TECHNISCHE UNIVERSITÄT MÜNCHEN

Lehrstuhl für Numerische Mechanik

LNM Seminar

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Modeling flowing polymer solutions: mesoscopic vis-á-vis microscopic approaches, with an eye to coupled multiscale simulations

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Complex flows of polymer solutions arise in many industrial and biological applications. In many cases, free surfaces and free boundaries are present, e.g., in coating, ink-jet printing, spraying, and flow in the deep pulmonary alveoli. When modeling flows of polymer solutions, two approaches are possible: a mesoscopic one, where the dynamic microstructure of the liquid is accounted for by one or more tensors which obey convection-diffusion-generation equations; and a microscopic one, where the liquid microstructure is represented by micromechanical elements obeying stochastic ordinary differential equations. The former approach is best suited for process modeling; the latter for studying fluid properties.

In the first part of this talk, I will focus on macroscopic models, where the structure of the polymer solution is represented by the gyration tensor of local ensembles of polymer molecules. Recent developments in mesoscopic non-equilibrium thermodynamics have yielded general theories that can include disparate microstructural models for polymer solutions. I will discuss how such theories can be incorporated into full three-dimensional finite element codes for free surface flows based on fully coupled formulations and full Newton's method with analytical Jacobian (and arclength continuation in parameter space), and I will show results on benchmark flows.

In the second part of this talk, I will discuss how microscopic models can be used to study the interesting interplay of of bending elasticity, viscous drag, and Brownian forces in shear flows of dilute solutions of rod-like macromolecules. I will show that flow-induced viscous tensions can cause rod-like macromolecules to buckle in dilute solutions; although buckling is controlled by the competition of viscous and bending forces, Brownian forces play a key role in whether such buckling affects macroscopic properties like solution viscosity and molecular size.

I will conclude the talk by discussing recent developments on using detailed microscopic models in process flows by representing the liquid microstructure with stochastic partial differential equations coupled to the macroscopic mass and momentum balances and mesh motion equations.

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