Rheology of Fluids: Newtonian to Non Newtonian

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Agenda:

- *Fluid: Definition*
- *Rheology: Elementary concepts*
- *Navier-Stokes Equation*
- *Basic Solutions*
- *Dilute Suspension*
- *Non Newtonian*
- *OldRoyd Model*

Fluid:

Deborah number, a measure of fluidity

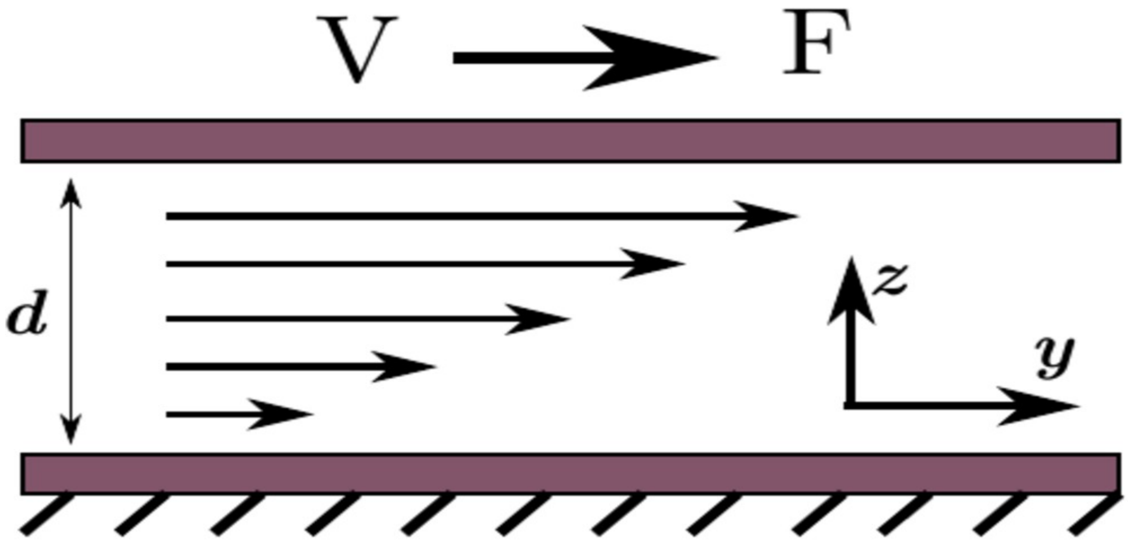
$$De = \frac{\tau_{relax}}{\tau_{exp}}$$

Relaxation time in response to an externally applied force

Observation time

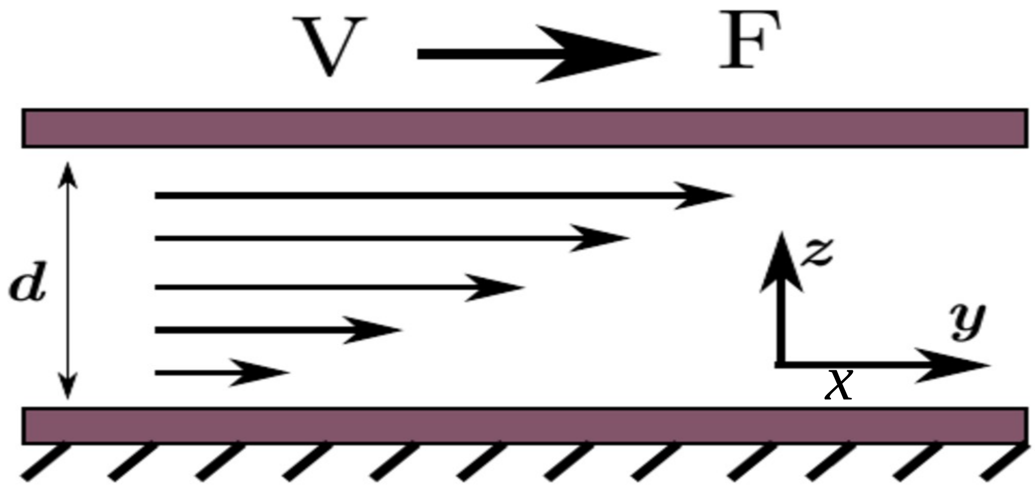
Rheology:

How does the system respond to an external force?



$$F = \Psi(V)$$

Viscosity: *How does the system respond to an externally applied force?*



$$\sigma_{yz} := \frac{F}{A}$$

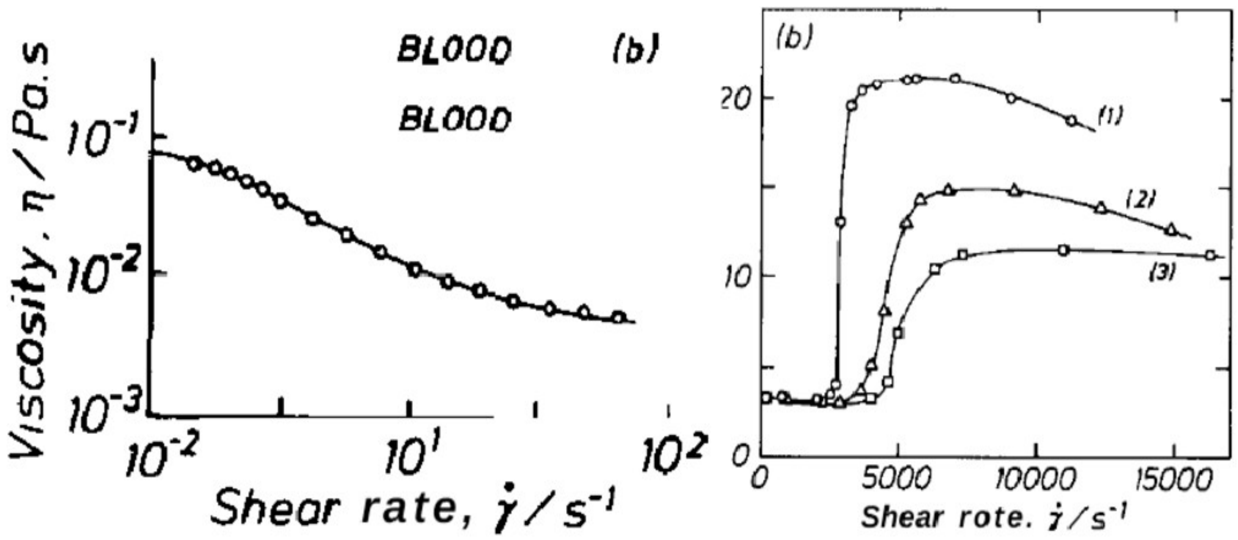
$$\sigma_{yz} = \Psi\left(\frac{\partial u_y}{\partial z}\right)$$

$$\frac{\partial u_y}{\partial z} = \dot{\gamma} = \frac{V - 0}{d}$$

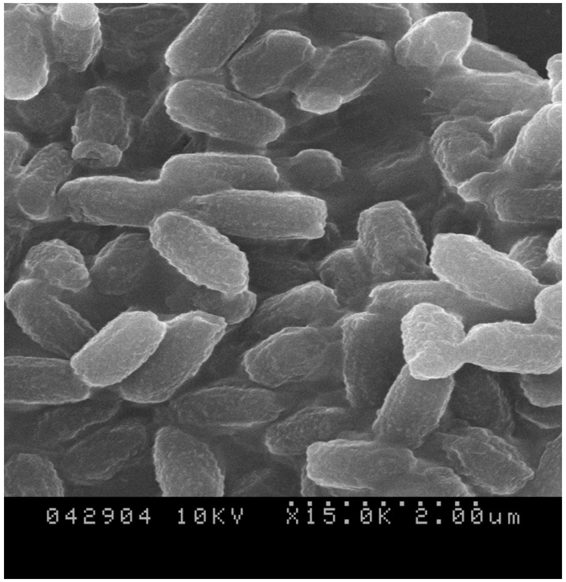
Linear .and. isotropic → Newtonian
Nonlinear .or. anisotropic → Non-Newtonian

$$\sigma_{yz} = \eta \frac{\partial u_y}{\partial z} = \eta \dot{\gamma}$$

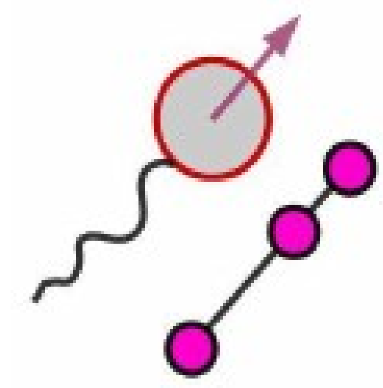
Some examples

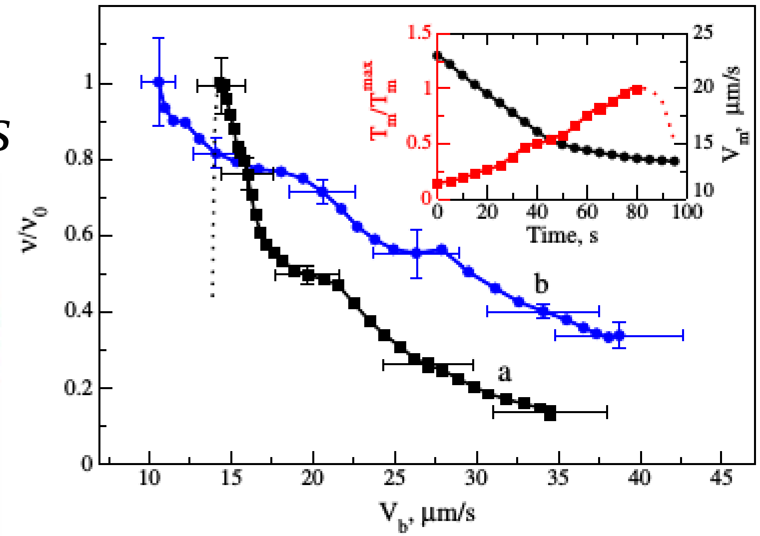


Active Suspensions:



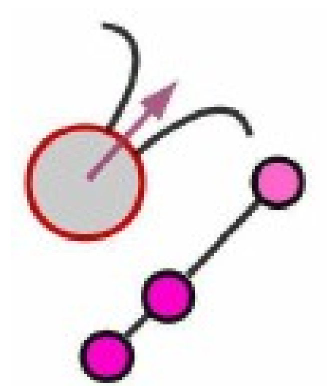
Bacillus Subtilis

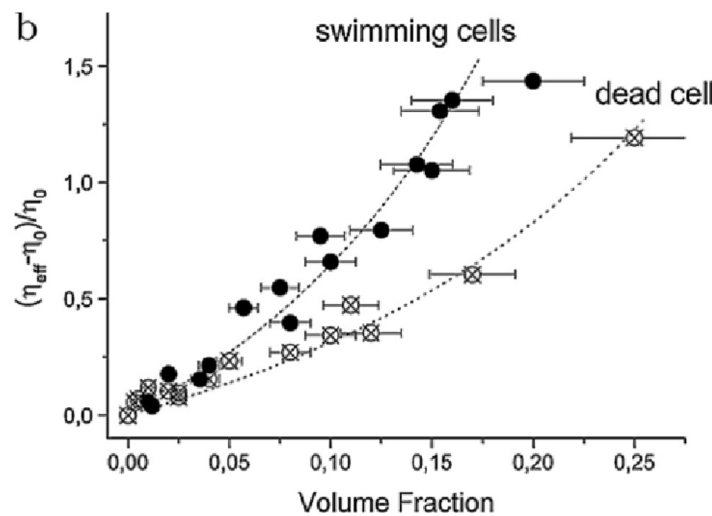




Aranson, PRL 2009

Chlamydomonas

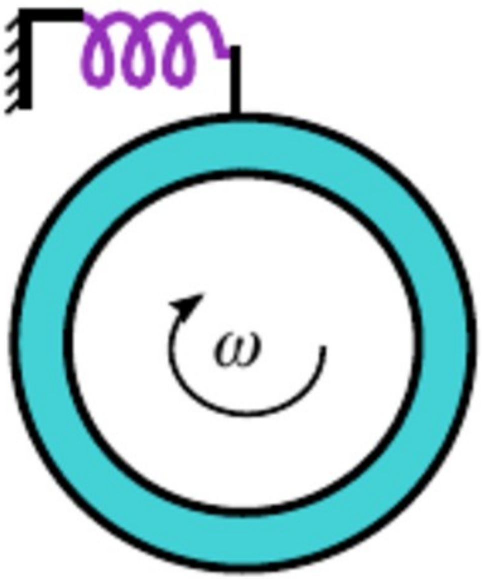


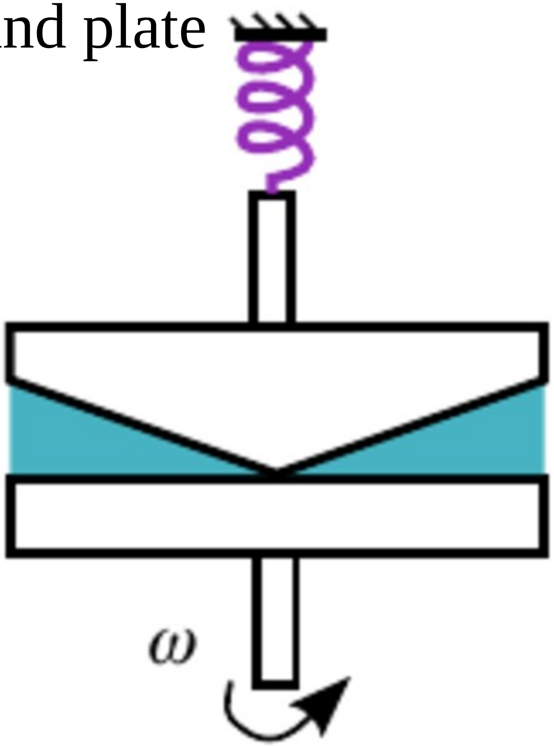


Rafai, PRL 2010

Rheometry: Elementary tools

Two cylinders, cone and plate





Dimensional Analysis for water

$$\eta \sim \frac{m}{lT}$$

Rheometry: Elementary tools

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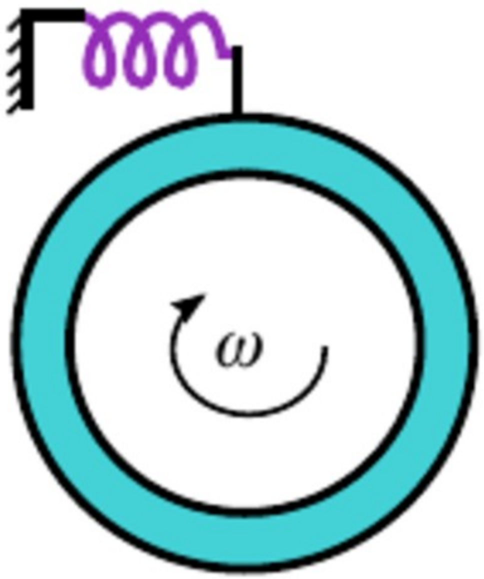

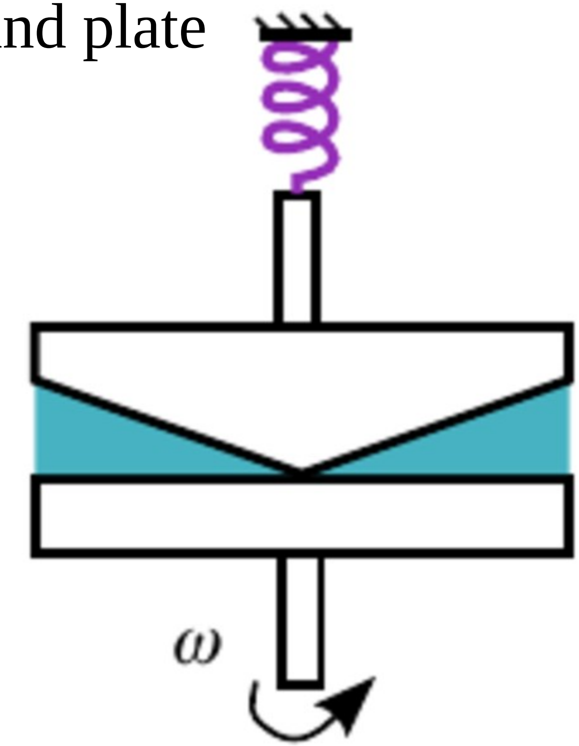

Dimensional Analysis for water

$$\eta \sim \frac{m}{lT}$$

$m \rightarrow ۱۰^{-۲۶} kg$

$l \rightarrow ۱۰^{-۹} m$

Rheometry: Elementary tools

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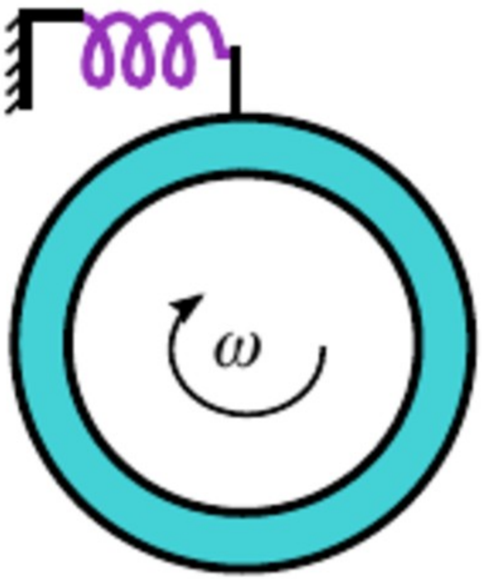
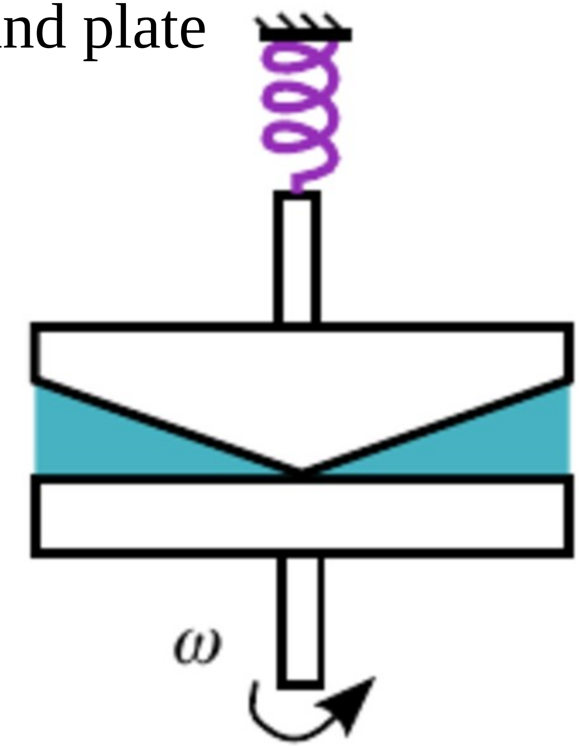




Dimensional Analysis for water

$$\eta \sim \frac{m}{lT}$$

m: $۱۰^{-۲۶} kg$

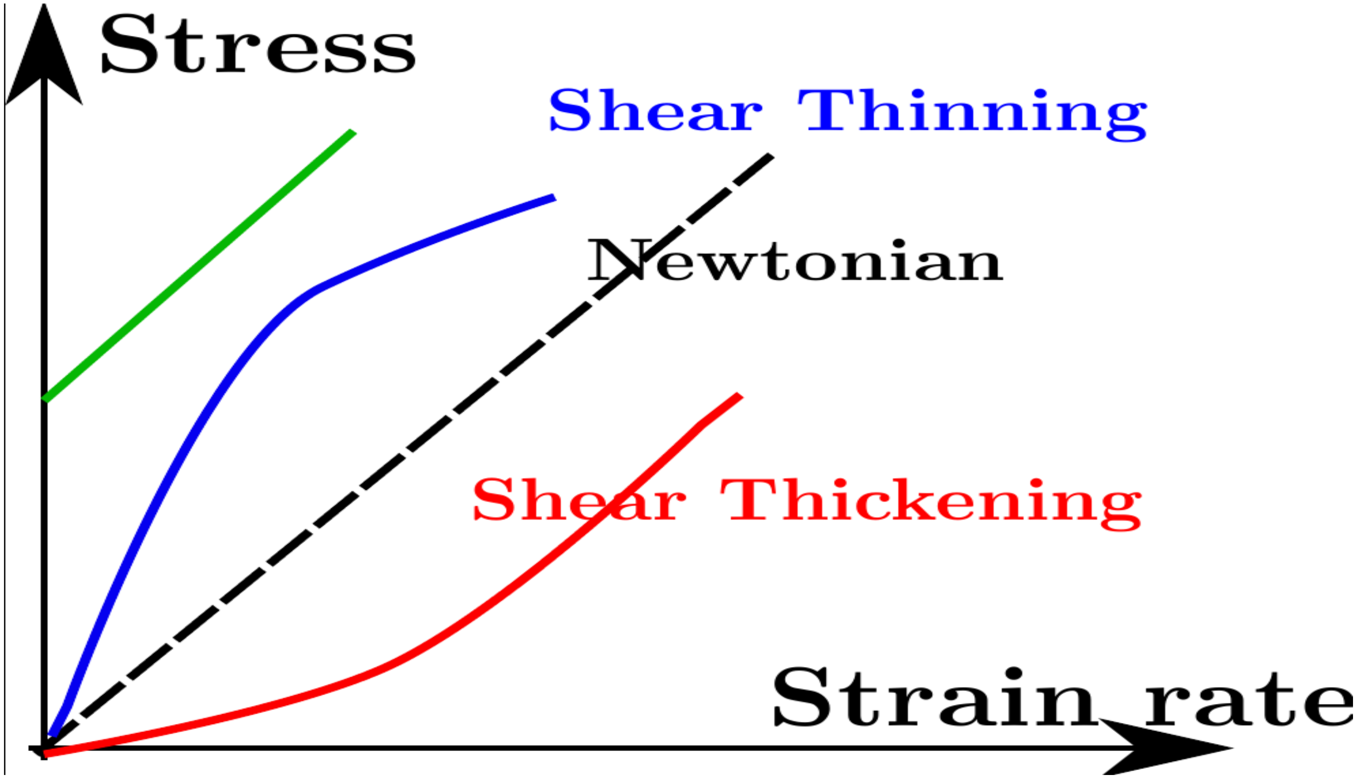
l: $۱۰^{-۹} m$

$\lambda \approx ۱\mu m \rightarrow \omega = c/\lambda \approx ۱۰^{۸}/۱۰^{-۶} = ۱۰^{۱۴}$

$T \approx ۱/\omega = ۱۰^{-۱۴} s$

$$\eta \approx \frac{m}{l\,T} \approx ۱۰^{-۳} Pa.s$$

Non-Newtonian



Toward the governing equations:

Velocity field $\mathbf{u}(\mathbf{x}, t)$

Acceleration field

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Acceleration field

$$a(x,t)=(u(x+\delta x,t+\delta t)-u(x,t))/\delta t=¿$$

$$\frac{d}{dt}\mathbf{u}(\mathbf{x}, t) = \left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{u}(\mathbf{x}, t)$$

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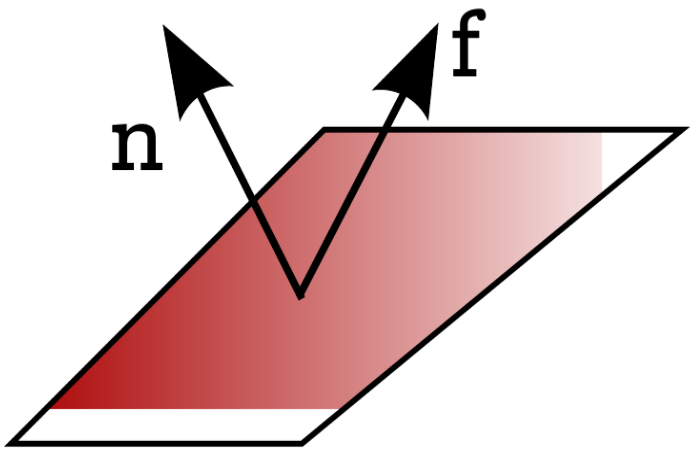
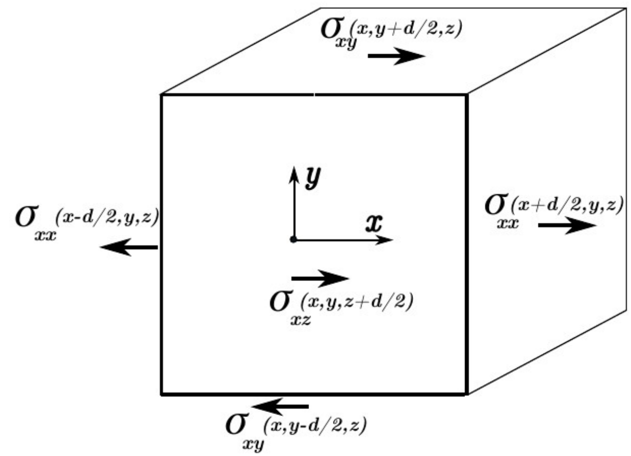
$\sigma_{ij}(\mathbf{x}, t)$ Stress Tensor: i'th component of the the force exerted on a surface that is pointed to j direction



$$df_x = \sigma_{xx} ds_x + \sigma_{xy} ds_y + \sigma_{xz} ds_z$$

$$\mathbf{f} = \oint \sigma \cdot d\mathbf{s}^T,$$

Governing equations



$$\mathbf{u}(\mathbf{x}, t) \qquad \sigma_{ij}(\mathbf{x}, t)$$

$$\nabla \cdot (\rho \mathbf{u}) + \frac{\partial}{\partial t}\rho = ۰$$ Continuity equation

$$\rho(\mathbf{x}, t) \times dv \times \frac{d}{dt}\mathbf{u}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x}, t) \times dv$$

$$\begin{aligned} F_x &= d^{۲} \times [\sigma_{xx}(x + \frac{d}{۲}, y, z) - \sigma_{xx}(x - \frac{d}{۲}, y, z) + \sigma_{xy}(x, y + \frac{d}{۲}, z) \\ &- \sigma_{xy}(x, y - \frac{d}{۲}, z) + \sigma_{xz}(x, y, z + \frac{d}{۲}) - \sigma_{xz}(x, y, z - \frac{d}{۲})]. \quad (۴.۴) \end{aligned}$$

Governing Equations:

$$\sigma_{yz} = \eta \frac{\partial u_y}{\partial z} = \eta \dot{\gamma}$$

Phenomenological model for stress tensor

$$\sigma_{ij} = -P\delta_{ij} + \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

$$\frac{d}{dt}\mathbf{u}(\mathbf{x}, t) = \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u}(\mathbf{x}, t)$$

Hydrodynamics:

Navier-Stokes Equation

$$\rho\left(\frac{\partial}{\partial t}+\mathbf{u}\cdot\nabla\right)\mathbf{u}(\mathbf{x},t)=\eta\nabla^2\mathbf{u}(\mathbf{x},t)-\nabla P(\mathbf{x},t),\qquad \nabla\cdot\mathbf{u}=0$$

The Millennium Prize: 10^6\$,The Clay Mathematics Institute of Cambridge, Massachusetts (CMI)

Colloid's Universe: Low Reynolds Regime:

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0$$

Colloid's Universe: Low Reynolds Regime:

$$\rho\left(\frac{\partial}{\partial t}+\mathbf{u}\cdot\nabla\right)\mathbf{u}=-\nabla p+\eta\nabla^2\mathbf{u},\quad \nabla\cdot\mathbf{u}=0$$

$$\mathcal{R}e=\frac{[\rho(\mathbf{u}\cdot\nabla)\mathbf{u}]}{\eta\nabla^{۲}\mathbf{u}}\approx\frac{\rho V/L}{\eta/L^{۲}}=\frac{\rho VL}{\eta}$$

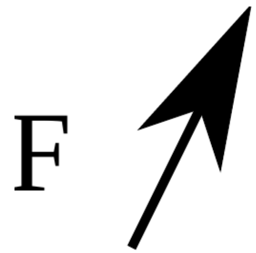
$$L=0.1\mu m,\quad V=1\mu m/S,\quad \eta=10^{-3}\,PaS,\quad \rho=10^{3}\,Kg/m^{3}$$

$$Re\ll 1$$

$$\eta\nabla^{۲}\mathbf{u}(\mathbf{x})-\nabla P(\mathbf{x})=\mathbf{f}(\mathbf{x}),\quad \nabla.\mathbf{u}(\mathbf{x})=۰$$

Hydrodynamics:

$$\eta\nabla^{۲}\mathbf{u}(\mathbf{x}) - \nabla P(\mathbf{x}) = \mathbf{f}(\mathbf{x}), \quad \nabla.\mathbf{u}(\mathbf{x}) = ۰$$



Point force:

$$\mathbf{f}(\mathbf{x}) = \mathbf{F}\delta(\mathbf{x})$$

$$u_i^{۰}(\mathbf{x}) = \sum_j G_{ij}F_j, \qquad \boxed{G_{ij} = \frac{۱}{۸\pi\eta r}(\delta_{ij} + \hat{r}_i\hat{r}_j)}$$

Hydrodynamics:

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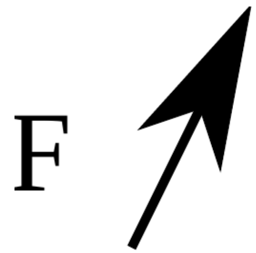
Point force:



$$\mathbf{f}(\mathbf{x}) = \mathbf{F}\delta(\mathbf{x})$$

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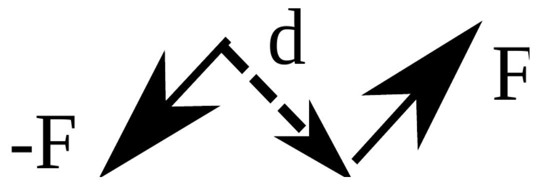
Force Dipole:



$$\mathbf{u}^D = (\mathbf{G}(\mathbf{x}+\mathbf{d}) - \mathbf{G}(\mathbf{x}))\cdot\mathbf{F}$$

$$u_i^D = \sum_{j,k} G_{ijk}^D P_{kj} \qquad P_{kj} = d_k F_j$$

$$G_{ijk}^D = \frac{\partial}{\partial x_k}G_{ij} = \frac{١}{٨\pi\eta r^{٢}}\left(\delta_{ij}\hat{r}_k - \delta_{ik}\hat{r}_j + \delta_{jk}\hat{r}_i + ٣\hat{r}_i\hat{r}_j\hat{r}_k\right)$$

Multipole Expansion:

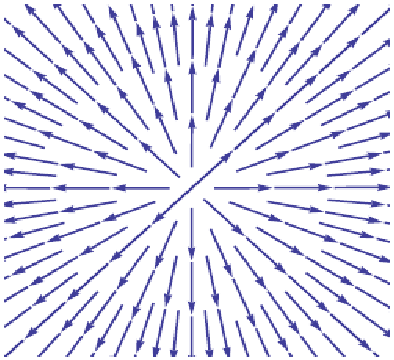
$$u_i(\mathbf{x}) = \sum_j G_{ij} b_j + \sum_{j,k} G^D_{ijk} p_{jk} + \sum_{j,k,l} G^Q_{ijkl} t_{jkl} + \text{چند قطبی‌های مراتب بالاتر}$$

$$G_{ij} = \frac{۱}{۸\pi\eta r}(\delta_{ij} + \hat{r}_i\hat{r}_j)$$

$$G^D_{ijk} = \frac{\partial}{\partial x_k} G_{ij}$$

$$G^Q_{ijlm} = \frac{\partial}{\partial x_m} G^D_{ijl}$$

Sink and Source another singular solutions:



$$u_i^s = \frac{\hat{r}}{۴\pi r^۲}$$

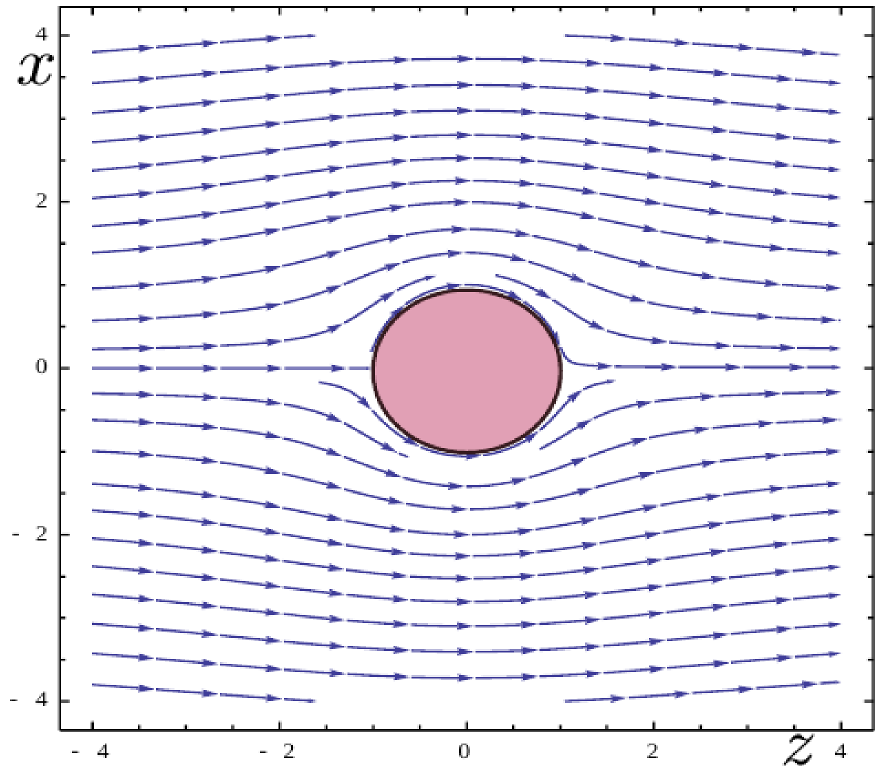
$$u_i(\mathbf{x}) = Q u_i^s + \sum_j P_j \frac{\partial}{\partial x_j} u_i^s + \sum_{j,k} T_{jk} \frac{\partial^۲}{\partial x_j \partial x_k} u_i^s + \cdots$$

$$\frac{\partial}{\partial x_j} u_i^s = \frac{۱}{۴\pi r^۳} (\delta_{ij} - ۳\hat{r}_i \hat{r}_j)$$

Moving Sphere:

$$u_i(\mathbf{x}) = \sum_j \left(b_j G_{ij} + P_j \frac{\partial}{\partial x_j} u_i^s \right)$$

$$\mathbf{u}(\mathbf{x})|_{\mathbf{x}=R} = \mathbf{V}。$$



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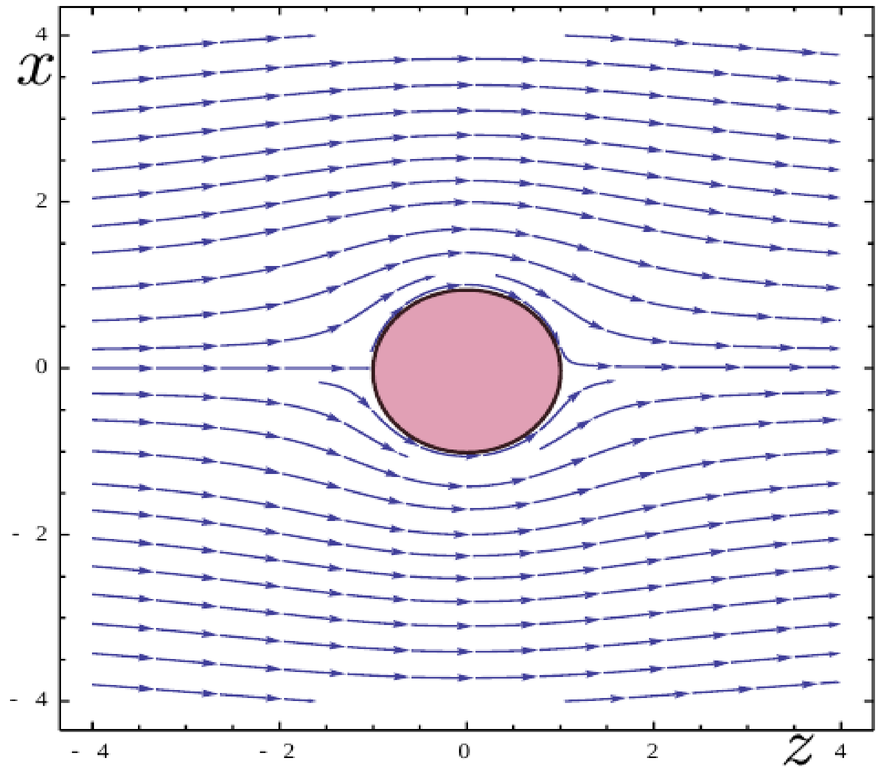


$$\mathbf{P} = \pi R^{۳} \mathbf{V}_{۰}, \quad \boxed{\mathbf{b} = ۶\pi\eta R \mathbf{V}_{۰}}$$

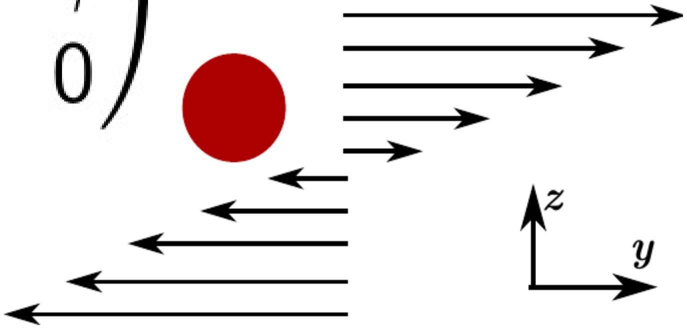
$$\mathbf{u}(\mathbf{r}) = \left(\frac{۳}{۴} \left(\frac{R}{r}\right) (I + \hat{r}\hat{r}) + \frac{۱}{۴} \left(\frac{R}{r}\right)^{۳} (I - ۳\hat{r}\hat{r}) \right) \cdot \mathbf{V}.$$

Sphere in shear flow:

$$\mathbf{u}^{\infty}(\mathbf{x}) = \mathbf{\Gamma} \cdot \mathbf{x}$$

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}^{\infty}(\mathbf{x}) + \mathbf{u}'(\mathbf{x})$$

$$\mathbf{\Gamma} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \dot{\gamma} \\ 0 & 0 & 0 \end{pmatrix}$$



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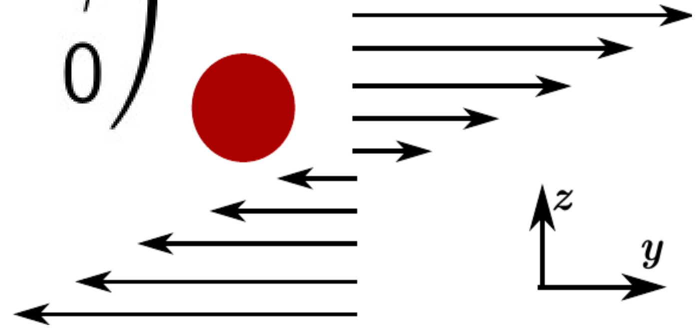

$$\mathbf{u}'(\mathbf{x}) = 0, \quad x \to \infty$$
$$\mathbf{u}'(\mathbf{x}) = -\mathbf{\Gamma} \cdot \mathbf{x}, \quad x \to a$$

$$\mathbf{u}'(\mathbf{x}) = \text{Force Dipole} + \text{Sourse Quadrapole}$$

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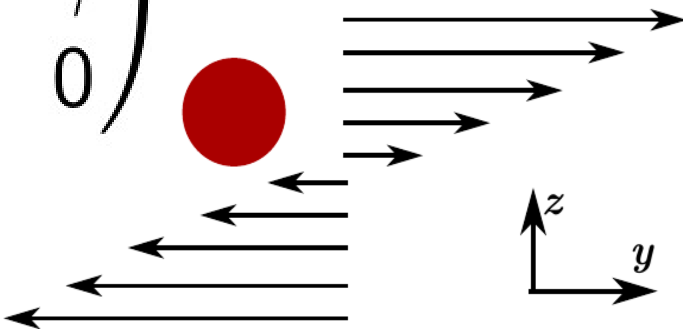

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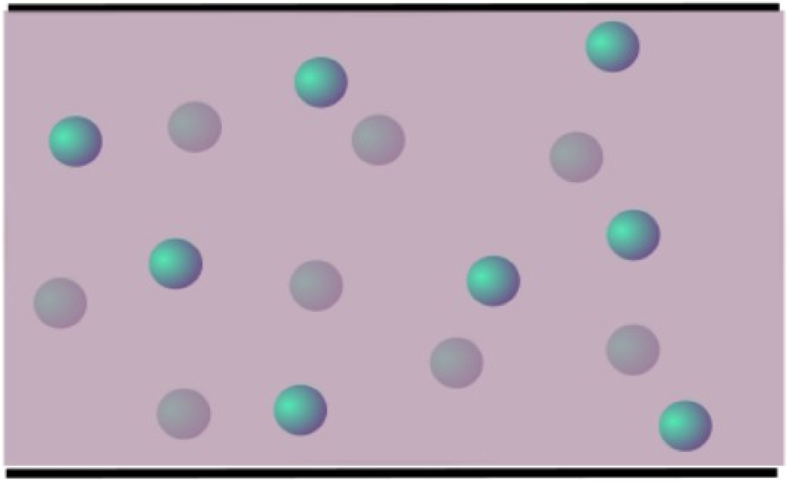
$$u'_i = G^D_{ijl} d_{jl} + Q_{ijl} q_{jl} \qquad G^D_{ijl} = \partial_l G_{ij} \quad Q_{ijl} = \partial_j \partial_l u^s_i$$

$$\mathbf{d} = -\frac{5}{a^2}\mathbf{q} = -\frac{a^3}{6}(4\mathbf{\Gamma} + \mathbf{\Gamma}^T)$$

$$S = 8\pi\eta\frac{1}{2}(\mathbf{d} + \mathbf{d}^T) = -\frac{20}{6}\eta a^3(\mathbf{\Gamma} + \mathbf{\Gamma}^T)$$

Passive suspension: Einstein's theory

$$\eta^{\mathrm{eff}} \sim \frac{\Sigma}{\nabla \mathbf{u}} \quad ?$$



In the presence of colloids, the applied force should do much work to establish the same velocity profile as in the bare fluid

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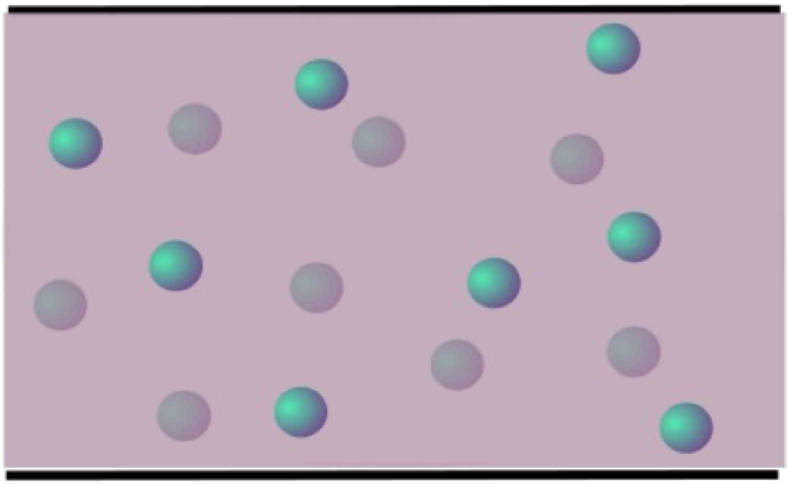

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Einstein 1906

$$\eta^{\text{eff}} = \eta\left(1 + \frac{5}{2}c + \mathcal{O}(c)^2\right)$$

Passive suspension: Einstein's theory

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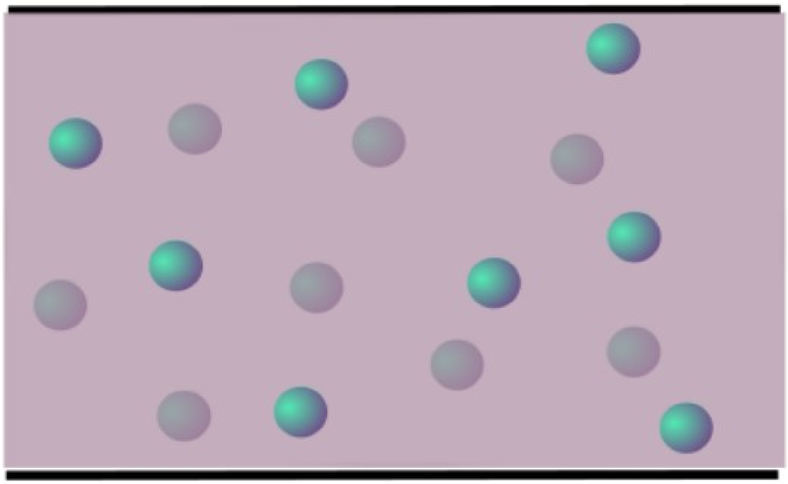
?



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Perrin+Einstein 1909

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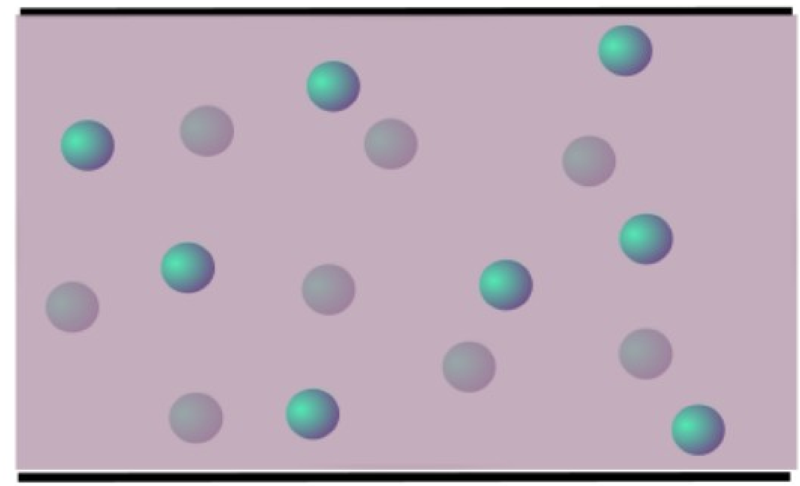

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Perrin+Einstein 1909

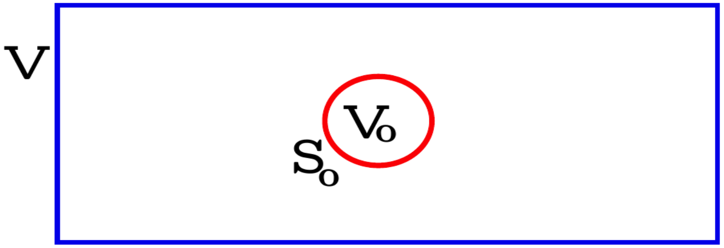
Einstein 1906

Interactions: Batchelor 1972

$$\eta^{\text{eff}} = \eta\left(1 + \frac{5}{2}c + \mathcal{O}(c)^2\right)$$

Fluctuations: Batchelor 1977

$$\sigma_{ij} = -P\delta_{ij} + \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$



$$\langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij} dv = \frac{1}{V} \int_{V-V_0} \sigma_{ij} dv + \frac{1}{V} \int_{V_0} \sigma_{ij} dv$$

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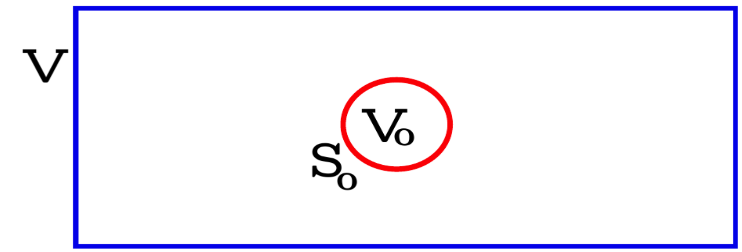

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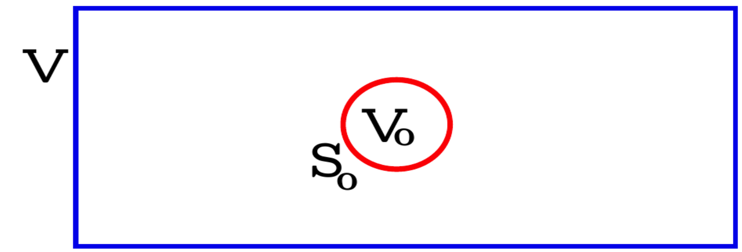
$$\int_V \partial_k (\sigma_{kj} x_i) = \int_V (\partial_k \sigma_{kj}) x_i + \int_V \sigma_{kj} \delta_{ki}$$

$$\oint_S \sigma_{kj} x_i n_k = 0 + \int_V \sigma_{ij}$$

$$= \frac{1}{V} \int_{V-V_0} \sigma_{ij} dv + \frac{1}{V} \int_{S_0} x_i \sigma_{jk} n_k ds$$

$$\sigma_{ij} = -P\delta_{ij} + \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$



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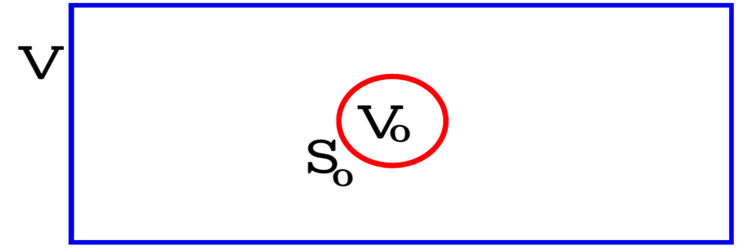
$$\oint_S \sigma_{kj} x_i n_k = 0 + \int_V \sigma_{ij}$$

$$= \frac{1}{V}\int_{V-V_0} \sigma_{ij} dv + \frac{1}{V}\int_{S_0} x_i \sigma_{jk} n_k ds$$

$$= \frac{1}{V}\int_{V-V_0} (-P\delta_{ij} + \eta(\partial_i u_j + \partial_j u_i)) dv + \frac{1}{V}\int_{S_0} x_i f_j ds \qquad f_i = \sigma_{ik} n_k$$

$$\sigma_{ij} = -P\delta_{ij} + \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$



$$\langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij} dv = \frac{1}{V} \int_{V-V_0} \sigma_{ij} dv + \frac{1}{V} \int_{V_0} \sigma_{ij} dv$$

$$\int_V \partial_k (\sigma_{kj} x_i) = \int_V (\partial_k \sigma_{kj}) x_i + \int_V \sigma_{kj} \delta_{ki}$$

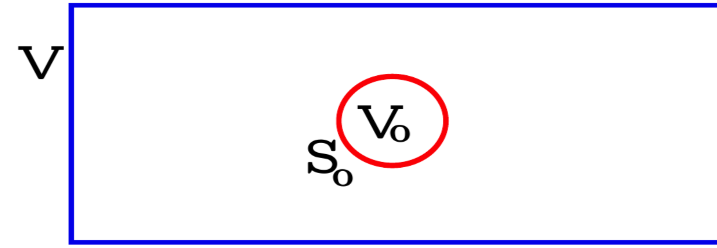
$$\oint_S \sigma_{kj} x_i n_k = 0 + \int_V \sigma_{ij}$$

$$= \frac{1}{V} \int_{V-V_0} \sigma_{ij} dv + \frac{1}{V} \int_{S_0} x_i \sigma_{jk} n_k ds$$

$$= \frac{1}{V} \int_{V-V_0} (-P\delta_{ij} + \eta(\partial_i u_j + \partial_j u_i)) dv + \frac{1}{V} \int_{S_0} x_i f_j ds \qquad f_i = \sigma_{ik} n_k$$

$$= \frac{1}{V} \delta_{ij} \int_{V-V_0} P dv + \eta \langle (\partial_i u_j + \partial_j u_i) \rangle + \frac{1}{V} \int_{S_0} (x_i f_j - \eta(u_i n_j + u_j n_i)) ds$$

$$\sigma_{ij} = -P\delta_{ij} + \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$



$$\langle\sigma_{ij}\rangle = \frac{1}{V}\int_V \sigma_{ij}dv = \frac{1}{V}\int_{V-V_0}\sigma_{ij}dv + \frac{1}{V}\int_{V_0}\sigma_{ij}dv$$

$$\int_V \partial_k(\sigma_{kj}x_i) = \int_V (\partial_k\sigma_{kj})x_i + \int_V \sigma_{kj}\delta_{ki}$$

$$\oint_S \sigma_{kj}x_i n_k = 0 + \int_V \sigma_{ij}$$

$$= \frac{1}{V}\int_{V-V_0}\sigma_{ij}dv + \frac{1}{V}\int_{S_0} x_i\sigma_{jk}n_k ds$$

$$= \frac{1}{V}\int_{V-V_0}(-P\delta_{ij} + \eta(\partial_i u_j + \partial_j u_i))dv + \frac{1}{V}\int_{S_0} x_i f_j ds \qquad f_j = \sigma_{jk}n_k$$

$$= \frac{1}{V}\delta_{ij}\int_{V-V_0} Pdv + \eta\langle(\partial_i u_j + \partial_j u_i)\rangle + \frac{1}{V}\int_{S_0}(x_i f_j - \eta(u_i n_j + u_j n_i))ds$$

$$= \frac{1}{V}\delta_{ij}\int_{V-V_0} Pdv + \eta\langle(\partial_i u_j + \partial_j u_i)\rangle + \frac{1}{V}S_{ij}$$

Force Dipole

Simple shear flow

$$\mathbf{u}(\mathbf{x}) = \mathbf{\Gamma} \cdot \mathbf{x}$$

$$\eta\langle(\partial_i u_j + \partial_j u_i)\rangle + \frac{1}{V} S_{ij} = \eta(\mathbf{\Gamma} + \mathbf{\Gamma}^T) + 0$$

Simple shear flow

$$\mathbf{u}(\mathbf{x}) = \mathbf{\Gamma} \cdot \mathbf{x}$$

$$\eta\langle(\partial_i u_j + \partial_j u_i)\rangle + \frac{1}{V} S_{ij} = \eta(\mathbf{\Gamma} + \mathbf{\Gamma}^T) + 0$$

Simple shear flow + Sphere

$$\eta\langle(\partial_i u_j + \partial_j u_i)\rangle + \frac{1}{V} S_{ij} = \eta(\mathbf{\Gamma} + \mathbf{\Gamma}^T) + \frac{1}{V}\frac{20\pi}{6}\eta a^3(\mathbf{\Gamma} + \mathbf{\Gamma}^T)$$

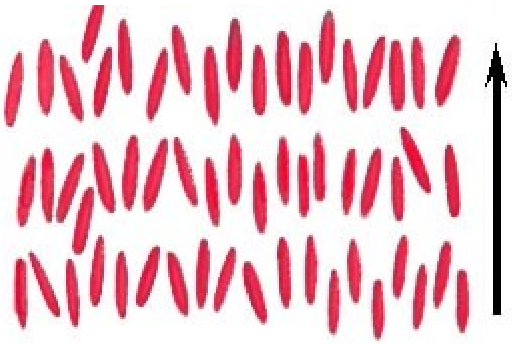
$$\boxed{\eta \to (1 + 5/2\phi)\eta}$$

$$\phi = N(\frac{4}{3}\pi a^3)/(V)$$

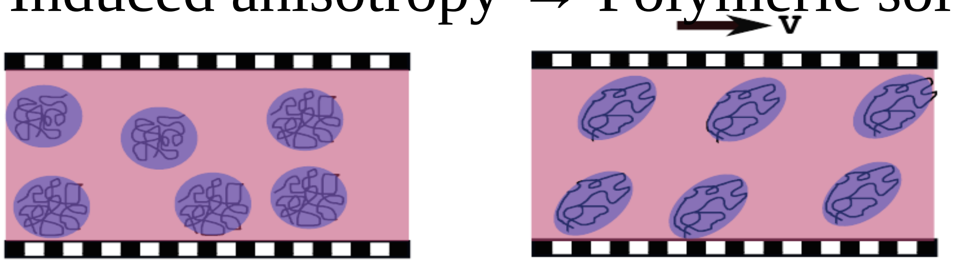
Non Newtonian Behavior:

Microscopic anisotropy

I: Intrinsic → Liquid Crystal



II: Induced anisotropy → Polymeric solutions



Non Newtonian Behavior:

Microscopic anisotropy

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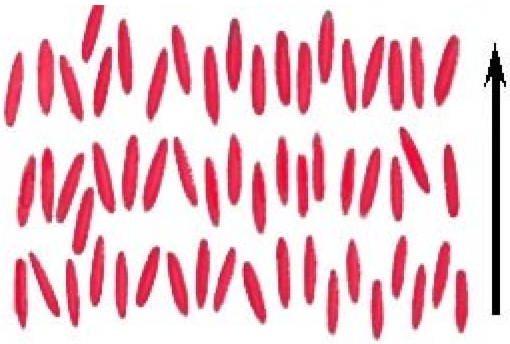
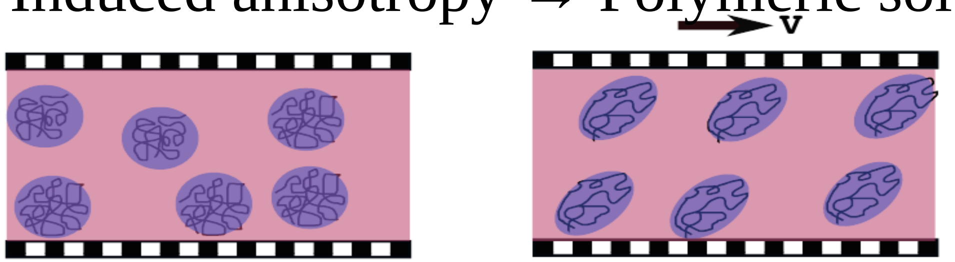


II: Induced anisotropy → Polymeric solutions



Molecular relaxation time

Time scale for external force

$\dot{\gamma}^{-۱} < \tau$ → N-N

Molecules will not have enough time to response and reach their isotropic structure

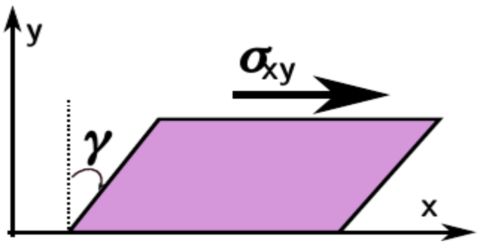
Relaxation time for water=$۱۰^{-۱۲} s$

We expect to see N-N behavior in water for frequencies >$۱۰^{۱۲} Hz$

Phenomenological Description:

$$\sigma_{xy} = \eta(\dot{\gamma})\dot{\gamma}, \qquad \sigma_{xz} = \sigma_{zy} = ۰,$$

$$\sigma_{xx} - \sigma_{yy} = N_{۱}(\dot{\gamma}), \qquad \sigma_{yy} - \sigma_{zz} = N_{۲}(\dot{\gamma})$$



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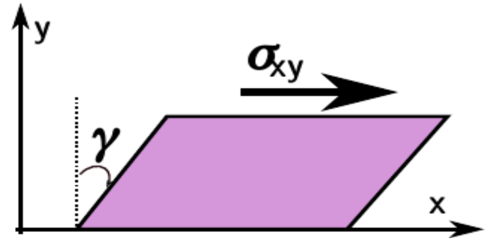
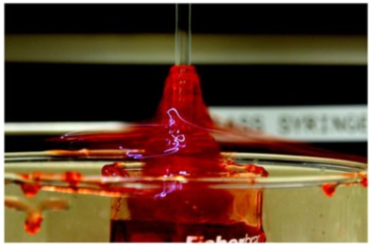


Normal Stress Differences

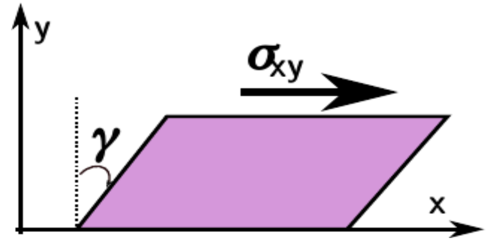
Macroscopic Manifestation:
Weisenberg Effect



Phenomenological Description:

$$\sigma_{xy} = \eta(\dot{\gamma})\dot{\gamma}, \qquad \sigma_{xz} = \sigma_{zy} = 0,$$

$$\sigma_{xx} - \sigma_{yy} = N_1(\dot{\gamma}), \qquad \sigma_{yy} - \sigma_{zz} = N_2(\dot{\gamma})$$



Normal Stress Differences Macroscopic Manifestation:
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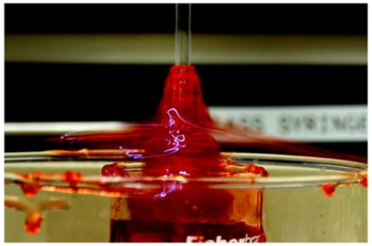


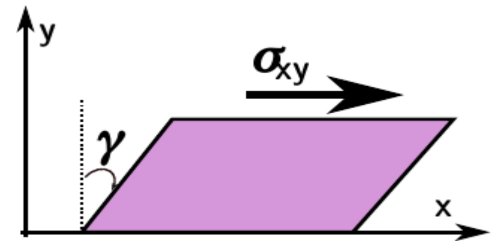
Shear thickening: Viscosity increases by increasing external shear
برش وشکسان: نشاسته ذرت و آب

Shear thinning: Viscosity decreases by increasing external shear
برش روان: سس گوجه

Phenomenological Description:

$$\sigma_{xy} = \eta(\dot{\gamma})\dot{\gamma}, \qquad \sigma_{xz} = \sigma_{zy} = 0,$$

$$\sigma_{xx} - \sigma_{yy} = N_1(\dot{\gamma}), \qquad \sigma_{yy} - \sigma_{zz} = N_2(\dot{\gamma})$$



Normal Stress Differences Macroscopic Manifestation:
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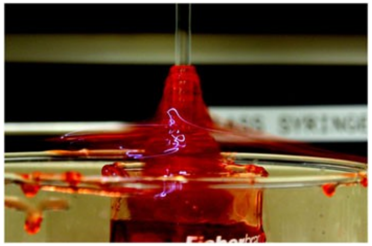

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Shear thinning: Viscosity decreases by increasing external shear
برش روان: سس گوجه

Viscoelastic Behavior → Kelvin Voigt Model

$$\sigma = G\gamma + \eta\dot{\gamma}$$

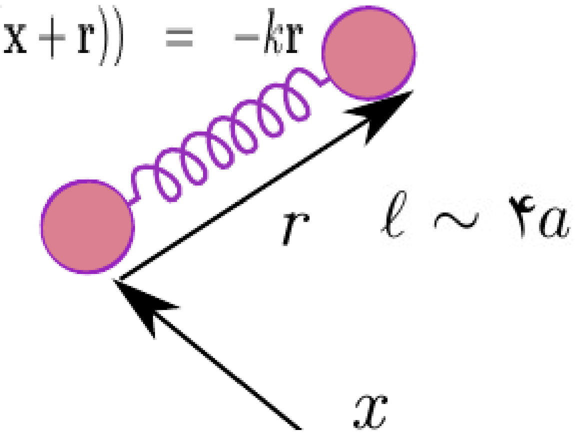
$$\gamma(t) = \gamma_0 e^{-i\omega t}$$

$$\sigma(t) = \tilde{G}(\omega)\gamma(t)$$
$$\tilde{G}(\omega) = G - i\omega\eta$$

Molecular Anisotropy: Microscopic Model

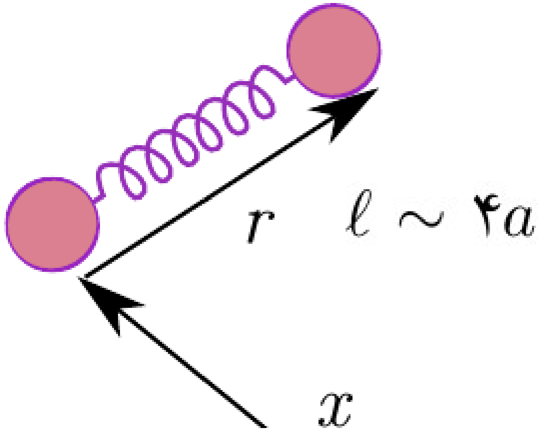
$$
\begin{aligned}
۶\pi\eta a(\mathbf{V}_۱ - \mathbf{u}(\mathbf{x})) &= k\mathbf{r}, \\
۶\pi\eta a(\mathbf{V}_۲ - \mathbf{u}(\mathbf{x}+\mathbf{r})) &= -k\mathbf{r}
\end{aligned}
$$

$$۶\pi\eta a(\mathbf{V}_۲ - \mathbf{V}_۱ - \mathbf{u}(x+\mathbf{r}) + \mathbf{u}(x)) = -۲k\mathbf{r}$$



Molecular Anisotropy: Microscopic Model

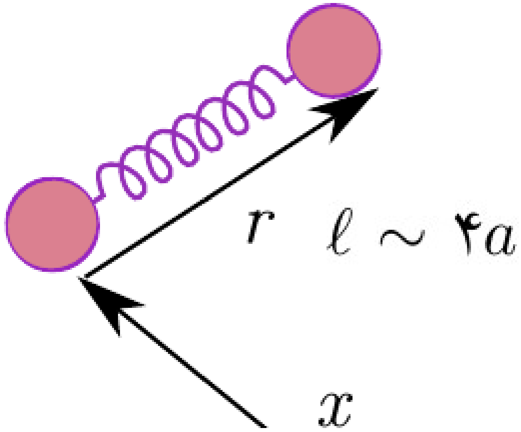
$$6\pi\eta a(\mathbf{V}_2 - \mathbf{V}_1 - \mathbf{u}(x+\mathbf{r}) + \mathbf{u}(x)) = -2k\mathbf{r}$$
$$6\pi\eta a\frac{d}{dt}\mathbf{r} = -2k\mathbf{r} + 6\pi\eta a(\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x})$$



Molecular Anisotropy: Microscopic Model

$$۶\pi\eta a(\mathbf{V}_۲ - \mathbf{V}_۱ - \mathbf{u}(x+\mathbf{r}) + \mathbf{u}(x)) = -۲k\mathbf{r}$$

$$۶\pi\eta a\frac{d}{dt}\mathbf{r} = -۲k\mathbf{r} + ۶\pi\eta a(\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x})$$



$$\frac{d}{dt}\mathbf{r} = -\frac{۱}{۲\tau}\mathbf{r} + (\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x}) + (\frac{۱}{۶\pi\eta a})\mathbf{f}(t)$$

$$\tau = ۶\pi\eta a/۴k$$

$$\langle f_i(t)f_j(t')\rangle = ۲\xi k_B T\delta_{ij}\delta(t-t')$$

Molecular Anisotropy: Microscopic Model

$$6\pi\eta a(\mathbf{V}_2 - \mathbf{V}_1 - \mathbf{u}(x+\mathbf{r}) + \mathbf{u}(x)) = -2k\mathbf{r}$$
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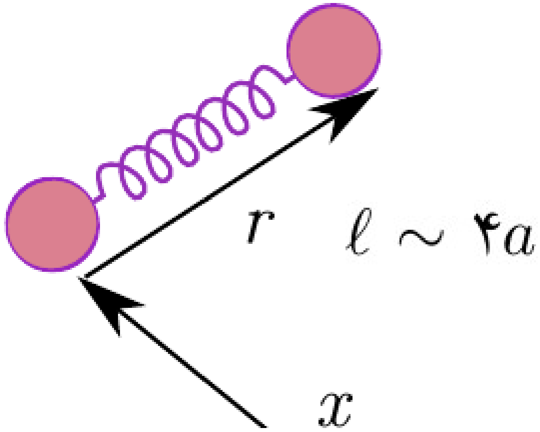

$$\frac{d}{dt}\mathbf{r} = -\frac{1}{2\tau}\mathbf{r} + (\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x}) + (\frac{1}{6\pi\eta a})\mathbf{f}(t)$$
$$\langle f_i(t) f_j(t')\rangle = 2\xi k_B T \delta_{ij}\delta(t-t')$$

$$\tau = 6\pi\eta a/4k$$

$$\sigma^P \cdot d\mathbf{s} = (k\mathbf{r})(\mathcal{N}\mathbf{r}\cdot d\mathbf{s}) \qquad \sigma^P = \mathcal{N}k\mathbf{r}\mathbf{r} \qquad \mathbf{r} = \mathbf{r}(\mathbf{x}, t)$$

Molecular Anisotropy: Microscopic Model

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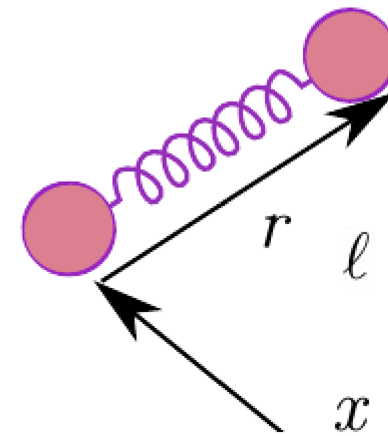

$$\ell \sim ۴a$$

$$\frac{d}{dt}\mathbf{r} = -\frac{۱}{۲\tau}\mathbf{r} + (\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x}) + (\frac{۱}{۶\pi\eta a})\mathbf{f}(t)$$

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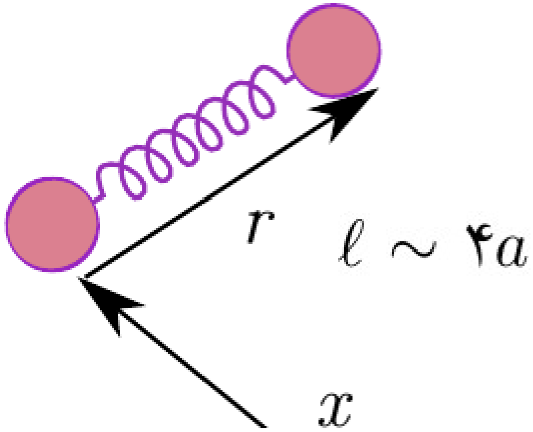

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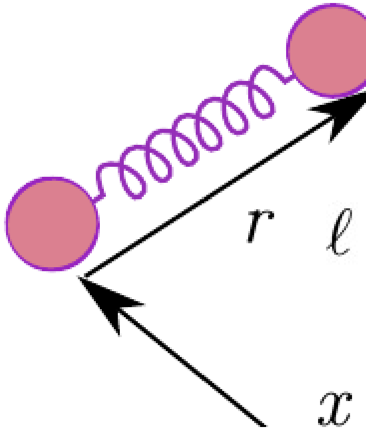

$$\frac{d}{dt}\mathbf{r} = -\frac{۱}{۲\tau}\mathbf{r} + (\mathbf{r}\cdot\nabla)\mathbf{u}(\mathbf{x}) + (\frac{۱}{۶\pi\eta a})\mathbf{f}(t)$$
$$\langle f_i(t)f_j(t')\rangle = ۲\xi k_B T\delta_{ij}\delta(t-t')$$

$$\tau = ۶\pi\eta a/۴k$$

$$\sigma^P\cdot d\mathbf{s} = (k\mathbf{r})(\mathcal{N}\mathbf{r}\cdot d\mathbf{s}) \qquad \sigma^P = \mathcal{N}k\mathbf{r}\mathbf{r} \qquad \mathbf{r} = \mathbf{r}(\mathbf{x},t)$$

After averaging over noise, it is easy to show: $\mathbf{\Sigma} = \frac{۲}{\mathcal{N}k_B T}\sigma^P$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{\Sigma} - \mathbf{\Sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\mathbf{\Sigma} = -\frac{۱}{\tau}(\mathbf{\Sigma} - I)$$

OldRoyd Model

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{u} = \nabla\cdot\sigma, \qquad \nabla\cdot\mathbf{u} = 0,$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\boldsymbol{\Sigma} - \boldsymbol{\Sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\boldsymbol{\Sigma} = -\frac{1}{\tau}(\boldsymbol{\Sigma} - I)$$

$$\sigma = -PI + \eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + g\boldsymbol{\Sigma} \qquad g = \frac{1}{2}\mathcal{N}k_B T$$

OldRoyd Model

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{u} = \nabla\cdot\sigma, \qquad \nabla\cdot\mathbf{u} = 0,$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{\Sigma} - \mathbf{\Sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\mathbf{\Sigma} = -\frac{1}{\tau}(\mathbf{\Sigma} - I)$$

$$\sigma = -PI + \eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + g\mathbf{\Sigma} \qquad g = \tfrac{1}{2}\mathcal{N}k_B T$$

Response to a simple shear flow:

$$\mathbf{u} = (\dot{\gamma}y, 0, 0) \qquad \nabla\mathbf{u} = \begin{pmatrix} 0 & 0 \\ \dot{\gamma} & 0 \end{pmatrix} \qquad \mathbf{\Sigma} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_{yy} \end{pmatrix}$$

OldRoyd Model

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{u} = \nabla\cdot\sigma, \qquad \nabla\cdot\mathbf{u} = \circ,$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{\Sigma} - \mathbf{\Sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\mathbf{\Sigma} = -\frac{\text{۱}}{\tau}(\mathbf{\Sigma} - I)$$

$$\sigma = -PI + \eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + g\mathbf{\Sigma} \qquad g = \tfrac{\text{۱}}{\text{۲}}\mathcal{N}k_B T$$

Response to a simple shear flow:

$$\mathbf{u} = (\dot{\gamma}y, \circ, \circ) \qquad \nabla\mathbf{u} = \begin{pmatrix} \circ & \circ \\ \dot{\gamma} & \circ \end{pmatrix} \qquad \mathbf{\Sigma} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_{yy} \end{pmatrix}$$

$$\dot{\gamma}\begin{pmatrix} \text{۲}\Sigma_{xy} & \Sigma_{yy} \\ \Sigma_{yy} & \circ \end{pmatrix} = \frac{\text{۱}}{\tau}\begin{pmatrix} \Sigma_{xx} - \text{۱} & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_{yy} - \text{۱} \end{pmatrix}$$

OldRoyd Model

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{u} = \nabla\cdot\sigma, \qquad \nabla\cdot\mathbf{u} = ۰,$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\mathbf{\Sigma} - \mathbf{\Sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\mathbf{\Sigma} = -\frac{۱}{\tau}(\mathbf{\Sigma} - I)$$

$$\sigma = -PI + \eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + g\mathbf{\Sigma} \qquad g = \tfrac{۱}{۲}\mathcal{N}k_BT$$

Response to a simple shear flow:

$$\mathbf{u} = (\dot\gamma y, ۰, ۰) \qquad \nabla\mathbf{u} = \begin{pmatrix} ۰ & ۰ \\ \dot\gamma & ۰ \end{pmatrix} \qquad \mathbf{\Sigma} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_{yy} \end{pmatrix}$$

$$\dot\gamma\begin{pmatrix} ۲\Sigma_{xy} & \Sigma_{yy} \\ \Sigma_{yy} & ۰ \end{pmatrix} = \frac{۱}{\tau}\begin{pmatrix} \Sigma_{xx} - ۱ & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_{yy} - ۱ \end{pmatrix}$$

$$\Sigma_{xx} = ۱ + ۲\dot\gamma^۲\tau^۲, \qquad \Sigma_{xy} = \dot\gamma\tau, \qquad \Sigma_{yy} = ۱ \qquad\qquad \tau = ۶\pi\eta a/۴k$$

$$\sigma = \begin{pmatrix} -P & \eta\dot\gamma \\ \eta\dot\gamma & -P \end{pmatrix} + g\begin{pmatrix} ۱ + ۲\dot\gamma^۲\tau^۲ & \dot\gamma\tau \\ \dot\gamma\tau & ۱ \end{pmatrix}$$

$$N_۱ = \sigma_{xx} - \sigma_{yy} = ۲g\dot\gamma^۲\tau^۲$$

$$\eta_e = \eta + g\tau = \eta(۱ + \epsilon)$$

$$\epsilon = (۳/۴)\pi\mathcal{N}k_BTa/k$$

Response to an harmonic shear flow:

$$\mathbf{u} = (\dot{\gamma} y, \circ, \circ)$$

$$\dot{\gamma}(t) = a\omega \cos \omega t$$

$$\sigma_{xy} = \tilde{G}(\omega)\gamma(t)$$

$$\tilde{G}(\omega) = G_r(\omega) + iG_i(\omega)$$

$$G_r(\omega) = ?$$

$$G_i(\omega) = ?$$

از توجه شما ممنونم