HIGH ORDER, RELIABLE COMPUTATIONS OF FLOW STRUCTURE IN NEMATIC POLYMERS

R. Zhou[a], **M.G. Forest**[b] and **Q. Wang**[c]

[a]Department of Mathematics
University of North Carolina at Chapel Hill
Chapel Hill, North Carolina 27599-3250
ruhai@amath.unc.edu

[b]Department of Mathematics
University of North Carolina at Chapel Hill
Chapel Hill, North Carolina 27599-3250
forest@amath.unc.edu

[c]Department of Mathematics
Florida State University
Tallahassee, Florida 32306
wang@math.fsu.edu

The Doi kinetic theory with a Marrucci-Greco distortional elasticity potential is the leading model for spatio-temporal structures created in plane shear flow of nematic liquid crystalline polymers (LCPs). These structures are critical to performance properties of LCP materials. The governing system of equations consists of a Smoluchowski equation for the evolution of the orientational probability distribution function at each location, coupled with a momentum flow balance equation, a constitution equation for the extra stress, and an incompressible continuity equation. The spatio-temporal structure of the polymer varies significantly and the integration of the Smoluchowski equation is computationally challenging.

In our numerical method, we first handle the variables for orientation by expanding the orientational distribution function in spherical harmonics and applying a Galerkin procedure. The Smoluchowski equation is thus reduced to a finite set of partial differential equations in time and space. Then we discretize the spatial variables (method of lines) using high-order finite differences, which reduces the full system to a large set of ordinary differential equations. Adaptive grid generation techniques are implemented. To provide an accurate and stable integration of these ordinary differential equations, we employ the newly developed spectral deferred correction algorithm.

We benchmark our method on the homogeneous dynamic of molecular orientation in imposed shear flow, where there are many complex bifurcations as molecular and flow parameters are varied. We confirm results by Larson, Ottinger, Faraoni, Maffettone and collaborators, and report our results on the full phase diagram for rigid rods and platelets. We then report simulations of structures that form in shear cells.