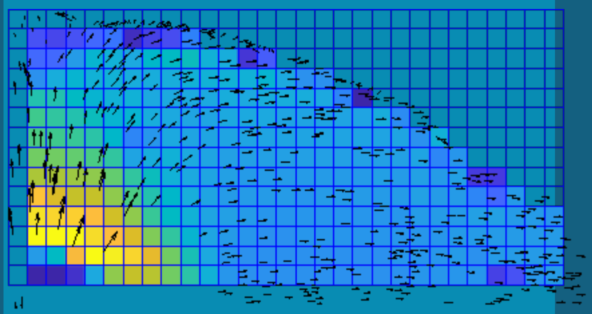
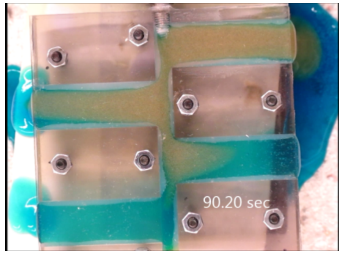
SAND2024-06674C

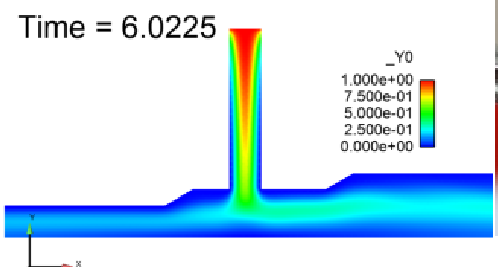
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

Elastoviscoplastic Models and Experiments for Yield Stress Fluids Filling a Thin Mold







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Lisbon, Portugal

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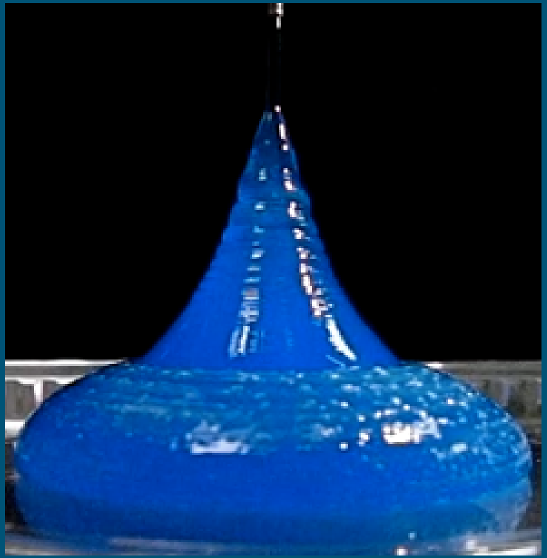
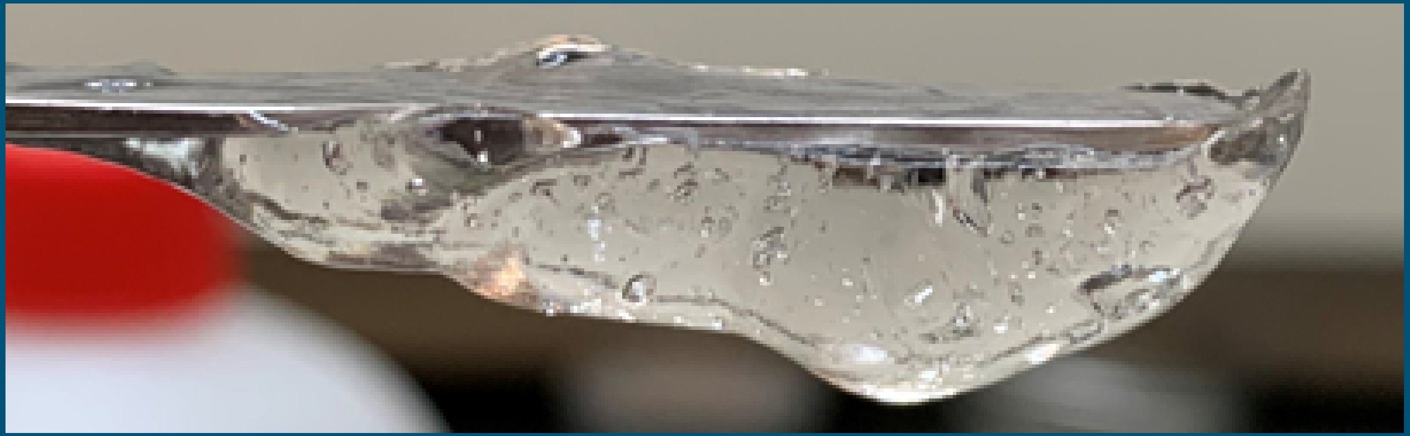
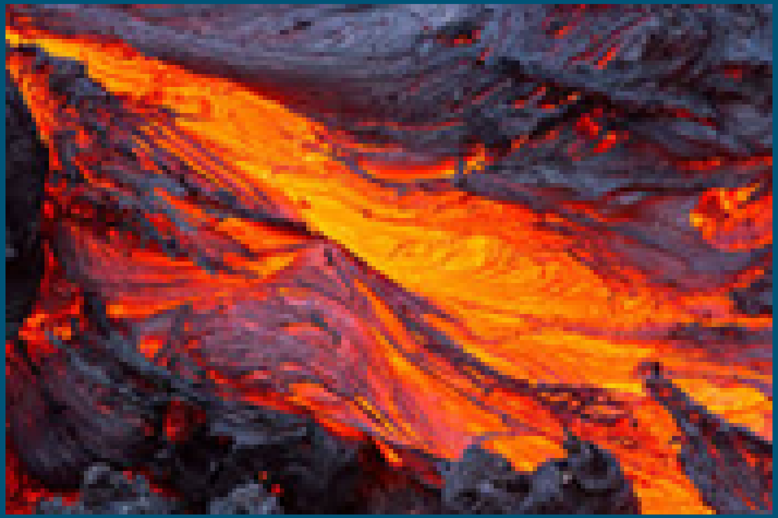
Objective: develop computational models for free-surface flows of yield stress fluids







Yield stress can be seen in wax, whipped cream, toothpaste, lava, ceramic pastes, and Carbopol

Models for Visco/elastic/plastic materials

- Viscoplastic (yield stress fluid) models
  - Bingham: $\sigma = \tau_y + \eta\dot{\gamma}$
  - Herschel Bulkley: $\sigma = \tau_y + k\dot{\gamma}^n$
- Viscoelastic models
  - Maxwell: $\lambda\dot{\sigma} + \sigma = 2\eta_p\dot{\gamma}$
  - Kelvin-Voigt: $\sigma = G\gamma + \eta_p\dot{\gamma}$
- Elastoviscoplastic (EVP) models
  - Saramito [1]: $\frac{1}{G}\dot{\sigma} + \max\left[\frac{|\sigma|-\tau_y}{k|\sigma|^n}\right]^{\frac{1}{n}}\sigma = 2\dot{\gamma}$
  - P&L model [2]: $\lambda\dot{\sigma} + \sigma = 2\eta_p(\dot{\gamma})\dot{\gamma}$
  - KDR [3]: $\lambda_1\dot{\sigma} + \sigma = \eta_p(\dot{\gamma})\dot{\gamma} + \lambda_2\ddot{\gamma}$

1. P. Saramito. *A new constitutive equation for elastoviscoplastic fluid flows.* J. Non-Newton. Fluid Mech., 145 (1) (2007), pp. 1-14
2. Y.S. Park, P.L.F. Liu. *Oscillitory pipe flows of a yield stress fluid.* . J. Fluid Mech. 658 (2010) 673-689
3. K. Krutarth, G.J. Donley, and S.A. Rogers. *Unification of the Rheological Physics of Yield Stress Fluids*. Phys. Rev. Lett. 126:21 (2021): 218002

Equations of motion and stress constitutive equations

Momentum and Continuity

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} - \dot{x}) \cdot \nabla \mathbf{u}\right) = -\nabla P + \nabla \cdot (2\mu\dot{\boldsymbol{\gamma}}) + \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$$

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

Oldroyd-B stress constitutive model + Saramito yield model

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overset{\nabla}{\boldsymbol{\sigma}}\right) + \left[\frac{1}{k|\boldsymbol{\sigma}_d|^{n-1}}\right]^{\frac{1}{n}} \mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\mu\dot{\boldsymbol{\gamma}}$$

$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)^{\frac{1}{n}}$$

Herschel-Buckley (HB)-Saramito yield model

The mesh motion is governed by a pseudo-solid model

$$\nabla \cdot \boldsymbol{T} = 0$$

Where $\boldsymbol{S}$ is the Cauchy stress tensor

$$\boldsymbol{T} = \lambda \epsilon_m \boldsymbol{I} + 2\mu_m \boldsymbol{E}$$

- Solve with DEVSS stress stabilization using the Finite Element Method for $\mathbf{u}$, P, $\mathbf{x}$, $\boldsymbol{\sigma}$ and $\boldsymbol{G}$ tensors
- LBB compliant form, 27 node hex, with quadratic $\mathbf{u}$ and linear $\boldsymbol{P}$
- $\boldsymbol{G}$ is a continuous projection of velocity gradients
- Arbitrary-Lagrangian Eulerian moving mesh equations with periodic remeshing/remapping

Guénette, R. and Fortin, M. *Journal of Non-Newtonian Fluid Mechanics* (1995) 60: 1, 27-52.

Saramito, P. *Journal of Non-Newtonian Fluid Mechanics* (2007) 145: 1, 1-14.

Saramito, P.. *Journal of Non-Newtonian Fluid Mechanics* 158.1-3 (2009): 154-161.

Fraggedakis, D et al. *Journal of Non-Newtonian Fluid Mechanics* (2007) 236, 104-122.

We also consider a generalized-Newtonian constitutive model

Momentum and Continuity

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u}\right) = -\nabla P + \nabla \cdot (2\mu\dot{\boldsymbol{\gamma}}) + \rho\mathbf{g}$$

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

Bingham-Carreau-Yasuda model

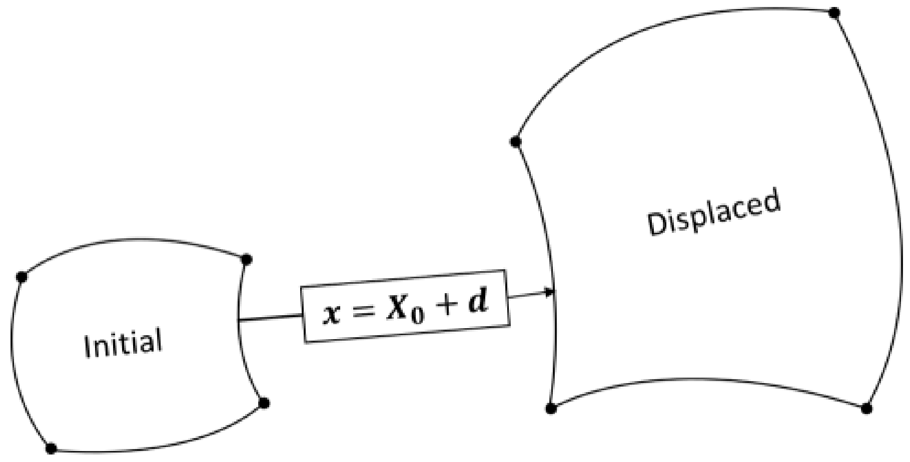
$$\mu = \mu_\infty + \left[\mu_0 - \mu_\infty + \tau_y \frac{1 - e^{F\dot{\gamma}}}{\dot{\gamma}}\right][1 + (\lambda\dot{\gamma})^a]^{\frac{n-1}{a}}$$

The mesh motion is governed by a pseudo-solid model

$$\nabla \cdot \boldsymbol{T} = 0$$

Where $\boldsymbol{S}$ is the Cauchy stress tensor

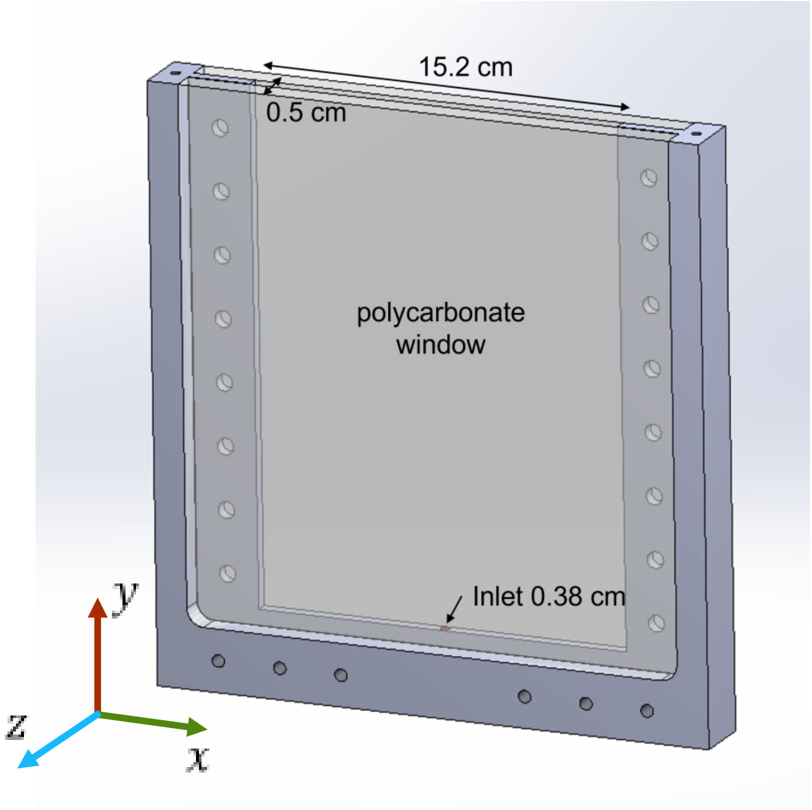
$$\boldsymbol{T} = \lambda\epsilon_m\boldsymbol{I} + 2\mu_m\boldsymbol{E}$$



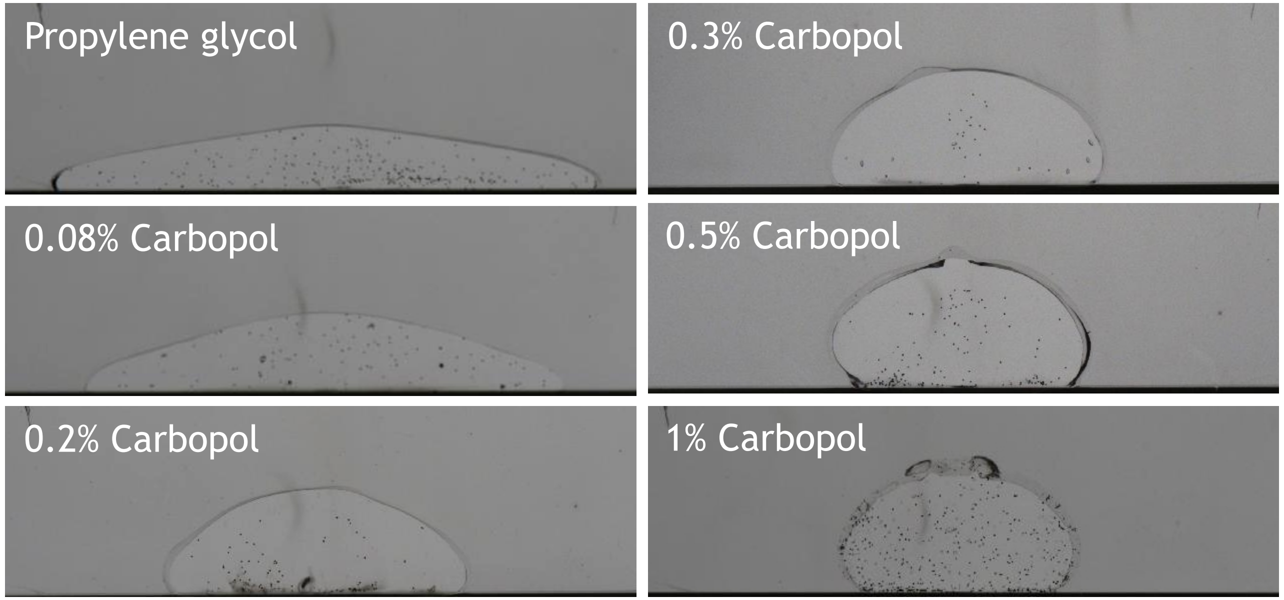
Solve with Finite Element Method for $\mathbf{u}, P, \mathbf{d}$

Mold filling geometry: flow between two thin plates

- **Apparatus dimensions**
  - Inlet diameter = 0.38 cm
  - (x) W = Width = 15.2 cm
  - (y) Height > Width
  - (z) Gap between plates = 0.5 cm



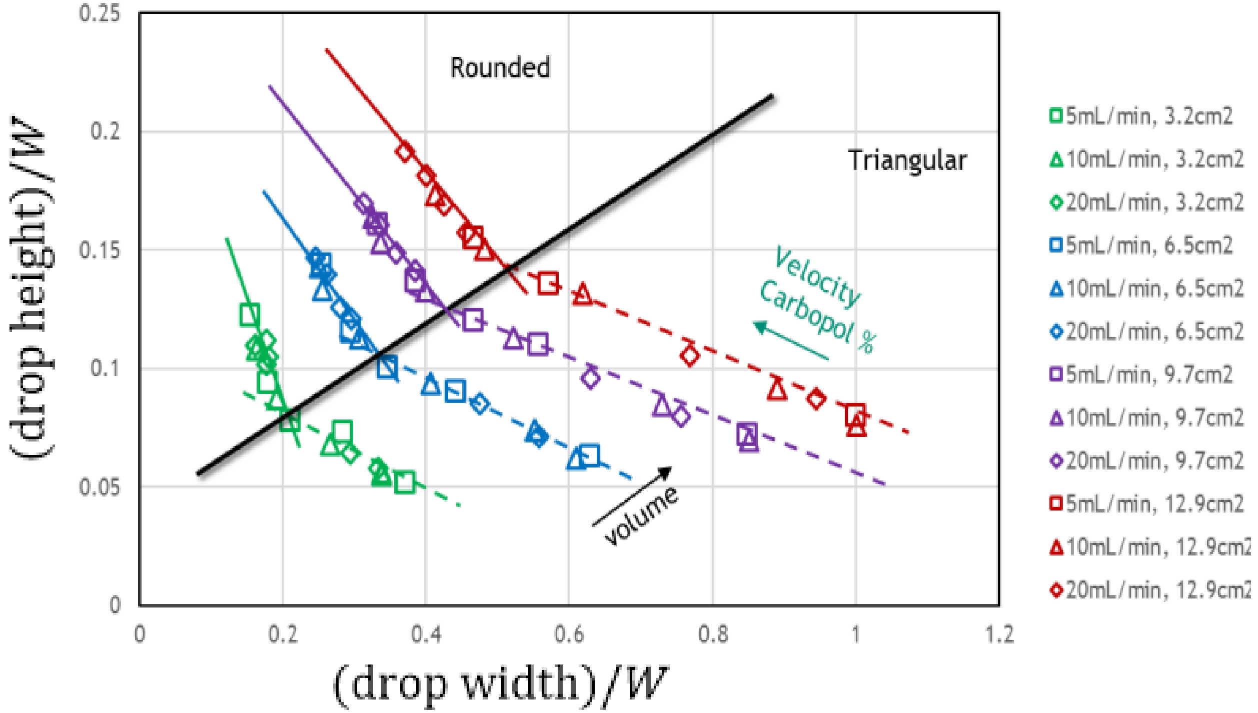
- **Experimental study considers**
  - inlet flow rate: 5-20 mL/min
  - 0-1 wt% Carbopol solutions

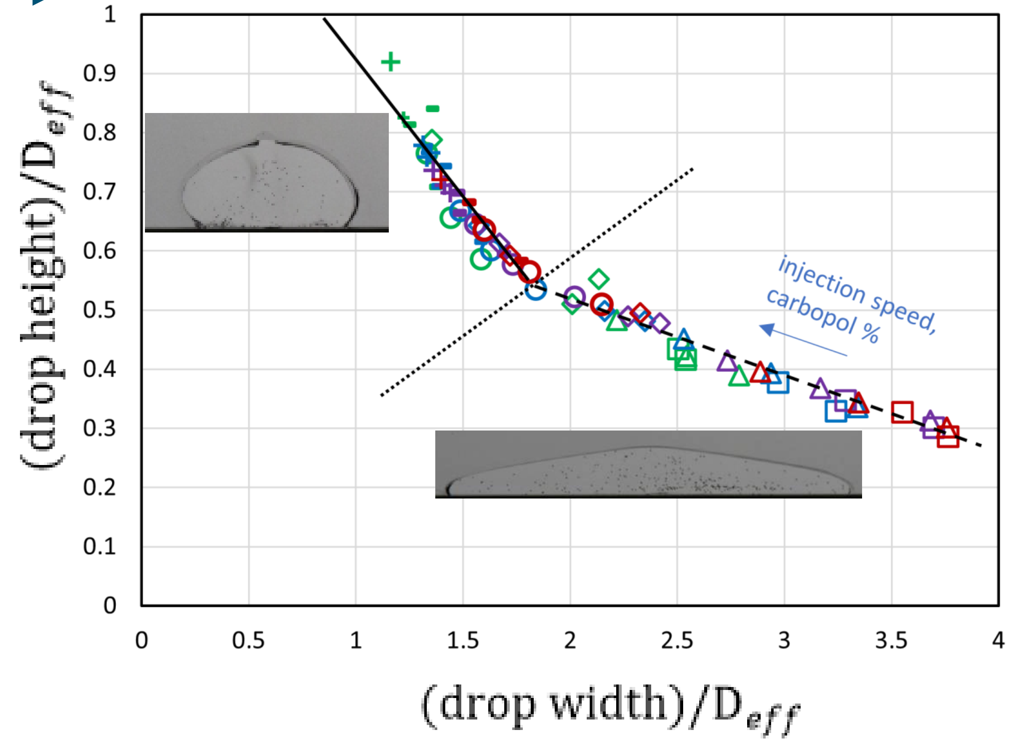


Trends for drop shape evolution

Scale by D_{eff}

$$D_{eff} = \sqrt{\frac{4}{\pi}(\text{cross} - \text{sectional area})}$$

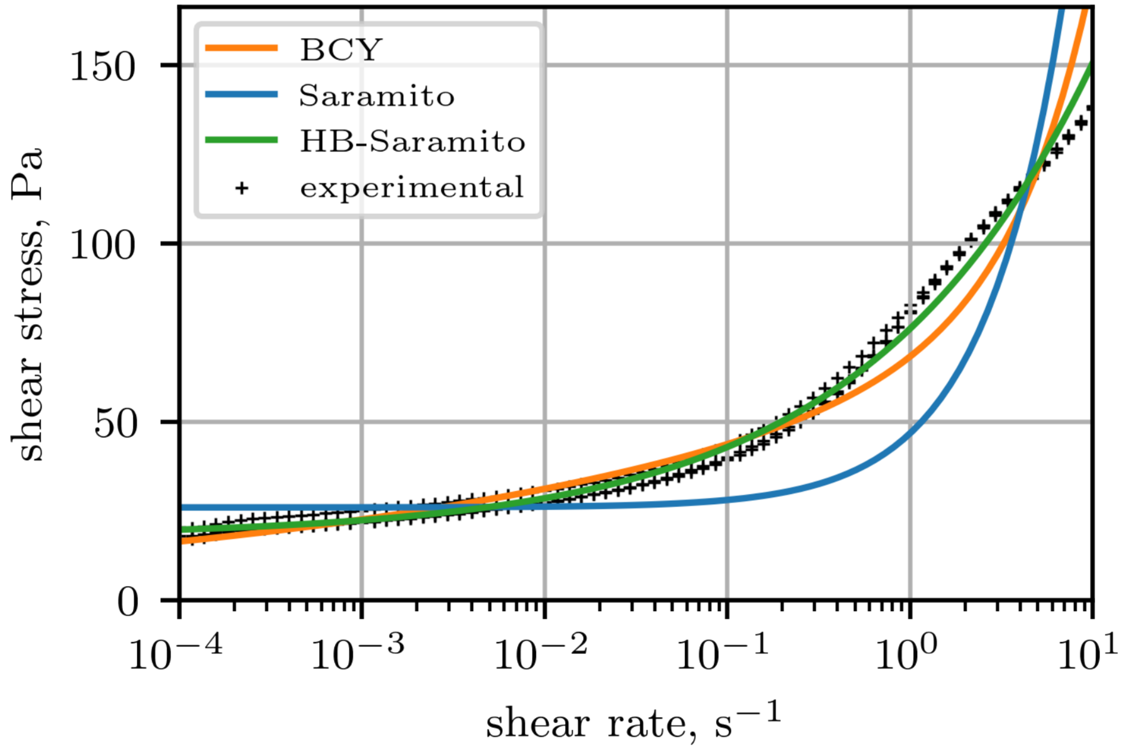




- Fluid drop changes from triangular to round with
  - increasing Carbopol concentration, injection flow rate
  - decreasing drop cross-sectional area

- Height, width collapse onto a single curve when scaled by effective diameter, D_{eff}

Several Constitutive Models for Carbopol Studied



Bingham-Carreau-Yasuda (BCY)

$$\mu = \mu_\infty + \left[\mu_0 - \mu_\infty + \tau_y \frac{1 - e^{-F\dot{\gamma}}}{\dot{\gamma}}\right] \left[1 + (b\dot{\gamma}^a)\right]^{\frac{n-1}{a}}$$

μ_0, (Pa•s)	μ_∞, (Pa•s)	b (s^{-1})	a	n	τ_y, (Pa)	R^2
217.15	0.018	3.112	0.966	0.190	31.21	0.954

Saramito-Oldroyd-B & HB-Saramito

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overset{\nabla}{\boldsymbol{\sigma}}\right) + \left[\frac{1}{k|\boldsymbol{\sigma}_d|^{n-1}}\right]^{\frac{1}{n}} \mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\dot{\gamma}$$

	n	k, (Pa•s^n)	τ_y, (Pa)	G, (s)	R^2
Saramito	== 1	52.85	32.10	576.9	0.889(*)
HB-Saramito	0.368	58.9	64.4	576.9	0.991

- Small amplitude oscillatory rheology gives the elastic modulus, *G*.
- Parameters fit to shear rheology with least squares.

- Saramito model predicts elastic solid response below yield and viscoelastic flow above yield
- Bingham model has yield stress and shear thinning but no elasticity

Mold filling simulations

Constitutive models

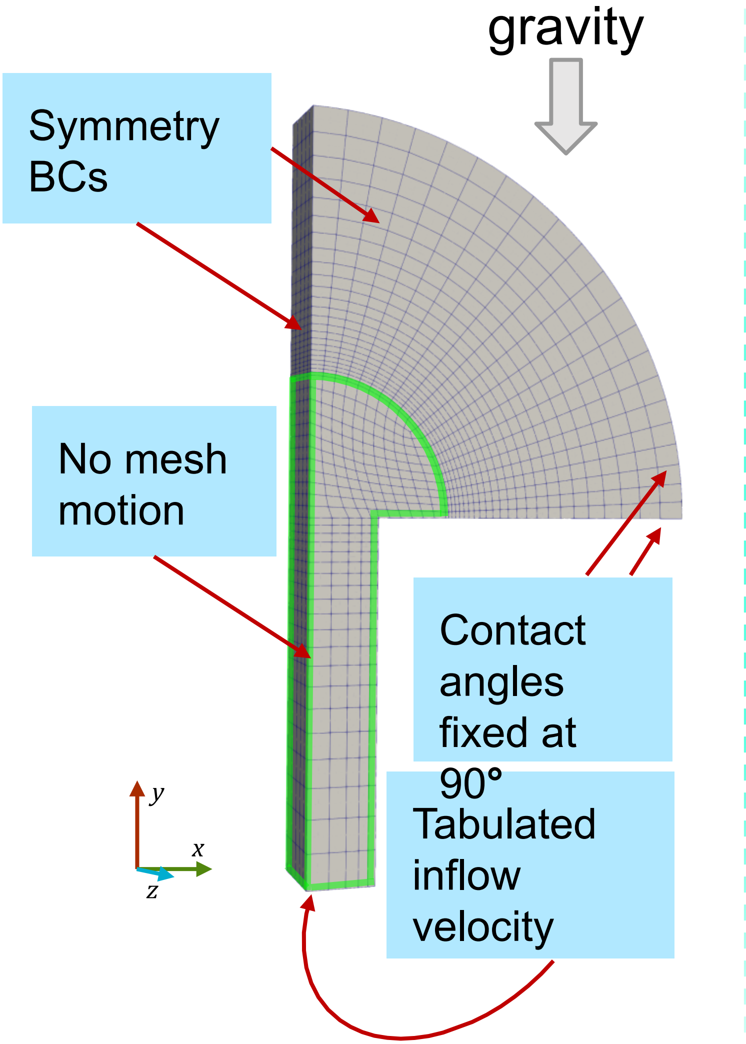
- Bingham-Carreau-Yasuda (generalized Newtonian)
- HB-Saramito

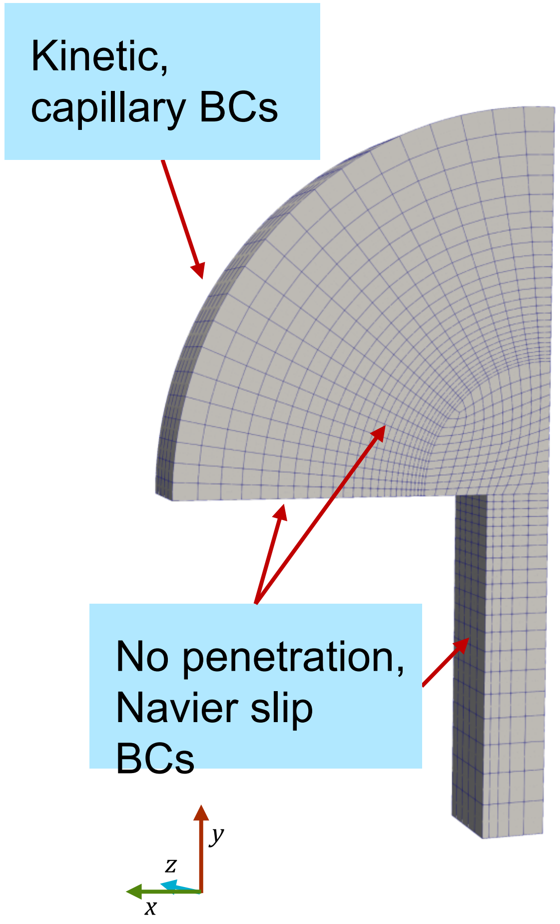
Computations

- Finite element method in Goma
- DEVSS stabilization for EVP models
- Monolithic solve in one matrix with LBB elements
- Arbitrary Eulerian-Lagrangian moving mesh framework
- Remeshing done every ~30 timesteps

Validation Experiments

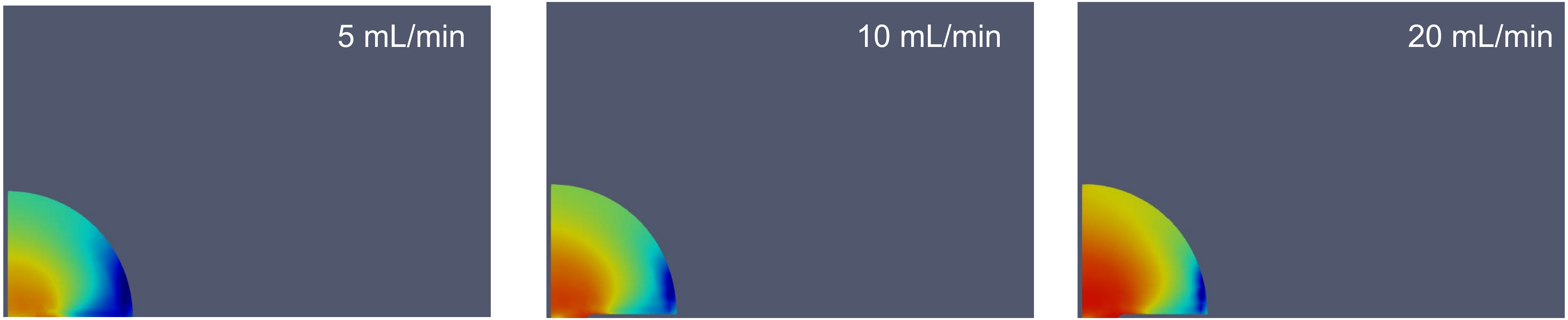
- 0.08, 0.30 wt.% Carbopol
- 5-20 mL/min inlet flow rate





Yield coefficient computed by HB-Saramito model

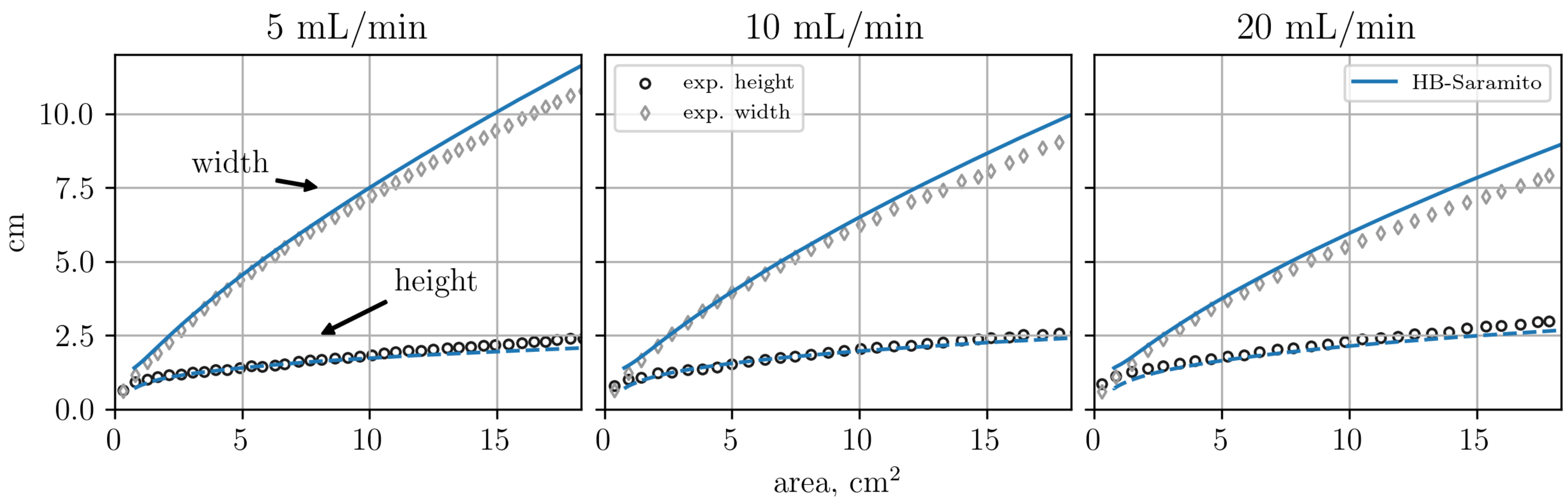
$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)^{\frac{1}{n}}$$



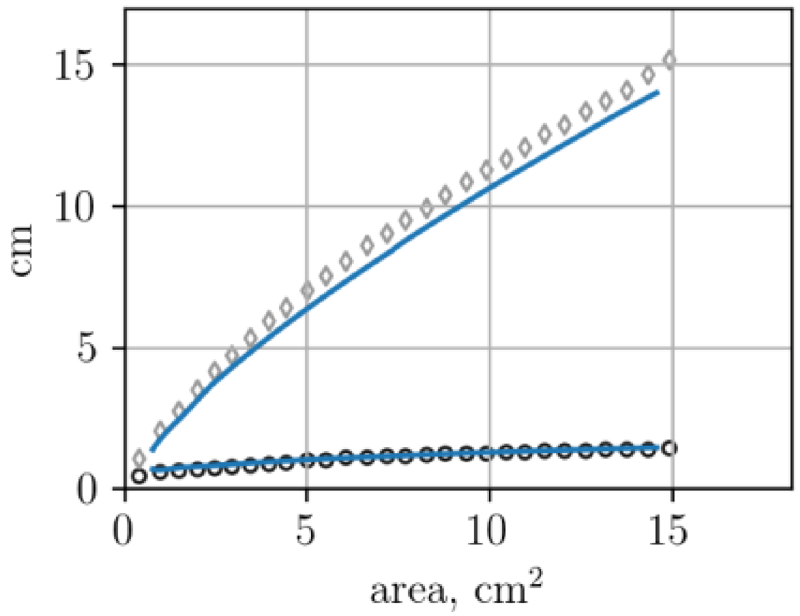
- $S = 0$ indicates solid-like behavior, $S > 0$ → fluid-like
- Unyielded region ($S = 0$) appears near the edges of the droplet and grows at the volume increases
- Increasing flow rate associated with a larger degree of fluid-like behavior, particularly near the fluid inlet.

HB-Saramito drop height/width

0.30%

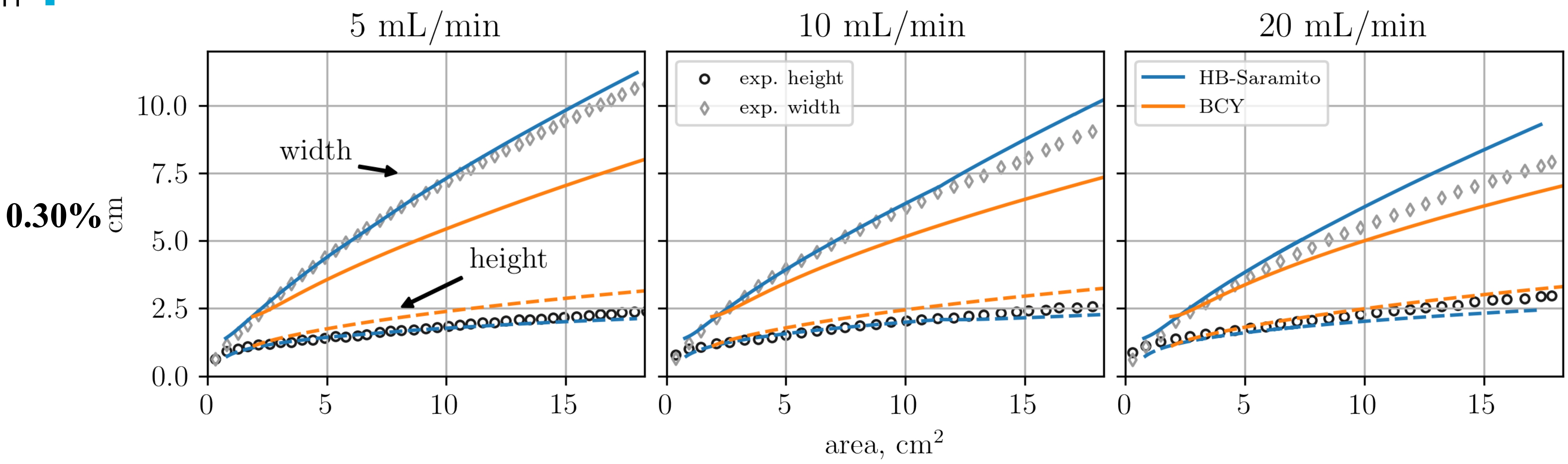


0.08%



- HB-Saramito model is predictive of both height and width, especially at the lowest inlet flow rate
  - Width tends to be over-estimated with growing flow rate and cross-sectional area

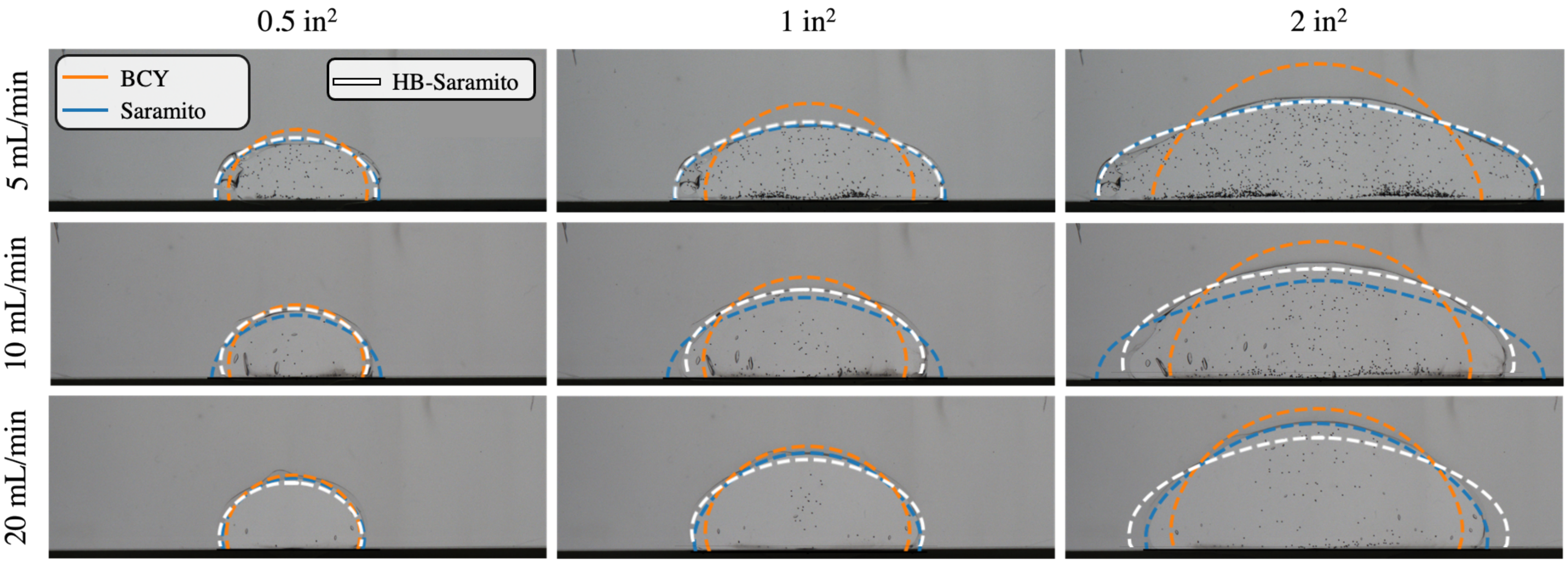
Computed drop height/width



- Overall, BCY model is less predictive of droplet dimensions, but accuracy improves for the largest flow rate considered

J. McConnell, W. Ortiz, J.C. Sutherland, P. Newell, A.M. Grillet, A.M. McMaster, R.B. Bhakta, R.R. Rao *Computational modeling and experiments of an elastoviscoplastic fluid in a thin mold-filling geometry*, Journal of Non-Newtonian Fluid Mechanics. 30 (2022), 104851

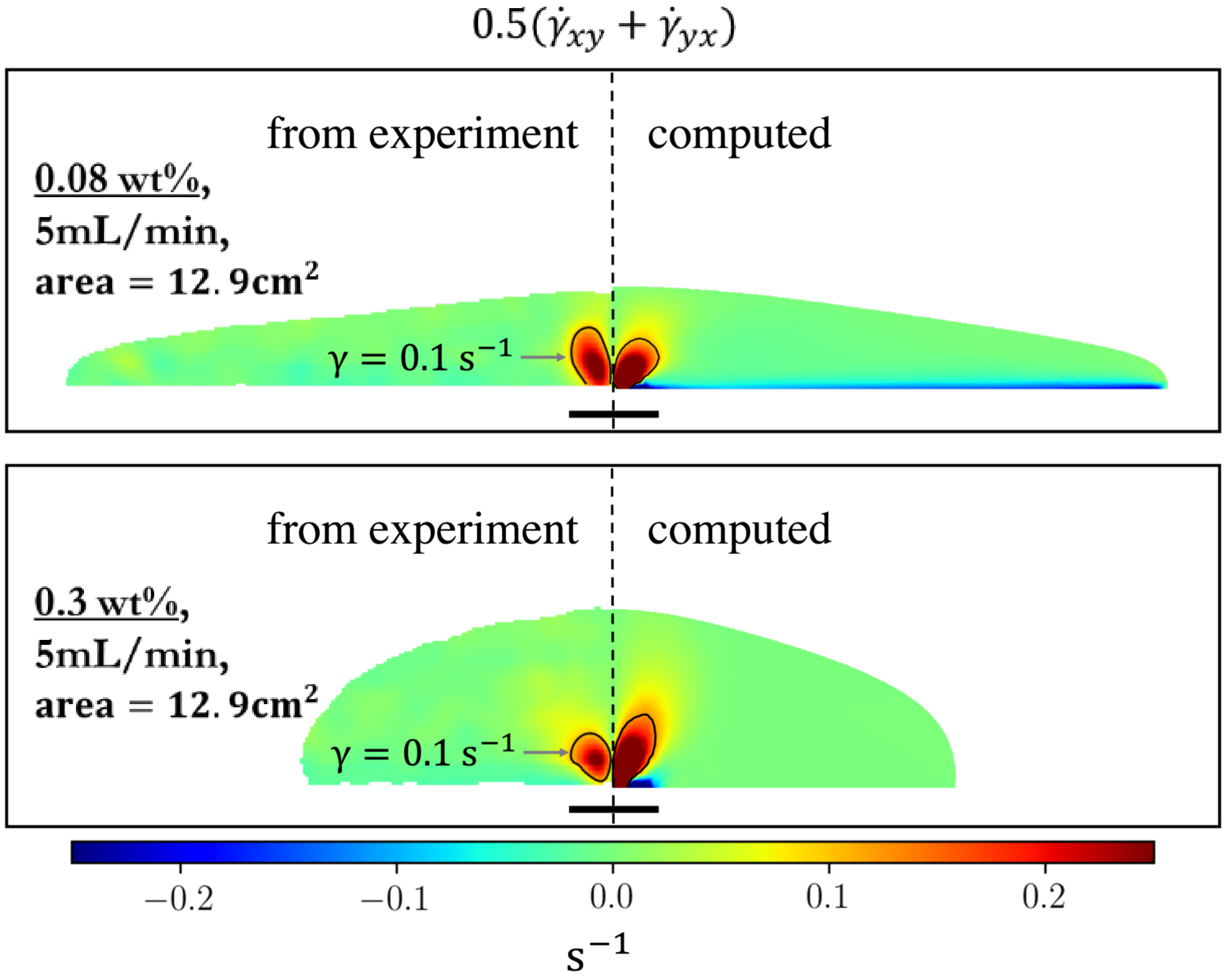
Droplet shape computed from 3D simulations



- Experimental droplet transitions from round triangular as volume is increased.
  - For a fixed droplet volume, higher flow rate leads to a rounder droplet.
- The Saramito and HB-Saramito models predict this behavior (though imperfectly).
  - BCY model struggles to show transition to a triangular shape at larger volumes.

Comparison of experimental and HB-Saramito shear rate

- For the available data, shear rate computed by the HB-Saramito model is generally in agreement with experimental values
- Largest differences manifest near the inlet region:
  - Magnitude of near-wall shear rate is overestimated – no slip BC near inlet doesn't reflect experimental observations
  - Experimental data pictured is smoothed – 8 pixel resolution over 10 images



Work in progress: flow simulations using the Kamani-Donley-Rogers (KDR) EVP model

$$\lambda_1 \overset{\nabla}{\boldsymbol{\sigma}} + \boldsymbol{\sigma} = \eta_f \dot{\boldsymbol{\gamma}} + \lambda_2 \overset{\nabla}{\dot{\boldsymbol{\gamma}}}$$

$$\lambda_1 = \lambda_2 + \lambda_3$$

$$\eta_f = \frac{\tau_y}{\dot{\gamma}} + k|\dot{\gamma}|^{n-1}$$

$$\lambda_2 = \frac{\eta_s}{G}, \quad \lambda_3 = \frac{\eta_f}{G}$$

Target problem:

Steady flow of a 0.3% Carbopol solution over a sphere in a cylindrical vessel

cylinder radius: $R_c = 10$ cm,

sphere radius: $R_s = 1$ cm

Avg. inlet velocity : $v_{inlet} = 0.8$ cm/s

No-slip BCs imposed on all solid surfaces

$n = 0.5$

$k = 71.5 \text{ Pa} \cdot \text{s}^n$

$\tau_y = 14$ Pa

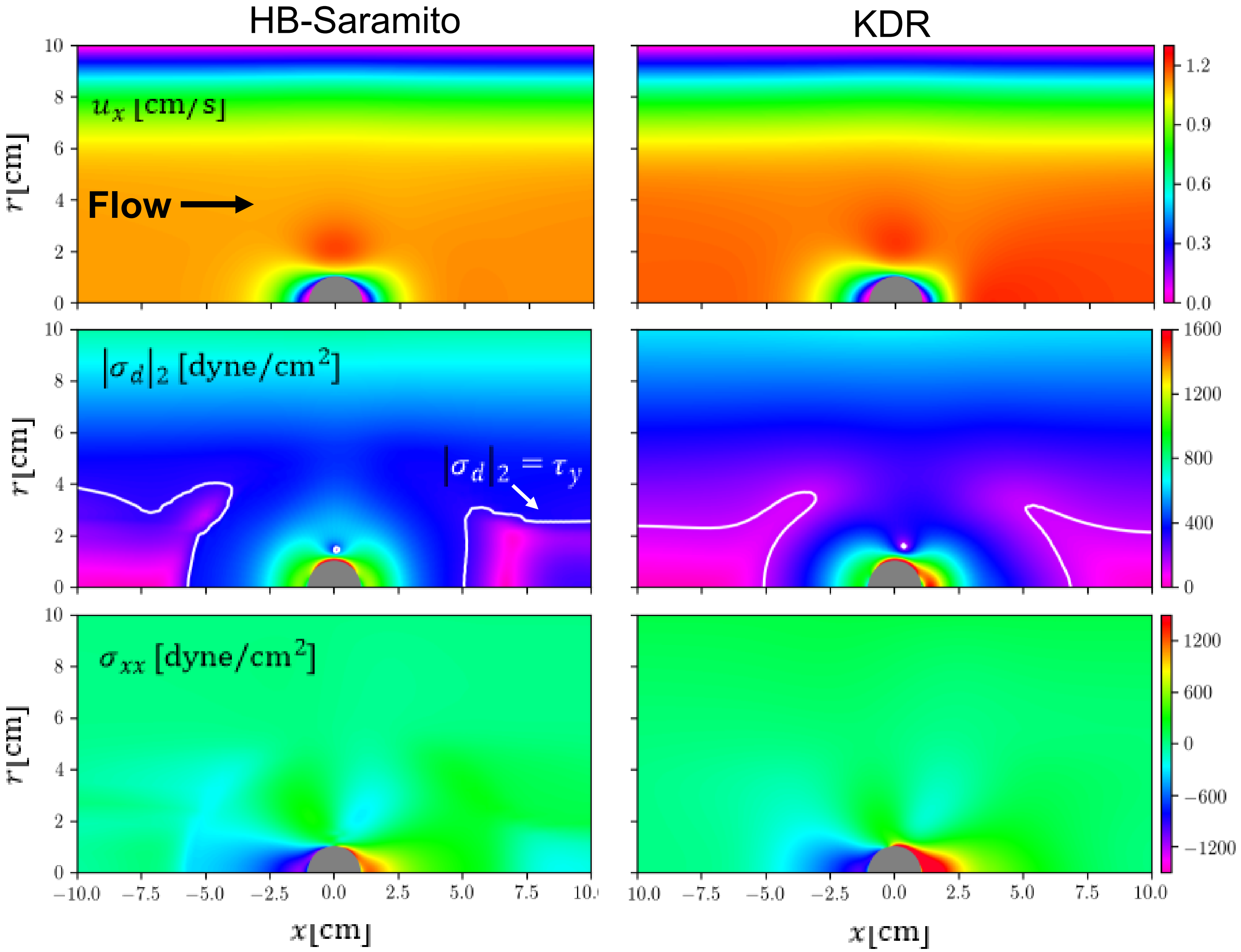
$G = 525$ Pa

$\eta_s = 30 \text{ Pa} \cdot \text{s}$

K. Krutarth, G.J. Donley, and S.A. Rogers. *Unification of the Rheological Physics of Yield Stress Fluids*. Phys. Rev. Lett. 126:21 (2021): 218002

Flow over a sphere: comparing the KDR and HB-Saramito models

- Both EVP models exhibit axial asymmetry of velocity field
  - This asymmetry is more apparent with the KDR model
- An unyielded ring around the sphere is predicted by both models
- $|\sigma_d|_2 = \tau_y$ boundary for both EVP models are similar
- Both models predict substantial normal stresses in the vicinity of the sphere



Summary and conclusions

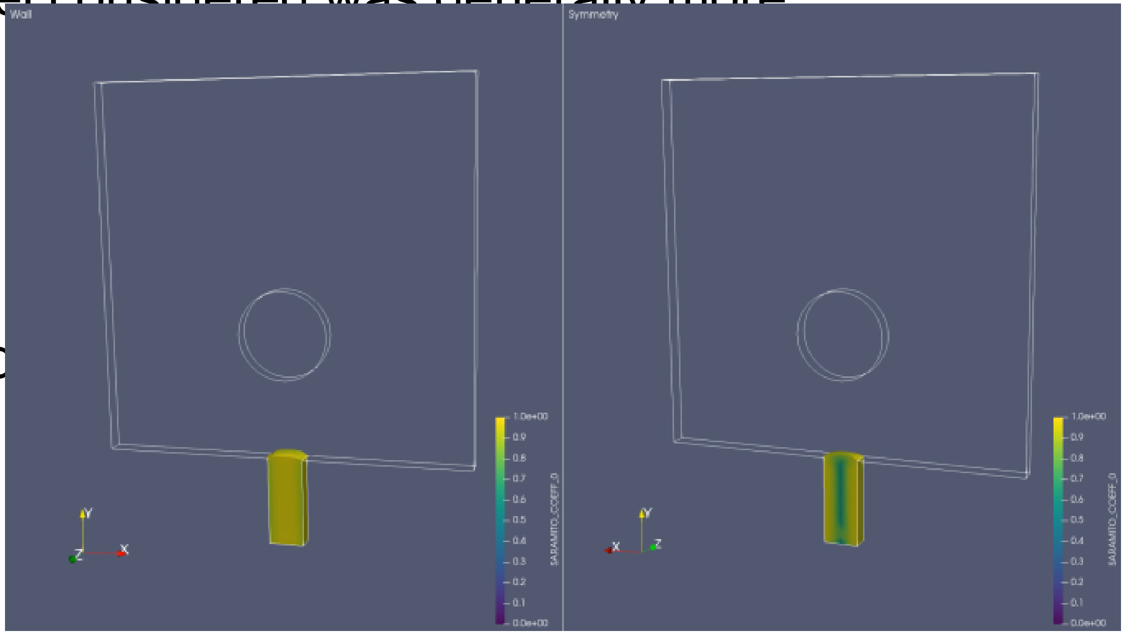
The numerical and modeling framework developed for this work predicts morphological changes of growing Carbopol drops observed in flow visualization

- Drop shape predicted by HB-Saramito model consistent with experimentally-observed drop shapes
- HB-Saramito model yields accurate predictions for fluid drop height over a range of flow rates.
- Predicting drop width is more difficult – the EVP model considered was generally more accurate than the BCY model.

- Ongoing efforts:
  - Level set implementations of EVP models
  - Unsteady flow simulations using the KDR mod

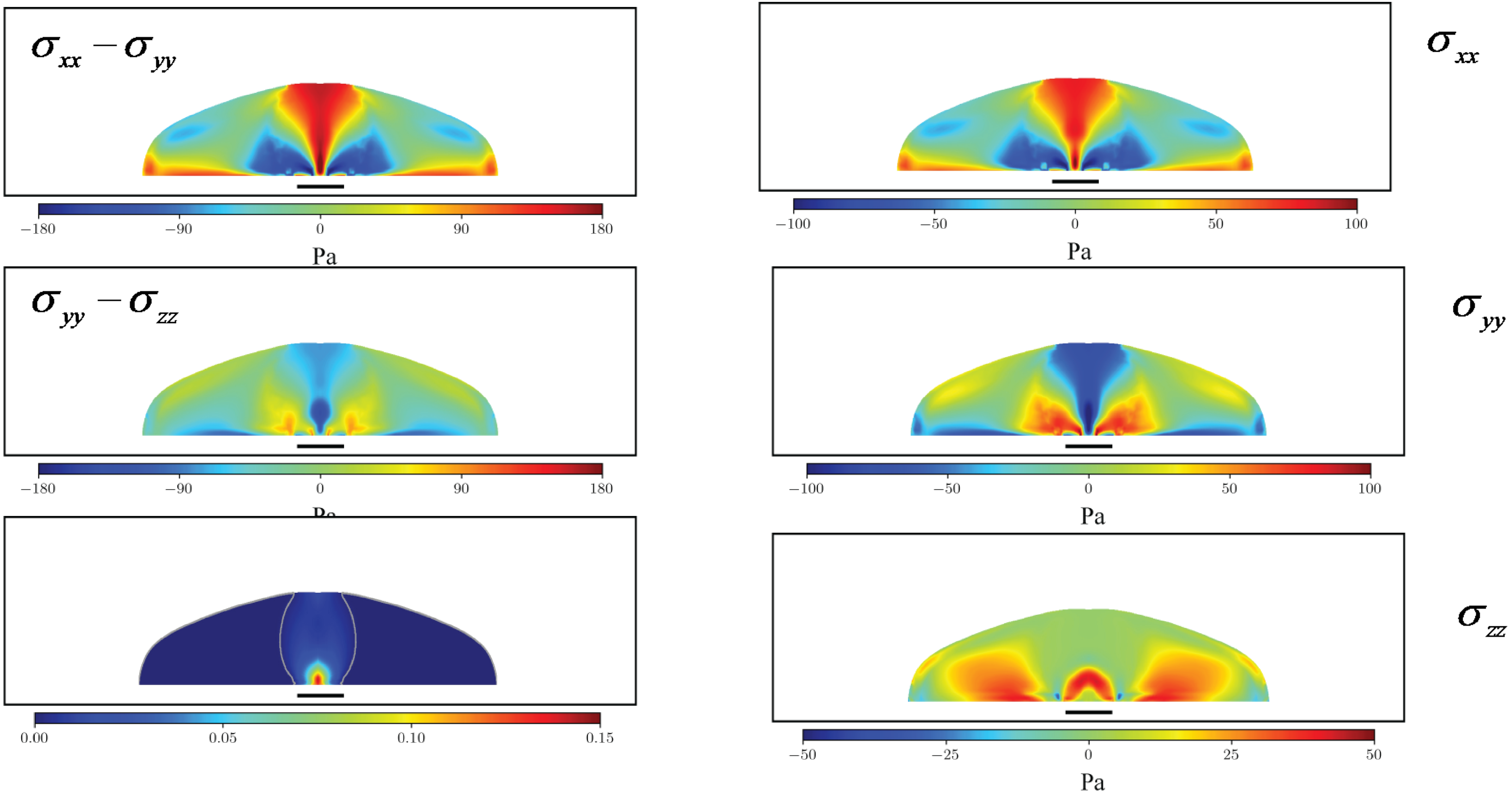
Acknowledgements: Simon Rogers Research Group (UIUC)

Grillet et al., “Non-Viscometric Flow of Yield Stress Fluids,” to be submitted, *Journal of Rheology*

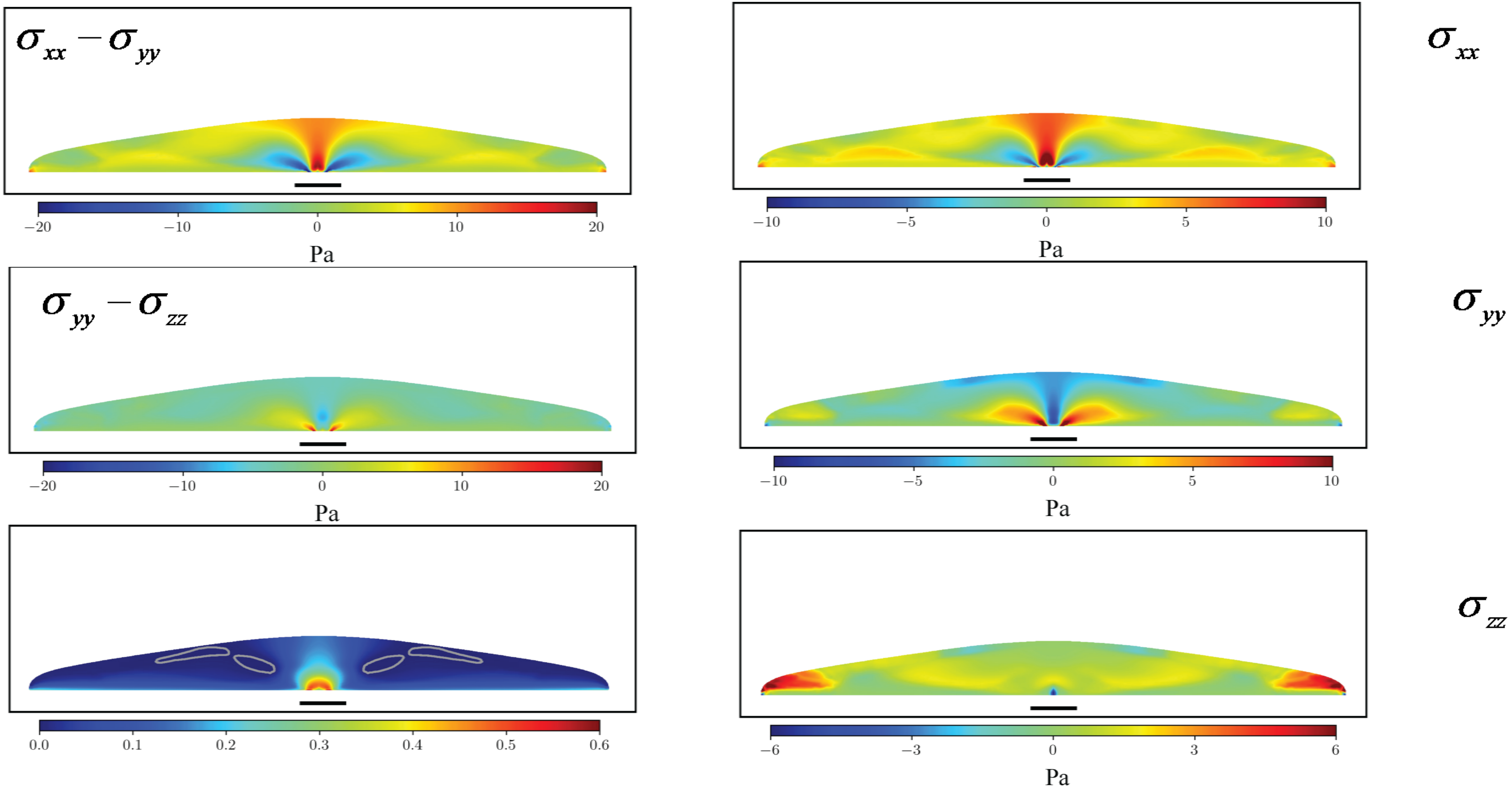


Backup Slides

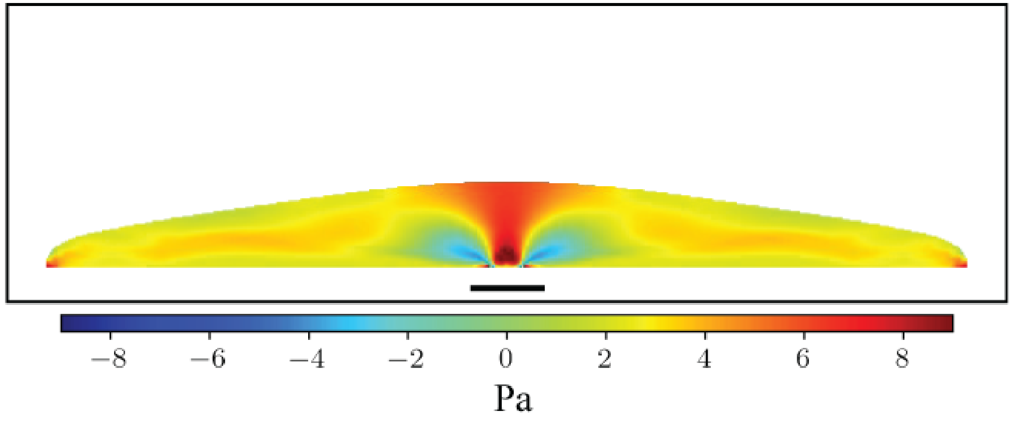
Centerline for normal stresses 0.30% Carbopol



Centerline for normal stresses for 0.08% Carbopol

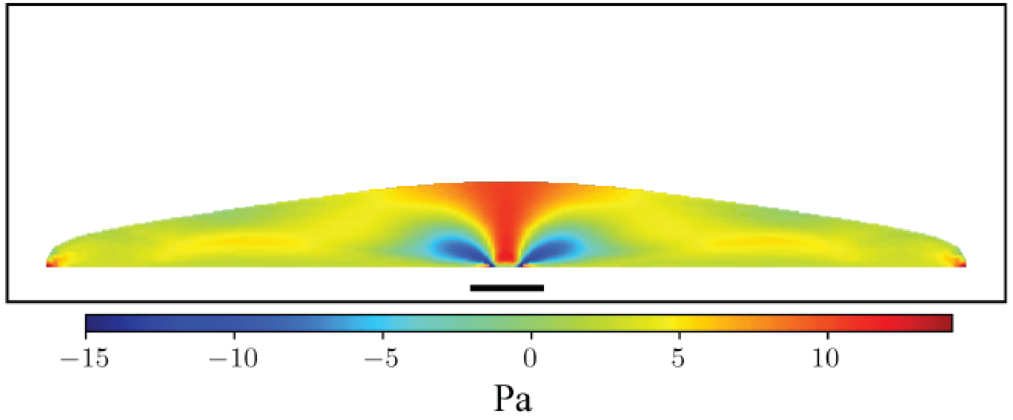


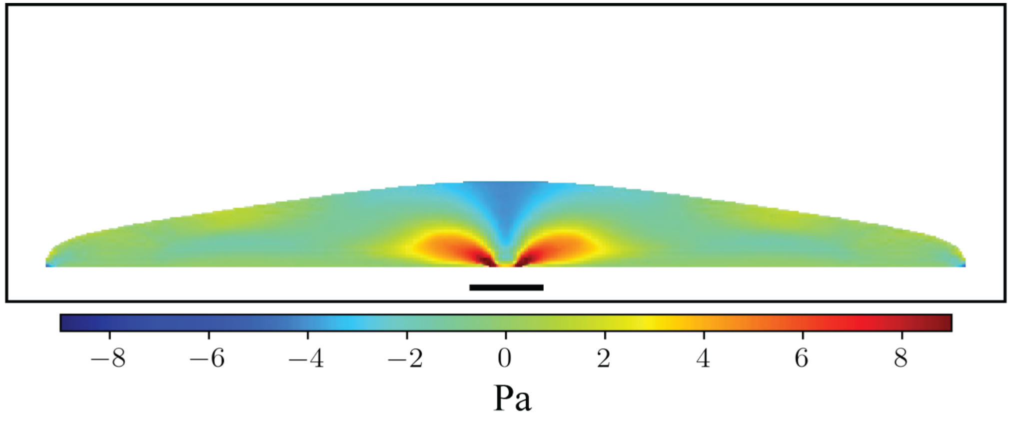
Josh Average of Stress: 0.08 Carbopol



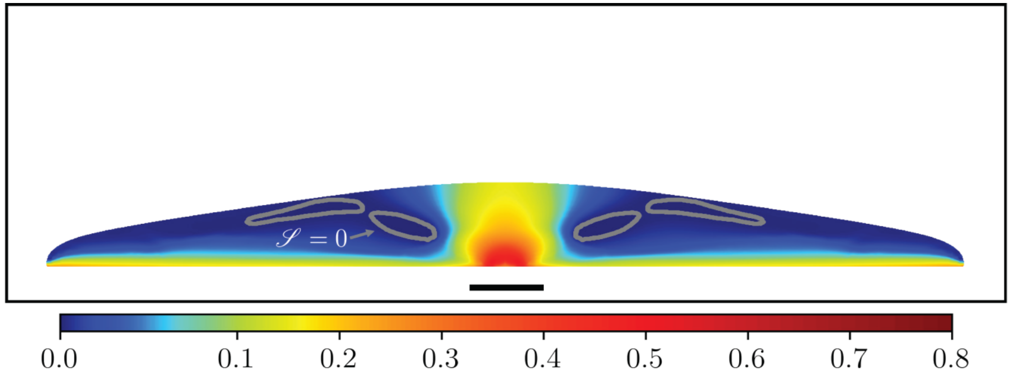
σ_{xx}

$\sigma_{xx} - \sigma_{yy}$





σ_{yy}



Josh Average of Stress: 0.3 Carbopol