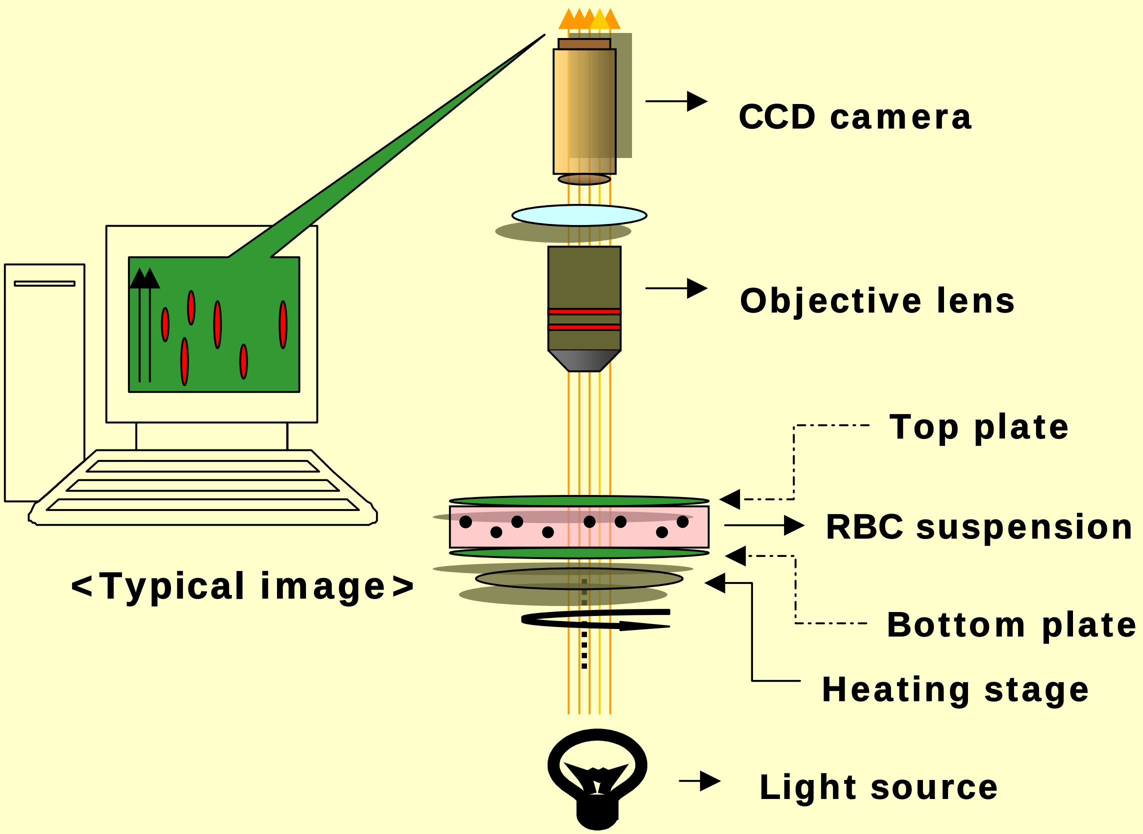
# Ch 03
# Methodology

# Structural probes

- Microscopy (w/ shearing system)
- Small angle light scattering
- Polarimetry (birefringence)
- Dichroism
- Light, X-ray, neutron scattering
- Others

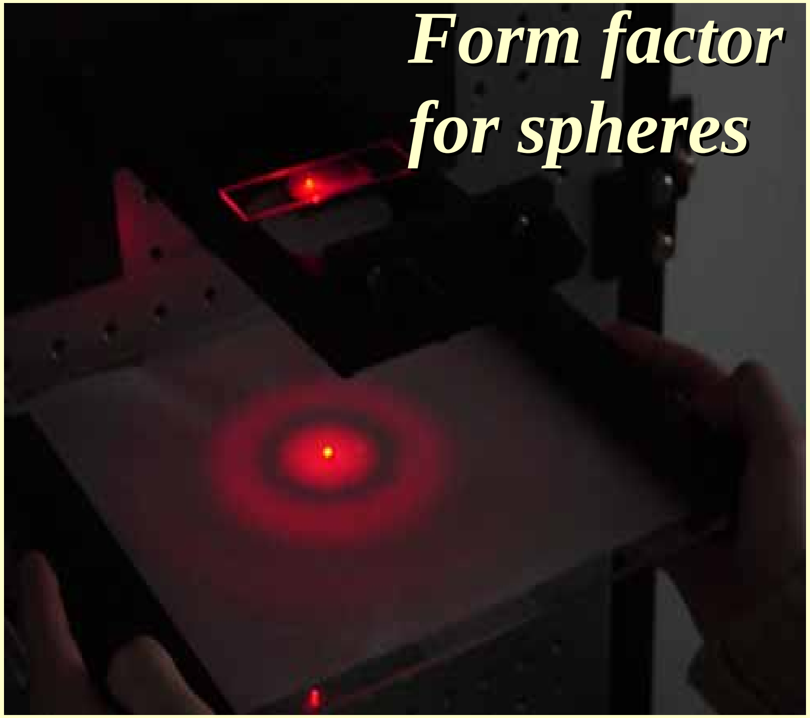
# *Shearing system*




10~100 μm

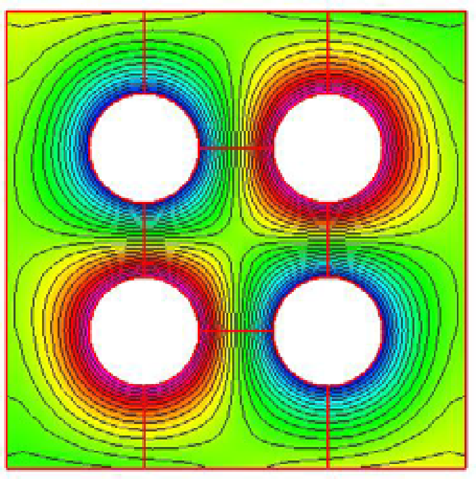
Shearing system

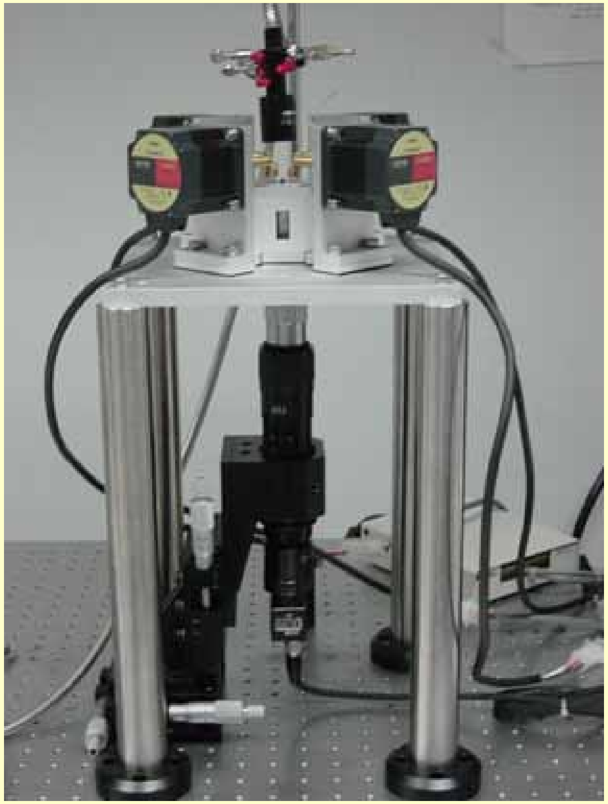
# SALS

# *Four roll mill*

- Relatively easy to control
- Flow type constant
  - Pure extensional flow: $\alpha=1$
  - Mixed flow : $0< \alpha <1$
  - Pure shear flow: $\alpha=0$





# Computational methods

- Macroscopic simulation
  - FEM, FVM, spectral…
- Microscopic simulation
  - BD, MD, MC, SD, FPD, DPD, LB…
- Micro-macro simulation

# Macroscopic simulation

- **Governing eqn's.**

$$\tau_p = f\left(\mathbf{u}, \tau_p, \lambda, \beta, \eta\right)$$

$$\mathrm{Re}\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \nabla \cdot \tau_p + (1-\beta)\nabla^2 u \qquad \boxed{\beta = \frac{\eta_p}{\eta_p + \eta_s}}$$

$$\nabla \cdot u = 0$$

$$\tau_p + We\left(\frac{\partial \tau_p}{\partial t} + u \cdot \nabla \tau_p - (\nabla u)^T \cdot \tau_p - \tau_p \cdot \nabla u\right) = \beta\left(\nabla u + (\nabla u)^T\right)$$

- **Dimensionless Group**

$$Re = \frac{LU\rho}{\eta} \;\square\; \frac{inertia}{viscous} \qquad We = \frac{U\lambda}{L} \;\square\; \frac{elastic}{viscous}$$

◈ **HWNP** **(High Weissenberg Number Problem)**

- coupled elliptic-hyperbolic system
- ill-posed problem
- geometry effect (singularity)

→ Numerical breakdown

# Microscopic modeling

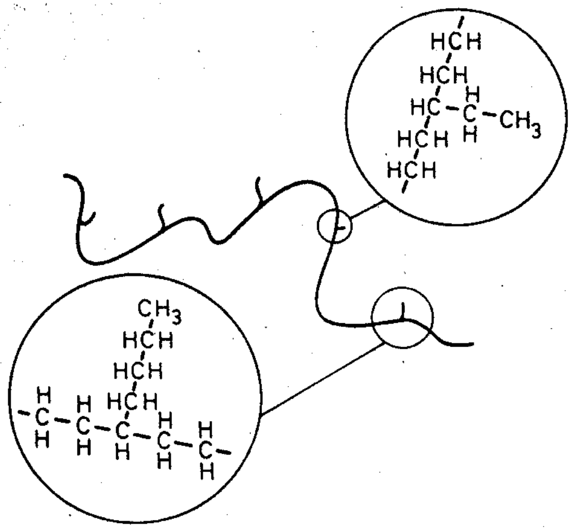
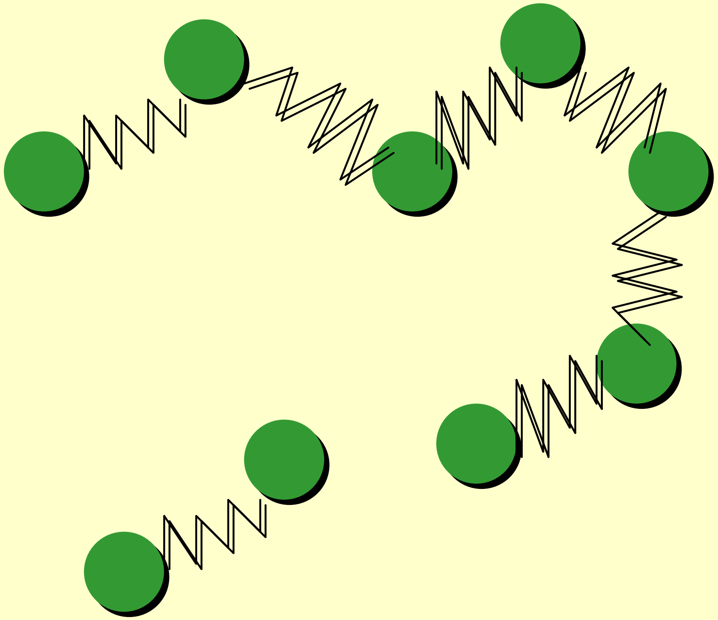
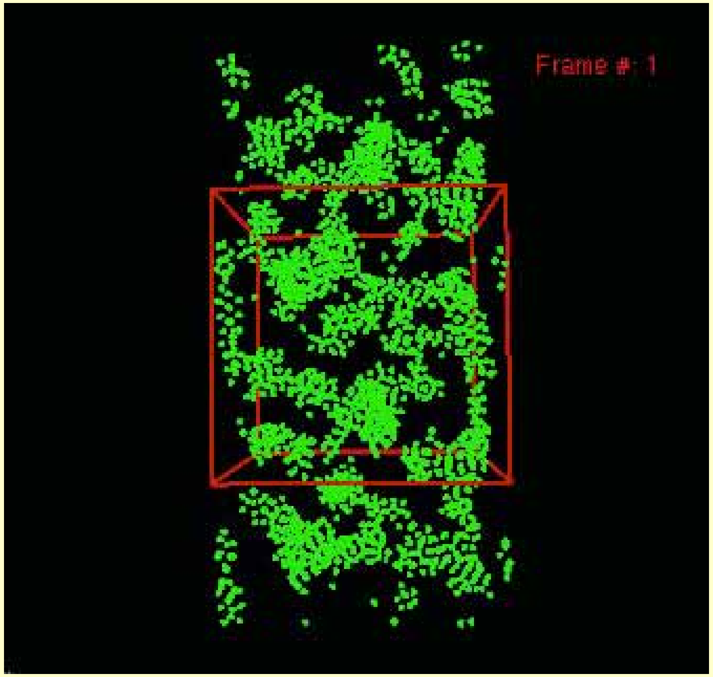
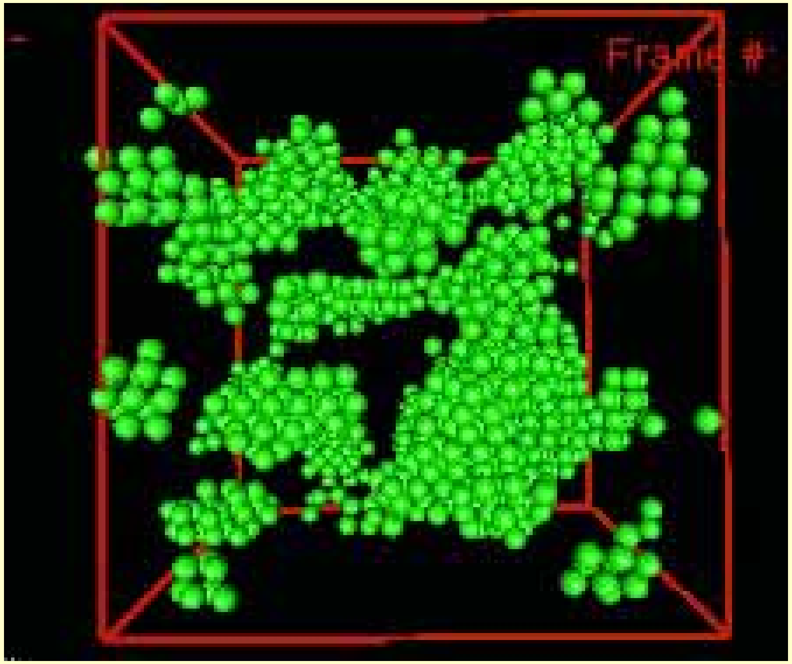


Fig. 1.1. Side branched polyethylene.

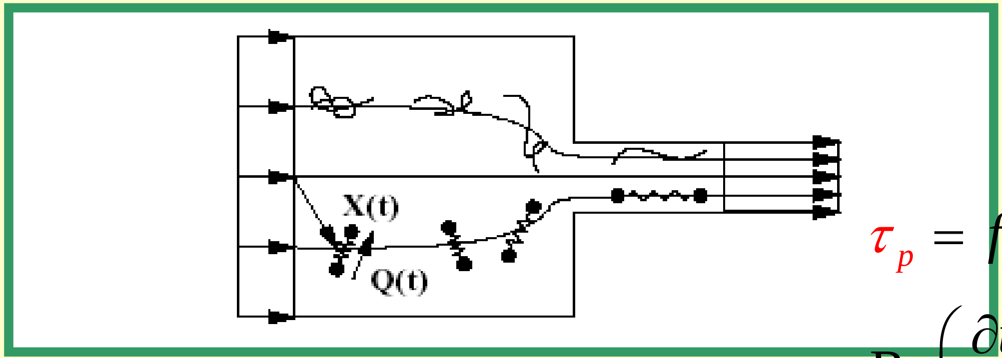


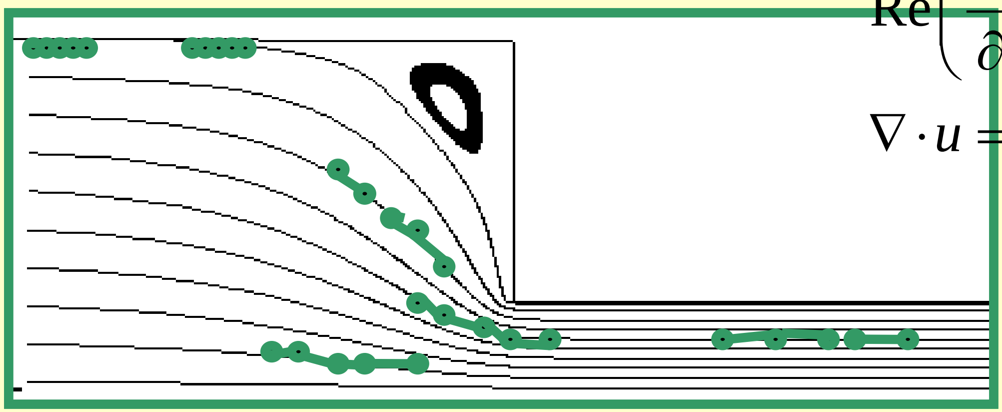
# <u>Modeling</u>: BD, DPD, FPD, LB,…



# Micro-macro simulation



$$\tau_p = f\left(\mathbf{u}, \tau_p, \lambda, \beta, \eta\right)$$

$$\mathrm{Re}\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \nabla \cdot \tau_p + (1-\beta)\nabla^2 u$$

$$\nabla \cdot u = 0$$

**Critical to precise process control**

- precision injection, coating, micro-channel flow …