

Viscoelasticity, Stochasticity, Non-Equilibrium Thermodynamics, and Non-Newtonian Fluid Mechanics.

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Abstract

Water and air are simple molecules with well-known evolution equations describing their macroscopic dynamics. Everything else is interesting. For example, if you stretch a rubber band, the tension can take an hour to equilibrate. If you quickly deform a polymer liquid and release it, it can recover more than half of its strain. Each of these substances is both elastic and viscous, or *viscoelastic*. Describing these viscoelastic responses is a decades old problem; but we are now making dramatic progress through molecular modeling, such that quantitative *predictions* are now possible. The class of models we find most successful are stochastic. Hence, description of non-Newtonian fluid mechanics will require combined macroscopic techniques, like finite element methods, and stochastic techniques, like Brownian dynamics. An additional complexity, is that these stochastic equations, aside from having white noise, also have a birth/death process. This latter effect renders state-of-the-art micro/macro simulations nearly useless.

In this talk I will try to get across (1) a successful philosophy for addressing such problems, (2) what sorts of equations we can expect to arise from this approach, and (3) what sorts of obstacles currently exist for their numerical solution. I will describe our slip-link theory for entangled polymers as a specific example. This model incorporates contemporary ideas of non-equilibrium thermodynamics. However, I will also argue that numerical techniques themselves should obey non-equilibrium thermodynamics.