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NUMERICAL APPROXIMATION OF THE SMOLUCHOWSKI EQUATION USING RADIAL BASIS FUNCTIONS*

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Abstract

The goal of this paper is to present a numerical method for the Smoluchowski equation, a drift-diffusion equation on the sphere, arising in the modelling of particle dynamics. The numerical method uses radial basis functions (RBF). This is a relatively new approach, which has recently mainly been used for geophysical applications. For a simplified model problem we compare the RBF approach with a spectral method, i.e. the standard approach used in related physical applications. This comparison as well as our other accuracy studies show that RBF methods are an attractive alternative for these kind of models.

Mathematics subject classification: 65M20, 65M70.
Key words: Smoluchowski equation, Spectral method, Radial basis function method.

1. Introduction

In this paper we study a numerical method which can be used in order to simulate the microstructure in a micro-macro model for suspensions of rod-like particles. Such mathematical models are used to describe complex fluids such as polymeric fluids. The full model is a time dependent, five dimensional system of partial differential equations. It consists of a three dimensional fluid flow equation which is coupled with a transport diffusion equation on the sphere describing the microscopic orientation of the suspended rod-like particles. Here we restrict our considerations to the description of the microscopic orientation, i.e. the partial differential equation on the sphere and provide a numerical method for this equation.

Numerical methods for such complex fluids are typically based on a fully macroscopic approach or on a stochastic approach using Monte-Carlo methods. We are instead interested in numerical methods which resolve the full multiscale problem. In Helzel and Otto [8], a finite difference method for the macroscopic flow equations was combined with a finite volume method for the microscopic equation. For a related model, Knezevic and Süli [10] combined finite element and spectral methods. In this paper we show that the use of radial basis function methods provides an attractive alternative for the resolution of the microscopic transport diffusion equation.

Radial basis functions provide a powerful tool for the grid-free approximation of multivariate functions, see for example the review by Buhmann [2]. Flyer and Wright [4, 5] introduced radial basis function methods for the approximation of transport dominated partial differential

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equations on the sphere. Since then such methods have successfully been used for several models, mainly motivated by geophysical applications as documented in the recent book by Fornberg and Flyer [6]. The method has also been extended to solve reaction-diffusion equations on surfaces (other than the sphere), see Piret [13] and Shankar et al. [14].

In what follows, we start in Section 2 with a description of the mathematical model. In Section 3 we restrict our considerations to a simplified one-dimensional model. For this model we derive a spectral method as well as a radial basis function method and compare their performance. In Section 4 we derive the radial basis function method for the full model and discuss numerical results for this method.

2. The Mathematical Model

We consider a mathematical model, which describes dilute suspensions of rod-like particles. With this model we can study the dynamics of a macroscopic flow which is influenced by suspended microscopic particles with a rigid rod-like structure.

Following the classical work of Doi and Edwards [3] and more recent work of Otto and Tzavaras [12], we consider a kinetic model which describes the orientation of microscopic rod-like particles. In this model $f(t,x,n)dn$ describes the time dependent probability that a rod with center of mass at the macroscopic position $x \in \mathbb{R}^d$ has at time $t \in \mathbb{R}^+$ an axis in the area element dn. Here $n \in S^{d-1}$ is a director on the unit sphere embedded in $\mathbb{R}^d$. The physical application we are interested in assumes $d = 3$. In order to verify our numerical methods we will also consider the case $d = 2$.

We assume that the relations

$$f \geq 0 \text{ and } \int_{S^{d-1}} f\, dn = 1$$

hold for all time. The evolution of the distribution function $f = f(t,x,n)$ is described by the Smoluchowski equation

$$\partial_t f + u \cdot \nabla_x f + \nabla_n \cdot (P_{n^\perp}, \nabla_x u n f) = D_r \Delta_n f + D \Delta_x f, \tag{2.1}$$

where $u : \mathbb{R}^d \times \mathbb{R}^+ \to \mathbb{R}^d$ is a macroscopic velocity field which depends on x and t. The second term on the left hand side describes the transport of the rods by the macroscopic velocity field u. The third term describes a rotation of the rod-like particles due to a macroscopic velocity gradient $\nabla_x u$. Here $P_{n^\perp} := \nabla_x u n - (n \cdot \nabla_x u n)\, n$ denotes the projection of the vector $\nabla_x u n$ on the tangent space in n. The terms on the right hand side model rotation and translation of the rod-like particles due to Brownian motion. Here $D_r \in \mathbb{R}^+$ is the rotational diffusion constant and $D \in \mathbb{R}^+$ is the translational diffusion constant.

A velocity gradient $\nabla_x u \neq 0$ distorts an isotropic distribution of f. This leads to an increase in entropy, which needs to be balanced (see [3, 12]) by a stress tensor of the form

$$\sigma(x,t) := \int_{S^{d-1}} (d\, n \otimes n - I)\, f\, dn. \tag{2.2}$$

This stress tensor appears as additional term in the macroscopic flow equation. The macroscopic flow is described by the Stokes or Navier-Stokes equation, i.e.

$$\begin{aligned} &Re\,(\partial_t u + (u \cdot \nabla_x)\, u) = \mu \Delta_x u + \nabla_x p + \nabla_x \cdot \sigma, \\ &\nabla_x \cdot u = 0. \end{aligned} \tag{2.3}$$