Using Simple Flows to Tie Knots in Flexible Fibers

STEVE KUEI, Princeton University, CHRIS SADLEJ1, Institute of Fundamental Technological Research, Polish Academy of Sciences, HOWARD A. STONE, Princeton University — Flexible fibers, such as DNA and other polymer chains, have sometimes been found to contain knotted regions. While such fibers are not strict, closed knots, they exhibit similar characteristics; the formation of these “open knots” and the effects they have on material properties are the subject of current research. We investigate the possibility that simple flows can generate open knots in sufficiently long and flexible elastic fibers. Using the HYDROMULTIPOLE algorithm, which solves the multipole expansion of Stokes equations, we use numerical simulations to study the time evolution of a bead-spring model fiber in a shear flow. The model is described by the dimensionless parameters $k$, $A$, and $l_0$, which account for the elastic forces, bending forces, and equilibrium distance between beads, respectively. We find that for certain systems, the characteristic tumbling motion of a fiber in shear flow will result in the formation of $3_1$ and $5_1$ knots, as identified by their Alexander polynomial knot invariants. Investigation of the knotting mechanism is ongoing.

1We dedicate this work to our collaborator Chris Sadlej who is recently deceased.