive sparse grid variant, the combination technique, to further reduce the enormous model complexity [2].

In this talk, we compare our multiscale bead-spring chain simulation results of three-dimensional contraction flows with experimental measurements from the literature and obtain a good agreement. Furthermore, we investigate the parallel scaling efficiency of our implementation and obtain close to optimal results.

REFERENCES

[1] Griebel, M. and Rüttgers, A. Multiscale simulations of three-dimensional viscoelastic flows in a square-square contraction. *J. Non-Newtonian Fluid. Mech.*, Vol. **205**, pp. 41–63, (2014).

[2] Rüttgers, A. and Griebel, M. Multiscale simulation of polymeric fluids using the sparse grid combination technique. *INS Preprint No. 1623, University of Bonn*, submitted to *Applied Mathematics and Computation.*