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NANO-ROD SUSPENSION FLOWS: A 2D SMOLUCHOWSKI-NAVIER-STOKES SOLVER

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Abstract. We present a numerical algorithm for nano-rod suspension flows, and provide benchmark simulations of a plane Couette cell experiment. The system consists of a Smoluchowski equation for the orientational distribution function of the nano-rods together with the Navier-Stokes equation for the solvent with an orientation-dependent stress. The rigid rods interact through nonlocal excluded-volume and distortional elasticity potentials and hydrodynamic interactions. The algorithm resolves full orientational configuration space (a spherical harmonic Galerkin expansion), two dimensional physical space (method of lines discretization), and time (spectral deferred corrections), and employs a velocity-pressure formulation of the Navier-Stokes equation. This method extends our previous solver [25] from 1D to 2D in physical space.

Key Words. Navier-Stokes, Smoluchowski equation, numerical methods, nano-rods, suspension flow

1. Introduction

Numerical simulations are critical for smart engineering of high-performance nano-composite materials. This paper is one step toward that goal, which we briefly explain in this introduction. While traditional composite engineering is replete with sophisticated control and optimization technology, based on accurate and fast direct and inverse solvers, nano-composites still remain unresolved with respect to various stages of the direct problem. There are fundamental limiting steps that must be overcome to reach a comparable level of simulation capability; the solver presented here addresses one of those steps.

Nano-rods and nano-platelets are too numerous and too small to image in statistically sufficient detail. Consider that nano-rod and nano-platelet macromolecules at 1% volume fraction and $1nm \times 100nm$ aspect ratio consist of 10^6 or greater particles in a cubic micron. Nano-clay platelets at this composition introduce football fields of new surface area in a raindrop [22]. The key to probing these nano-scale composites is high-fidelity resolved simulations combined with sparse data to interpret the dataset, to validate the model, and to perform inverse characterization of the modeling parameters. We have not reached that level of cross-talk and confirmation between theory and experiment.

The targets of nano-composite technology are the remarkable property enhancements that have been achieved in model systems. Properties range from conductivities to permeabilities to mechanical. Post-processed properties and performance

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features of nano-composite materials are a direct consequence of the orientational probability distribution (PDF) of the nano-particles; this is an empirical fact. But, *how* flow-processing, composition, and effective properties are related remains an open and difficult challenge. There are not sufficient quantities and resources to span experimental parameter space. The modeling state of affairs has been restricted to highly idealized limits where the rods or platelets are either perfectly aligned or random [19], with no ability to link the role of composition and flow to volume-averaged and percolation induced property enhancements. Our research group has made partial inroads into this problem, and the algorithms presented here take us yet another step further.

For the processing phase, the theoretical and computational obstruction is related to anisotropy: inherently due to the high aspect ratio of individual particles, but which then passes upscale to the ensemble distribution function. Otherwise, advanced sphere-viscous solvent dispersion codes would have resolved this problem long ago. Molecular dynamics simulations with parametrized Gay-Berne potentials have not yet been successful even in the homogeneous limit of orientational distributions for aspect ratios greater than 10; nano-particles typically have aspect ratios in the hundreds if not thousands. Because of nonlocal particle excluded-volume interactions, which require tracking of particle orientations with respect to their neighbors, rigid rod suspensions are extremely sensitive to low-moment closure models ([7]). This requires a resolved simulation of the Smoluchowski equation of Doi [3] and Hess [16] for the orientational probability distribution function (PDF). Following Larson and Ottinger [18], Grosso et al. [13], and Faraoni et al. [5], we first developed a Galerkin spherical harmonic expansion algorithm of the Smoluchowski equation in the longwave limit, together with a spectral deferred correction method for the dynamics. This formulation posits a linear flow, suppresses flow feedback, and computes how the PDF is modified by the coupling of excluded volume, torque and translation of spheroidal particles due to flow, and the geometry and volume fraction of the rods or platelets. With this code, we implemented continuation software (AUTO) [2] and thereby mapped out phase diagrams of PDF attractors versus linear flow type and strength, volume fraction of the rigid rods, and particle aspect ratio [9, 8, 11, 10]. Next, we generalized the method to 1D in physical space [25], allowing for hydrodynamic feedback, a fixed experimental geometry with wall confinement and driving conditions. Simulations of this code allowed us to map out space-time attractors versus flow and material elasticity parameters [12], and that numerical study continues. The output yields structure morphology in films, both in the orientational PDF of the rod ensemble and in the flow profile. Furthermore, the heterogeneous ensemble distributions are directly transferred to homogenization and new percolation methods to predict effective properties. This brings us to the present paper and the algorithms presented for 2D in physical space. With them, we can study stability of the 1D film composites to higher physical space perturbations, and we can simulate fully 2D flow and orientational structures. These are immediate applications of the algorithm developed here; for this paper, we provide only benchmark simulations.

2. Kinetic model equations

We consider an ensemble of high aspect ratio, rigid rods in a viscous solvent, confined between two parallel plates which are moving at the same speed in opposite directions. The rods are modeled as spheroids with aspect ratio r and axis of