Accepted for publication in SIAM Journal on Scientific Computing December 2009

A CERTIFIED REDUCED BASIS METHOD FOR THE FOKKER–PLANCK EQUATION OF DILUTE POLYMERIC FLUIDS: FENE DUMBBELLS IN EXTENSIONAL FLOW

DAVID J. KNEZEVIC* AND ANTHONY T. PATERA†

Abstract. In this paper we present a reduced basis method for the parametrized Fokker–Planck equation associated with evolution of Finitely Extensible Nonlinear Elastic (FENE) dumbbells in a Newtonian solvent for a (prescribed) extensional macroscale flow. We apply a POD–Greedy sampling procedure for the stable identification of optimal reduced basis spaces and we develop a rigorous finite–time *a posteriori* bound for the error in the reduced basis prediction of the two outputs of interest — the optical anisotropy and the first normal stress difference. We present numerical results for stress–conformation hysteresis as a function of Weissenberg number and final which that demonstrate the rapid convergence of the reduced basis approximation and the effectiveness of the *a posteriori* error bounds.

Key words. Reduced basis methods, POD, greedy algorithm, *a posteriori* error estimation, Fokker–Planck equation, FENE dumbbells, polymeric fluids, micro-macro model.

1. Introduction. The flow of polymeric fluids can be described by a variety of mathematical models from purely phenomenological macroscale approaches to multi-scale kinetic-theory based approaches [8, 9, 37]. The latter often take the form of the (Navier–)Stokes equation for the macroscale coupled to a Fokker–Planck description of the microscale: Stokes provides Fokker–Planck with strain rate; Fokker–Planck provides Stokes with an "extra polymeric stress" [9]. The microscale description includes both a spring–mass model and Brownian effects (reflected in the convective and diffusive components of the Fokker–Planck equation): the spring model will typically include $n_{\rm s}$ springs each described by a prescribed force law — most simply Hookean, but more realistically FENE (Finitely Extensible Nonlinear Elastic) [43].

There are two approaches to the numerical solution of the Stokes Fokker–Planck system: in the first approach, the Fokker–Planck equation is replaced by the equivalent stochastic differential equations that are then treated by Monte Carlo techniques [36]; in the second approach, the Stokes Fokker–Planck system is retained in deterministic form and treated by numerical techniques for partial differential equations (PDEs) [23, 28, 31]. The first approach can more readily treat high–dimensional systems ($n_{\rm s}$ large) but provides relatively slow convergence; variance reduction techniques [10, 11, 26] can at least partially address the latter issue. The second approach can not readily treat high–dimensional systems but provides relatively faster convergence; recent "dimension-adaptive" proposals can at least partially address the former issue [2, 3]. In this paper our interest is in the second, or "PDE," approach to the Stokes Fokker–Planck system. We restrict our attention here to the dumbbell model ($n_s = 1$) such that we can apply a standard finite element discretization; extension of our methodology to the $n_s > 1$ case is a topic of interest for future work, as described briefly at the conclusion.

Even in the $n_s = 1$ case the main difficulty with the PDE approach is dimensionality: in particular, the Fokker–Planck equation is posed over physical–configuration space — a $d \times d$ dimensional space.[1] To simplify the problem physical and configura-

*Department of Mechanical Engineering, MIT (dknez@mit.edu), corresponding author.
†Department of Mechanical Engineering, MIT (patera@mit.edu).

[1]Throughout this paper, d refers both to the dimension of physical space and the dimension of configuration space for a single dumbbell, either 2 or 3.