M2 Internship Proposal

Microscopic theory of the stress tensor in dense materials

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Thesis possibility after internship : YES

The **stress tensor**, introduced by Cauchy in 1822, quantifies the local distribution of forces within materials and links them to deformations, forming the basis of continuum mechanics. Over the years, stress has become a unifying concept across physics and engineering, governing elasticity and fracture in solids, viscous flow in fluids via the Navier-Stokes equations, and appearing as the stress-energy tensor in relativity and field theories. In modern statistical and condensed matter physics, stress connects microscopic dynamics to macroscopic transport. It determines pressure and shear in molecular simulations, enters Green-Kubo relations for transport coefficients, and controls the mechanical response of disordered materials like glasses and amorphous solids[1,2] (Fig. 1, left). The stress tensor also plays a key role in active matter, with active realizations of stress driving nonequilibrium dynamics[3,4] (Fig. 1, right).

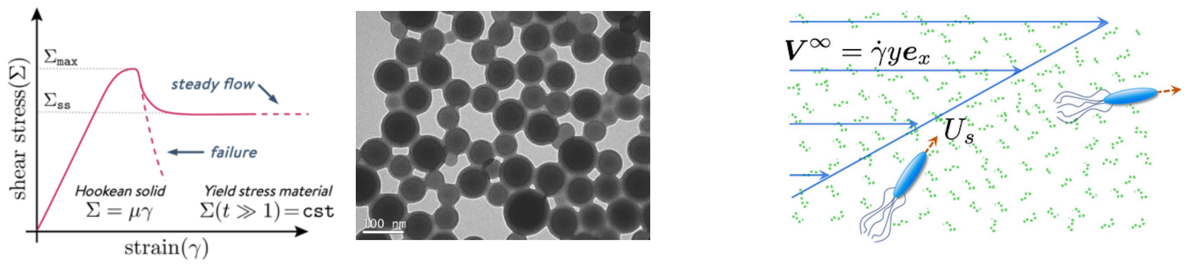

Figure 1. *Left: Yield stress material (Stress/strain curve and TEM picture of PLLA and PS particles, Fig. from Nicolas et al[2]). Right: Schematic view of active stress stemming from active swimmers (Fig. from Choudhary et al[5]).*

Theoretical descriptions of the stress span multiple scales, reflecting the level of coarse-graining. **Macroscopic models**[6] describe stress via continuum constitutive equations (viscoelastic, viscoplastic, or viscoelastoplastic models), reproducing experimental rheology but with parameters fitted rather than derived. **Mesoscopic models**, such as elastoplastic approaches, represent materials as assemblies of elastic regions undergoing stochastic plastic rearrangements, capturing intermittent flow and stress redistribution but relying on empirical rules like in the Hébraud-Lequeux model[7]. **Microscopic formulations**, including microstructural[8] and mode-coupling theories[9], express stress in terms of interparticle forces and correlations, offering a first-principles link between microscopic dynamics and macroscopic response. The challenge lies in handling many-body correlations and achieving consistent closures.

The aim of this internship is to develop a **first-principles microscopic theory of the stress tensor in dense materials**. Starting from the Irving-Kirkwood formulation of the stress tensor for a system of interacting particles, the project will focus on achieving a closure of the microscopic stress equation by building on recent theoretical developments[10,11]. The methodology will integrate advanced analytical techniques including effective and mean field theory, stochastic approaches, and projection operator methods. This analytical framework will be complemented by numerical simulations, such as event driven algorithms of hard spheres or hard disks, to validate and extend the theory. The resulting phenomenology, covering stress fluctuations and redistribution, will emerge from the combined insights of both analytical derivations and numerical analysis. This framework will provide new tools for analyzing stress fluctuations and redistribution in disordered and nonequilibrium systems.

References

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