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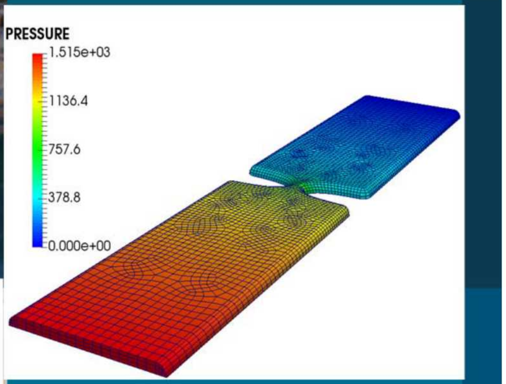

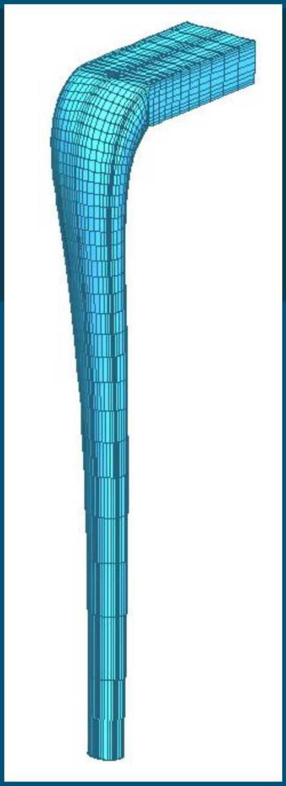

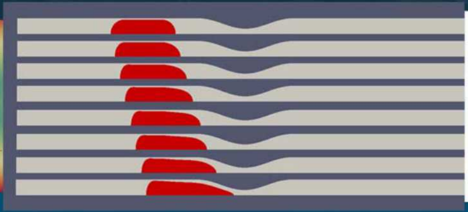

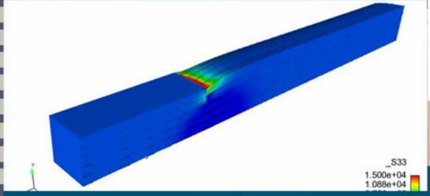

A Comparison of Viscoelastic Level Set Formulations: Property Averaging versus Equation Averaging

PRESENTED BY Rekha Rao (Sandia National Labs), Weston Ortiz, Kristianto Tjiptowidjojo, Richard Martin (University of New Mexico)

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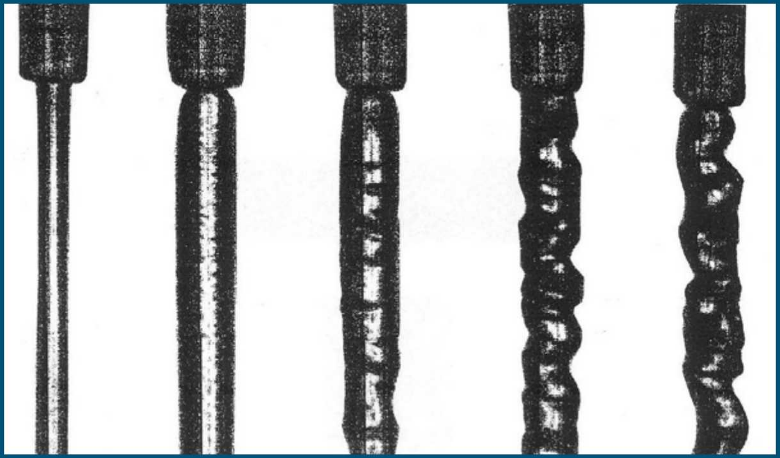
Motivation: Examples of Free Surface Flows of Viscoelastic Fluids

Bottle filling of non-Newtonian fluids



Melt Fracture during viscoelastic extrusion www.Lorentz.leidenuniv.nl

Coextrusion instabilities

Governing Equations, Navier-Stokes

- Equations for incompressible Newtonian fluid
- Conservation of momentum and mass

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho\mathbf{u}\cdot\nabla\mathbf{u}-\nabla\cdot T=\mathbf{f}$$

$$\nabla\cdot\mathbf{u}=0$$

- Where ρ is the density, $\boldsymbol{u}$ is the velocity, $\boldsymbol{f}$ is a body force, and T is the stress tensor:

$$\mathbf{T}=-p\mathbf{I}+\mu_s(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$$

- Where p is the pressure, and μ_s is the solvent viscosity

Governing Equations, Viscoelastic Constitutive Equation

For Oldroyd-B

$$\lambda[\frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \mathbf{u} - \nabla \mathbf{u}^T \cdot \boldsymbol{\sigma}] + \boldsymbol{\sigma} = \mu_p (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

Where σ is the polymer stress, μ_p is the polymer viscosity, and λ is the polymer time constant

$$\mathbf{T} = -p\mathbf{I} + \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \sigma$$

The extra stress tensor for our fluid equations becomes:

Governing Equations, Level Set

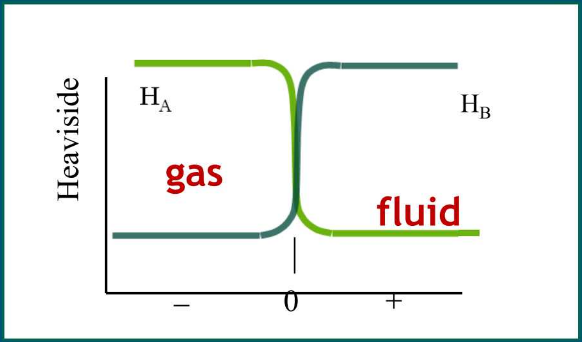
Level set method offers a convenient method to track the liquid-liquid interface

- We track an interface using a signed distance function where the level set zero represents the interface
- The level set is represented in an Eulerian fashion, which allows us to use fixed meshes for multimaterial problems
- The level set advection equation, where ϕ is the level set:

$$\boxed{\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0}$$

•Purely hyperbolic equation … fluid particles on $\phi(x,y,z) = 0$ should stay on this contour indefinitely

- Does not preserve $\phi(x,y,z)$ as a distance function
- Introduces renormalization step.



Material Properties in Level Set Method

- Represent property differences by a Heaviside function, $H = 0$ when the level set is negative, and $H = 1$ when the level set is positive. Example for density:

$$\rho(\phi) = \rho_- + (\rho_+ - \rho_-)H(\phi)$$

- Typically smoothing is required as instabilities occur when properties are discontinuous across the interface
- Smoothed Heaviside function: α represents an interface width

$$H(\phi) = \begin{cases} o & if\ \phi < \alpha \\ 0.5(1 + \frac{\phi}{\alpha} + \frac{\sin\left(\frac{\pi\phi}{\alpha}\right)}{\pi}) & if\ \alpha \leq \phi \leq \alpha \\ 1 & if\ \phi > \alpha \end{cases}$$

- We also represent Dirac delta's in this fashion for relevant boundary conditions:

$$\delta(\phi) = \partial H/\partial\phi$$

Extension of Level Set Method to VE Problems

Two Approaches:

- First is the same property split approach as described before, we just apply these to the viscoelastic properties λ and μ_p e.g.

$$\lambda(\phi) = \lambda_{-} + (\lambda_{+} - \lambda_{-})H(\phi)$$

- Second version instead of applying the Heaviside to properties we instead assume properties are constant in the entire domain and only apply the Heaviside to polymer stress contribution to momentum
- This assumes that only material is viscoelastic and the other is Newtonian

$$\lambda[\frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \mathbf{u} - \nabla \mathbf{u}^T \cdot \boldsymbol{\sigma}] + \boldsymbol{\sigma} = \mu_p (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

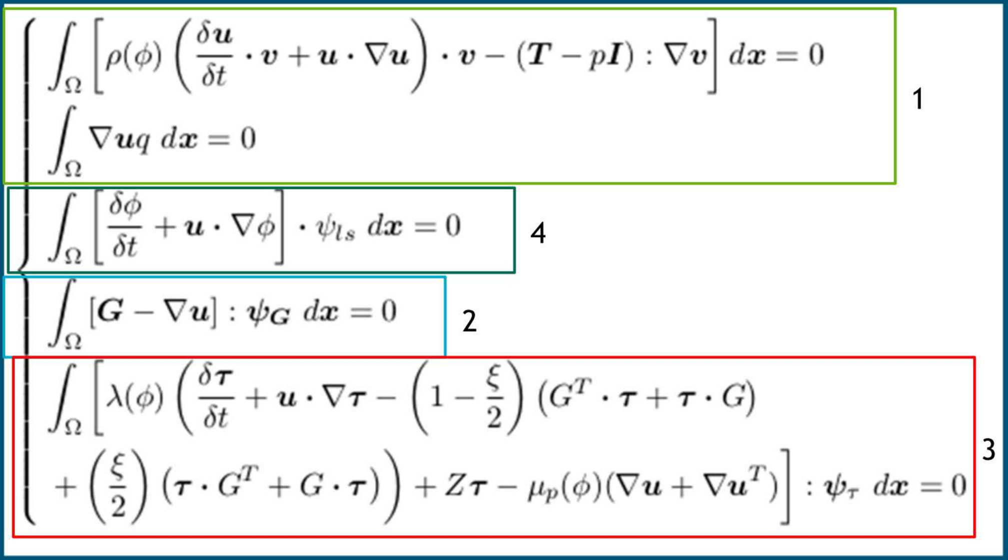
$$\boldsymbol{T} = -p\boldsymbol{I} + \mu_s(\phi)\left(\nabla \boldsymbol{u} + \nabla \mathbf{u}^{\mathrm{T}}\right) + \sigma H(\phi)$$

Equations in Finite Element Weak Form with DEVSS-G and PTT Constitutive Equation

$$
\begin{cases}
\displaystyle\int_\Omega \left[\rho(\phi)\left(\frac{\delta \boldsymbol{u}}{\delta t}\cdot \boldsymbol{v} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)\cdot \boldsymbol{v} - (\boldsymbol{T} - p\boldsymbol{I}) : \nabla \boldsymbol{v}\right] d\boldsymbol{x} = 0 \\
\displaystyle\int_\Omega \nabla \boldsymbol{u} q \; d\boldsymbol{x} = 0 \\
\displaystyle\int_\Omega \left[\frac{\delta \phi}{\delta t} + \boldsymbol{u}\cdot\nabla\phi\right]\cdot \psi_{ls} \; d\boldsymbol{x} = 0 \\
\displaystyle\int_\Omega [\boldsymbol{G} - \nabla \boldsymbol{u}] : \boldsymbol{\psi_G} \; d\boldsymbol{x} = 0 \\
\displaystyle\int_\Omega \left[\lambda(\phi)\left(\frac{\delta \boldsymbol{\tau}}{\delta t} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} - \left(1 - \frac{\xi}{2}\right)(G^T\cdot\boldsymbol{\tau} + \boldsymbol{\tau}\cdot G)\right.\right. \\
\displaystyle\left.\left.+\left(\frac{\xi}{2}\right)(\boldsymbol{\tau}\cdot G^T + G\cdot\boldsymbol{\tau})\right) + Z\boldsymbol{\tau} - \mu_p(\phi)(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)\right] : \boldsymbol{\psi}_\tau \; d\boldsymbol{x} = 0
\end{cases}
$$

Unknowns are $\boldsymbol{u}$ (velocity), p (pressure), ϕ (level set), **G** (velocity projection), and $\boldsymbol{\tau}$ polymer stress

Decoupling Equations in Lagged Manner



$$\begin{cases} \displaystyle\int_\Omega \left[\rho(\phi)\left(\frac{\delta \boldsymbol{u}}{\delta t}\cdot \boldsymbol{v} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)\cdot\boldsymbol{v} - (\boldsymbol{T} - p\boldsymbol{I}) : \nabla \boldsymbol{v}\right] d\boldsymbol{x} = 0 \\ \displaystyle\int_\Omega \nabla \boldsymbol{u} q \; d\boldsymbol{x} = 0 \\ \displaystyle\int_\Omega \left[\frac{\delta\phi}{\delta t} + \boldsymbol{u}\cdot\nabla\phi\right]\cdot \psi_{ls} \; d\boldsymbol{x} = 0 \\ \displaystyle\int_\Omega [\boldsymbol{G} - \nabla\boldsymbol{u}] : \boldsymbol{\psi_G} \; d\boldsymbol{x} = 0 \\ \displaystyle\int_\Omega \Bigg[\lambda(\phi)\left(\frac{\delta\boldsymbol{\tau}}{\delta t} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} - \left(1 - \frac{\xi}{2}\right)(G^T\cdot\boldsymbol{\tau} + \boldsymbol{\tau}\cdot G)\right. \\ \displaystyle\quad \left. + \left(\frac{\xi}{2}\right)(\boldsymbol{\tau}\cdot G^T + G\cdot\boldsymbol{\tau})\right) + Z\boldsymbol{\tau} - \mu_p(\phi)(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)\Bigg] : \boldsymbol{\psi_\tau} \; d\boldsymbol{x} = 0 \end{cases}$$

Unknowns are $\boldsymbol{u}$ (velocity), p (pressure), ϕ (level set), **G** (velocity projection), and $\boldsymbol{\tau}$ polymer stress

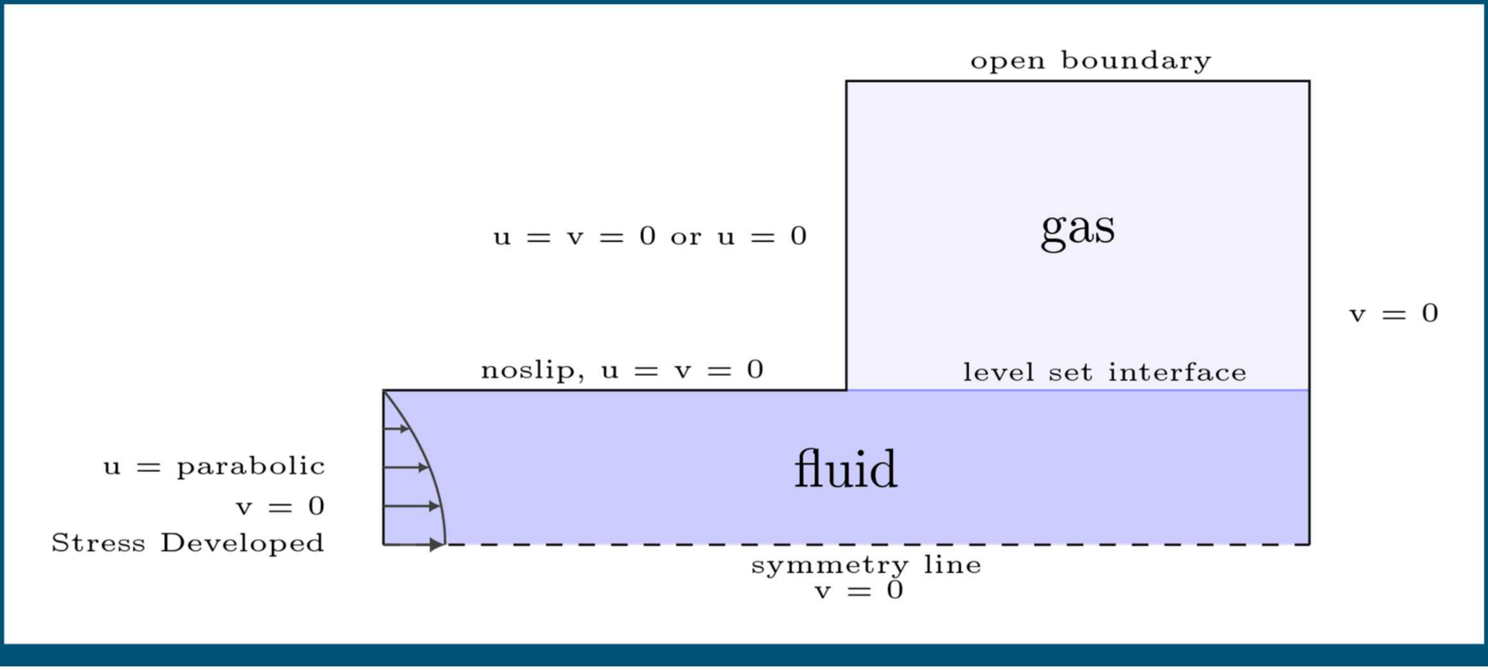
Now we solve in a set of 4 matrices:

Time step loop

1. Solve for $(\boldsymbol{u}, p)$
2. Solve for $\boldsymbol{G}$
3. Solve for $\boldsymbol{\tau}$
4. Solve for ϕ

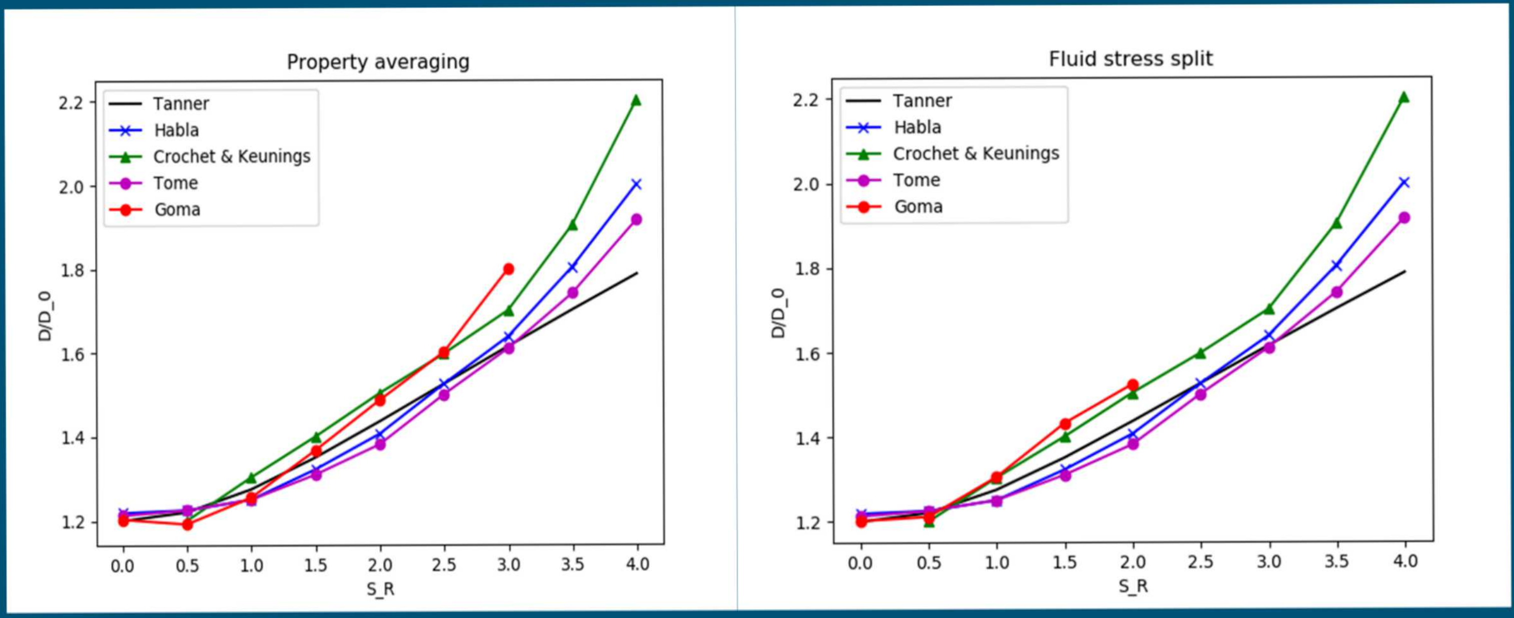
Viscoelastic Die Swell

- Compare with results to Tanner's theory and other numerical simulations where swell sized is measured with respect to recoverable shear
- From Habla et al 2011



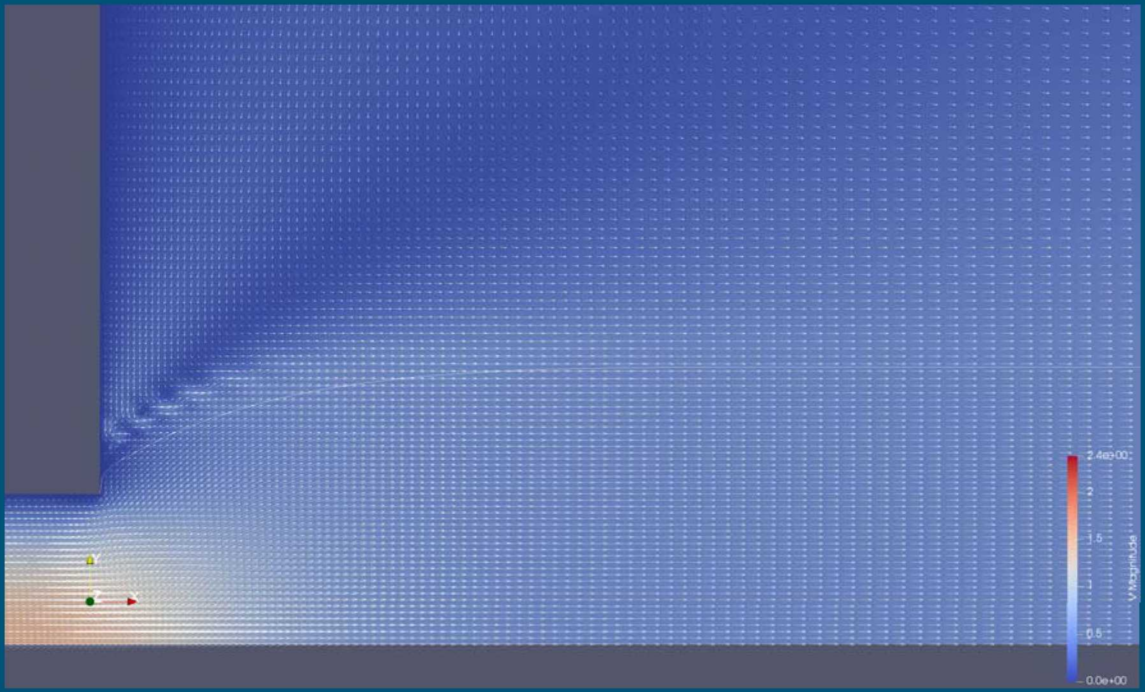
Results of Two Formulations

- Both formulations follow the trends reported by others and the analytical solution from Tanner et al.
- Failure to reach higher recoverable shear occurs because interface breaks down near the sharp change in geometry representing opening/die wall

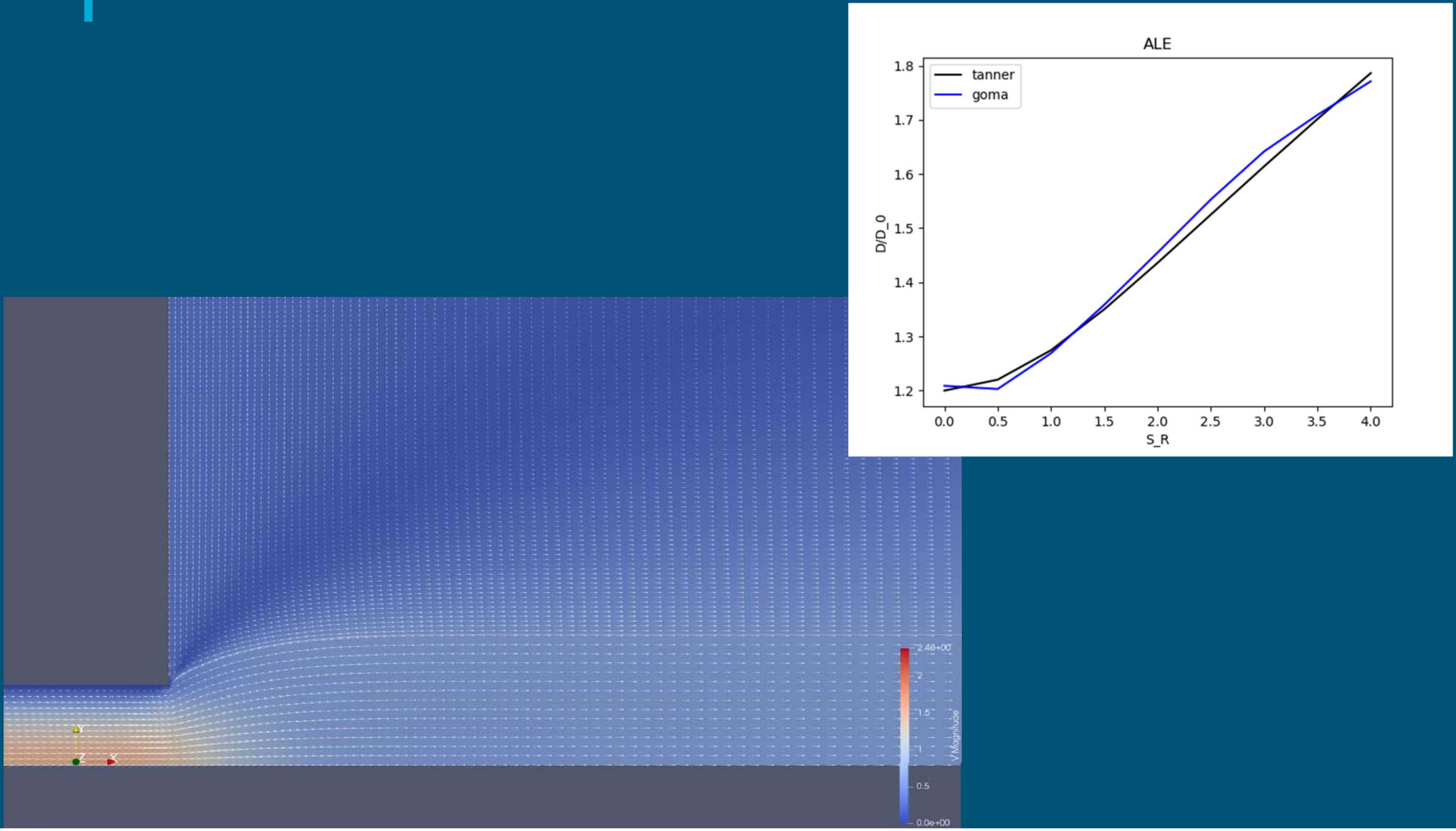


Example of Spurious Currents near Interface

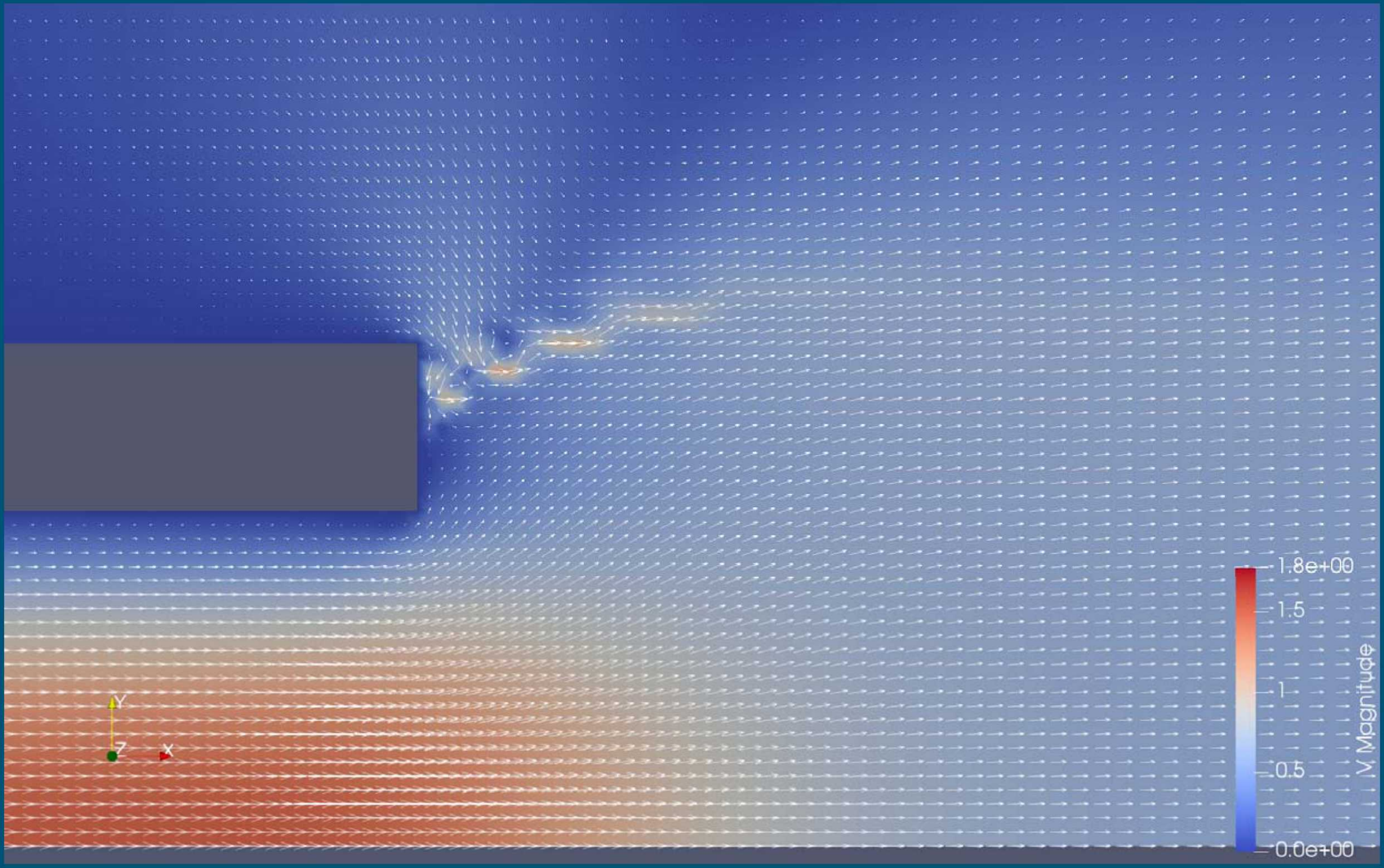
- Re-circulation appears near interface in the gas phase
- Appears to follow interface width and dissipates with large interface width (however the die swell does not behave correctly at large widths)



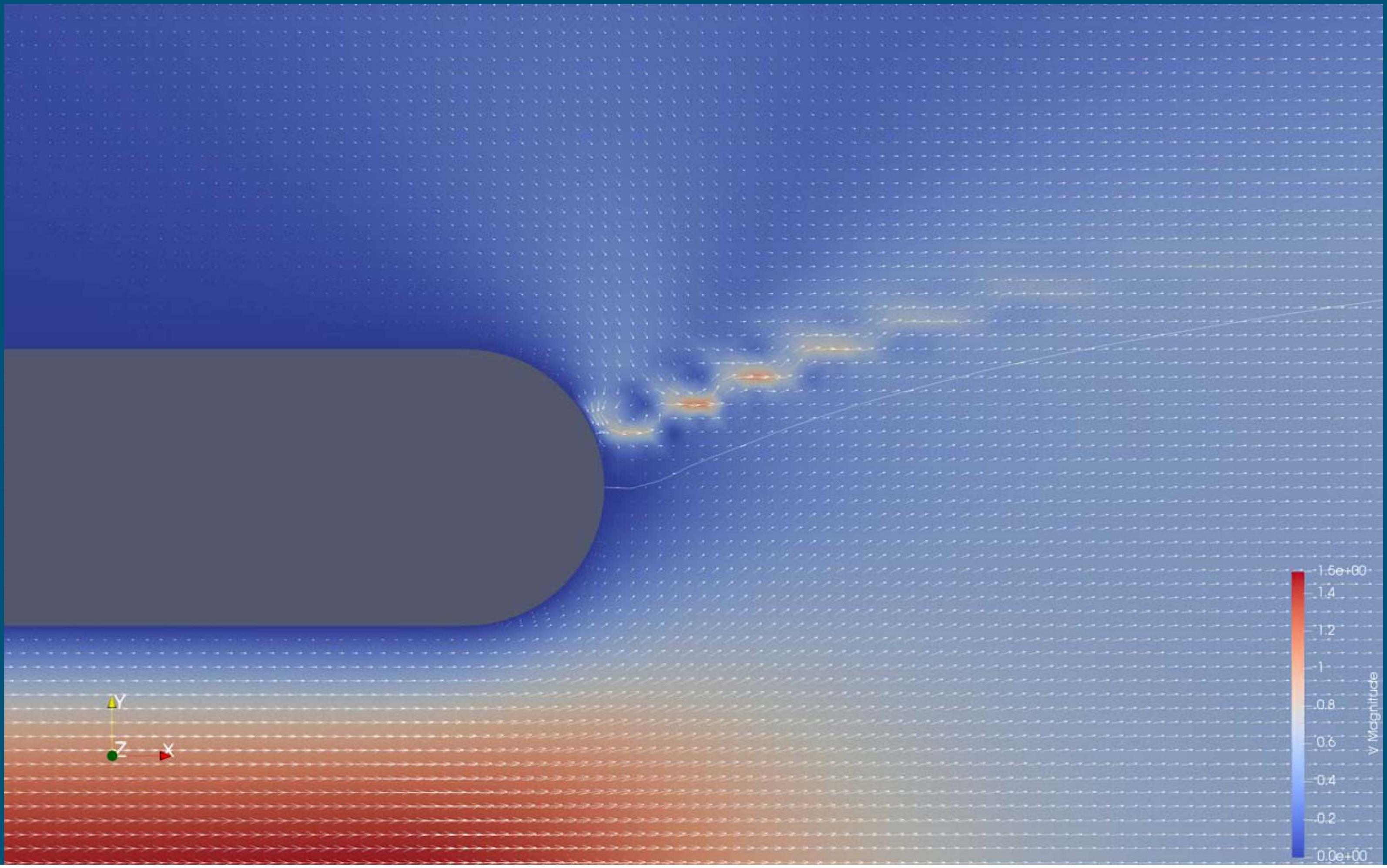
ALE Behavior with Same Properties



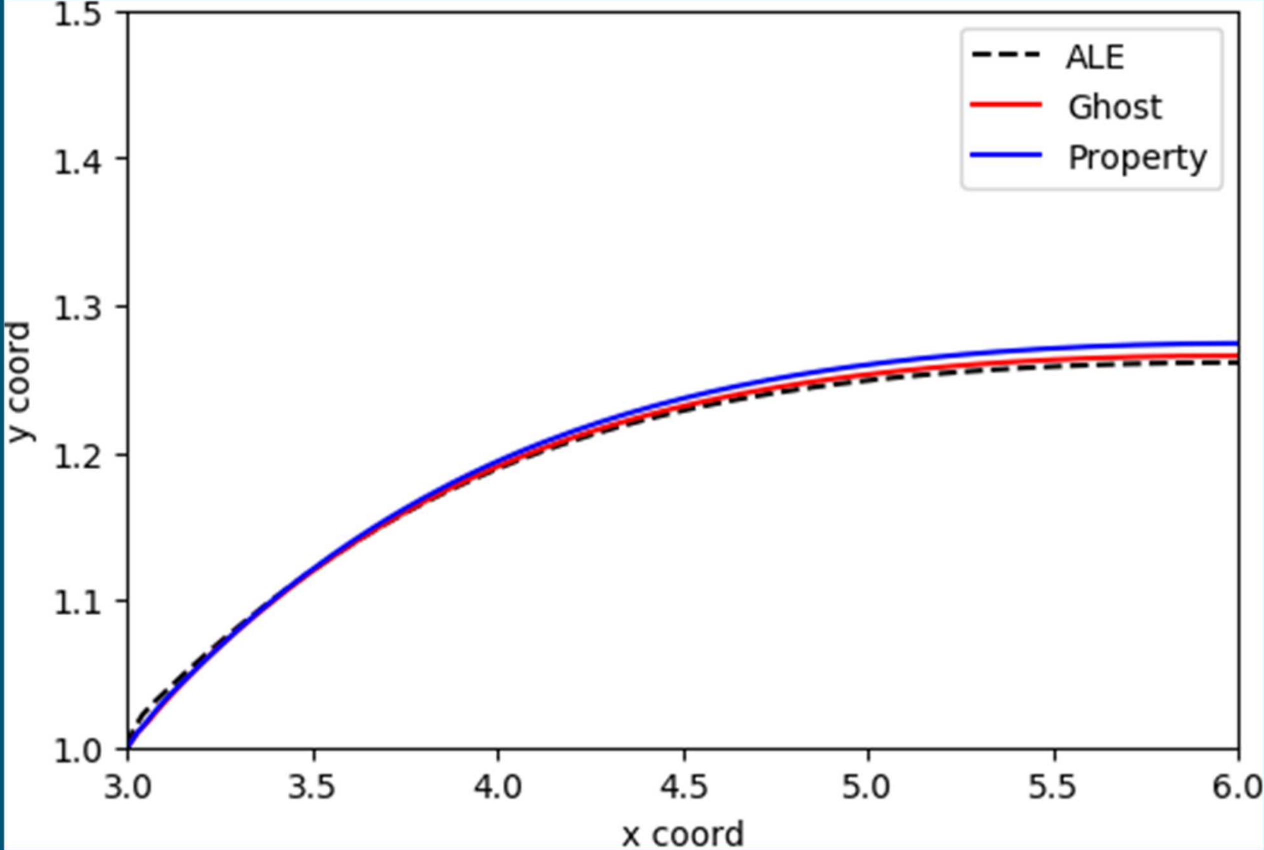
Die Swell with Extra Cavity



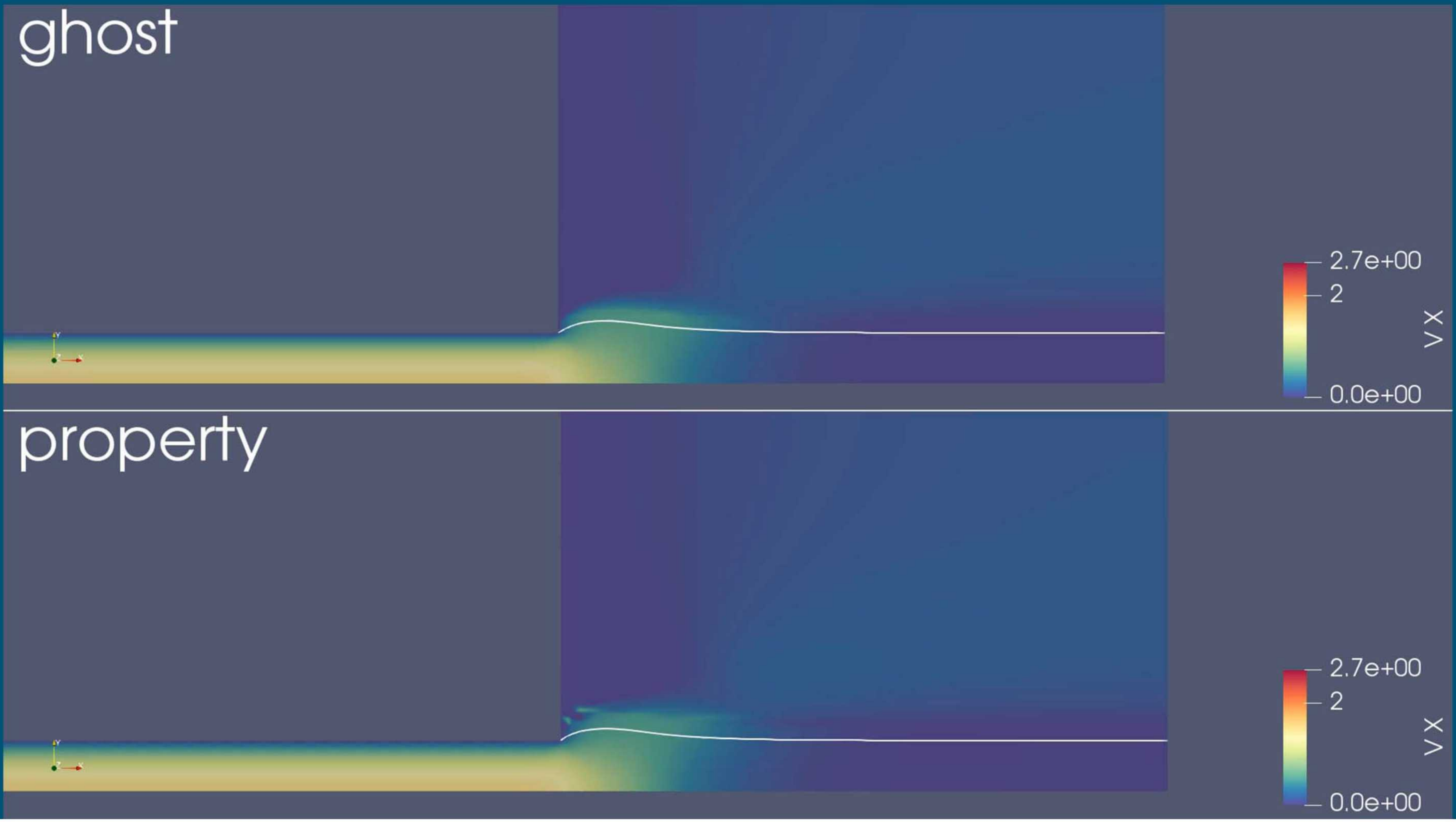
Extra Cavity with a Circular Die Wall



Die Swell Initial Comparison of Methods



Property Versus Stress Only Split



Level Set Surface Tension

Traditional Continuum Surface Stress (CSS) in Goma
Surface tension is added as a body force tensor to the momentum equation

$$\nabla \cdot T = \nabla \cdot (\sigma(\boldsymbol{I} - \boldsymbol{nn})\delta(\phi))$$

Hysing (2006) introduced using Laplace-Beltrami operator on the identity mapping in order, which results in an artificial diffusion term

$$\Delta_s id_\Gamma = \kappa \boldsymbol{n}, \qquad (id_\Gamma)^{n+1} = (id_\Gamma)^n + \Delta t^{n+1}\boldsymbol{u}^{n+1}, \qquad \Delta \mathrm{t}^{\mathrm{n+1}} = \mathrm{t}^{\mathrm{n+1}} - \mathrm{t}\text{\^{}}\mathrm{n}$$

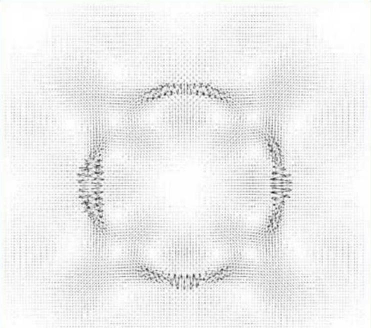
$$f_\sigma = \sigma\kappa\boldsymbol{n}\delta(\phi) \rightarrow f_\sigma^{n+1} = \sigma(\Delta_s(id_\Gamma)^n + \Delta t^{n+1}\Delta_s\boldsymbol{u}^{n+1})$$

This alternative formulation reduces spurious currents generated from the capillary force

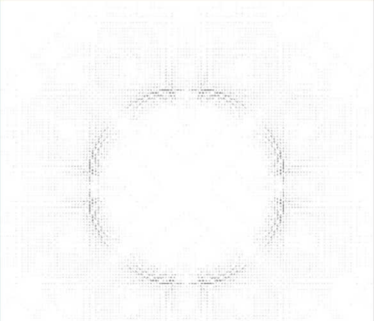
$\Delta_s\boldsymbol{u}$ term acts as artificial diffusion

$\nabla_s = (I - nn)\nabla$
$\Delta_s = \nabla_s \cdot \nabla_s$
$\sigma = surface\ tension$
$\phi = level\ set$
$\delta(\phi) = smoothed\ Dirac\ delta$

- Tested on a static drop problem which is a drop placed in equilibrium with no forces acting on it other than surface tension.
- The results to the right show velocity vectors for the CSS and Hysing version of surface tension.
- We can see that spurious currents are improved in Hysing's formulation



CSS 1X magnification



Hysing 10X magnification

Static drop example problem tests formulation

S. Hysing (2006) A new implicit surface tension implementation for interfacial flows

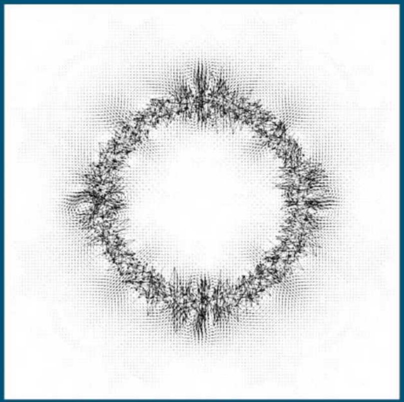
Diffusion/Artificial Viscosity to Stabilize the Spurious Currents

- Both Hysing 2011 and Denner (2015, 2017) describe an additional term which can be used to stabilize these spurious currents
- Both take the form of:

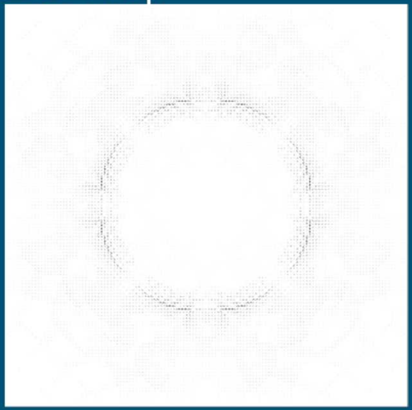
$$f_\Gamma = \Gamma \Delta t \delta(\phi) \nabla_s^2 \boldsymbol{u}$$

- Where ∇_s^2 is the Laplace-Beltrami operator
- This gives us an artificial diffusion which is scaled by the time step

Hysing/Denner comparison
10X time step size



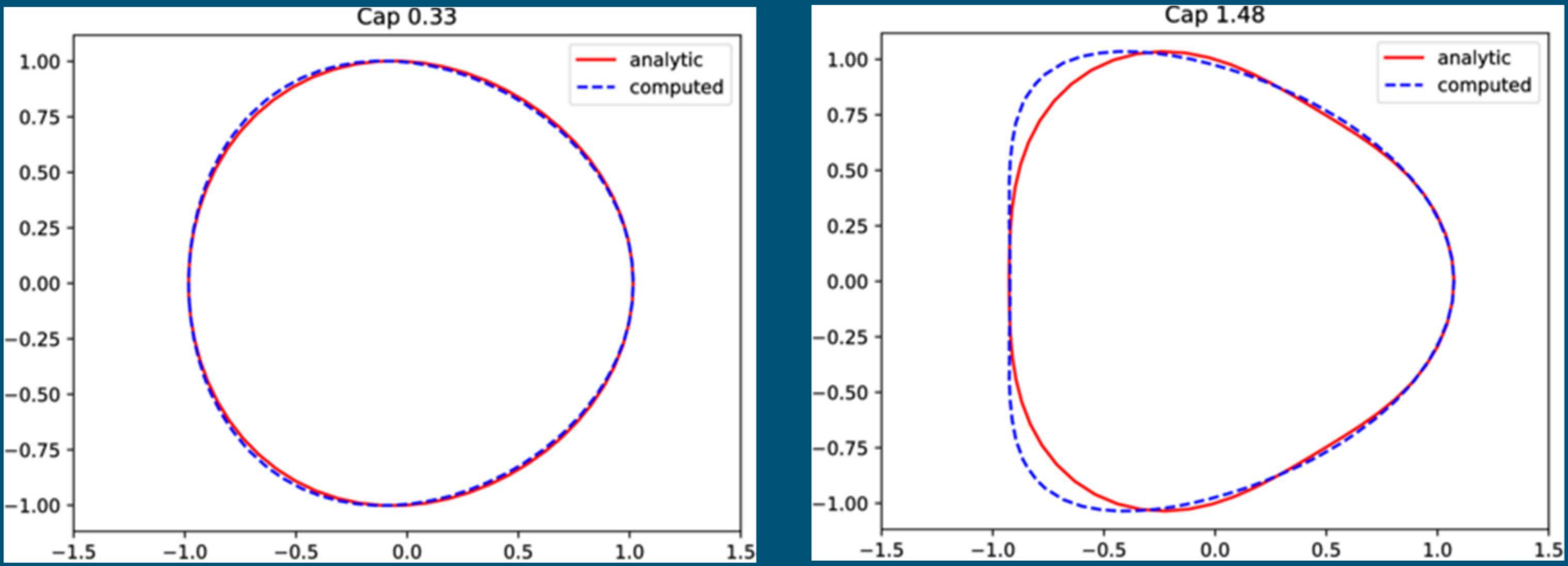
CSS 1X magnitude (after 9 seconds)



Hysing after 90 seconds 10X

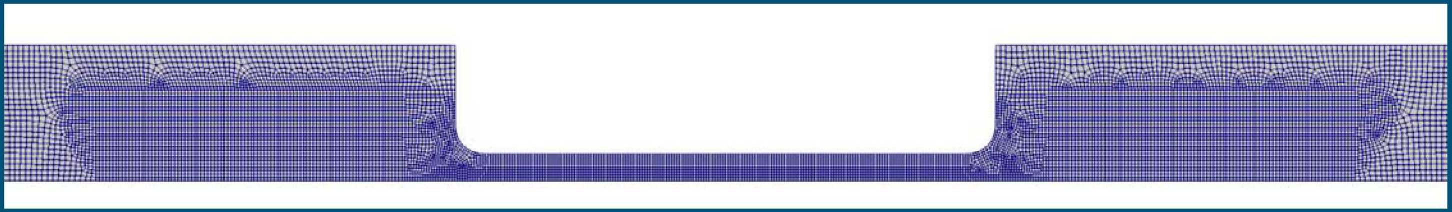
Drop in Planar Poiseuille Flow Comparison

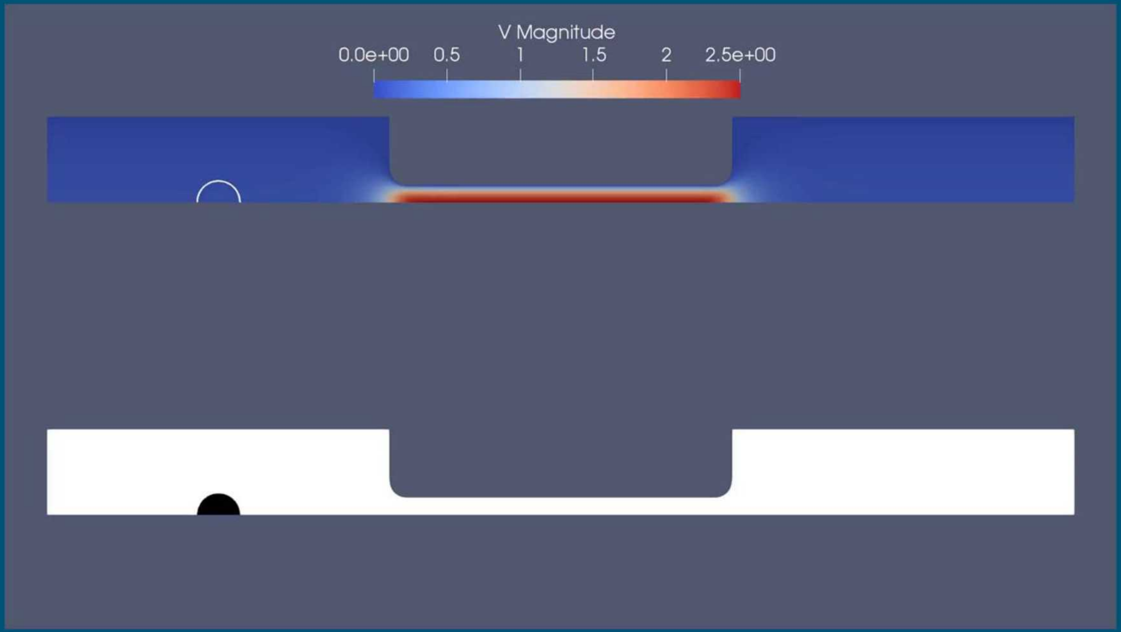
Add image of Poiseuille flow



Common benchmark problem, Compare to analytic function from Nadim and Stone 1991

Newtonian Drop in Constriction Ca~0.2

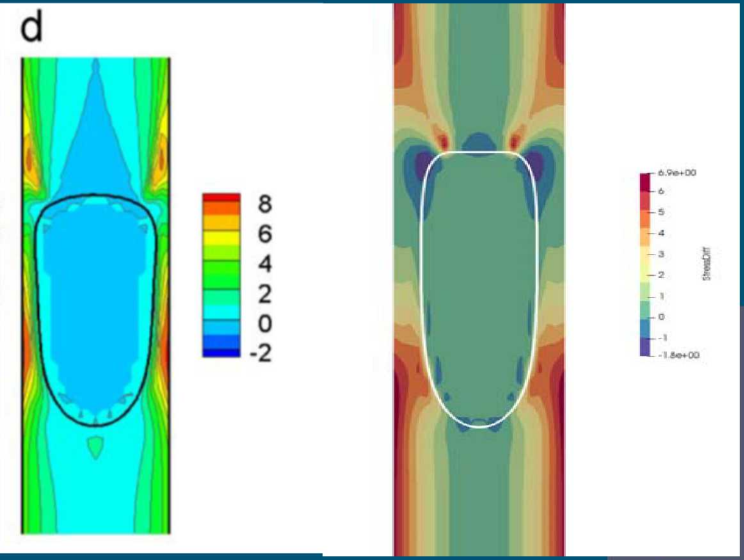




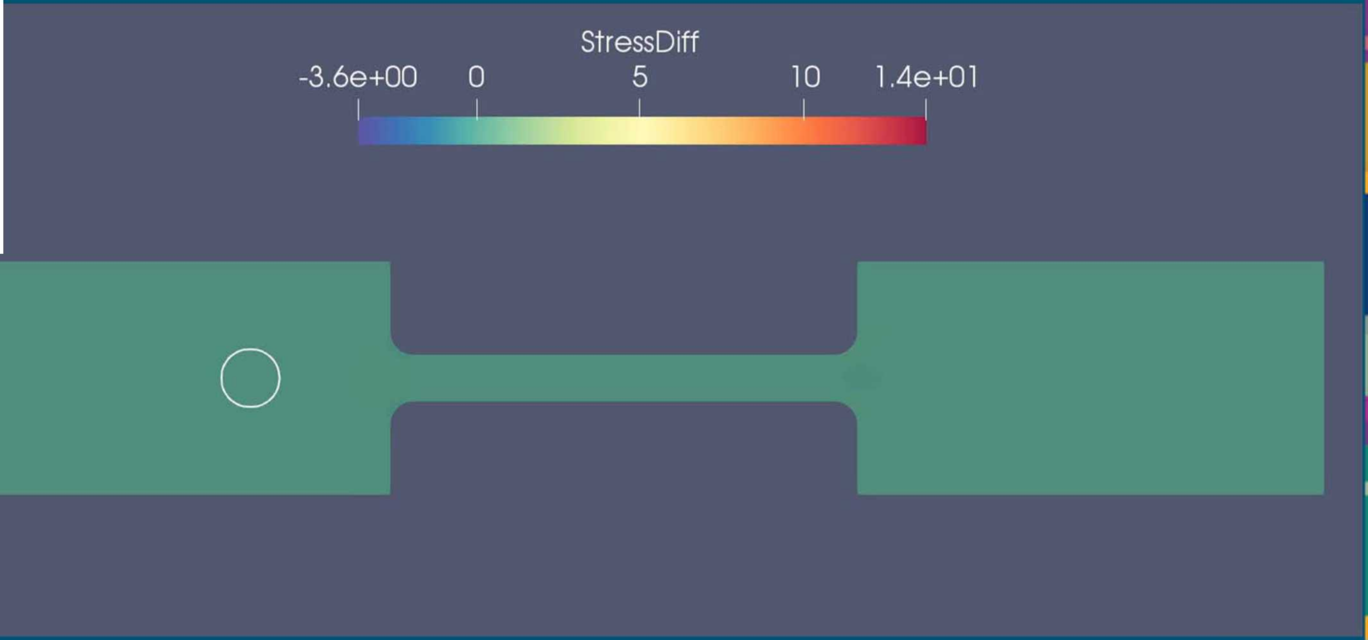
- An initial comparison with another millifluidic simulation by Chung et al. 2009
- Newtonian drop in 5 to 1 contraction in a Newtonian media
- As capillary is increased the drop elongates more in the constricted area

Chung et al., "Effect of viscoelasticity on drop dynamics in 5:1:5 contraction/expansion microchannel flow, Chem. Eng. Sci, 2009

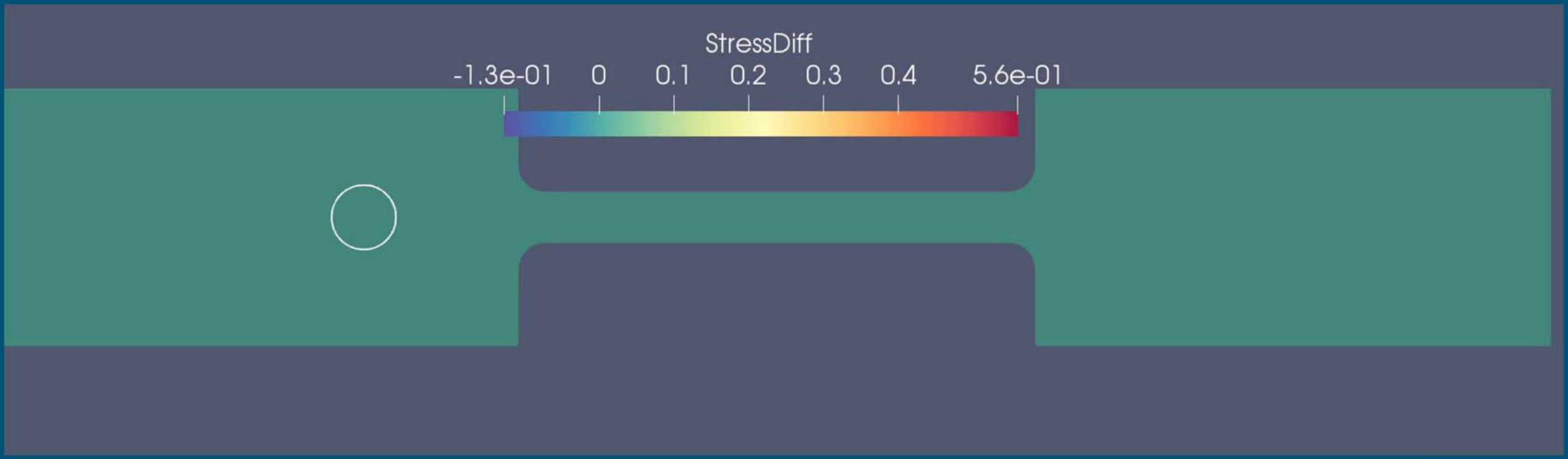
Newtonian Drop in a Viscoelastic Fluid: Constriction Ca~0.1 De~0.4



Verification test: Compare to results from Chung et al., 2009



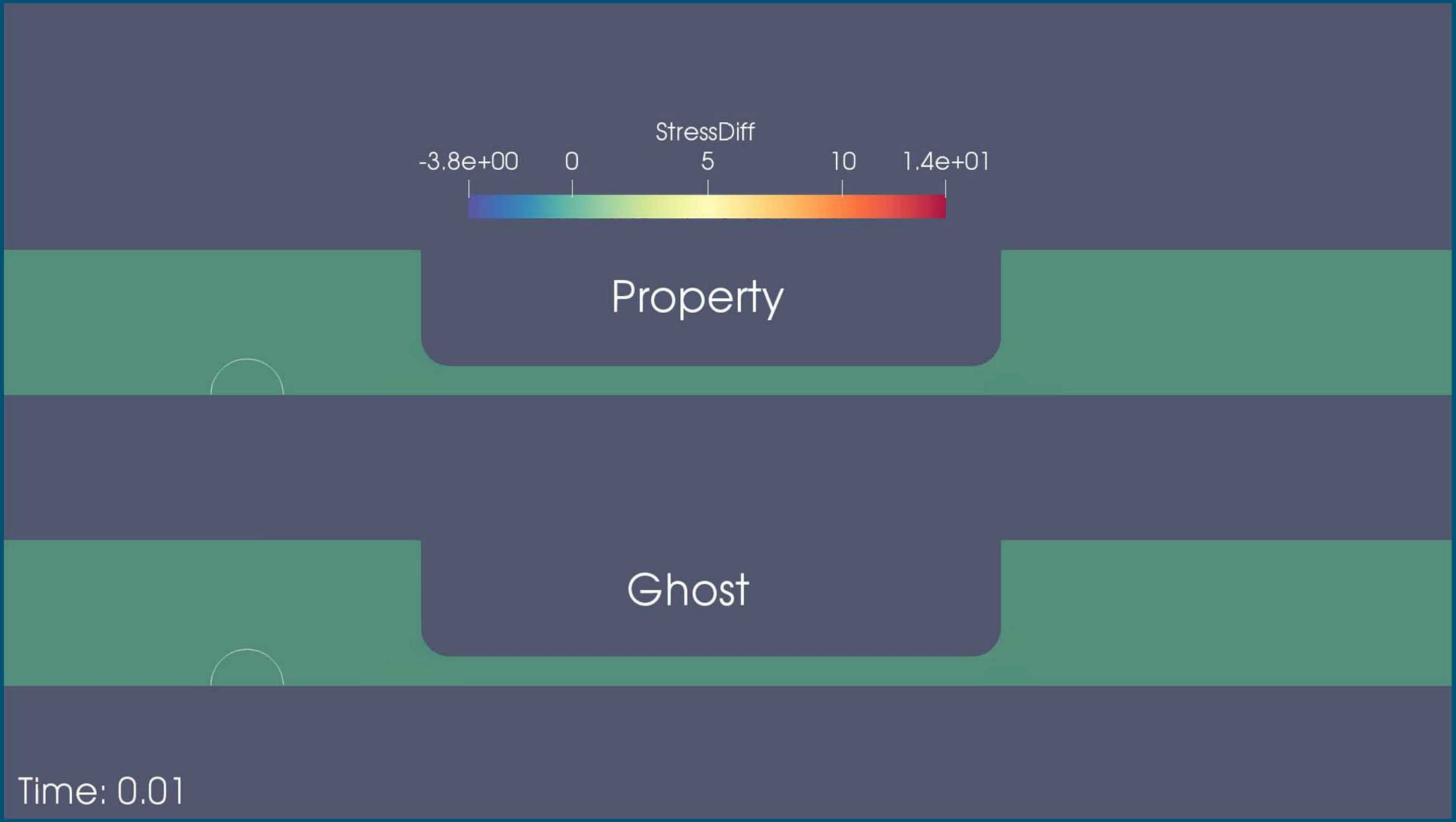
Viscoelastic Drop in a Newtonian Fluid: Constriction Ca~0.1 De~0.4



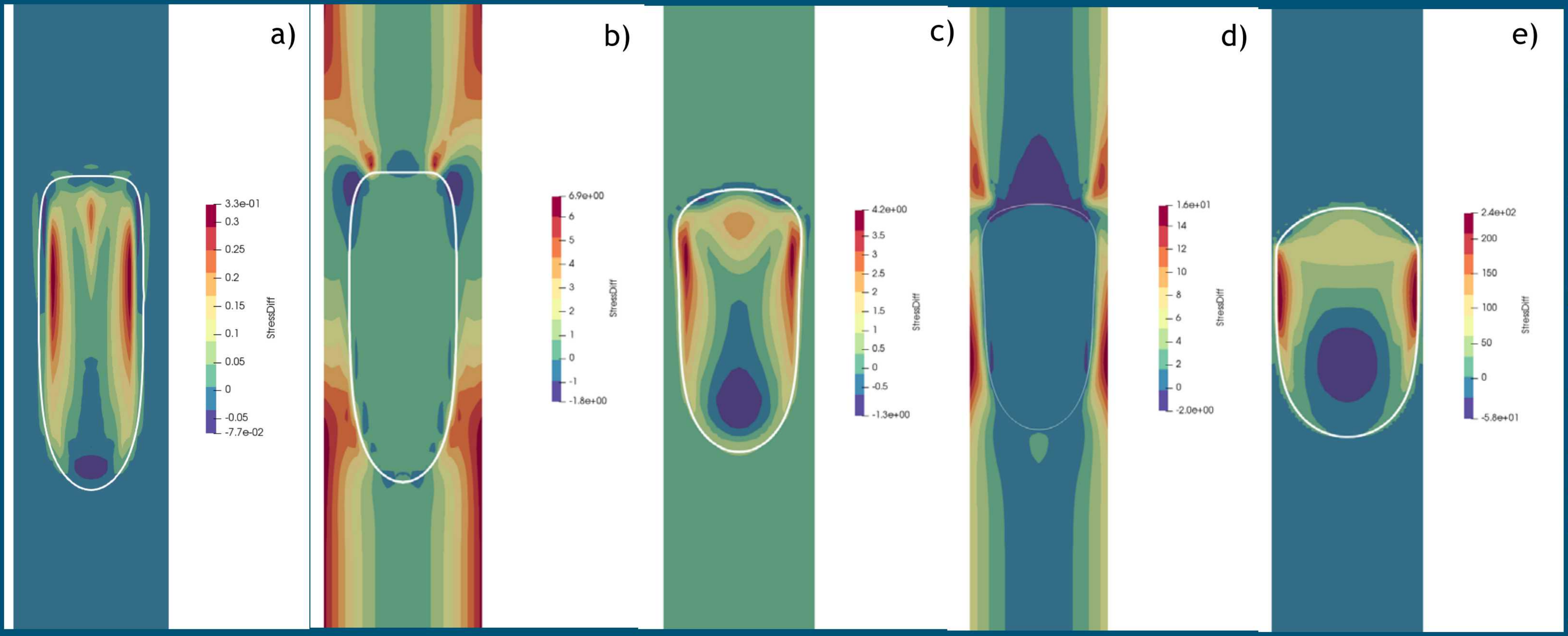
Verification test: Compare to results from Chung et al., 2009

Newtonian Drop in a Viscoelastic Fluid: Constriction Ca~0.1 De~0.4

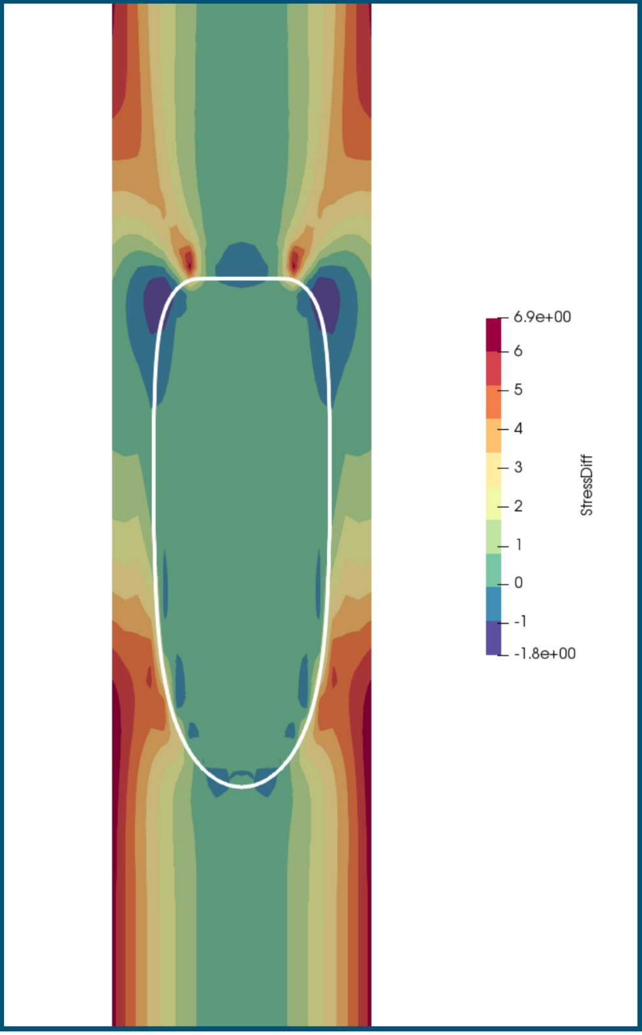
10b

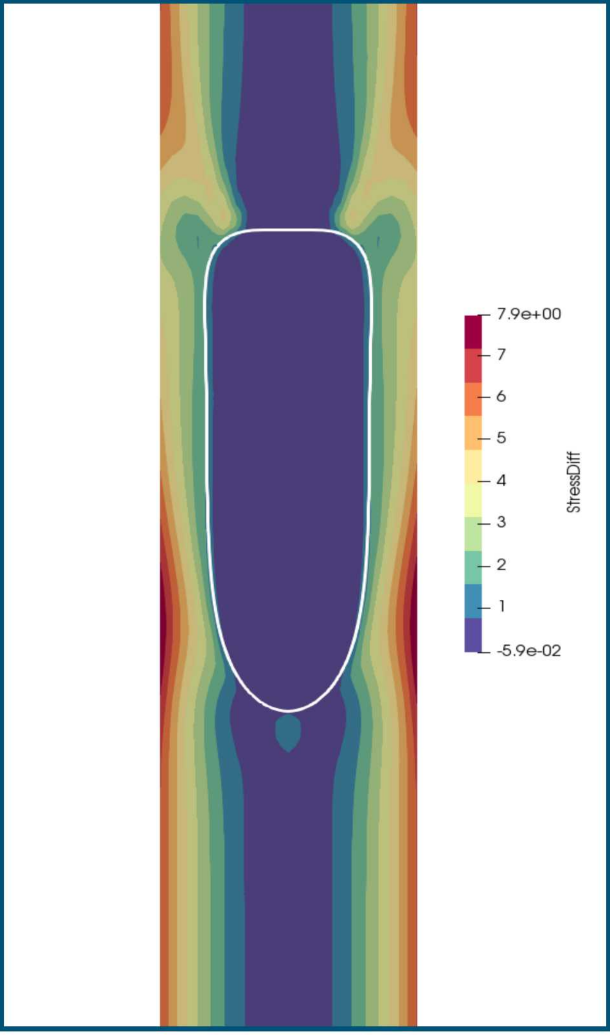


Droplet Shapes and Stress Profiles for Various Scenarios

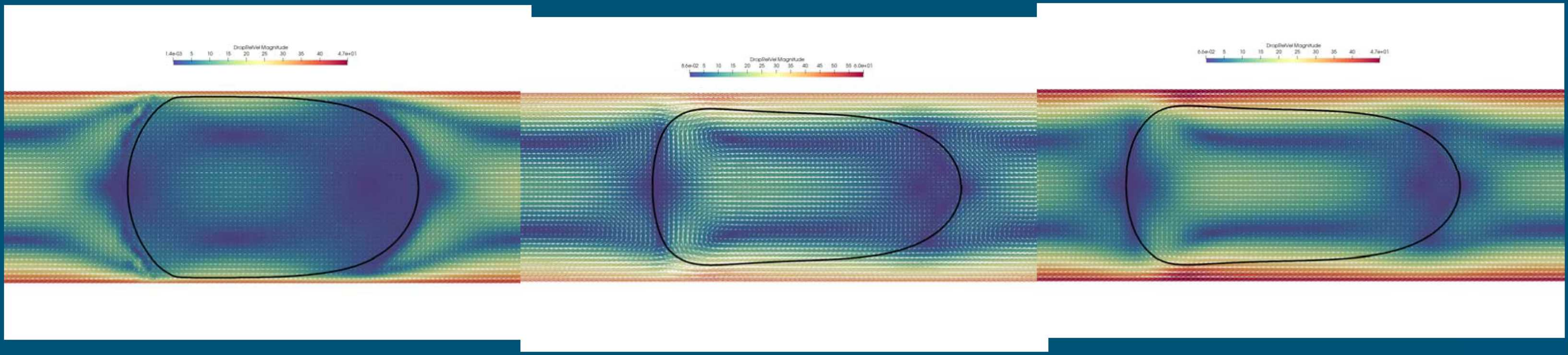


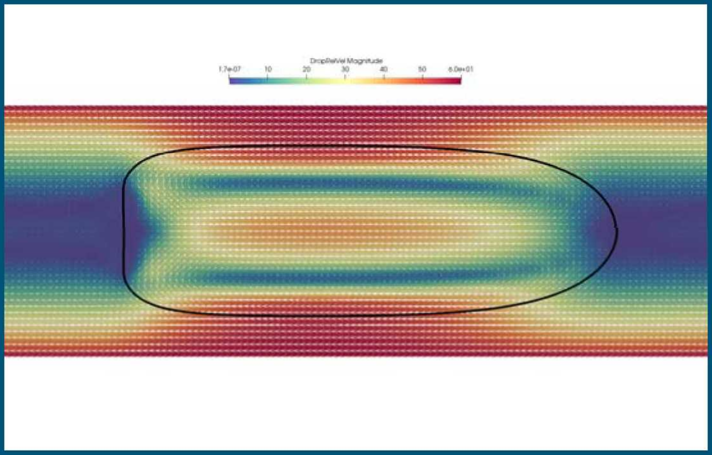
Property Averaging versus Ghost Method for Case b

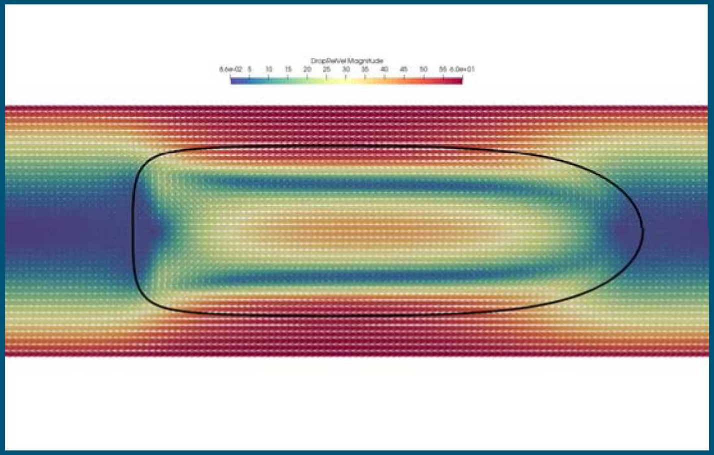




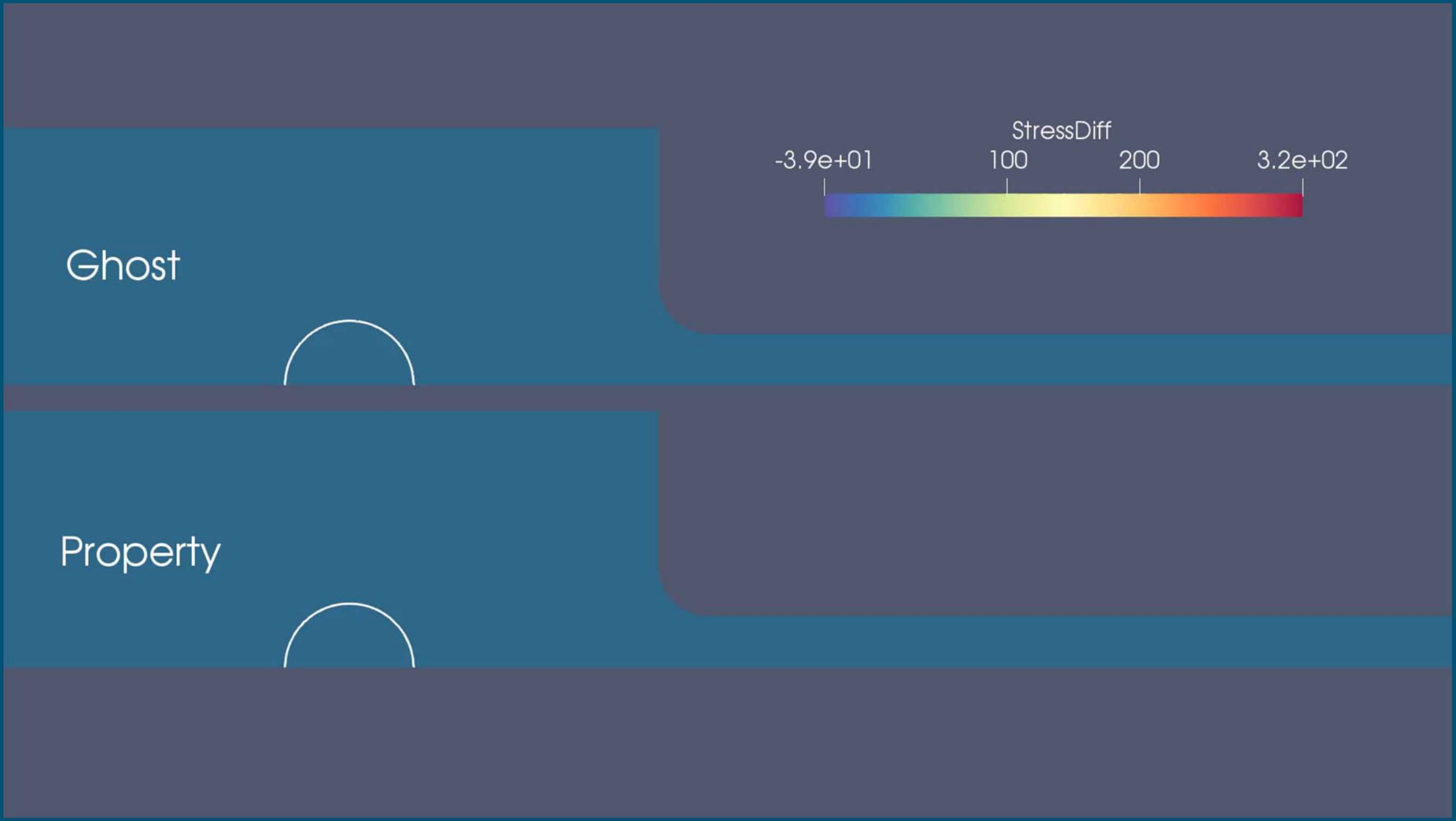
Drop Recirculation for Different Scenarios



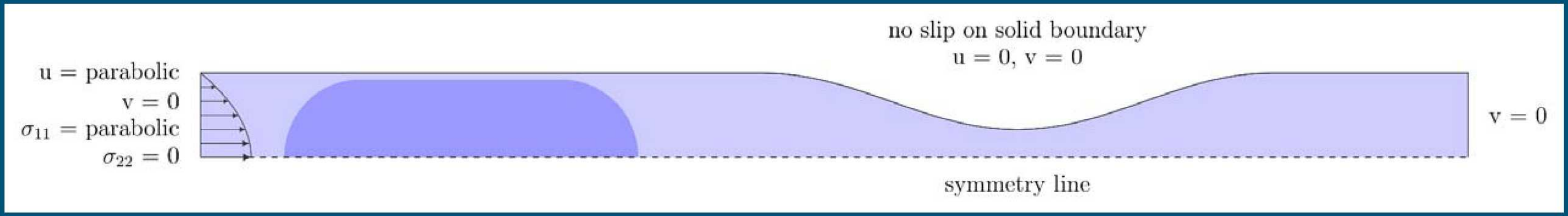




Ghost More Robust for Viscoelasticity in Thin Gaps (10f failure)

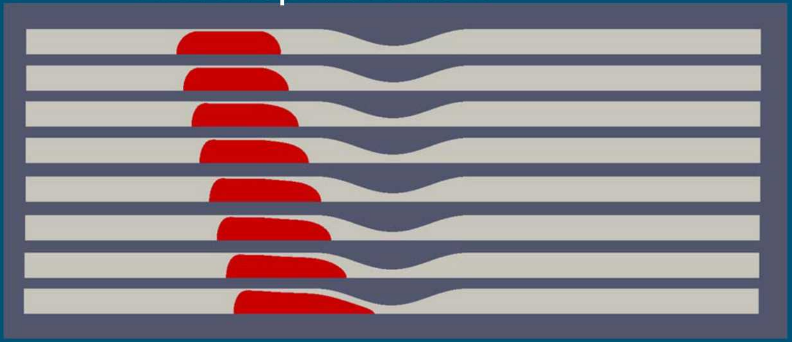


Millifluidic Drop in Constriction



- Newtonian drop in PTT viscoelastic fluid is moved through a narrow constriction.
- ALE requires remeshing often due to mesh movement
- Level set does not require remeshing
- Level set requires stricter time step size limitations due to the Courant limit and Capillary number
- Video on next shows level set flow through the constriction
- ALE was increasingly difficult to remesh at the constriction and we were not able to follow a drop completely through the constriction

ALE Drop Movement

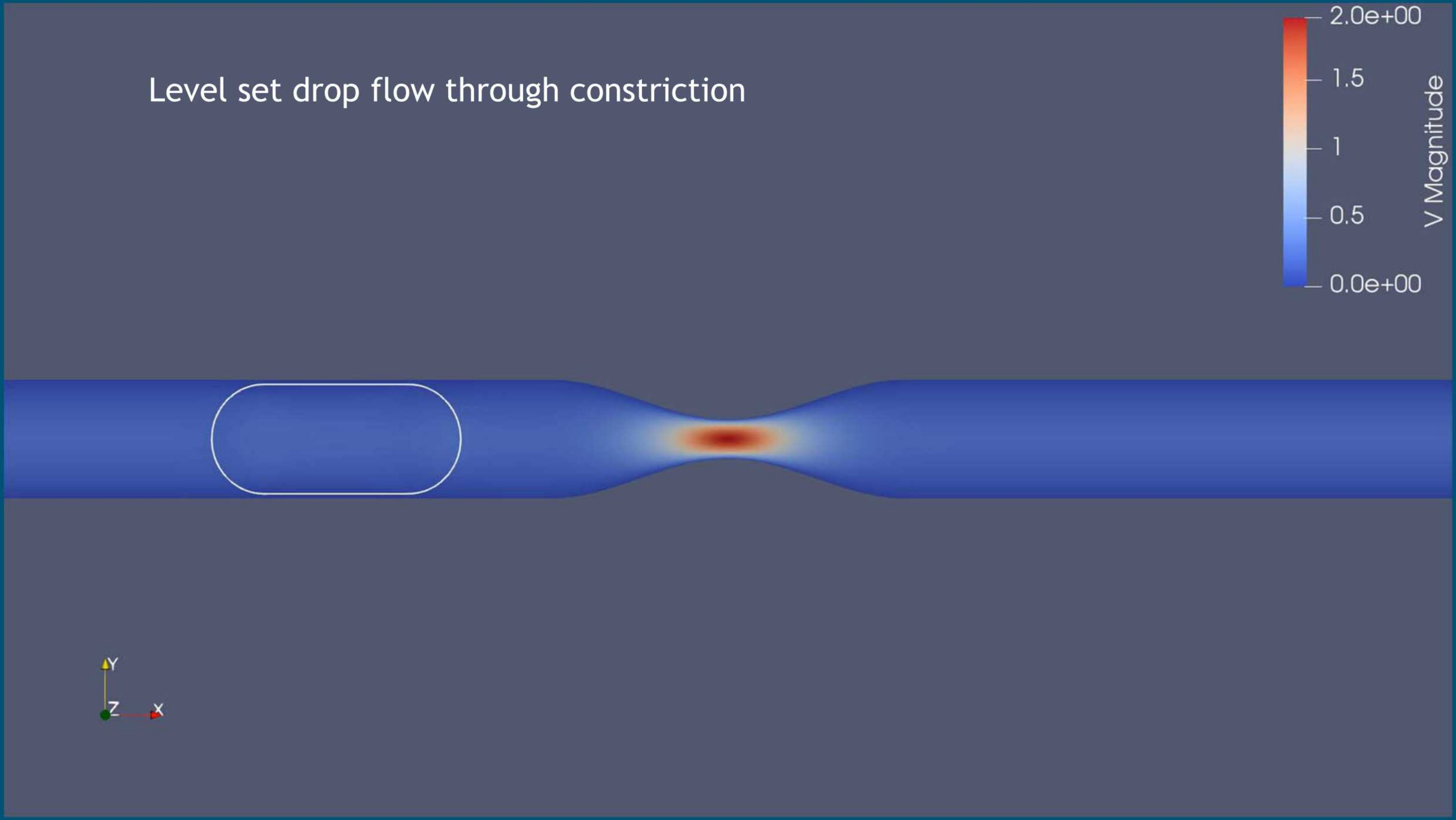


Example of the number of separate meshes required for moving the drop to the constriction in ALE, each step is a separate mesh

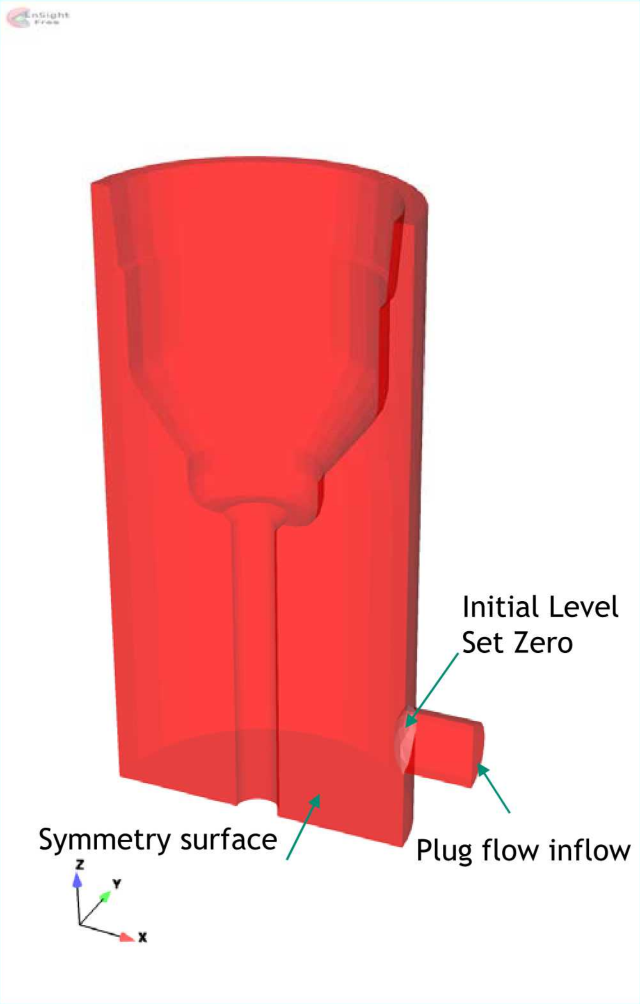
Difficulties increase at the constriction because element size is reduced requiring remeshing more often

Millifluidic Drop in Constriction

Level set drop flow through constriction



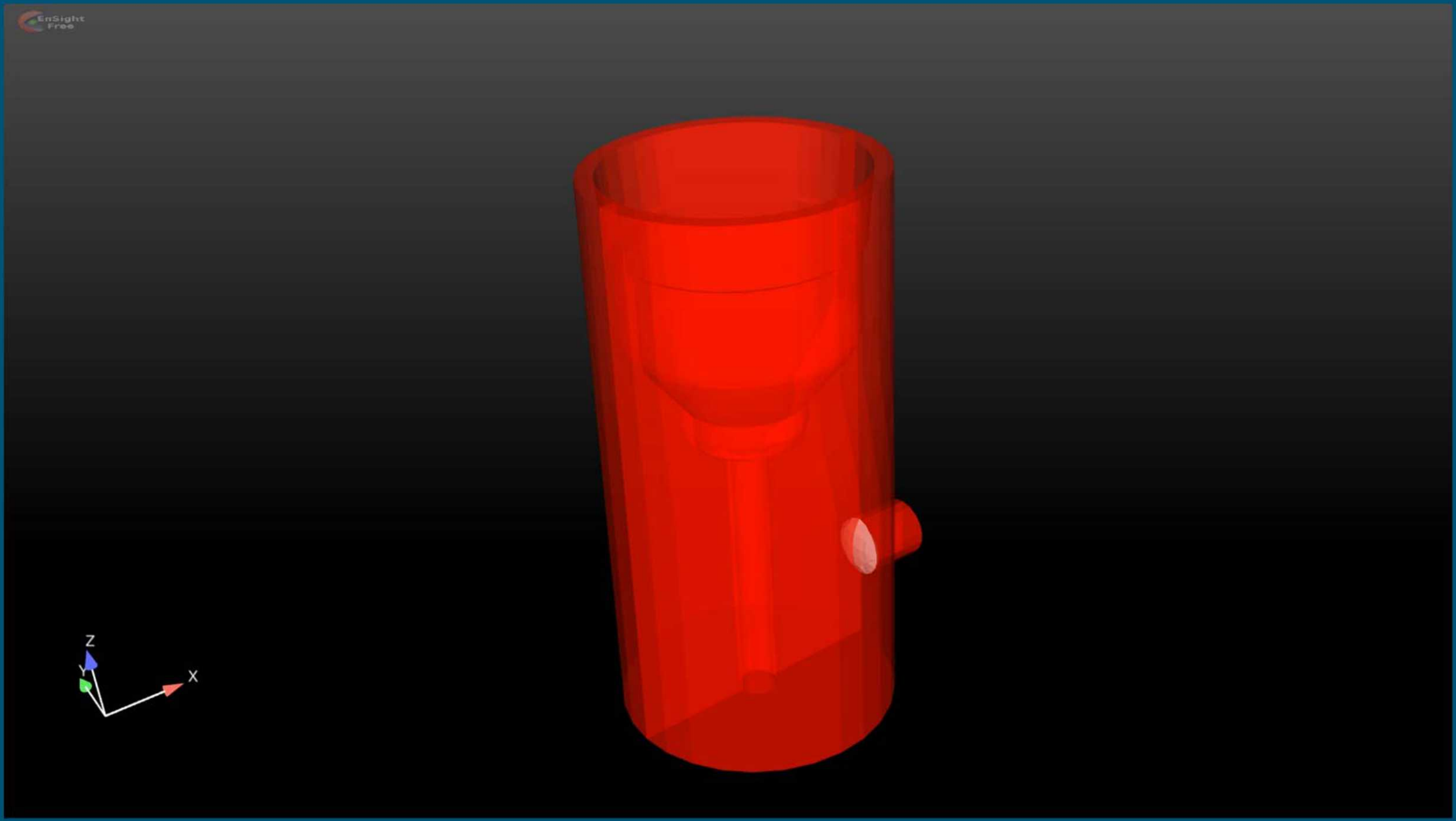
3D Level Set Mold Fill



- 3D Newtonian Level Set problem
- Runs both Fully Coupled and Segregated
- Segregated separates Level Set Equation from Momentum and Continuity solve
- Iterative solver (GMRES + ILUT) behavior is much faster and better behaved in Segregated version
- Iterative solver time for Segregated is near half the Fully Coupled version per time step
- Assemble time is about the same

- Using Direct solver the same benefit in speed is not seen ~15% faster solve time for Segregated
- However the number of Newton iterations required per time step is much fewer for Segregated version
- This reduction means for a similar number of time steps the segregated version is around 1.5X faster (for this 3D problem)

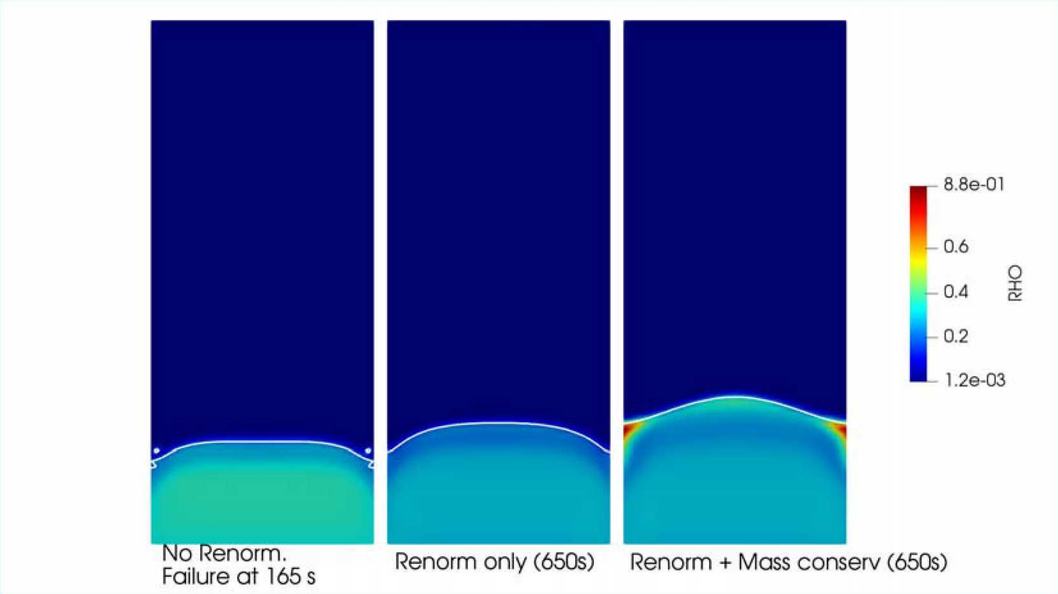
3D Level Set Mold Filling



Conclusions and Future Work

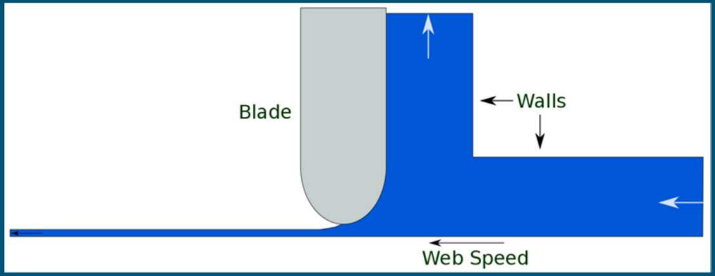
- We have demonstrated a viscoelastic free surface method using a level set to track the free surface
- Two formulations were compared
  - Equation and property averaging
- For problems with a VE fluid and a gas phase, spurious currents occur in the gas phase and grown until simulation dies
  - Spurious currents are worse with large viscosity, density jumps, and lower Ca
  - Equation averaging works slightly better than property averaging

- Still investigating improvements to VE level set formulation
  - Issue may be related to renormalization and the need to advect fields to catch up to the new material interface



Viscoelastic Modeling of Blade Coating

GOMA 6.0 with log-conformation formulation to improve stability at high Weissenberg Number



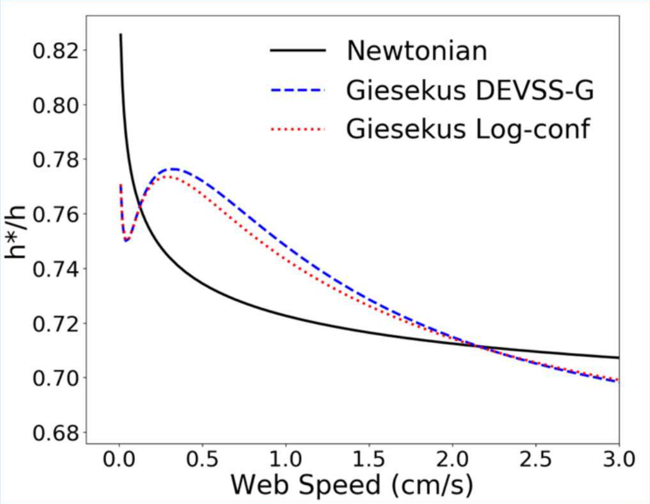
- For Newtonian fluids, the film thins as the web speed increases.
- Viscoelastic film thickness is non-monotonic, thickens and then thins
- Log conformation greatly increased maximum web speed

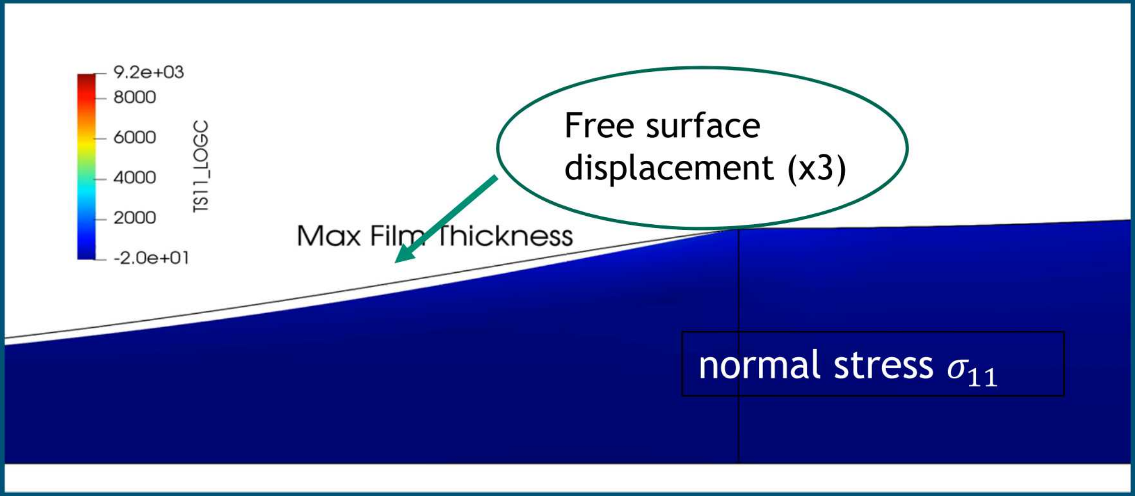
Maximum Web Speed

Giesekus
DEVSS-G: 18.2 cm/s
DEVSS-G Log Conf: 35.5 cm/s

Phan Thien Tanner
DEVSS-G: 4.6 cm/s
DEVSS-G Log Conf: 28.8 cm/s

Log-conformation tensor increases maximum web speed obtained for blade coating





Free surface displacement (x3)

Max Film Thickness

normal stress σ_{11}

Reference: Fattal and Kupferman, *J. Non-Newtonian Fluid Mech.* **123** (2004)

Martin et al, Viscoelastic Blade Coating, submitted C&F, 2018