Constitutively Complex Fluids: Transport Properties and Simulations

Multiscale Nonlinearity Protocols for Highly Entangled Polymers

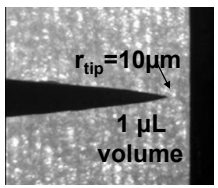
M.G. FOREST,[a] G. MILLER,[b] S. MITRAN,[a] D. TREBOTICH,[c] P. VASQUEZ,[a]

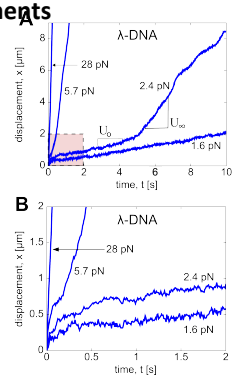
[a]*Department of Mathematics, University of North Carolina, Chapel Hill, NC 27516*

[b]*Department of Applied Science, University of California, Davis, CA 95616*

[c]*Lawrence Berkeley National Laboratory, Berkeley, CA 94720*

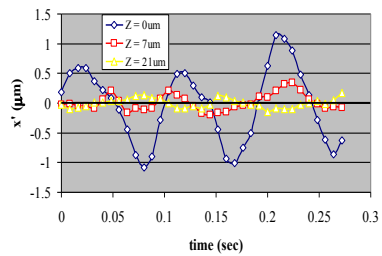
Micron-scale driven magnetic microbead experiments

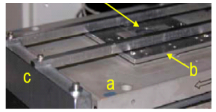




The experimental signature, a bead acceleration phase, is captured by Rolie-Poly model stress-dynamics simulations. The phenomenon is thereby: understood as a nonlinear stress overshoot & relaxation due to a tunable competition between molecular entanglement force and time scales.

Millimeter scale shear wave experiments w/ passive tracer beads





The observable signature of nonlinearity is harmonic generation by FFT of passive tracer bead tracking. With RP model simulations of shear stress-velocity waves in finite depth layers, we fit to tracer time series to infer entanglement timescales and determine nonlinear penetration depth in millimeter thick layers.

•Conservation of momentum

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = \frac{1}{\mathrm{Re}}\nabla\cdot(-p\mathbf{I}+\boldsymbol{\tau})$$

•Variables

$$p = p(y,t), \quad v_x = v_x(y,t), \quad v_y = 0, \quad v_z = 0$$

$$X(y,t) = \int_0^t v_x(y,t')dt' + X(y,0)$$

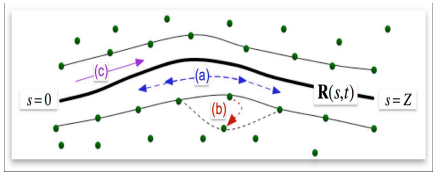
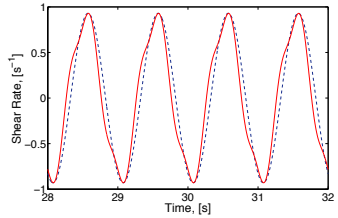
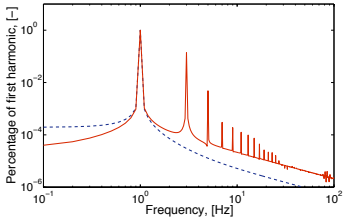
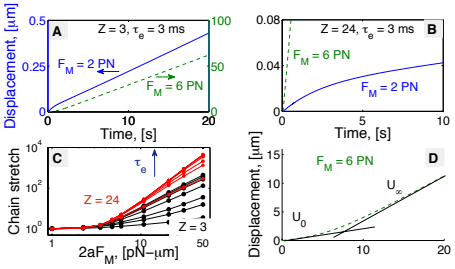
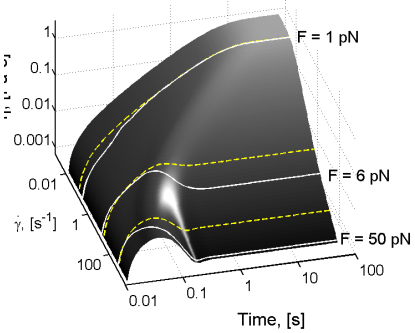
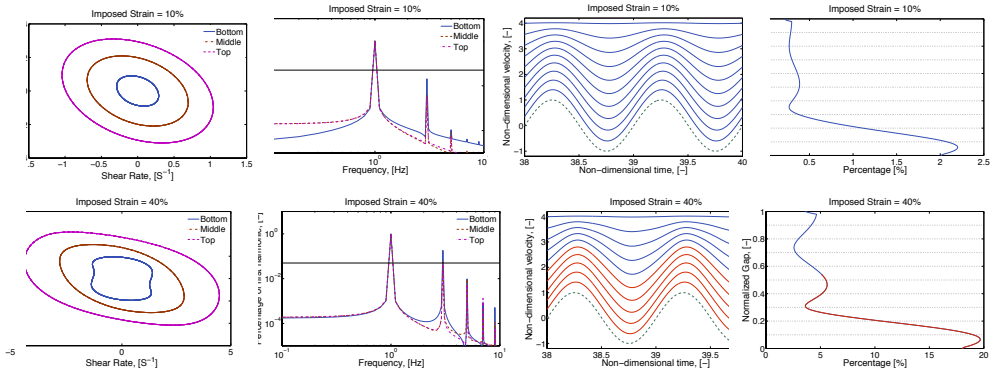
Mitran, Forest et al. JNNFM 154 (2008)
Lindley, Forest et al. JNNFM 156 (2009)

Rolie Poly Model

$$\frac{\boldsymbol{\tau}}{G_0} = \int_0^Z \left\langle \frac{\partial R_\alpha}{\partial s}\frac{\partial R_\beta}{\partial s}\right\rangle ds$$

Likhtman et al. JNNFM 114 (2003)
Teixeira et al. Macromolecules 40 (2007)
Cribb, Vasquez, Forest, et al. Preprint

$$\overset{\nabla}{\lambda\boldsymbol{\tau}} = \eta_p\dot{\boldsymbol{\gamma}} - \boldsymbol{\tau} - \frac{2}{\lambda_R}\left(1-\frac{1}{\sqrt{\mathrm{tr}(\boldsymbol{\tau})/3+1}}\right)\left[\boldsymbol{\tau}+\mathbf{I}+\beta\,\boldsymbol{\tau}\sqrt{\mathrm{tr}(\boldsymbol{\tau})/3+1}\right]$$



a) Reptation
b) Convective constraint release
c) Retraction