Adapting the 2.29 FV Framework for Simple Non-Newtonian Fluid Flows

2.29 Numerical Fluid Mechanics
Spring 2018

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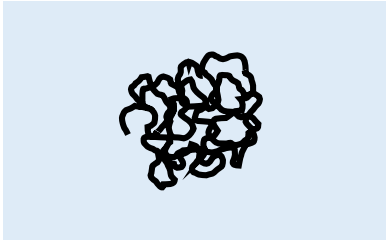
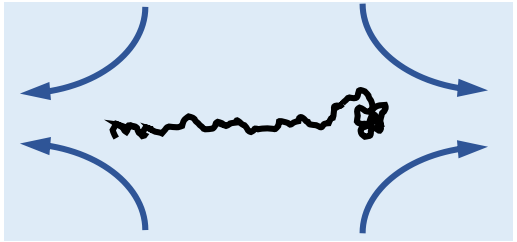
Non-Newtonian Fluids

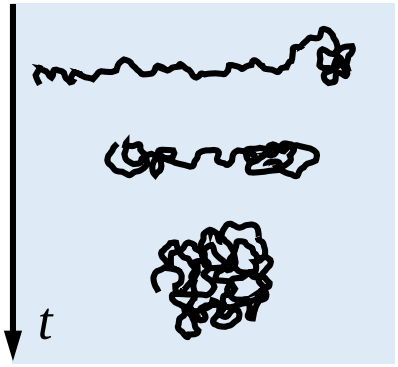
- Many non-Newtonian fluids consist of dissolved polymer molecules – very long chains of high molecular weight. These act as an "entropic spring" that gives rise to elasticity.



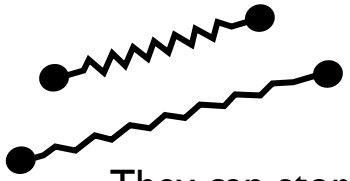
Molecules are initially coiled …



… but are stretched and deformed by flow …



… and relax back to the coiled state by thermal motion.



They can store energy via their configuration.

- A few distinctively non-Newtonian phenomena:
- Shear thinning

- Viscoelasticity

"Open Siphon" effect
0.5% Polyethylene oxide

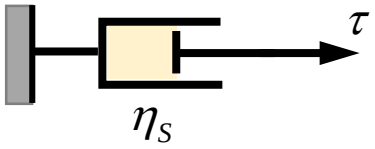
- Normal stresses under shear

"Rod climbing" effect

Credits: Ewoldt group, UIUC
McKinley group, MIT

Constitutive Equations for Polymeric Liquids

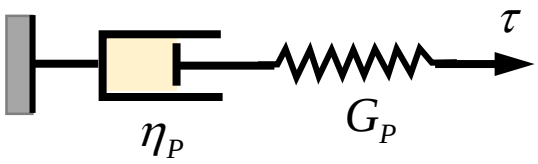
❑ Newtonian fluid



Purely viscous

$$\tau_S = \eta_S \, \dot{\gamma}$$

❑ Viscoelastic fluid
"Maxwell liquid"



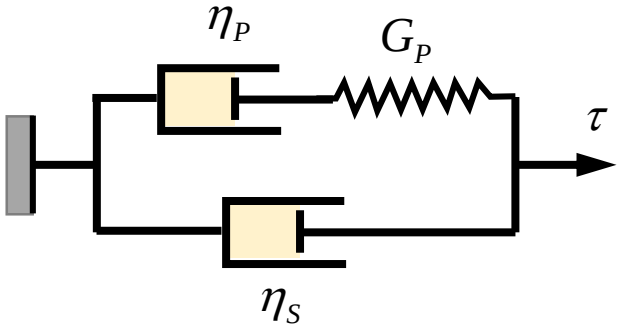
$$\dot{\gamma} = \frac{\tau_P}{\eta} + \frac{\dot{\tau}_P}{G}$$

$$\Rightarrow \tau_P + \lambda \frac{d\tau_P}{dt} = \eta \dot{\gamma}$$

Relaxation time

$$\lambda = \frac{\eta_P}{G_P}$$

❑ A simple model for a polymer solution



$$\tau = \tau_S + \tau_P$$

❑ Differential Constitutive Equations

❑ Upper Convected Maxwell (Oldroyd-B) Model

$$\tau = \tau_S + \tau_P \qquad \tau_S = \eta \, \dot{\gamma} \qquad \tau_P + \lambda \overset{\nabla}{\tau}_P = \eta_P \, \dot{\gamma}$$

Shear rate tensor

$$\dot{\gamma} = \left\{ \nabla u + (\nabla u)^T \right\}$$

Upper convected (contravariant) derivative:

$$\overset{\nabla}{\tau}_P = \left\{ \frac{\partial}{\partial t} \tau_P + u \cdot \nabla \tau_P - (\nabla u)^T \cdot \tau_P - \tau_P \cdot \nabla u \right\}$$

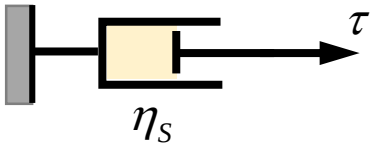
❑ Giesekus Model

Nonlinear term removes stress singularity due to unbounded extension of the polymer "spring".

$$\tau_P + \lambda \overset{\nabla}{\tau}_P = \eta_P \dot{\gamma} + \frac{\alpha \lambda}{\eta_P} \{ \tau_P \cdot \tau_P \} \qquad 0 \le \alpha \le \frac{1}{2}$$

Constitutive Equations for Polymeric Liquids

❑ Newtonian fluid



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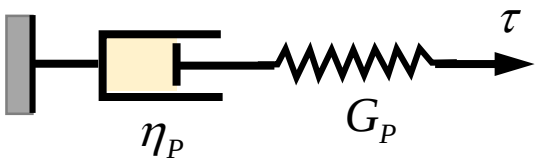

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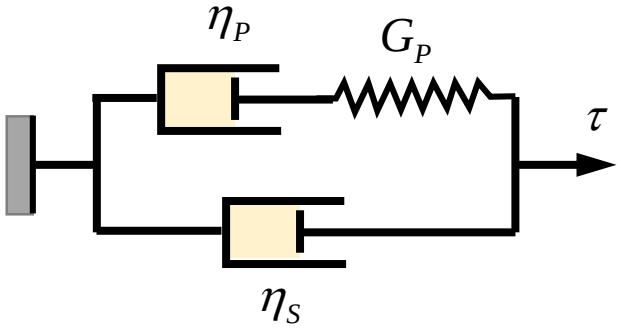


$$\tau = \tau_S + \tau_P$$

❑ Conformational Constitutive Equations

Utilizes a conformation tensor that tracks "how deformed polymer chains are" on average.

❑ FENE-CR Model (Chilcott and Rallison, 1988)

$$\tau_P = \frac{G_P}{\left(1 - \frac{\mathrm{tr}\, A}{L^2}\right)}\{A - I\} \qquad \overset{\nabla}{A} = -\frac{1}{\eta_P}\tau_P$$

Specifically formulated for computations to remove unphysical infinite stresses.

❑ FENE-P Model (Peterlin, 1966)

$$\tau_P = G_P\left\{\left(1 - \frac{\mathrm{tr}\, A}{L^2}\right)^{-1} A - I\right\} \qquad \overset{\nabla}{A} = -\frac{1}{\eta_P}\tau_P$$

Derived from a molecular dumbbell model.

Numerical Implementation – Differential Models

- Although a single evolution equation for extra stress tensor can be derived, the solvent and polymeric stresses were kept separate. This "Elasto-Viscous Stress Splitting" (EVSS) helps in stability.

$$\tau = \tau_S + \tau_P$$

$$\tau_S = \eta_S \dot{\gamma}$$

- Three stress components in 2D evolved as unknowns at the pressure node locations.

$$\frac{\partial \tau_{xx}}{\partial t} = -\left(u\frac{\partial \tau_{xx}}{\partial x} + v\frac{\partial \tau_{xx}}{\partial y} \right) + \left\{ -\frac{\tau_{xx}}{\lambda} + \frac{2\eta_P}{\lambda}\frac{\partial u}{\partial x} + 2\left(\tau_{xx}\frac{\partial u}{\partial x} + \tau_{xy}\frac{\partial u}{\partial y} \right) \right\}$$

$$\frac{\partial \tau_{yy}}{\partial t} = -\left(u\frac{\partial \tau_{yy}}{\partial x} + v\frac{\partial \tau_{yy}}{\partial y} \right) + \left\{ -\frac{\tau_{yy}}{\lambda} + \frac{2\eta_P}{\lambda}\frac{\partial v}{\partial y} + 2\left(\tau_{yy}\frac{\partial v}{\partial y} + \tau_{xy}\frac{\partial v}{\partial x} \right) \right\}$$

$$\frac{\partial \tau_{xy}}{\partial t} = -\left(u\frac{\partial \tau_{xy}}{\partial x} + v\frac{\partial \tau_{xy}}{\partial y} \right) + \left\{ -\frac{\tau_{xy}}{\lambda} + \frac{\eta_P}{\lambda}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \tau_{yy}\frac{\partial u}{\partial y} + \tau_{xx}\frac{\partial v}{\partial x} \right\}$$

Initially zero polymer stress at all locations: true if material is fully relaxed at time zero.

- AB2 Time Marching

$$\tau_P^{n+1} = \tau_P^n + \frac{\Delta t}{2}\left(3\frac{\partial \tau_P^n}{\partial t} - \frac{\partial \tau_P^{n-1}}{\partial t} \right)$$

- Advection using mexed scalar advection routines
- Red terms not directly available on a staggered grid.

Grad2D_uv2.m

- The incremental projection method with rotational correction is used.
  - No changes needed for (Newtonian) solvent stress.
  - Additional polymer stress term added as source term in the predictor step.

$$\frac{3\left(\rho u^*\right)^{n+1} - 4\left(\rho u\right)^n + \left(\rho u\right)^{n-1}}{2\Delta t} - \eta_S\frac{\partial^2\left(u^*\right)^{n+1}}{\partial x^2} = -\frac{\partial}{\partial x}\left(\rho u u\right)^n - \frac{\partial p^n}{\partial x} + \frac{\partial \tau_P^{n+1}}{\partial x}$$

Grad2D_T.m

  - The corrector steps are unchanged.

Numerical Implementation – Conformational Models

- Three conformation tensor components are evolved as unknowns at the pressure node locations.

$$\frac{\partial A_{11}}{\partial t} = -\left(u\frac{\partial A_{11}}{\partial x} + v\frac{\partial A_{11}}{\partial y} \right) + \left\{ -\frac{\tau_{xx}}{\eta_P} + 2\left(A_{11}\frac{\partial u}{\partial x} + A_{12}\frac{\partial u}{\partial y} \right) \right\}$$

$$\frac{\partial A_{22}}{\partial t} = -\left(u\frac{\partial A_{22}}{\partial x} + v\frac{\partial A_{22}}{\partial y} \right) + \left\{ -\frac{\tau_{yy}}{\eta_P} + 2\left(A_{22}\frac{\partial v}{\partial y} + A_{12}\frac{\partial v}{\partial x} \right) \right\}$$

$$\frac{\partial A_{12}}{\partial t} = -\left(u\frac{\partial A_{12}}{\partial x} + v\frac{\partial A_{12}}{\partial y} \right) + \left\{ -\frac{\tau_{xy}}{\eta_P} + A_{22}\frac{\partial u}{\partial y} + A_{11}\frac{\partial v}{\partial x} \right\}$$

Initially, conformation at all locations set to identity.

- AB2 Time Marching

$$A_{ij}^{n+1} = A_{ij}^{n} + \frac{\Delta t}{2}\left(3\frac{\partial A_{ij}^{n}}{\partial t} - \frac{\partial A_{ij}^{n-1}}{\partial t} \right)$$

- Advection using mexed scalar advection routines
- Red terms not directly available on a staggered grid.

Grad2D_uv2.m

- Stresses are computed from the conformation tensor, and inserted into the predictor step as a source term.

$$\tau_{xx}^{n+1} = \frac{\eta_P}{\lambda}\left(1 - \frac{A_{11}^{n+1} + A_{22}^{n+1}}{L^2} \right)^{-1} \left(A_{11}^{n+1} - 1 \right)$$

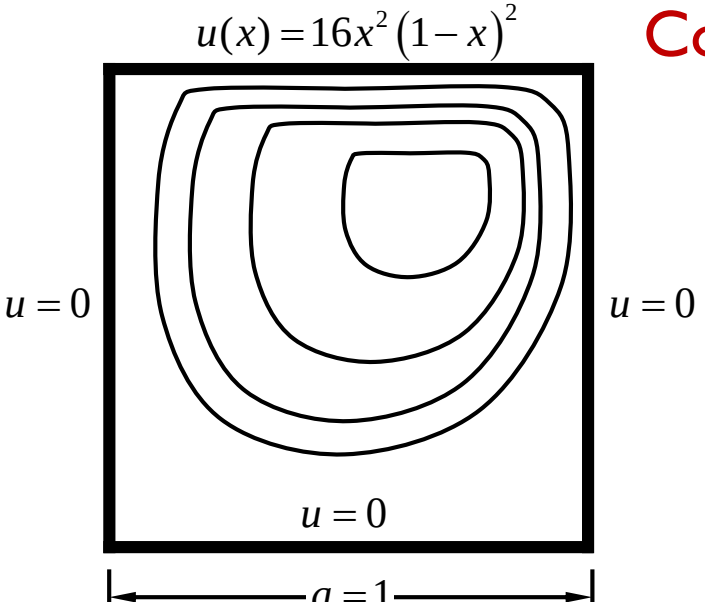
$$\tau_{yy}^{n+1} = \frac{\eta_P}{\lambda}\left(1 - \frac{A_{11}^{n+1} + A_{22}^{n+1}}{L^2} \right)^{-1} \left(A_{22}^{n+1} - 1 \right)$$

$$\tau_{xy}^{n+1} = \frac{\eta_P}{\lambda}\left(1 - \frac{A_{11}^{n+1} + A_{22}^{n+1}}{L^2} \right)^{-1} A_{12}^{n+1}$$

$$\frac{3\left(\rho u^*\right)^{n+1} - 4\left(\rho u\right)^{n} + \left(\rho u\right)^{n-1}}{2\Delta t} - \eta_S\frac{\partial^2\left(u^*\right)^{n+1}}{\partial x^2} = -\frac{\partial}{\partial x}\left(\rho u u\right)^{n} - \frac{\partial p^{n}}{\partial x} + \frac{\partial \tau_P^{n+1}}{\partial x}$$

Grad2D_T.m

Convergence: LDC



Time step:

$T = 25 \qquad \Delta t = 2 \times 10^{-3}$

Reference solution:

$N_x = N_y = 160$

Reynolds number

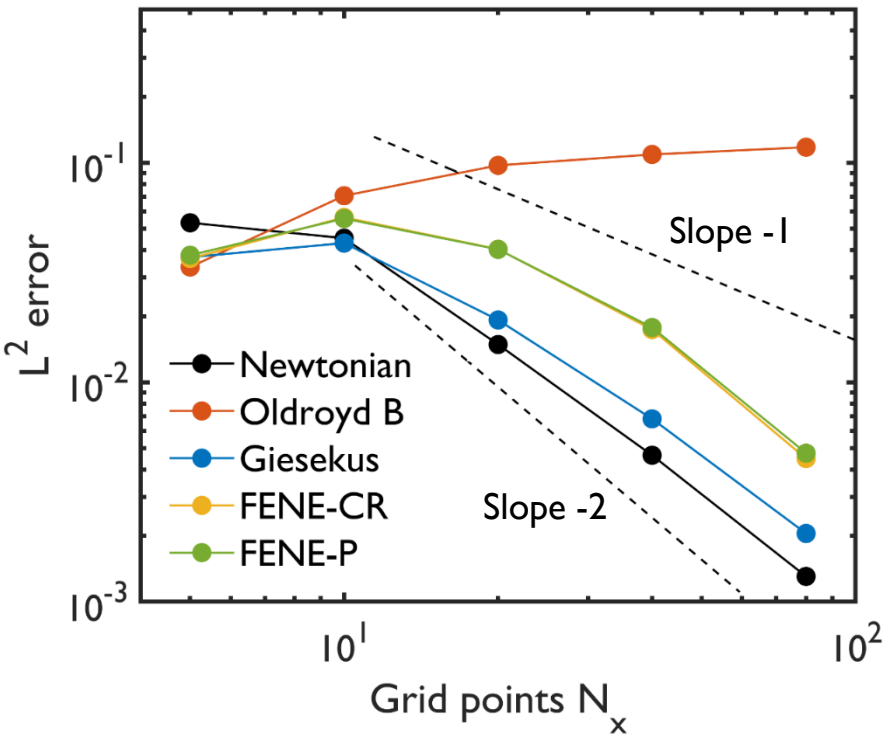
$$\mathrm{Re} = \frac{\rho \bar{U} a}{\eta_S + \eta_P} = 27$$

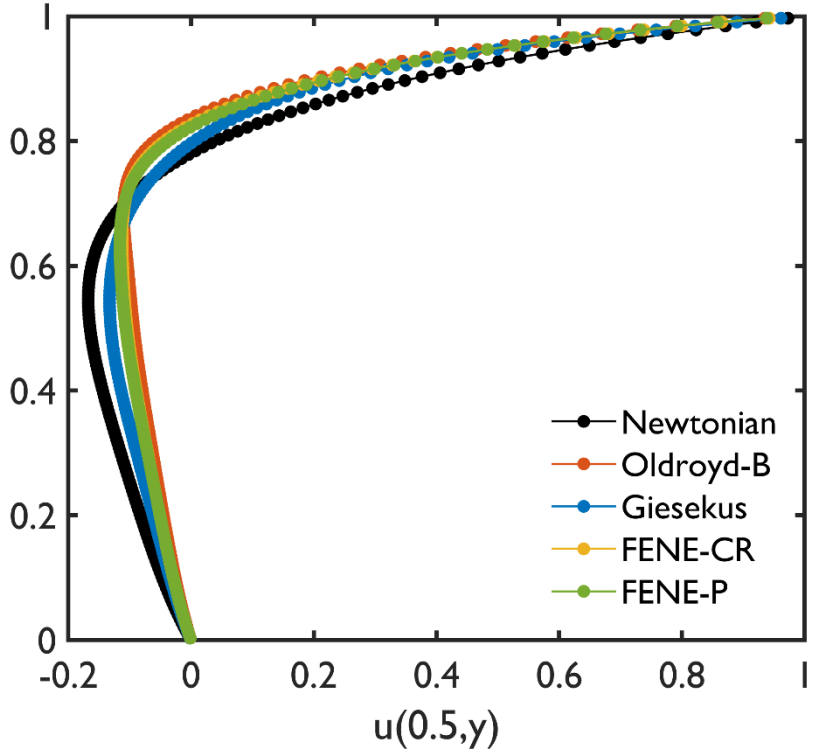
Weissenberg number

$$\mathrm{Wi} = \frac{\bar{U}\lambda}{a} = \frac{8}{15} = 0.533$$

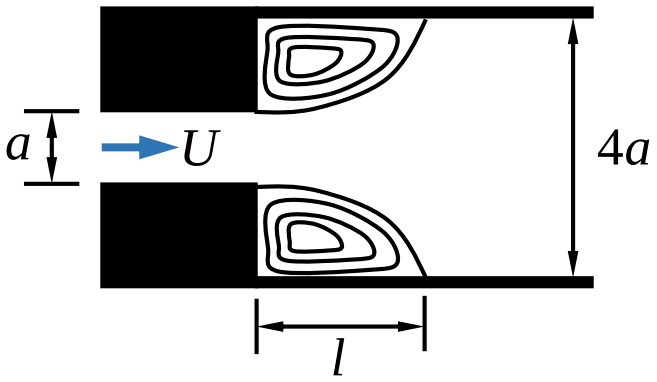
Viscoelastic parameters:

$\rho = 1 \quad \eta_S = \eta_P = 0.01 \quad \alpha = 1/3 \quad L^2 = 100 \quad \lambda = 1$





Test Case 1: Sudden Expansion



Reynolds number $\mathrm{Re} = \dfrac{\rho U a}{\eta_S + \eta_P}$

Weissenberg number $\mathrm{Wi} = \dfrac{U\lambda}{a}$

Geometry parameters:

$a = 0.5 \quad L_x = 10$

$N_x = 125 \quad N_y = 25$

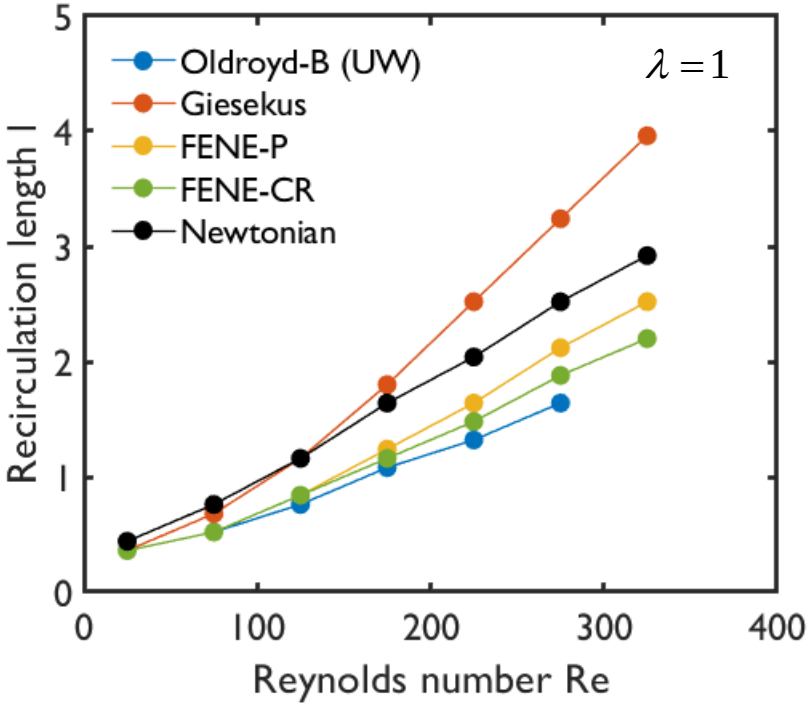
$T = 50 \quad \Delta t = 5\times10^{-3}$

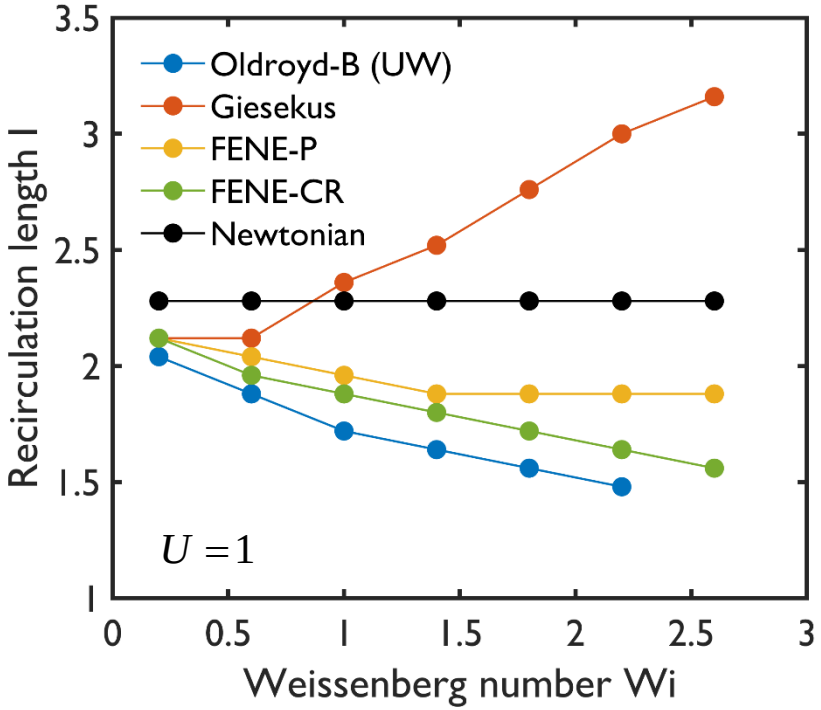
Viscoelastic parameters:

$\rho = 1 \quad \eta_S = \eta_P = 0.01 \quad \alpha = 1/3 \quad L^2 = 100$

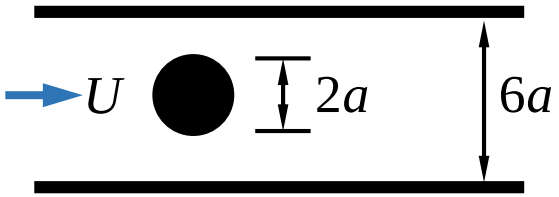
The Oldroyd-B solver was used with UW advection for stability.

The recirculation length decreases due to viscoelasticity, except for Giesekus model.





Test Case II: Flow Past Cylinder



The Oldroyd-B solver was unstable even with UW.

Reynolds number $\mathrm{Re} = \dfrac{\rho U a}{\eta_S + \eta_P} = 50$

Weissenberg number $\mathrm{Wi} = \dfrac{U\lambda}{a} = 4$

Geometry parameters:

$a = 0.5 \quad L_x = 20$

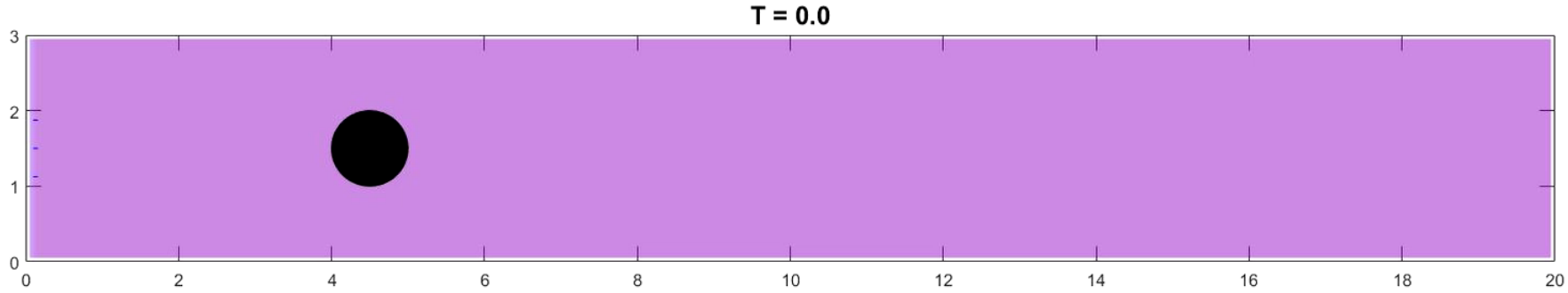
$N_x = 200 \quad N_y = 30$

$T = 100 \quad \Delta t = 0.01$

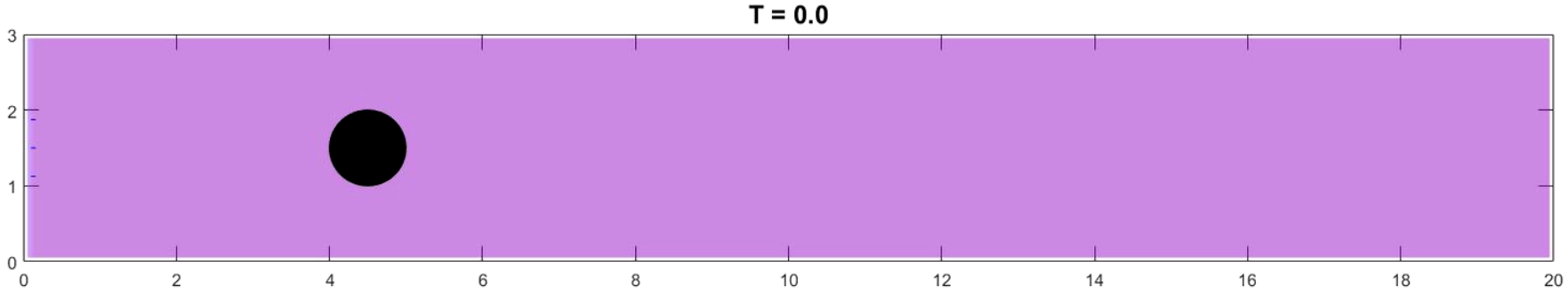
Viscoelastic parameters:

$\rho = 1 \quad \eta_S = \eta_P = 0.01 \quad \alpha = 1/3 \quad L^2 = 100 \quad \lambda = 1$

- Newtonian



- Giesekus



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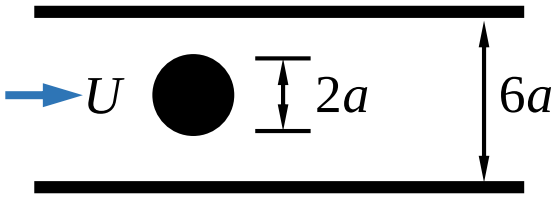

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Geometry parameters:

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$N_x = 200 \quad N_y = 30$

$T = 100 \quad \Delta t = 0.01$

Viscoelastic parameters:

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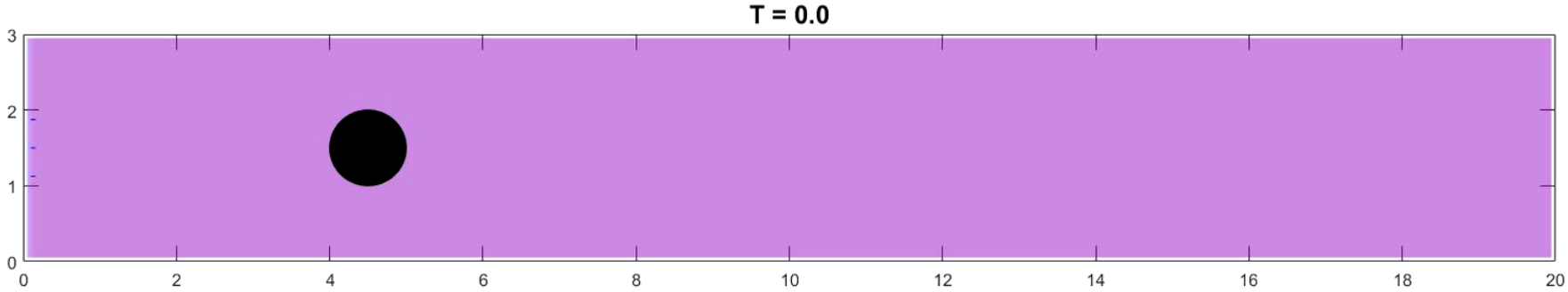
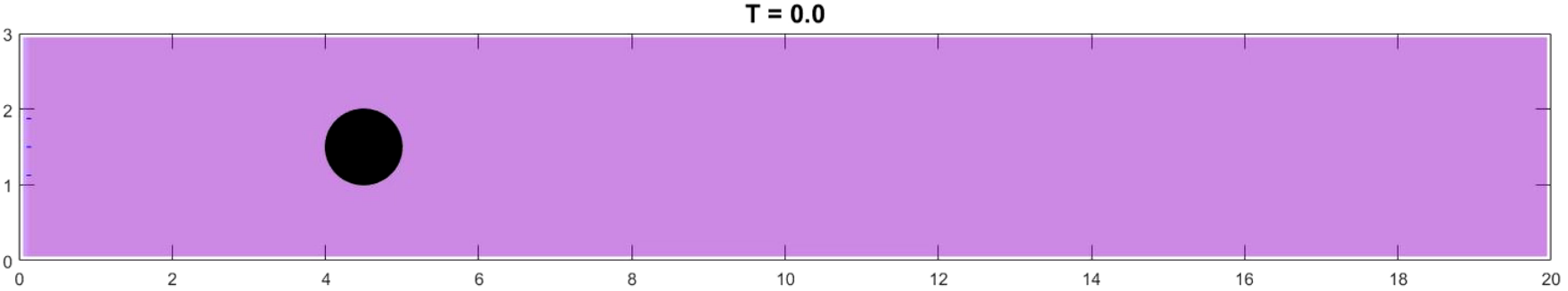
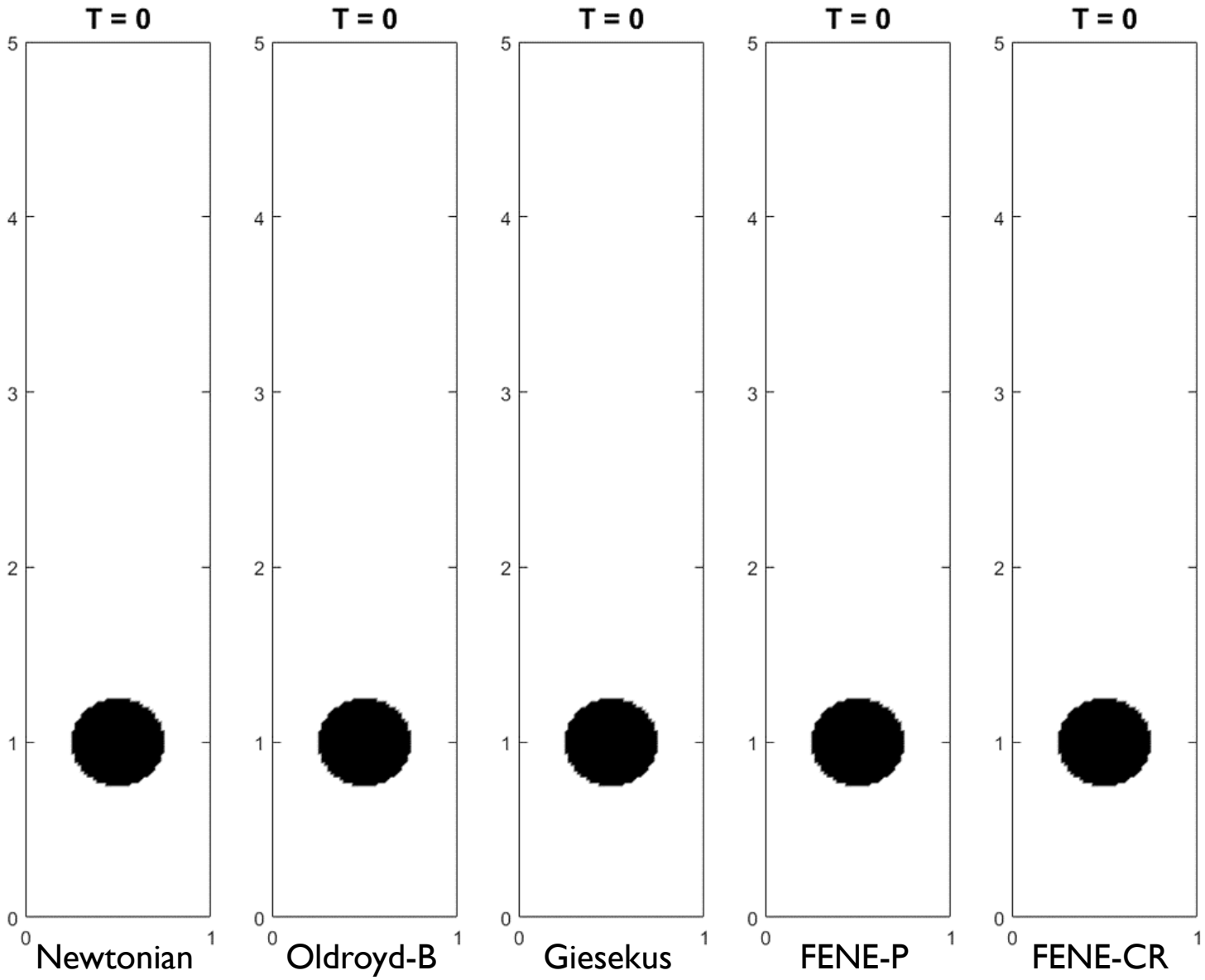
- FENE-P



- FENE-CR



Test Case III: Rising Buoyant Bubble



Geometry parameters:

$a = 0.25$

$L_x = 1$

$L_y = 5$

$N_x = 60$

$N_y = 300$

$T = 400$

$\Delta t = 0.1$

Viscoelastic parameters:

$\eta_S = \eta_P = 0.01$

$\alpha = 1/3$

$L^2 = 100$

Buoyancy and Diffusivity:

$\kappa = 0$

$g = 1$

$\Delta\rho = 0.01$

Test Case IV: Lock Exchange

Geometry parameters:

$L_x = 1$ $\quad L_x = 1$

$N_x = 200$ $\quad N_y = 200$

$T = 8$ $\quad \Delta t = 1 \times 10^{-4}$

Viscoelastic parameters:

$\eta_S = \eta_P = 1 \times 10^{-4}$

$\lambda = 10$

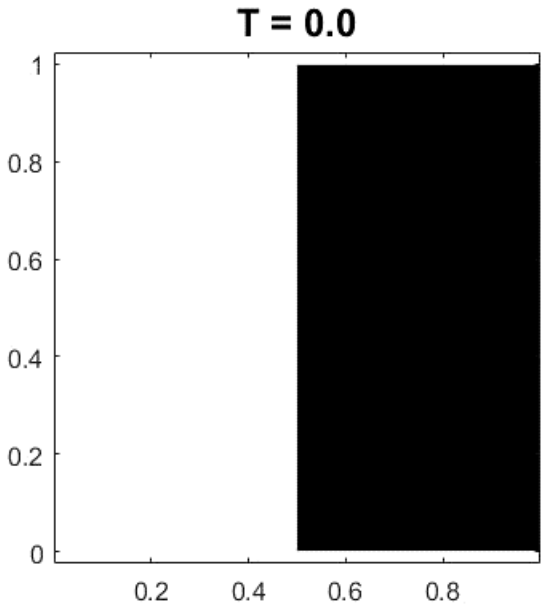
$L^2 = 100$

Density and Diffusivity:

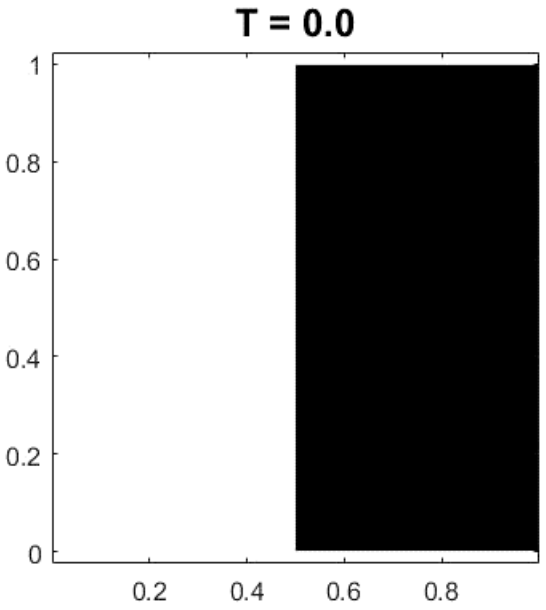
$\kappa = 0$

$g = 1$

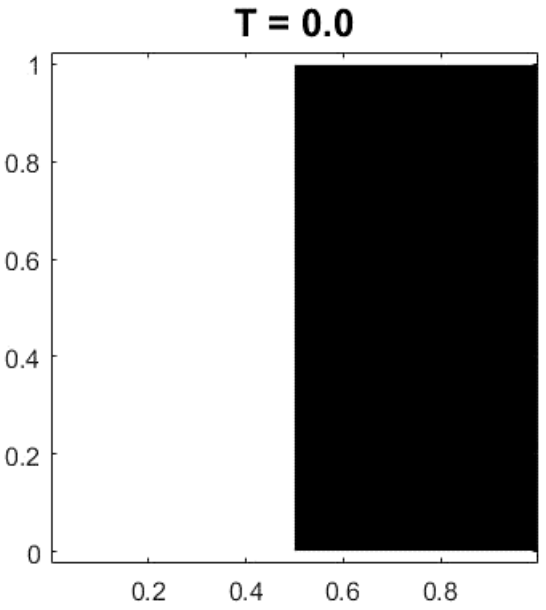
$\Delta\rho = 1$



Newtonian



FENE-CR



FENE-P

High Weissenberg Number Problem

- Many FE, FV and FM methods fail at modest Wi values – between 1 and 10.
- Called the High Weissenberg Number Problem or HWNP.
- Due to the inability of simple polynomial approximations to capture exponential profiles in polymer stress.

Even a linear velocity profile can lead to exponential stress profiles in viscoelastic fluids!

$$u(x) = \dot{\varepsilon}\, x$$

$$\Rightarrow \quad \Delta l(t) = \Delta l(0)\, e^{\dot{\varepsilon} t}$$

Stagnation points, sharp corners, discontinuous BC's are all potentially problematic.

Solution is to evolve the logarithm of the conformation tensor, rather than the tensor itself.

Log Conformation Formulation (Fattal and Kupferman, 2004).

- Involves additional cost of diagonalizing the conformation tensor, and decomposing the velocity gradient along the principal directions of the conformation tensor.

Summary

- Modified the 2.29 FV Code to implement two differential and two conformational viscoelastic constitutive equations:
  - Oldroyd B
  - Giesekus model
  - FENE-P
  - FENE-CR
- Simulated simple test cases of steady and unsteady flows.
- Can be easily extended to include polymer diffusion and spatial variation in viscoelastic properties.
- Overcoming the HWNP would probably require using a log conformation approach.