

DETERMINISTIC NUMERICAL METHODS FOR THE MICRO–MACRO MODEL OF DILUTE POLYMERIC FLUIDS

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ABSTRACT

Modelling polymer molecules as either Finitely Extensible Nonlinear Elastic (FENE) dumbbells or rigid-rod dumbbells, we arrive at a coupled Stokes Fokker–Planck (micro-macro) PDE system governing the non-Newtonian flow of dilute polymeric fluids. The primary challenge in solving this micro-macro system of PDEs in a deterministic fashion (as opposed to applying stochastic techniques) is dimensionality: the Fokker–Planck equation is posed on a high-dimensional domain that is the tensor product of the macroscopic flow domain and a microscopic “configuration space.” We present two different computational approaches that ameliorate the computational complexity of this task: (i) a heterogeneous alternating-direction method, and (ii) a certified reduced basis approach.

In the first approach, we formulate an alternating-direction (or dimension-splitting) method for the Fokker–Planck equation in which we perform a series of lower-dimensional solves — one at each “grid-point” in physical space and configuration space — instead of a single high-dimensional solve. Applying this alternating-direction scheme, however, is still a computationally intensive task and we exploit the “embarrassingly parallel” nature of our algorithm on a supercomputer in order to make large-scale problems tractable.

In the second approach, we recast the Fokker–Planck equation as a family of parametrized PDEs — parametrized by strain-rate histories associated with Lagrangian particle trajectories — and develop a reduced basis scheme with *a posteriori* error bounds that is highly efficient in this “many-query” context.

REFERENCES

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