Computer Simulation and Statistical Physics of Complex Fluids

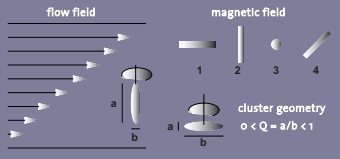
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Martin Kröger

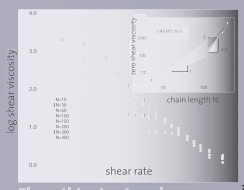
Polymer Physics

Goal

In order to predict the macroscopic material behavior of complex, macromolecular fluids based on the molecular topology of their constituents, we study physical models which capture essential features of these structures (connectivity, semiflexibility, functionality, densities, etc.). We focus on the understanding and prediction of the dynamical, rheological, and optical behaviors of complex fluids subjected to external (flow or electromagnetic) fields.

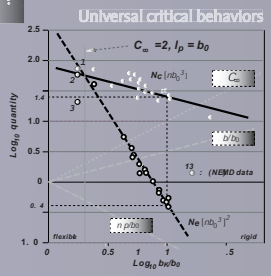


polymer melts

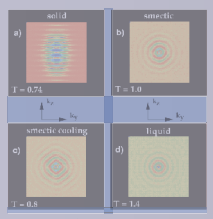


Shear thinning in polymer melts, rheological crossover

Universal critical behaviors

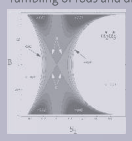


polymer solutions

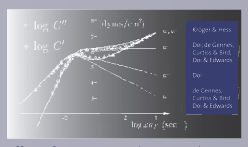


Structure factor for a simulated polymeric liquid crystal

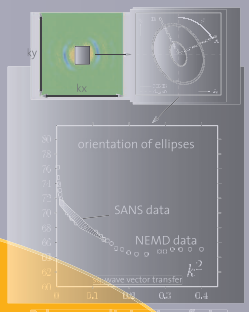
Tumbling of rods and disks



liquid crystals



Effect of anisotropic tube renewal on linear viscoelastic properties of melts



Polymer melt structure factor: local vs global anisotropy

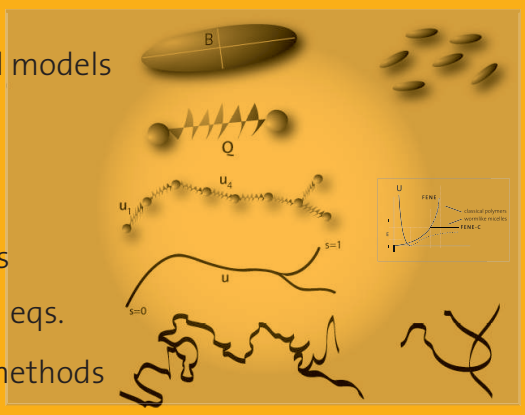
coarse-grained models

nonequilibrium molecular and brownian dynamics simulation

smothed particle dynamics

stochastic differential eqs.

Monte Carlo methods

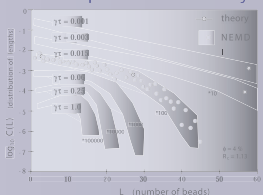


dynamics

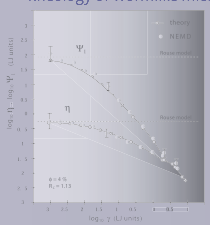
structure

rheology

Growth processes in micellar systems



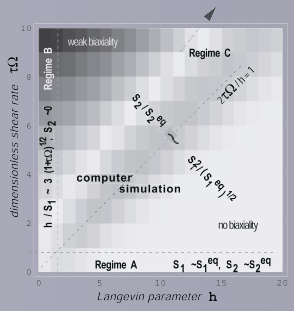
Rheology of wormlike micelles



wormlike micelles

ferrofluids

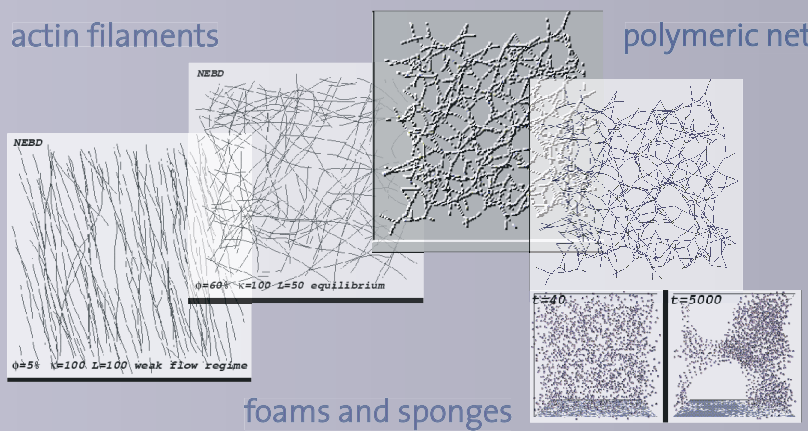
magnetorheological fluids



Uniaxial vs biaxial shear-induced ferrofluid phases

actin filaments

polymeric networks



foams and sponges

Further reading

MK, W Loose, S Hess, J Rheol 37 (1993) 1057
MK, A Alba, M Laso, HC Öttinger, JCP 113 (2000) 4767
MK, S Hess, Phys Rev Lett 85 (2000) 1128
MK, Phys Rep (review) (2003) in press.

Running projects

DFG Priority Program 1104 *Colloidal magnetic fluids*
DFG project HE 1100/7-1 *Smoothed particle dynamics*

Contact / Manuscripts available at **www.ar.ethz.ch/mk/**

13 Nov 2003