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Moving Mesh Kinetic Simulation for Sheared Rodlike Polymers with High Potential Intensities

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Abstract. The Doi-Hess equation that describes the evolution of an orientational distribution function is capable of predicting several rheological features of nematic polymers. Since the orientational distribution function becomes sharply peaked as potential intensity increases, powerful numerical methods become necessary in the relevant numerical simulations. In this paper, a numerical scheme based on the moving grid techniques will be designed to solve the orientational distribution functions with high potential intensities. Numerical experiments are carried out to demonstrate the effectiveness and robustness of the proposed scheme.

Key words: Orientational distribution function; moving mesh method; spherical geometry; Smoluchowski equation; potential intensity.

1 Introduction

The rheological behavior of rod-like polymers in the nematic phase is analyzed by the Doi-Hess kinetic theory (Doi [5], Hess [9]). A homogeneous population of equal rods is described with an orientational distribution function (ODF). The evolution of the ODF is modeled by the Smoluchowski equation (Doi and Edwards [4]). Once the ODF is known, the rheological response will be determined. It was demonstrated in [10] that under shear flows this theory can give a variety of behaviors for the dynamics of the rod population. The existing numerical schemes include a spectral type method with spherical harmonic functions as basis functions, see, e.g., [7,10,12]. More precisely, the expansion of the ODF in spherical harmonics is truncated at some level l_{max}, and the Smoluchowski equation is reduced to a system of $l_{max}(l_{max}+3)/2$ first-order ordinary differential equations through a Galerkin procedure.

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The intensity of the excluded volume potential U is proportional to the concentration of polymers. When the intensity increases, the ODF becomes sharply peaked and behaves more or less like a δ function. In this case, it is expected that the accuracy of the spherical-harmonic scheme with fixed l_{max} is degraded. Since the accuracy and efficiency of the spectral Galerkin methods rely highly on the solution regularity, higher-order spherical-harmonic functions have to be used in the spectral expansion. However, this may involve a large amount of computational time. In fact, earlier works did not explore high-intensity situations due to computer limitations ([6, 7, 11]).

The main purpose of this paper is to apply the moving grid technique to resolve the ODF with large potential intensities. In the past few years, it has been demonstrated that the moving mesh methods are very useful in solving problems with singularity, layers, or spikes (see, e.g., [13, 14, 17]). In this paper, we will also pay particular attention to the rheological features and phase transitions with high potential intensities.

The finite element method on a sphere [15] is used where the basis function is carefully chosen to guarantee the conservation of the ODF. Using the properties of the ODF, we will propose a special moving mesh method for solving the Smoluchowski equation on a sphere. In this respect, it is useful to introduce a vector as the average orientation of the population, the director [4], that serves as a reference for mesh moving. The goal of moving mesh methods is to resolve the small scale of the ODF by clustering more grid points in the smallest scale areas, i.e., around the director. To this end, a two-step scheme is designed: Firstly find the director, rotate the mesh according to the director orientation; this is called 0-d moving; secondly, adjust the mesh according to the numerical solution for ODF; this is called 1-d moving. It is pointed out that the mesh on the sphere is structured in this approach.

The present paper is built up as follows. The Doi-Hess model is introduced in Section 2. The finite element method on the sphere is presented in Section 3. The moving mesh strategy will be described in Section 4. Numerical experiments for high intensities are given in the final section.

2 The Smoluchowski equation

In recent years, the microscopic model has been introduced to study polymeric fluids successfully. Especially, for the rod-like polymer, the Doi-Hess model (Doi [4]) is the most commonly used model, which is capable of predicting several rheological features of rod-like polymers in the nematic phase. In the Doi model, the orientation of a rod is determined by a pseudo-vector $\mathbf{u}$ on the unit sphere, or equivalently by two angles θ and ϕ. A homogeneous population of rod-like, rigid, extremely high-aspect-ratio molecules is described with an orientational distribution function $\Psi(\mathbf{u}, t)$. The ODF gives the probability density that a rod is oriented along $\mathbf{u}$ at time t. The evolution of the ODF is modeled with the Smoluchowski equation or the Fokker-Planck equation [4]:

$$\frac{\partial \Psi}{\partial t} = \frac{1}{De}\mathcal{R} \cdot (\mathcal{R}\Psi + \Psi \mathcal{R} V_{ev}) - \mathcal{R} \cdot (\mathbf{u} \times \kappa \cdot \mathbf{u}\Psi), \quad \text{on } \Omega = \mathcal{S}^2 \tag{2.1}$$