Advanced Scientific Computing Research
Applied Mathematics
FY 2007 Accomplishment

"Instabilities and Mixing in Complex Fluids"

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Summary

A central activity of our group has been modeling and simulating the dynamics of bodies – flexible or active or moveable – immersed in fluids. Many complex fluids are fluids with suspended microstructural bodies such as fibers, or macromolecules both synthetic (e.g. PEO) and biological (e.g. DNA)). We have developed new simulation methods for analyzing the dynamics of complex fluids in the Stokesian limit (when fluid inertia is negligible, the regime of interest in micro-fluidic applications). We have also found new instabilities in flexible fiber suspensions, with application to mixing and transport. These phenomena are made quite different in complex fluids by the presence of elastic responses and nonlinearities. We are also exploring the dynamics of ``active suspensions''.

While the dynamics of complex fluids are central to materials science, biophysics, and chemical, mechanical, and bio- engineering, very little is understood theoretically of their transport, instability, and mixing properties. Simple shearing and straining flows are often used to probe mechanical response of deformable media, and for a complex fluid even such simple forcing can induce nontrivial dynamics in the fluid's micro-structure. For example, our simulations of of flexible fiber suspensions show that shearing beyond a critical shear-rate can induce fiber buckling, and the appearance of normal stress differences [*Becker & Shelley, PRL (2001); Tornberg & Shelley, JCP (2004)*].

We have been analyzing and simulating the dynamics of viscoelastic fluids in more complicated situations, and discovering new phenomena in both continuum and microstructural descriptions. In one study we have discovered a new instability at hyperbolic stagnation points -- the *stretch-coil transition* -- which is an analogue to the coil-stretch transition of floppy polymer suspensions [*Young & Shelley, PRL (2007)*]. Using slender-body theory for Stokes flow, we show that there is a critical dimensionless viscosity (combining strain-rate, filament length and rigidity, and fluid viscosity), beyond which an elastic fiber near a hyperbolic stagnation point is unstable to buckling. There a filament transits from being straight (stretched) to buckled (coiled), thus storing elastic stresses which are then released as the fiber moves away from the fixed point.

Our simulations show that this instability yields surprising transport properties in more complex background flows. The figure below shows the path of a fiber moving through a simple periodic cellular flow. In essence, the fiber is moving as a random walker across the flow. This occurs because

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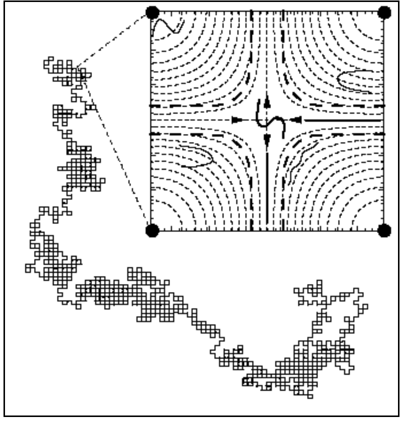
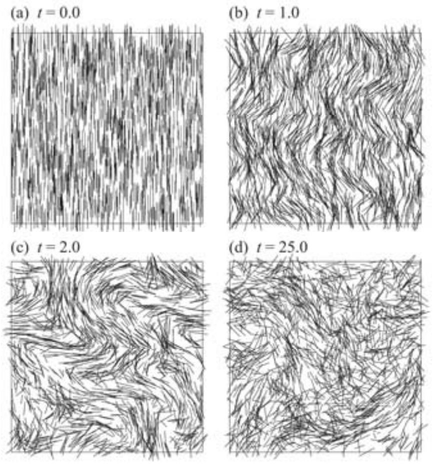
the fiber can become entrained along the stable manifolds of the fixed point, transported there where it then buckles. The buckling allows it to act as a test particle extended over the fixed point, and it randomly chooses a direction from which to exit, and thence moving along to the next fixed point.



We are currently studying fiber-fiber interactions, and stress production. In a companion study, we show that in the Oldroyd-B continuum model, such stagnation point flows can produce attractive singular stress distributions and strong mixing [*Thomases and Shelley (2007)*].

Active suspensions are those whose microstructure changes shape or exerts stress on the surrounding fluid due to internal forces. One important example is a bath of swimming microorganisms. Their collective dynamics in bulk can be characterized by strong fluctuations and correlated motions on scales much larger than an individual organism, presumably resulting from many-body hydrodynamic interactions. The relevance to basic biology and to bio-remediation efforts is clear, as these larger-scale flows increase mean particle transport, mixing, and diffusion, with consequences for nutrient and material uptake.

Shelley and D. Saintillan (a DOE postdoc) have developed numerical tools for simulating active suspensions. They adapt nonlocal slender body theory for rigid rods [*Saintillan et al, Phys. Fluids (2005); Tornberg & Gustavsson, JCP (2006)*] to incorporate a propulsive surface stress. The figure below shows a 3d simulation of 2500 self-locomoting rods, with periodic boundary conditions, using spectral expansions of force distributions and a smooth particle-mesh Ewald algorithm to efficiently calculate hydrodynamic interactions. These simulations show the development of orientational instabilities, and the emergence of strongly mixing, random flows [*Saintillan & Shelley, PRL (2007)*]. We are currently developing and analyzing nonlinear kinetic theory descriptions of such systems.



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