Thermodynamically Guided Nonequilibrium Simulations

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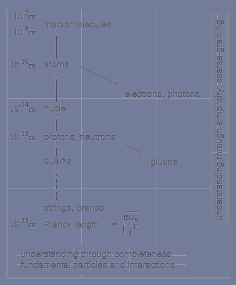
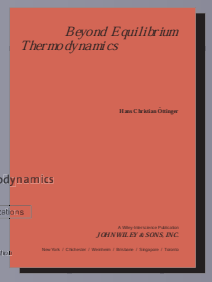
Polymer Physics

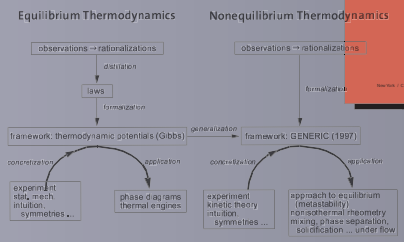
Facing levels of description for bridging scales

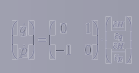
Thermodynamically guided simulations - based on GENERIC and its projection-operator justification - rely on a statistical nonequilibrium ensemble, which is defined in terms of the variables of some coarse-grained description of the system of interest. The availability of an appropriate coarse-grained level of description is thus absolutely crucial for thermodynamically guided simulations.

The new methods are devoted establishing a connection between different levels of description of complex fluids and offer insight into the effect of varying the molecular structure on the macroscopic behavior









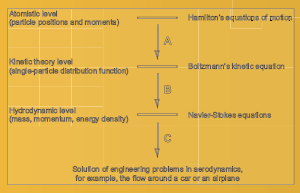
Approach to Nonequilibrium Thermodynamics

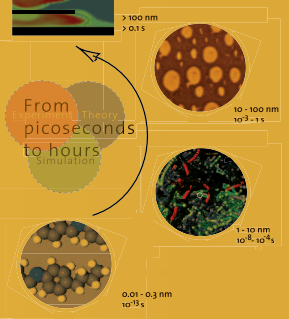
Step	Equilibrium	Nonequilibrium
1	"work" vs "heat"	"reversible" vs "irreversible" dynamics
2	$dE = \delta W + \delta Q$	$\frac{dx}{dt} = v_{\text{reversible}} + v_{\text{irreversible}}$
3	$TdS = pdV + \mu dN + \delta Q$	$\frac{dx}{dt} = L \cdot \frac{\delta H}{\delta x} + v_{\text{irreversible}}$
4	$dE = -pdV + \mu dN + TdS$	$\frac{dx}{dt} = L \cdot \frac{\delta H}{\delta x} + M \cdot \frac{\delta S}{\delta x}$

$$\frac{dx}{dt} = L\frac{\delta E}{\delta x} + M\frac{\delta S}{\delta x}$$

General Equation for the NonEquilibrium Reversible-Irreversible Coupling

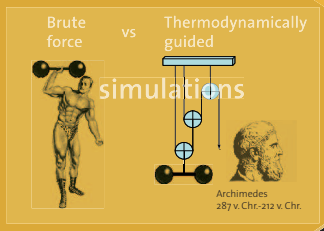
Beyond-equilibrium statistical mechanics

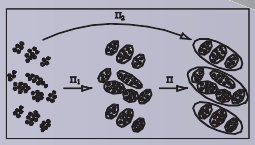




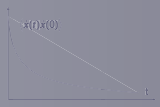
- Monte-Carlo simulations
  - Molecular and Brownian dynamics
    - Finite element calculations for complex flows

Bridging scales

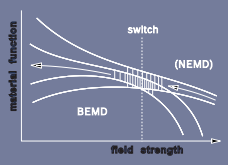




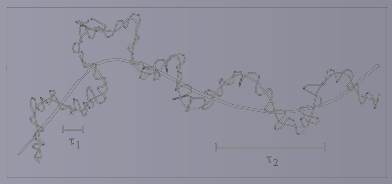
Entropy on different levels of description



Examples

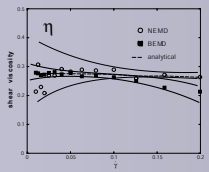


(A) In an exemplary guided beyond-equilibrium molecular dynamics study we treated a rarefied gas by facing it with Grad's 10-moment method, where the set of distinguished moments consists of five hydrodynamic moments and five components of the traceless stress tensor. Promising results are obtained at small shear rates, where conventional molecular dynamics usually fails.
(B) In another examplary study, so called GENERIC Monte Carlo has been adopted to study single and multiple conformation tensor viscoelastic models for unentangled and also long-chain branched polymers.



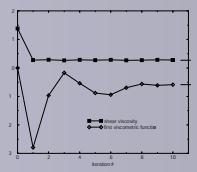
Coarse-graining to separate time and length scales

(A)



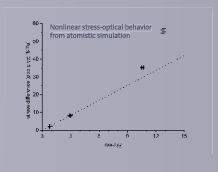
viscosity for a rarefied gas via BEMD

(A)



convergence behavior of BEMD

(B)



Thermodynamically guided melt simulation

Further reading

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www.nonequilibrium-thermodynamics.org

17 Nov 2003