Guided Simulations for Bridging the Gap in Time Scales

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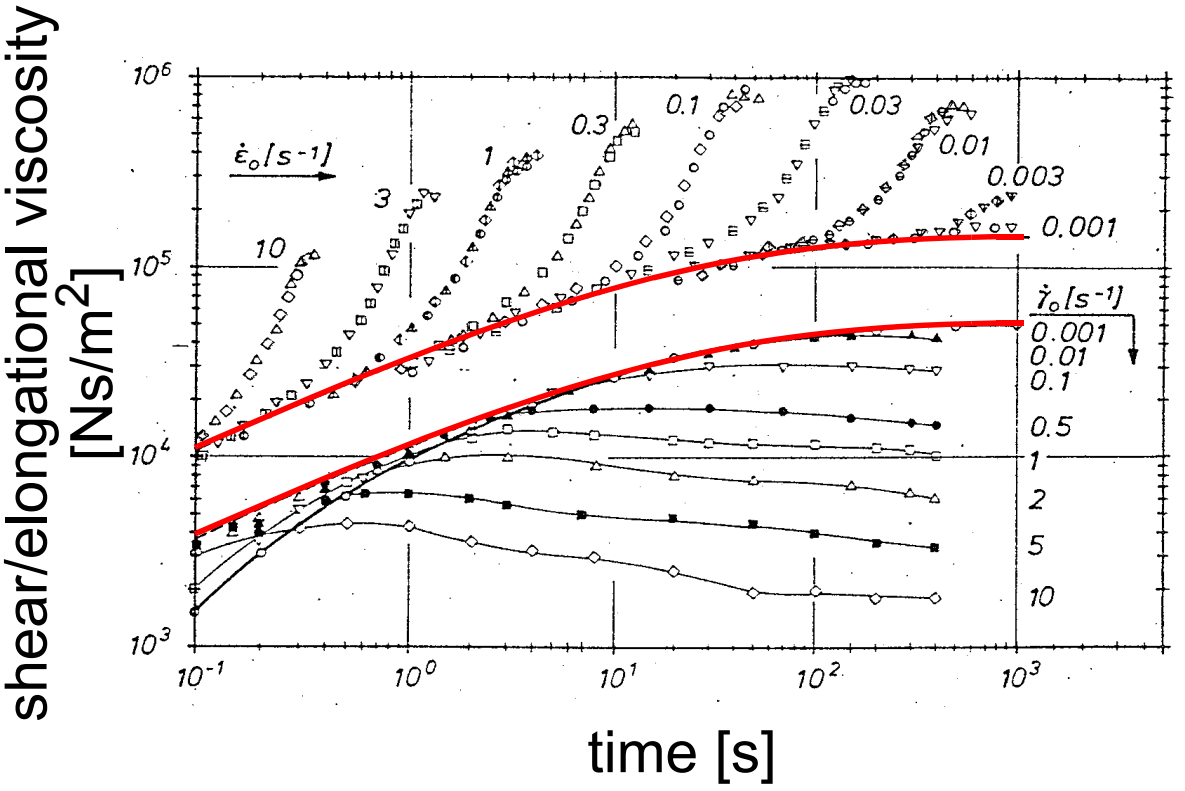
The Challenge

(LDPE at T=150°C)



A Beyond-Equilibrium Ensemble

Ensemble after integrating out momentum variables:

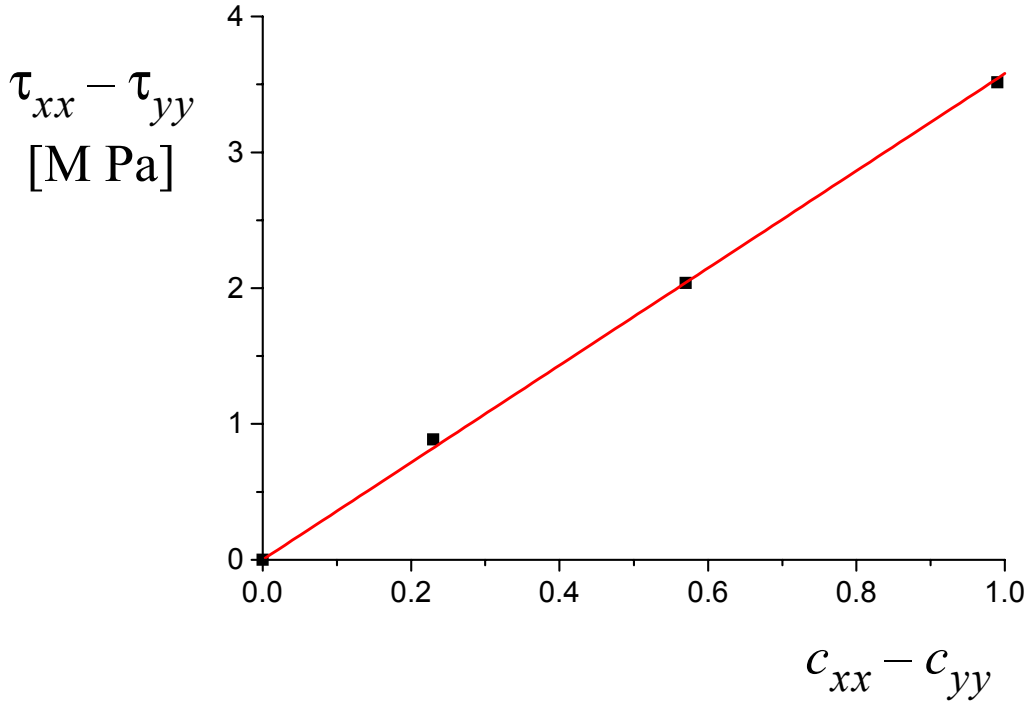
$$\propto \exp\left\{-\frac{p}{kT}V(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) - \frac{1}{kT}\phi(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) - \lambda_c : \sum_{k=1}^{N_p} \boldsymbol{Q}'_k \boldsymbol{Q}'_k\right\}$$

Slowest vibration mode: $$\boldsymbol{Q}'_k = \sqrt{\frac{2}{N_k}} \sum_{j=1}^{N_k - 1} (\boldsymbol{r}_{j+1} - \boldsymbol{r}_j) \sin\frac{j\pi}{N_k}$$

Systematic coarse-graining instead of computer experiments!

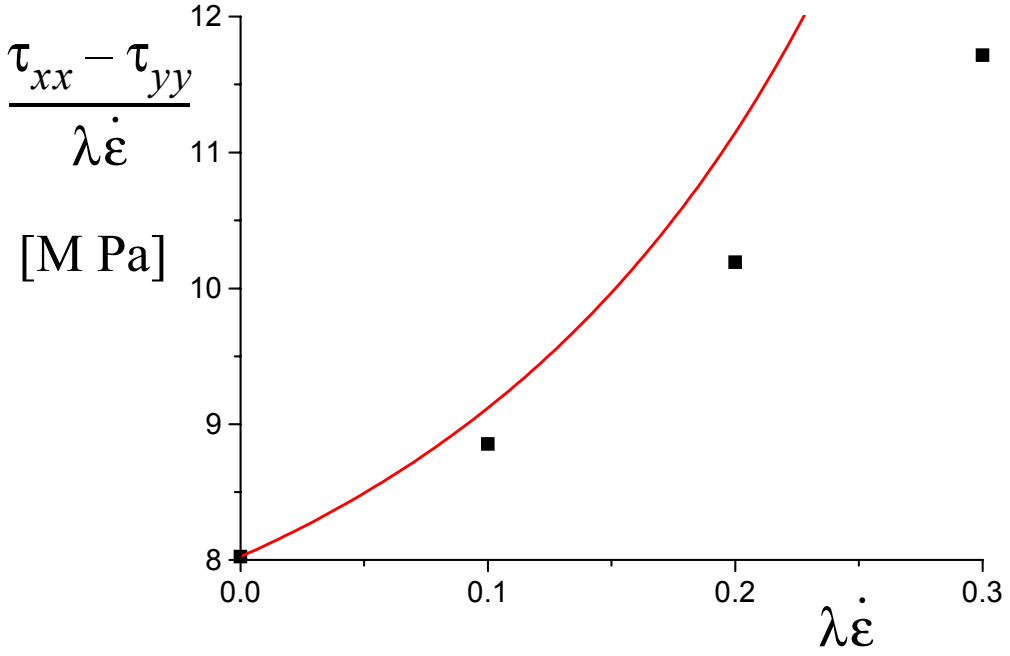
Stress-Optical Rule

Polyethylene, C_{78}



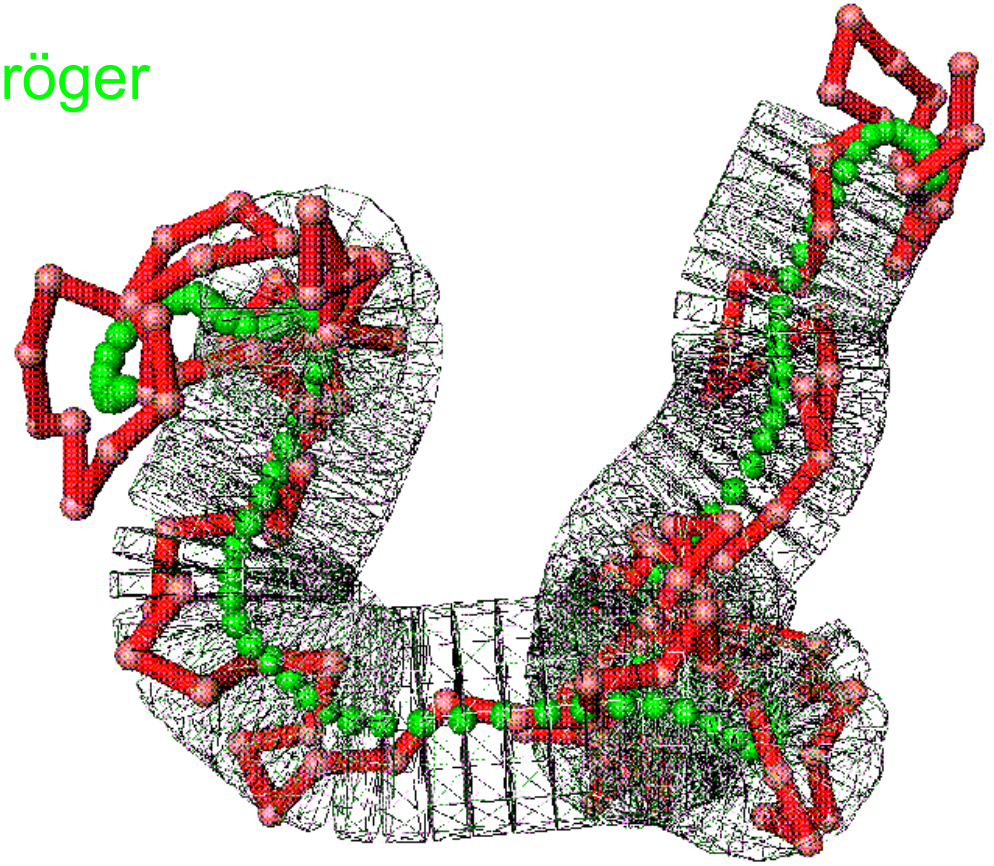
Elongational Viscosity

Polyethylene, C_{78}

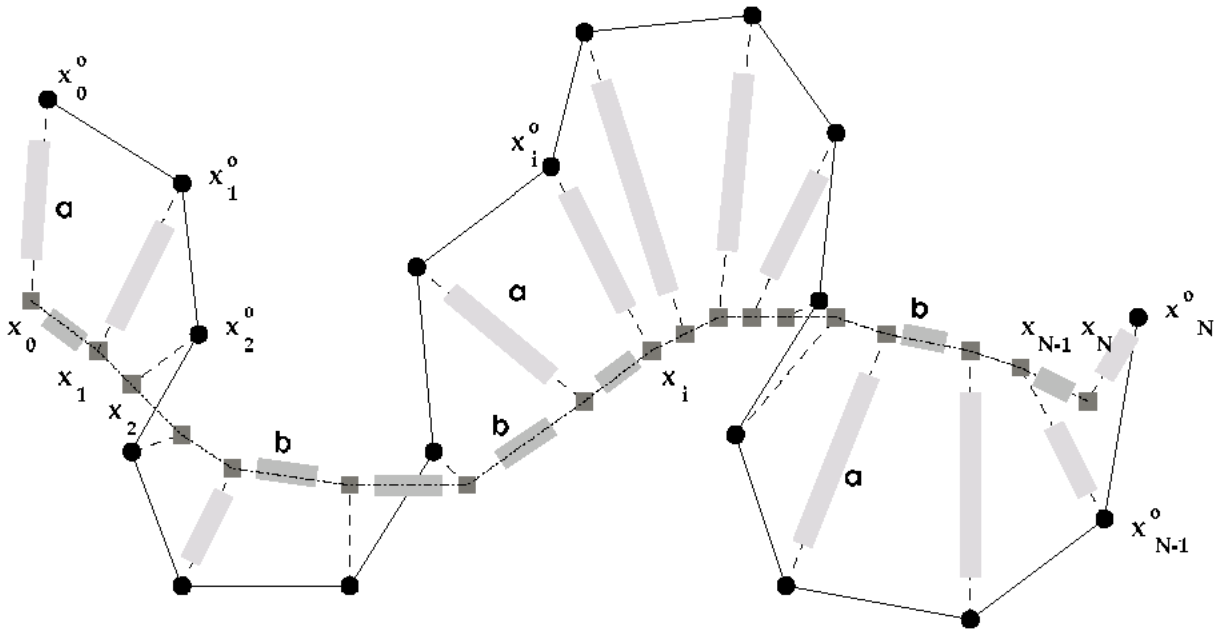


Polymer Melts: Smoothed Chain

Martin Kröger



Polymer Melts: Smoothing



Thermodynamics and Anisotropic Tube Cross Sections

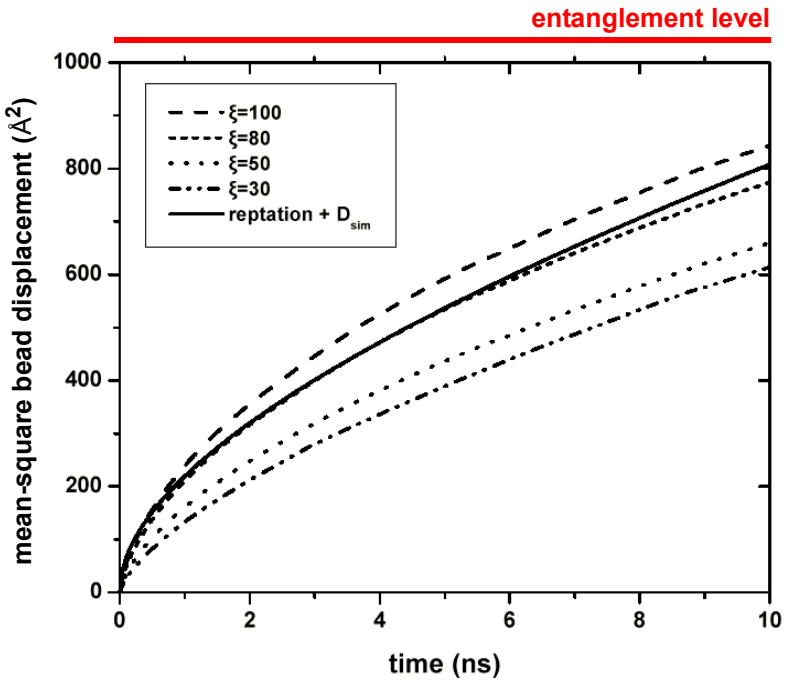
Pino Marrucci: stress tensor $\Rightarrow$ Thermodynamics: time-evolution

stress tensor in shear flow: $\begin{bmatrix} p_{11} & p_{12} & 0 \\ p_{12} & p_{22} & 0 \\ 0 & 0 & p_{33} \end{bmatrix}$ $\quad \Phi = -\dfrac{p_{22} - p_{33}}{p_{11} - p_{22}}$

famous values for Φ: 0.28, 0.14, 0.25
simulations based on the theory of coarse-graining: 0.17 ... 0.21

- How to complete and clarify a picture?
  (From Turner to high-resolution graphics)
- How to get maximum results from minimum simulation efforts?
  (From Italian/Dutch to German soccer)

Polymer Melts: Diffusion



Vlasis Mavrantzas