Numerical Simulations of Thin Viscoelastic Films

Valeria Barra
Advisor: Shahriar Afkhami
Collaborator: Shawn Chester

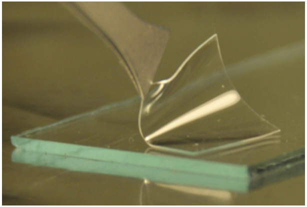
Department of Mathematical Sciences, NJIT

Januray 12, 2018

Introduction

Applications:

- Food Industry: ketchup, custard, starch suspensions
- Chemical and Pharmaceutical Industries: toothpaste, shampoo
- Biomedical Industry: blood, mucus, saliva
- Materials Science: glue, solar cells, liquid crystal polymers



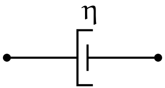
Constitutive Models

- Hookean: incompressible elastic solids

$\sigma_{ij} = 2G\epsilon_{ij}$
G the shear elastic modulus

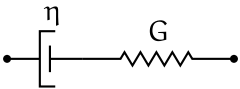
- Newtonian: viscous fluids

$\sigma_{ij} = 2\eta\dot{\epsilon}_{ij}$
η dynamic (shear) viscosity



- Maxwell: viscoelastic fluids

$\sigma_{ij} + \lambda\partial_t\sigma_{ij} = 2\eta\dot{\epsilon}_{ij}$
λ relaxation time, s. t. $\lambda = \eta/G$.



Mathematical formulation

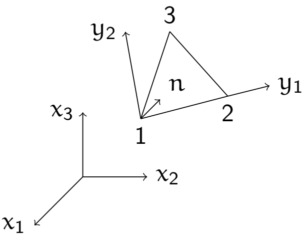


Figure: The surface coordynate system on triangular elements.

$\mathbf{x}_i$ global coordinate system

$\mathbf{y}_i$ current state surface coordinate system
$\widetilde{\mathbf{x}}^i$ current nodal positions
$\mathbf{e}_{ij} = \widetilde{\mathbf{x}}^j - \widetilde{\mathbf{x}}^i$ current state edge vectors

$\mathbf{Y}_i$ reference state surface coordinate system
$\widetilde{\mathbf{X}}^i$ reference nodal positions
$\mathbf{E}_{ij} = \widetilde{\mathbf{X}}^j - \widetilde{\mathbf{X}}^i$ reference state edge vectors

$\xi_1 + \xi_2 + \xi_3 = 1$, area (baricentric) coordinates

Deformation gradient on triangles

Let $\mathbf{u}$ be the displacement vector field, the deformation gradient tensor is

$$\mathbf{F}_{(2\times 2)} = \frac{\partial \mathbf{y}}{\partial \mathbf{Y}} = \mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{Y}}, \qquad (1)$$

Denoting $H_{ij} = \partial u_i / \partial x_j$, given by $\mathbf{H}_{(2\times 2)} = \mathbf{F} - \mathbf{I}$, we have the (small deformations) strain tensor in 2D

$$\boldsymbol{\epsilon}_{(2\times 2)} = \frac{1}{2}\left(\mathbf{H} + \mathbf{H}^T\right).$$

Note: $\epsilon_{vol} = \epsilon_{kk} \neq 0 \Leftrightarrow \nabla \cdot \mathbf{u} \neq 0$

Strong and weak equation of motion

Connservation of momentum, for a continuum medium with constant density ρ, is

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{F_b} = \rho \ddot{\mathbf{u}}, \qquad \text{on } \Omega \tag{2}$$

where $\mathbf{F_b}$ are the body forces, that comprise applied loads and gravitational force, and Ω is the surface of the membrane, and $\mathbf{u} = (u_1(x,y,z,t), u_2(x,y,z,t), u_3(x,y,z,t))$ is the displacement vector field. The weak form, for each element e, using the virtual work formulation, is

$$\delta\Pi = \int_{\Omega^{(e)}} \delta\mathbf{u}^T \rho \ddot{\tilde{\mathbf{u}}} dV - \int_{\Omega^{(e)}} \delta\boldsymbol{\epsilon}^T \boldsymbol{\sigma} dV - \int_{\Omega^{(e)}} \delta\mathbf{u}^T \mathbf{F_b}\, dV = 0\,, \tag{3}$$

with $dV = h\, dA$, h constant thickness of membrane.

Constitutive Laws

Newtonian (viscous) liquids:

$$\sigma_{ij} = 2\eta\dot{\epsilon}'_{ij} + \widehat{K}\dot{\epsilon}_{kk}\delta_{ij}\,, \tag{4}$$

Maxwellian (viscoelastic) liquids:

$$\sigma_{ij} + \lambda\partial_t\sigma'_{ij} = 2\eta\dot{\epsilon}'_{ij} + \widehat{K}\dot{\epsilon}_{kk}\delta_{ij}\,, \tag{5}$$

Where $\boldsymbol{\sigma}'$ and $\boldsymbol{\epsilon}'$ are the deviatoric stress and strain, respectively

$$\sigma'_{ij} = \sigma_{ij} - \frac{1}{2}\sigma_{kk}\delta_{ij}\,, \tag{6}$$

$$\epsilon'_{ij} = \epsilon_{ij} - \frac{1}{2}\epsilon_{kk}\delta_{ij}\,, \tag{7}$$

and where $\widehat{K}$ is the penalty constant, such that

$$\dot{\epsilon}_{kk} + p_{hyd}/\widehat{K} = 0\,, \text{ with } \widehat{K} \gg \eta. \tag{8}$$

Time Discretization of constitutive models

Discrete Newton model:

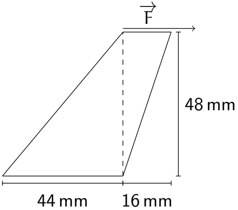
$$\sigma_{ij}^{n+1} = \frac{2\eta}{\Delta t}\left\{\left(\epsilon_{ij} - \frac{1}{2}\epsilon_{kk}\delta_{ij}\right)^{n+1} - \left(\epsilon_{ij} - \frac{1}{2}\epsilon_{kk}\delta_{ij}\right)^{n}\right\} + \frac{\widehat{K}}{\Delta t}\left\{\epsilon_{kk}^{n+1}\delta_{ij} - \epsilon_{kk}^{n}\delta_{ij}\right\}, \tag{9}$$

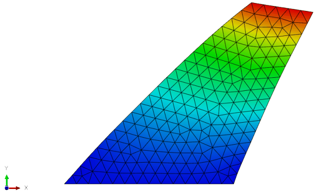
Discrete Maxwell model:

$$\boldsymbol{\sigma}^{n+1} = \left(1 + \frac{\Delta t}{\lambda_1}\right)^{-1}\left\{\boldsymbol{\sigma}^{n} + \frac{2\eta}{\lambda}\left[\left(\epsilon_{ij} - \frac{1}{2}\epsilon_{kk}\delta_{ij}\right)^{n+1} - \left(\epsilon_{ij} - \frac{1}{2}\epsilon_{kk}\delta_{ij}\right)^{n}\right] + \frac{\widehat{K}}{\lambda}\left[\epsilon_{kk}^{n+1} - \epsilon_{kk}^{n}\right]\delta_{ij}\right\}. \tag{10}$$

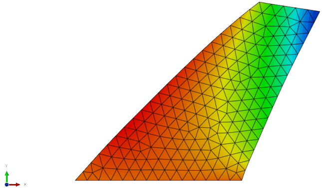
Numerical Results

Cook's membrane: a convergence test





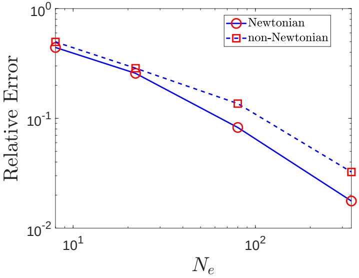
$u_{1_{max}} =$
5.686×10^{-3} m



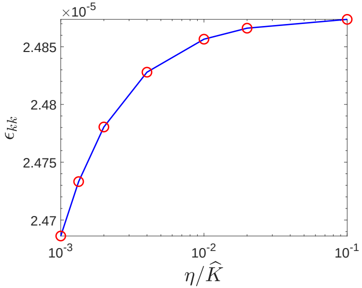
$u_{2_{min}} =$
-3.275×10^{-3} m

Cook's membrane (cont'd)

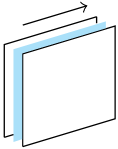
Mesh independence test



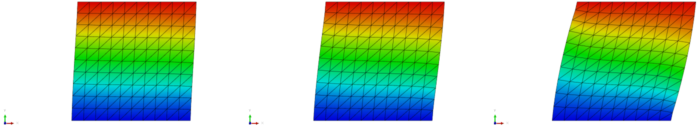
Pressure validation (tension test)



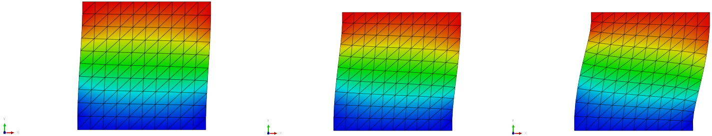
Shear flow (cont'd)



$\lambda = 0$

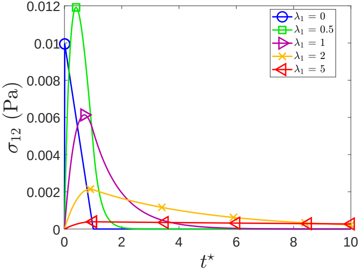


$\lambda = 5$

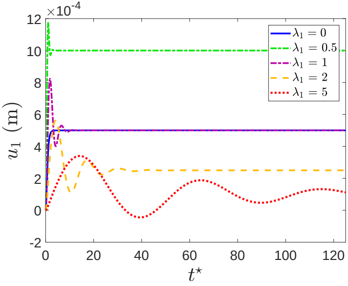


Shear Flow (cont'd)

Imposing a time-dependent velocity, e. g. $\mathbf{v}(\mathbf{t}=\mathbf{0}\,\mathbf{s}) = (0.001, 0)\,\mathrm{m}/s$



Applying a time-dependent load $\mathbf{F} = (10^{-2}, 0)$ N,



Extensional Flow

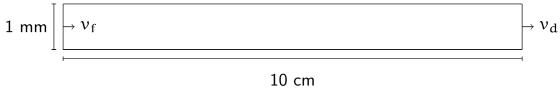
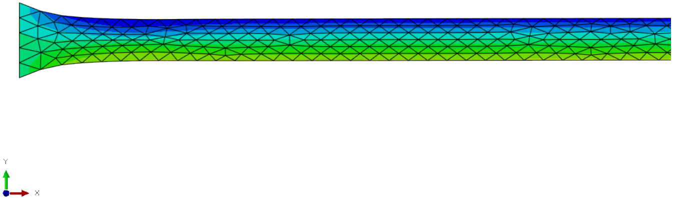
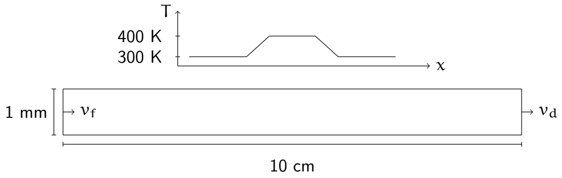
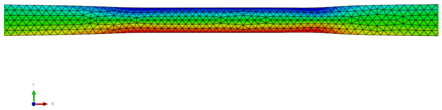


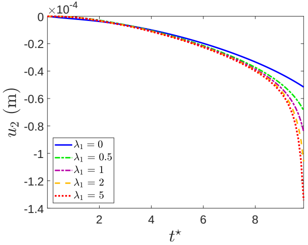
Figure: Set-up of the drawing process of a thin viscoelastic sheet



Extensional flow (cont'd)







Conclusions

- We have provided a general Finite Element framework for the simulations of the dynamics of viscoelastic membranes with applications in shearing and extensional flow (redrawing process)
- We have validated the penalty formulation for the pressure with a tension test
- We have found that viscoelasticity affects not only the dynamics but also the final configurations

Thank you.