SAND2022-7259C

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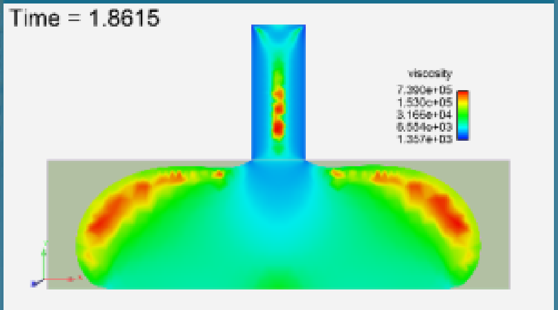
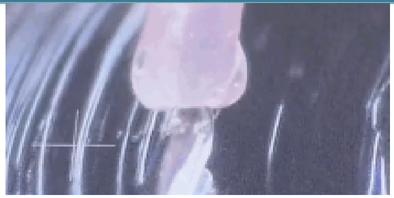
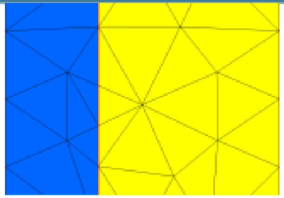
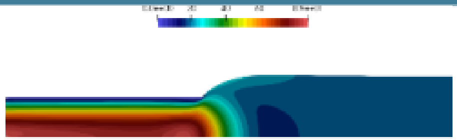
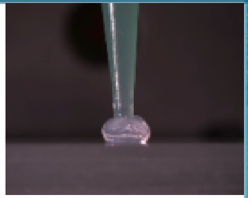
Simulation of the direct ink write process using finite elements and cThruAMR











Presented By:

Alec Kucala, Rekha Rao, Anne Grillet & Jessica Kopatz

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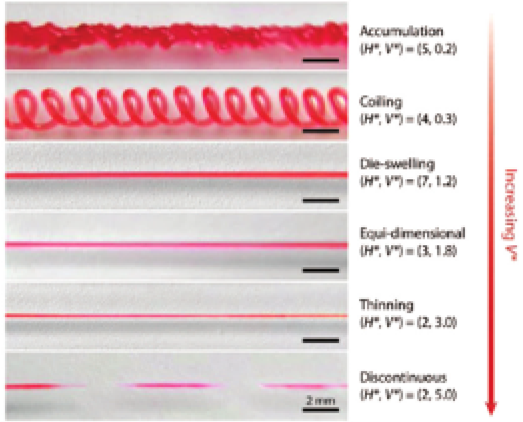
Direct Ink Write Process

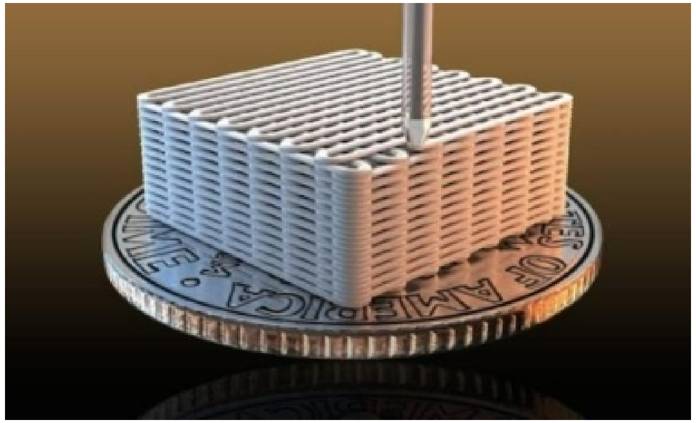
- Direct Ink Write (DIW) is an additive manufacturing (AM) process which involves the deposition of a viscous material from a syringe onto a substrate
- Often the “ink” or material is non-Newtonian (in our cases shear thinning)
- Desire to model this using finite-elements
  - Predict behavior of non-Newtonian inks for printing
- Capturing the interface between the ink material and air/substrate is a difficult modeling problem
  - Capture surface tension
  - Viscous effects
  - Topology
- cThruAMR – a sharp-interface capturing method in the Krino library is used

Examples of Direct Ink Write



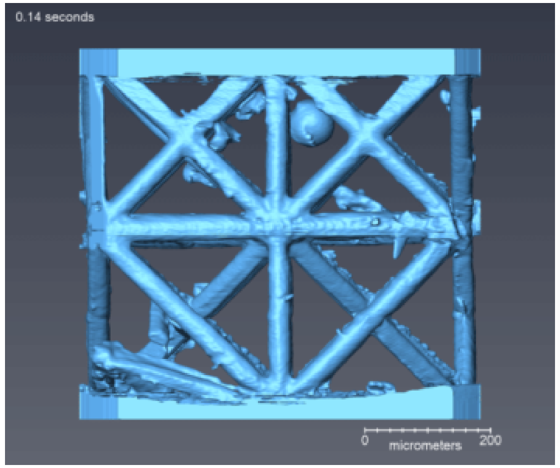
(a)

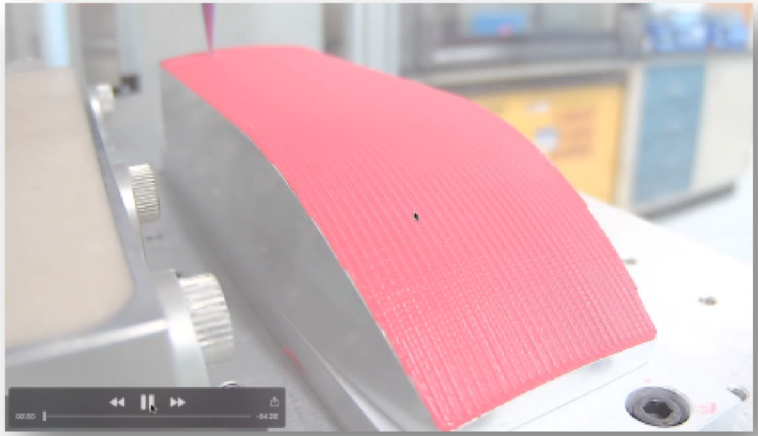
Bioink printability
Zhang et al, 2018



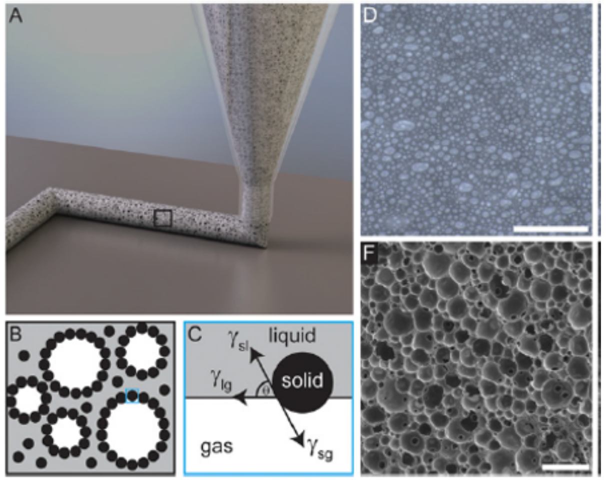
Graphene aerogel microlattices
Ryan Chen (LLNL)

Printing an Ear
www.think3d.in/researchers-use-biobot-3d-bioprinter-for-nerve-cell-engineering





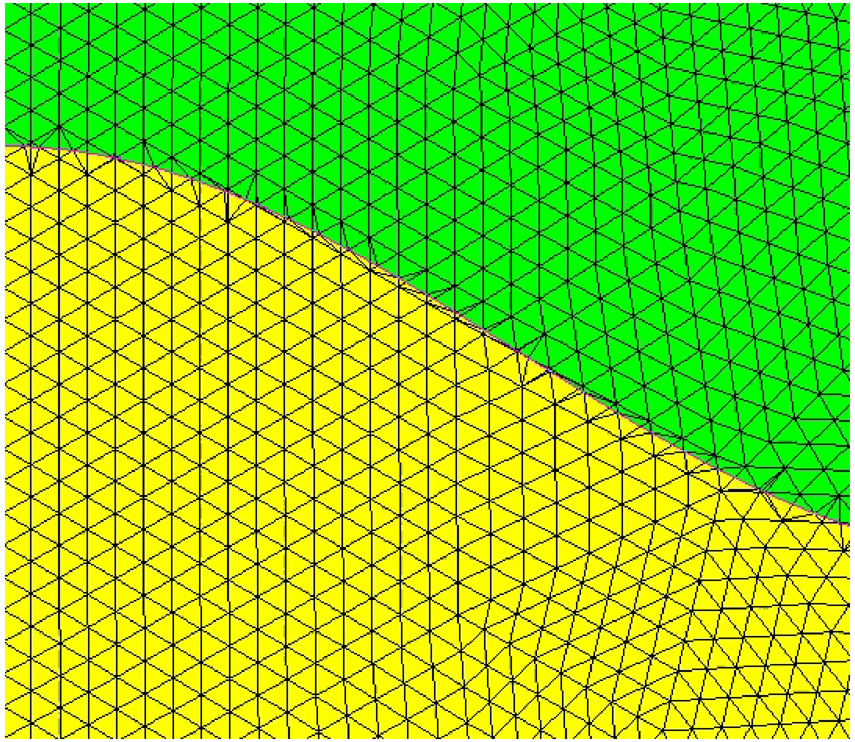
Silicone Engineered Foam
Adam Cook (SNL)



Direct Foam Writing
Muth et al., 2017

Conformal Decomposition Finite Element Method (CDFEM)

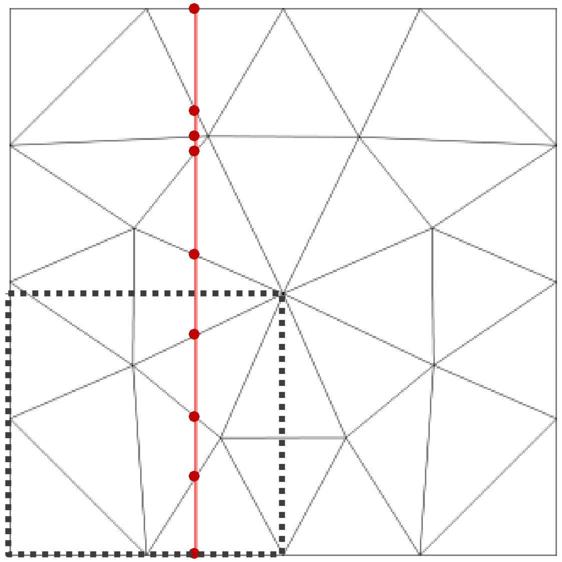
- Relatively new method (Noble et al., 2010) used to discretize moving interfaces that do not conform to static finite element meshes
- Used in conjunction with level sets to track interface motion
- Adds degrees of freedom by adding nodes to mesh which lie on the exact interface location
- Can apply boundary conditions directly at interface
  - Surface tension
  - Wetting line models
- Caveat: Creates sliver elements which can create nearly-singular matrices

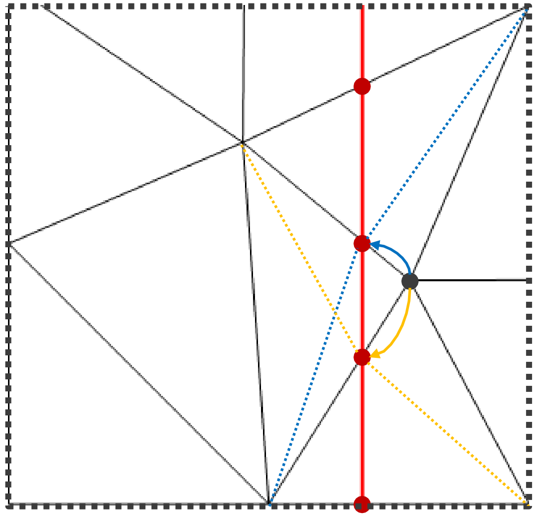


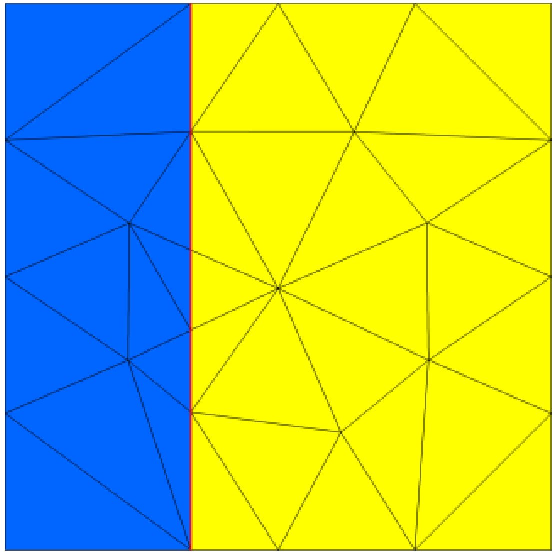
Simpler and More Robust Snapping Algorithm: Snap When Quality is Better than Cutting

Snap when element quality of snapping is better than the element quality if the intersection points are cut into the mesh

- The estimated cutting quality for a node is the minimum quality of the elements that would be produced by cutting each edge using the node at its intersection point
- The snapping quality for a node and intersection point is the minimum quality of the elements if the node is moved to that intersection point
- If the snapping quality is better than the estimated cutting quality, then the node is a candidate for snapping to that intersection point
- Select and snap the candidates that are higher quality than any of the neighboring snap candidates, reintersect edges, repeat until all candidate snaps are performed



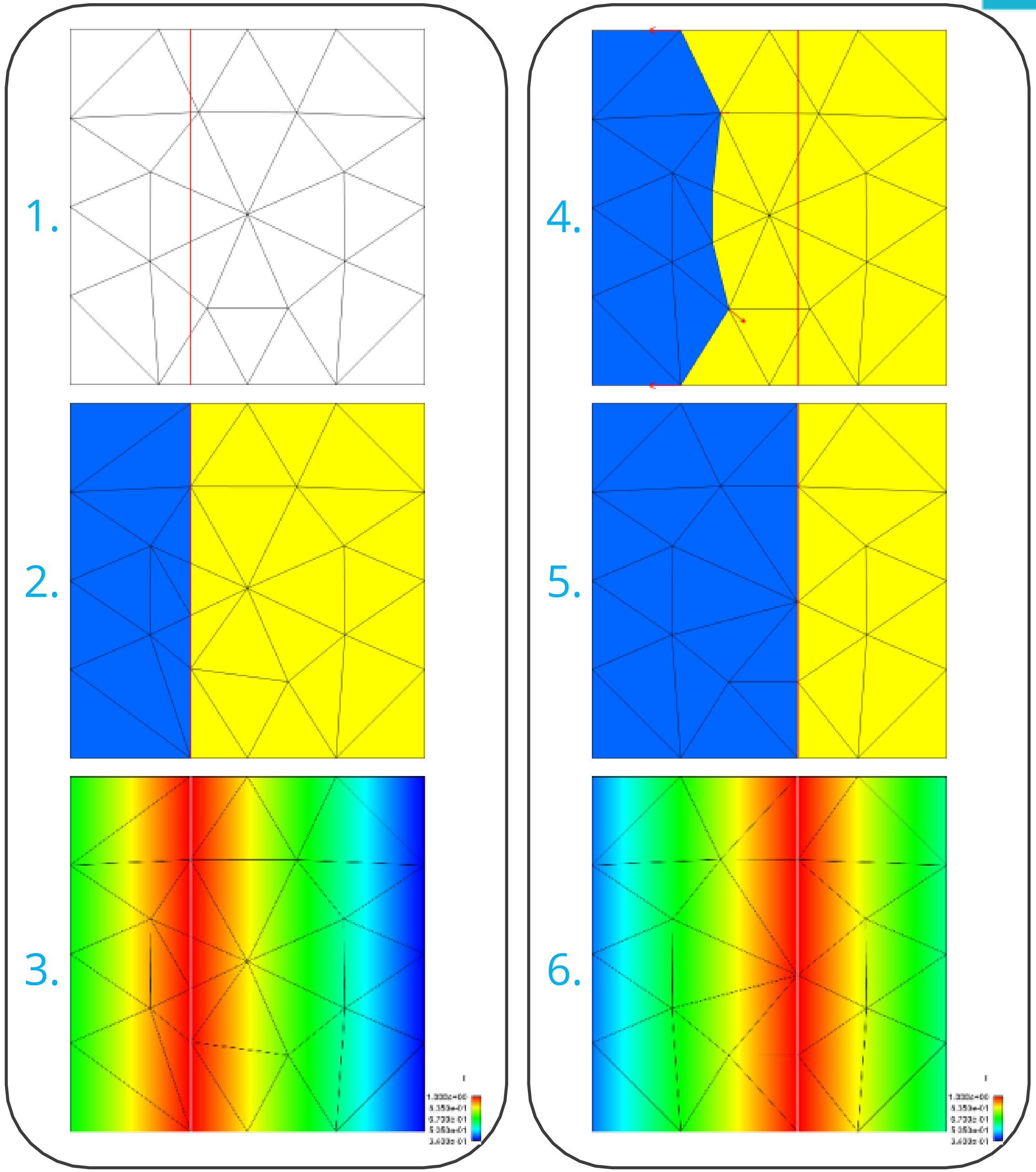




cThruAMR Algorithm

Integrate snapping and cutting for transient level set problems: conforming transient h-r unstructured adaptive mesh refinement (cThruAMR)

1. Initialize level sets on input mesh
2. Create conforming mesh by snapping and cutting
   - Snap whenever quality is higher than cutting quality
3. Initialize physics on conforming mesh
4. Advect level sets while "reversing" snap displacements
5. Create new conforming mesh by snapping and cutting
6. Solve physics on conforming mesh
   - Include moving mesh term where interface nodes and nodes that have changed material are considered to have advected from the nearest point on the old interface



Finite element model

- Use Sierra/Aria to model the deposition of an ink material onto a substrate for various configurations
- Galerkin finite-element method
  - P1 tetrahedron elements (P1 tri elements in 2D)
- BDF2 time discretization
- Compare to experimental videos
  - Moving substrate
  - Stationary drop
  - Newtonian vs non-Newtonian
- Simulations will be two- and three-dimensional

Governing Equations

Conservation Equations

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

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u}\right) = -\nabla p + \nabla \cdot \left(\mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right)\right)$$

$$\rho C_{\mathrm{P}}\left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) - \nabla \cdot (k \nabla T) = \dot{q}$$

Level Set Equation

$$\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\,\phi = 0$$

Interface Boundary Conditions

$$[\mathbf{u}]_{\Delta} = 0, \qquad \mathbf{x} \in \Gamma_{\mathrm{F}}$$

$$[-p\mathbf{I} + \mu(\mathbf{x})\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right)]_{\Delta} \cdot \hat{\mathbf{n}} = -\gamma \kappa \hat{\mathbf{n}}, \qquad \mathbf{x} \in \Gamma_{\mathrm{F}}$$

Ink material and viscosity model

Variable	Value
μ_0	29740
μ_∞	10
τ_y	9520
λ	7.542
F	200
α	2.764
n	0.633586

Ink material used in our simulations is DowSil SE1700

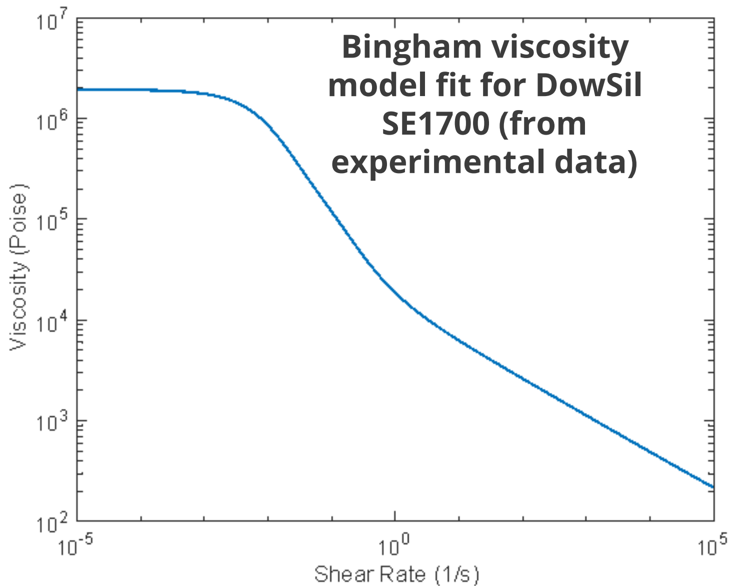
Bingham–Carreau-Yasuda model is used to model the shear-rate dependent viscosity

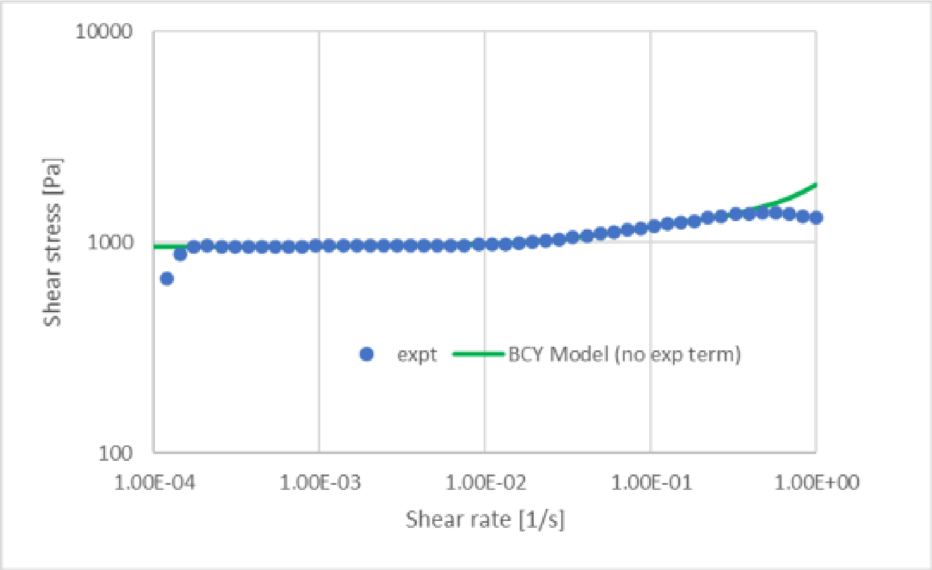
Papanastasiou regularization

Model includes yield stress and explicit shear thinning

Fit to model experimental data

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

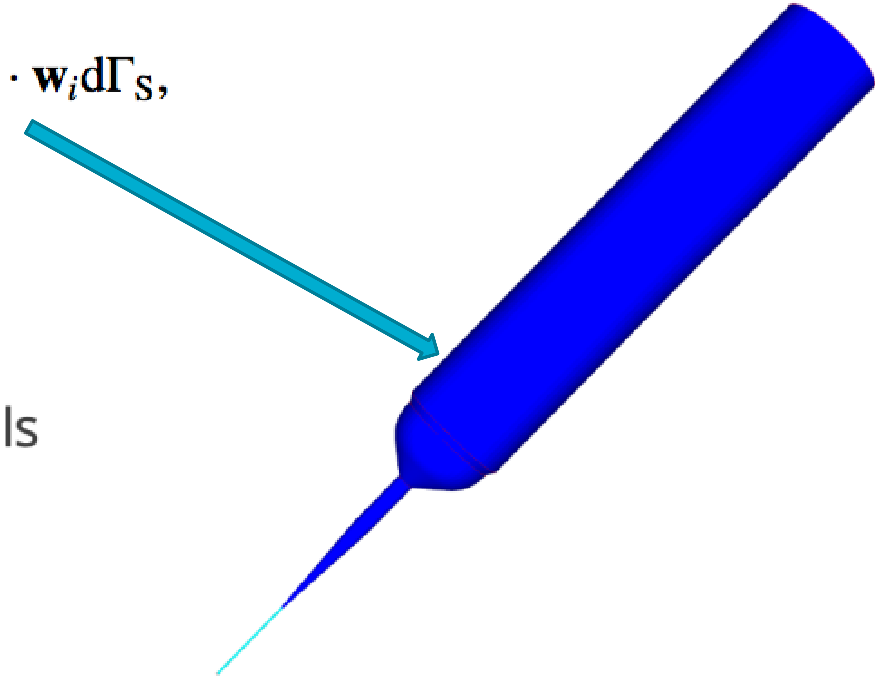




Slip condition

- In order to model the movement of the interface through the syringe "tip", a slip model must be used in lieu of a no-slip model
  - This allows the contact line between the syringe wall, air, and ink material interface to advect along the surface wall
- The Navier-slip condition is used to model the interface slip at the wall

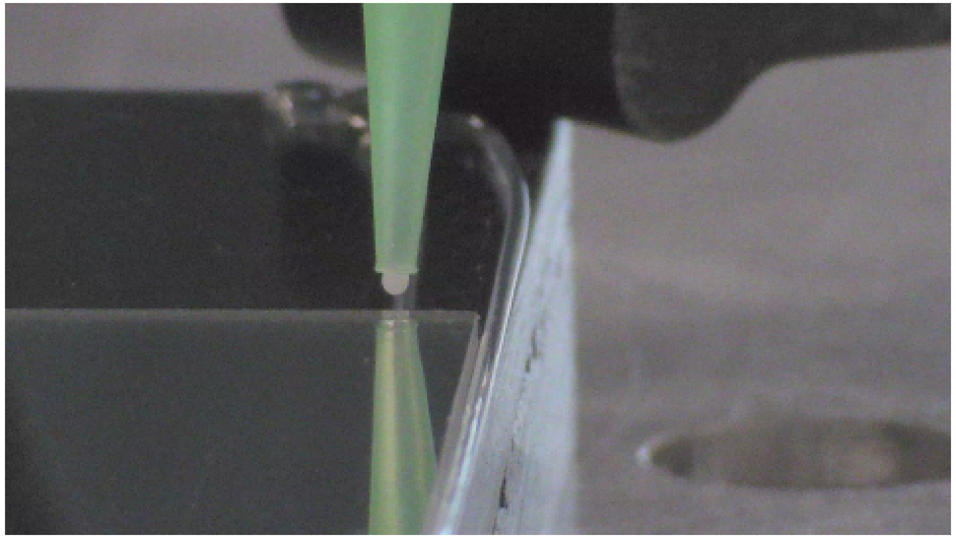
$$\int_{\Gamma_S^{n+1}} \left(\left(-p\mathbf{I} + \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right)^{n+1}\right)\cdot\hat{\mathbf{n}}\right) w_i \mathrm{d}\Gamma_S = \int_{\Gamma_S^{n+1}} \frac{\mu_{\mathrm{m}}}{\beta}\left(\mathbf{u}_{\mathrm{w}} - \mathbf{u}^{n+1}\right)\cdot\mathbf{w}_i \mathrm{d}\Gamma_S,$$



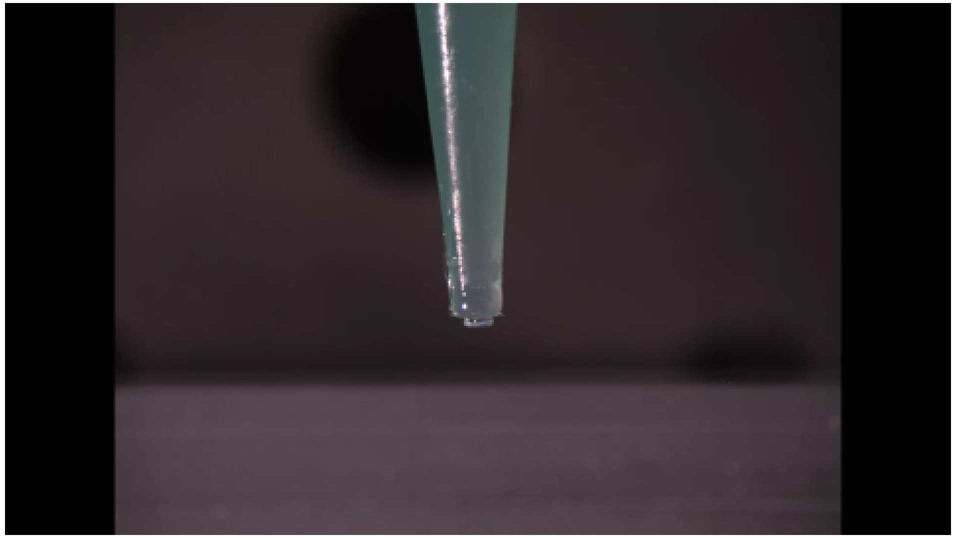
- Can recover the no-slip condition as $\beta \to 0$
- We will investigate the effect of the slip on the syringe walls

Experiments

Serpentine Printing Pattern

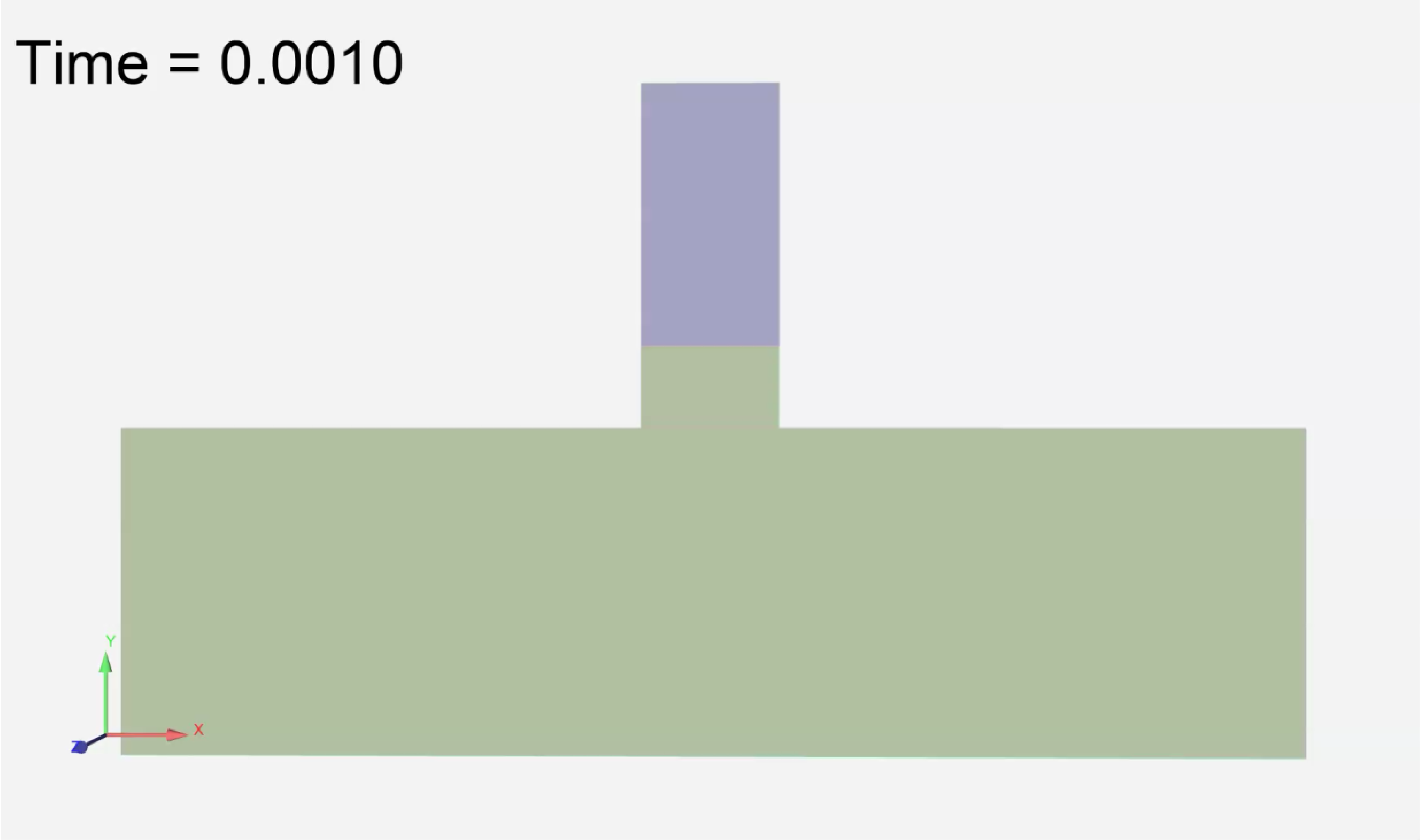


Stationary Drop

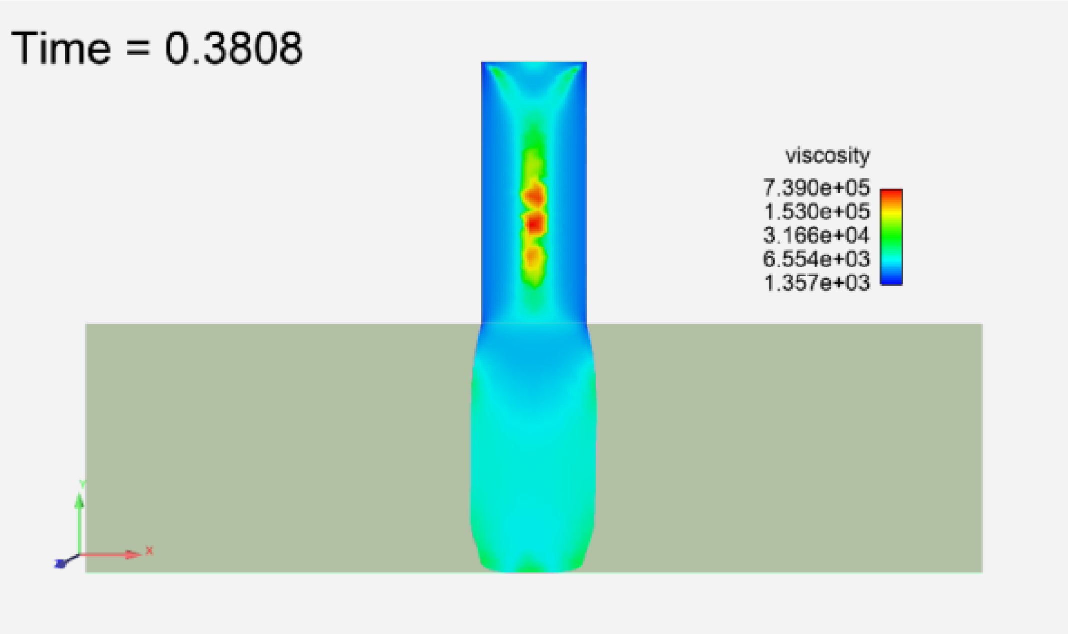


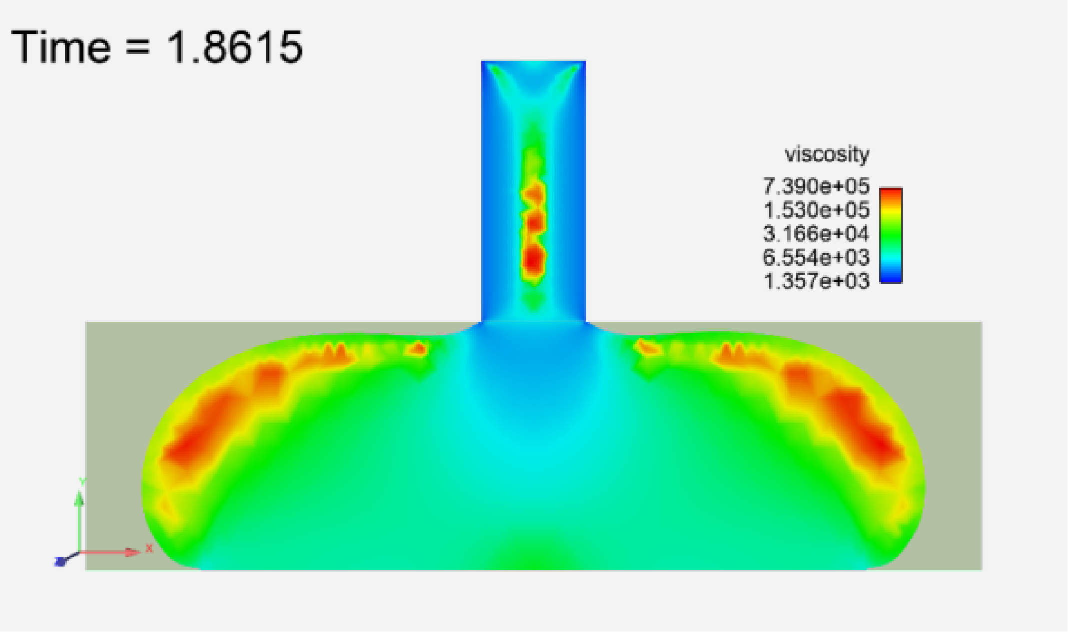
Printer designed by Adam Cook & Derek Reinholtz

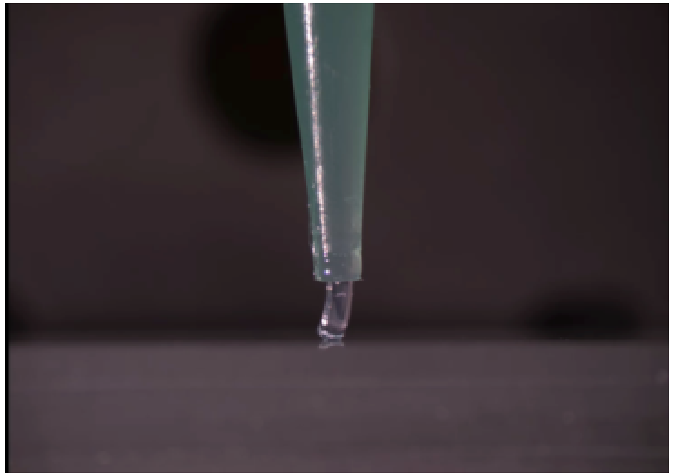
Simulations – Stationary Extrudate

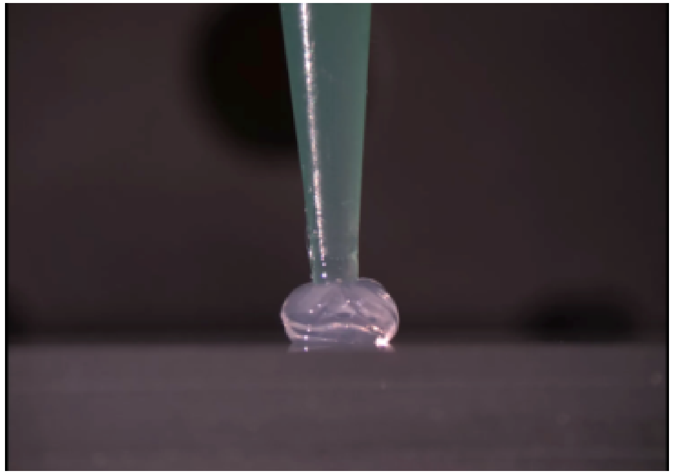


Stationary Extrudate



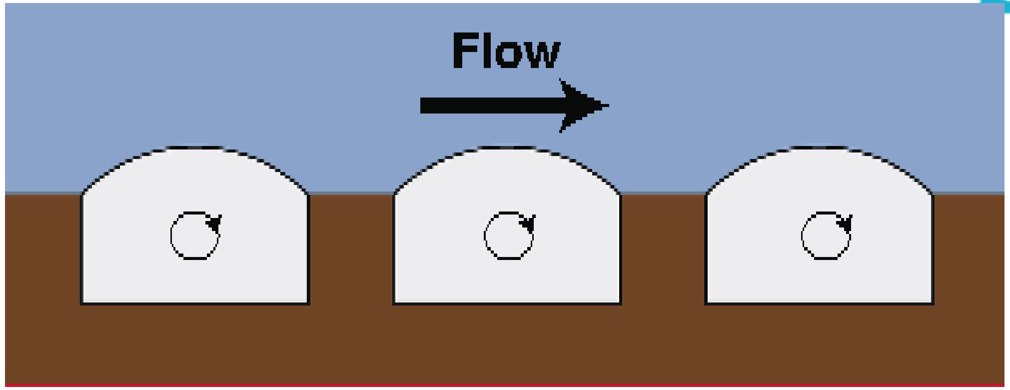


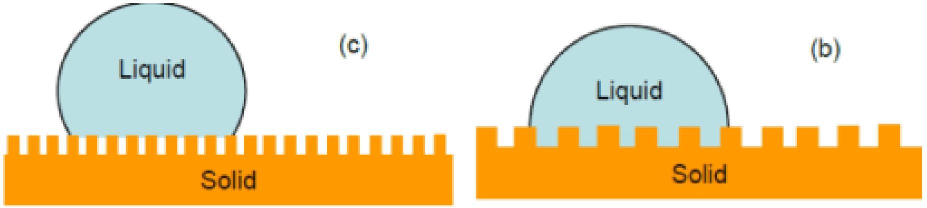




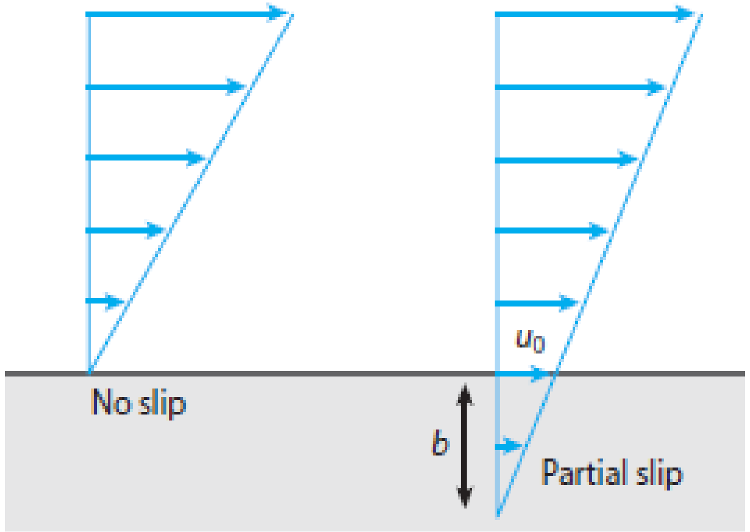
Stationary Extrudate

- Comparison of the 2mm extrudate between experiment and simulation agree qualitatively
- Non-uniform forcing might be present due to the coiling of the material in the experimental video
  - For a uniform forcing, would expect shear forces equal on both sides of syringe, creating a symmetric outflow of material as seen in the simulations
- Asymmetry may be explained by surface roughness effects on the walls of the syringe tip
- Depending on the properties of the syringe and ink material, fluid may slip along the trapped air phases in the trapped pores
  - Wenzel
  - Cassie-Baxter
- Can be modeled as an asymmetric slip condition
  - Each side wall in the simulation can have unique slip length

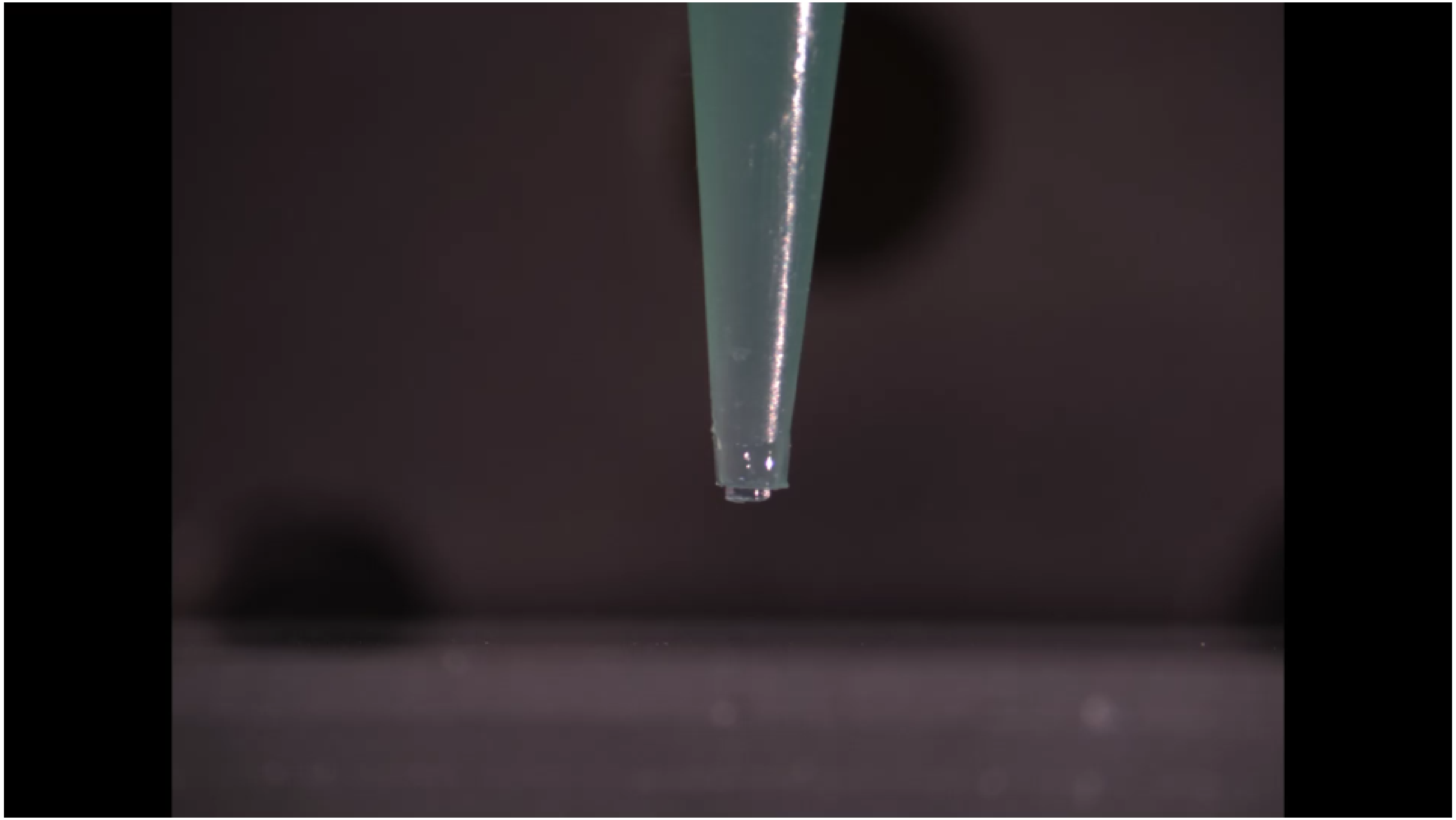




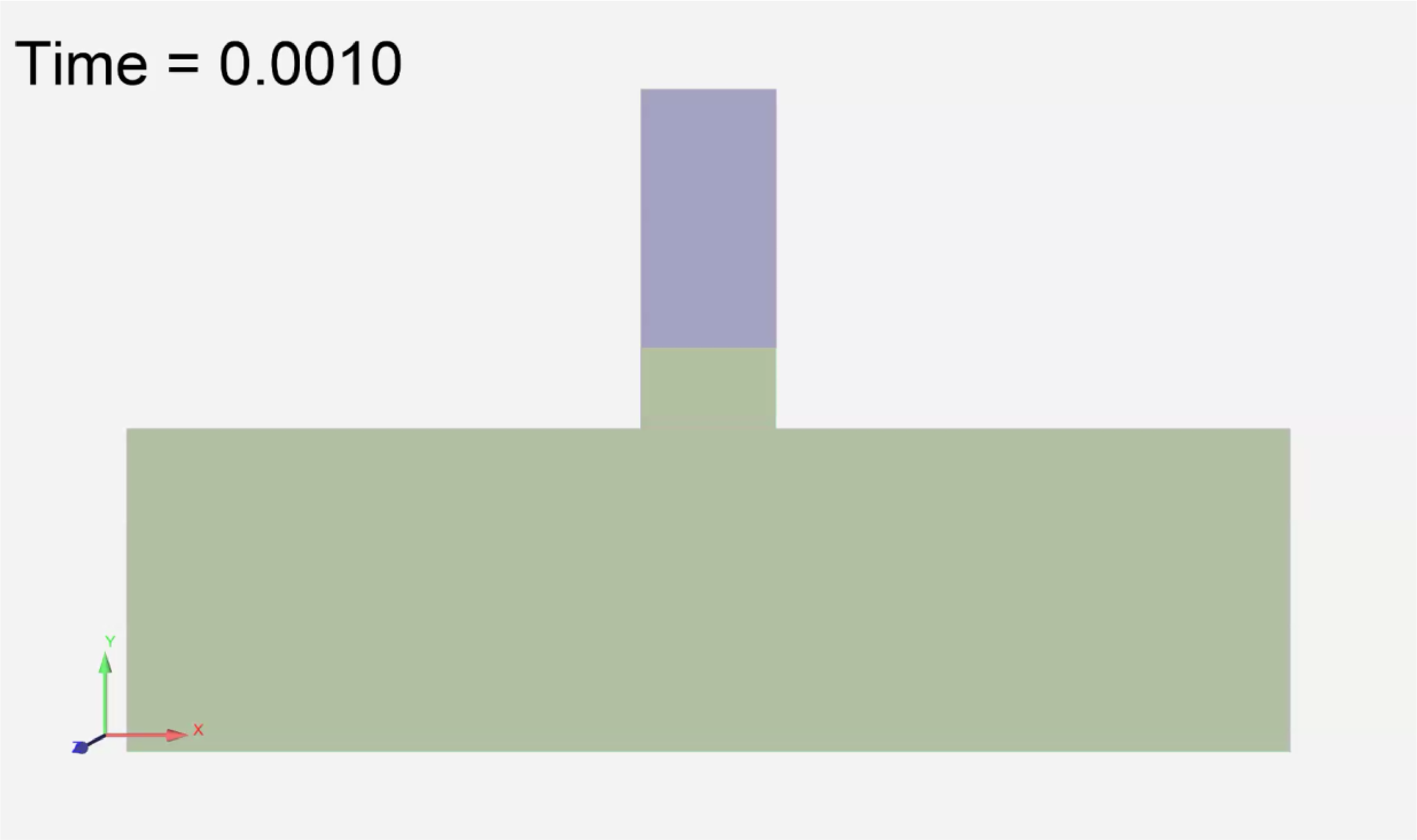
Wenzel State Cassie-Baxter State



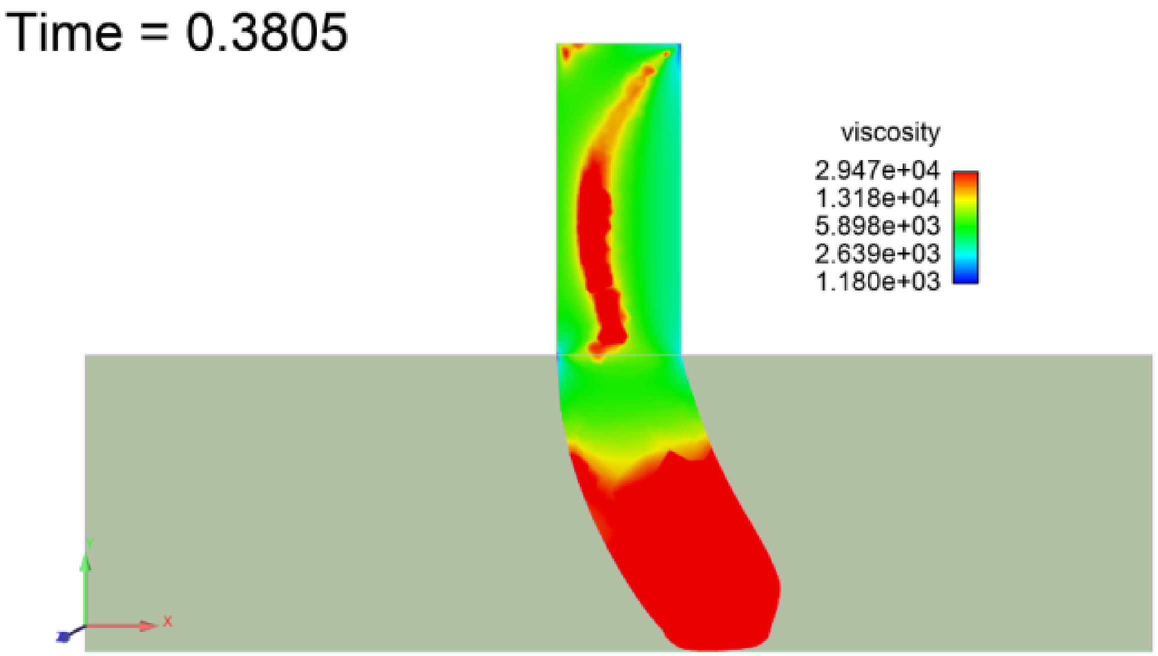
Experiment – Asymmetric outflow



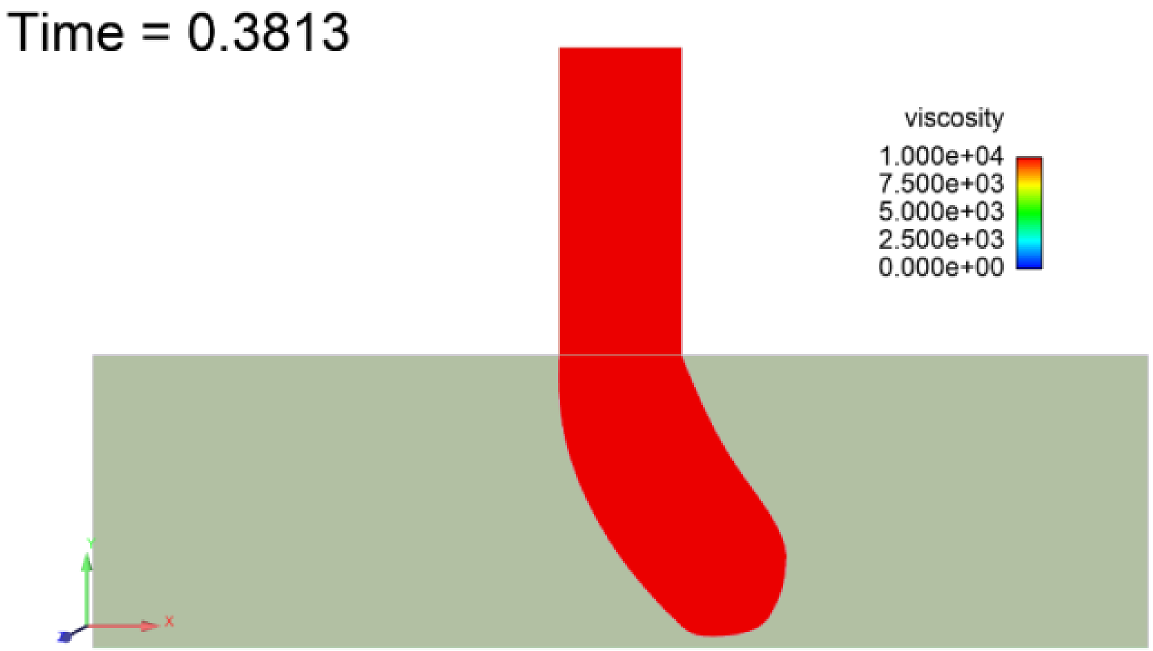
Simulation – Asymmetric outflow



Non-Newtonian viscosity vs Newtonian



Non-Newtonian

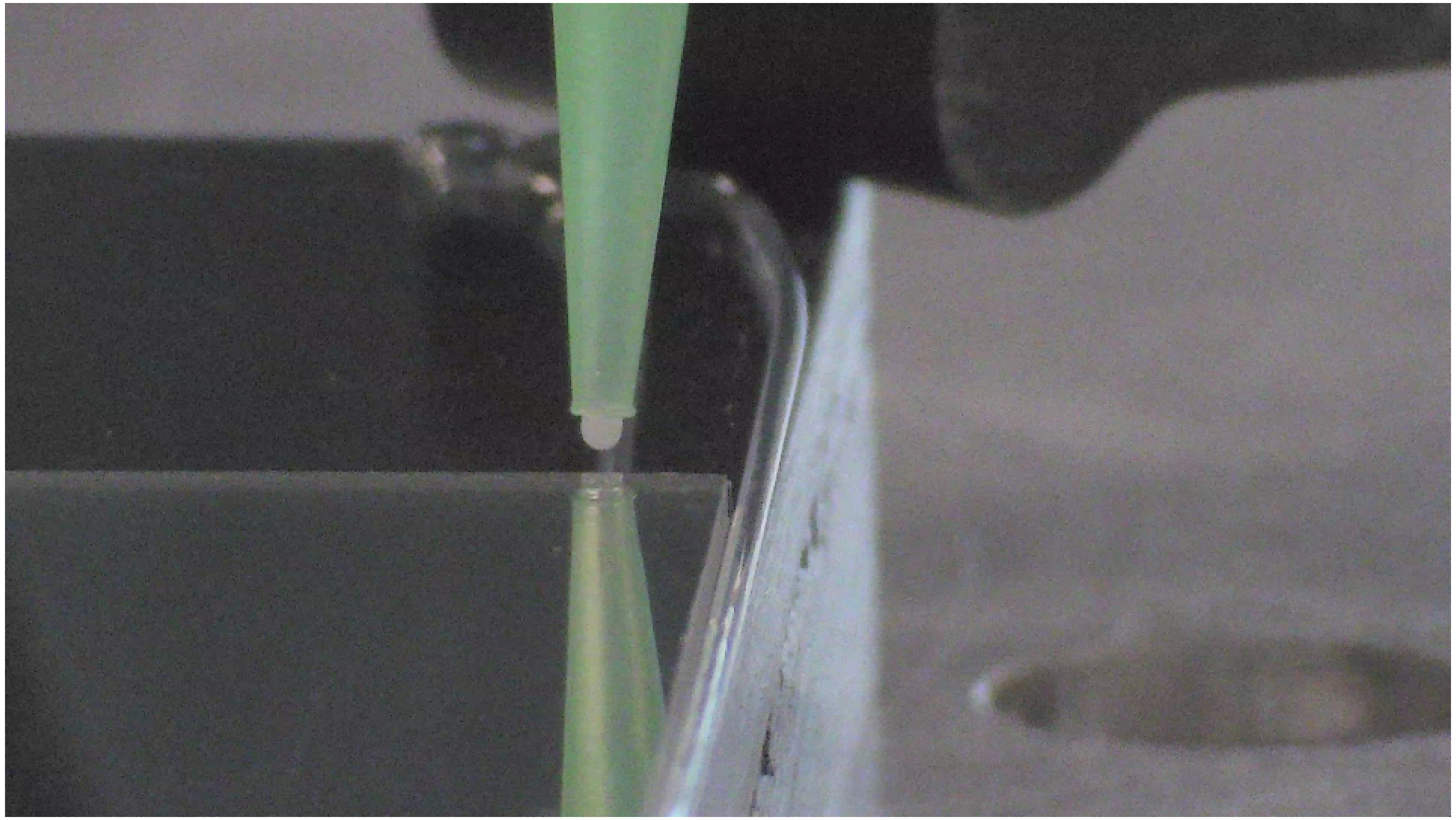


Newtonian

Stationary – Summary

- Simulations comparing the stationary case have been made
- When flow is symmetric through syringe tip, we have good qualitative agreement
- Asymmetric flow captured by model when applying non-uniform slip condition on each wall
- Does not appear to be an artifact of the shear-thinning properties of the ink material
  - Some qualitative differences are observed though
- Initial startup effects appear to be the culprit, may not be completely explained by the fluid slip due to rough pores

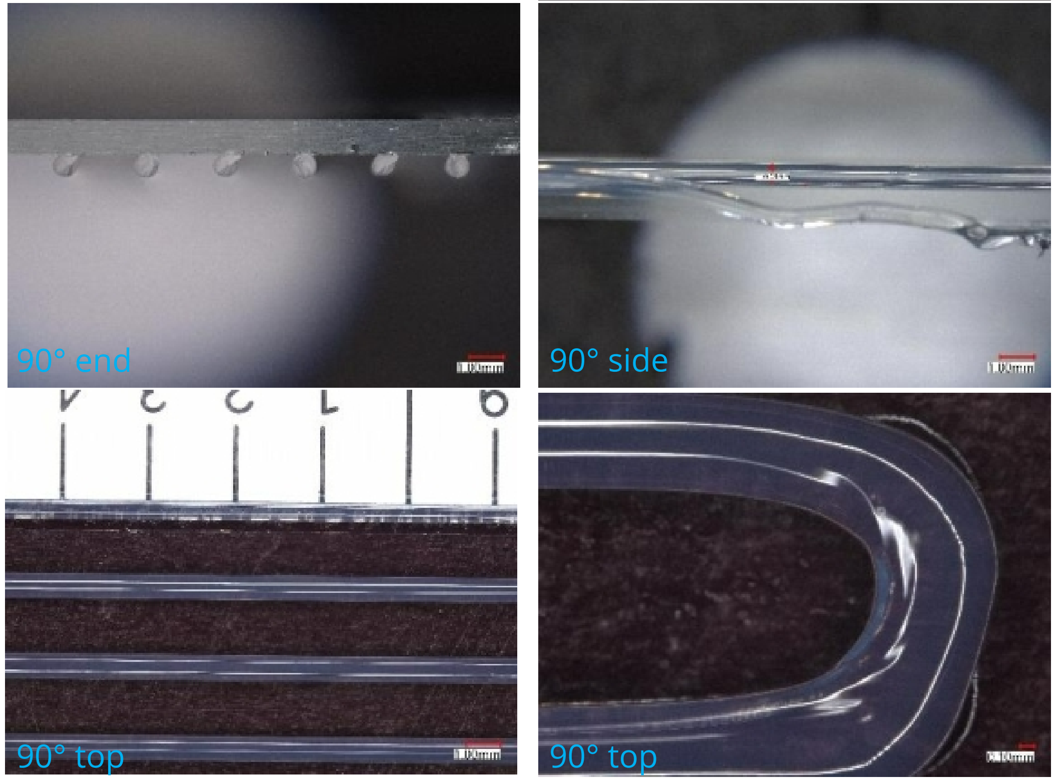
DIW printing



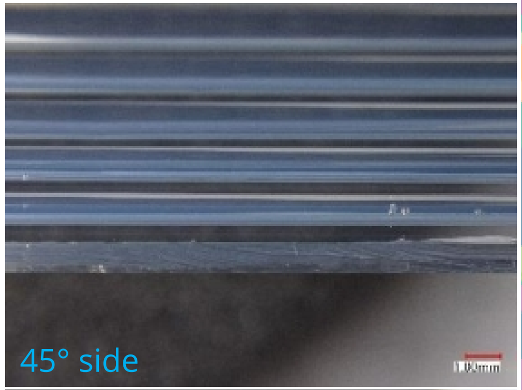
- Will model by moving the substrate at constant velocity
- Will run 2D model and compare topology
  - Newtonian vs non-Newtonian (BCY model)
- 3D model (Newtonian)

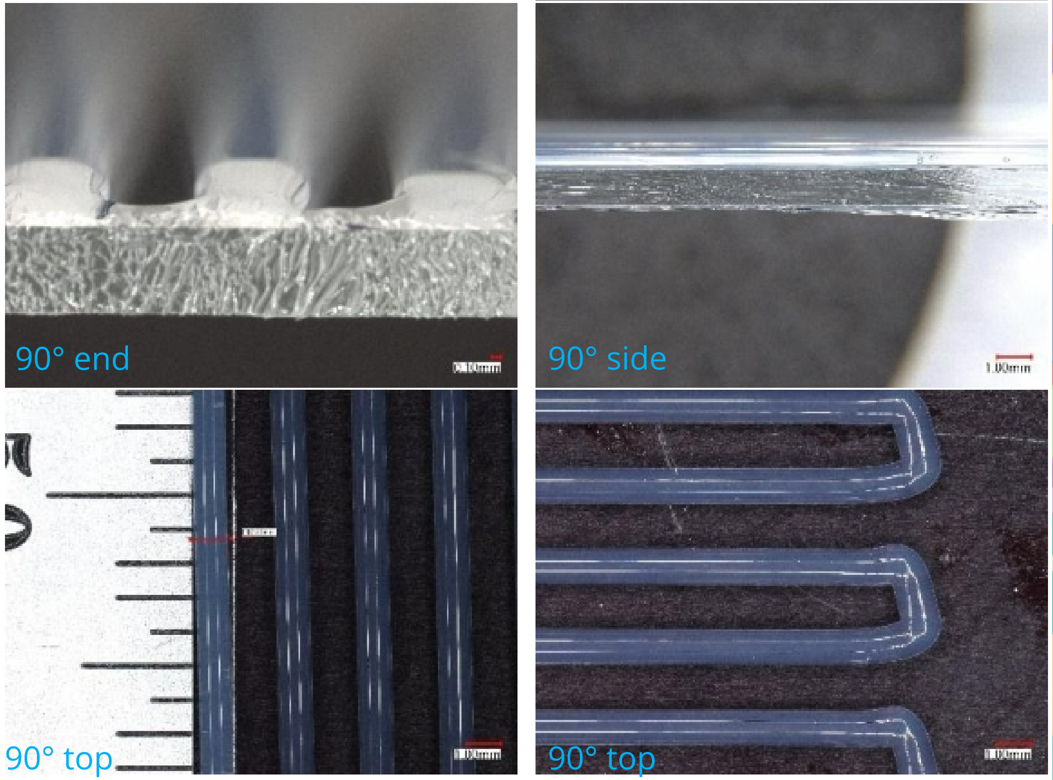
DowsilSE1700 validation data-Dynamic Printing (Goliath)

0.84 mm nozzle
0.25 mL/min



0.84 mm nozzle
0.5 mL/min



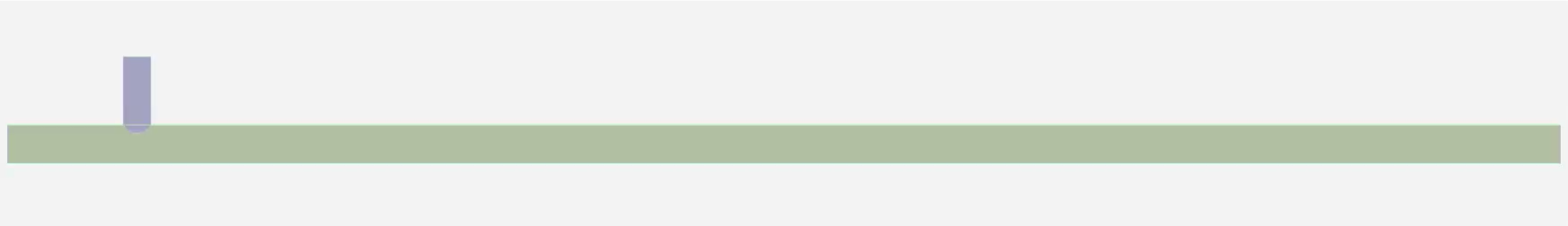


Higher flow rates resulted in oval/oblong bead shapes due to over-extrusion

2D moving substrate

Newtonian

Non-Newtonian (BWLF)



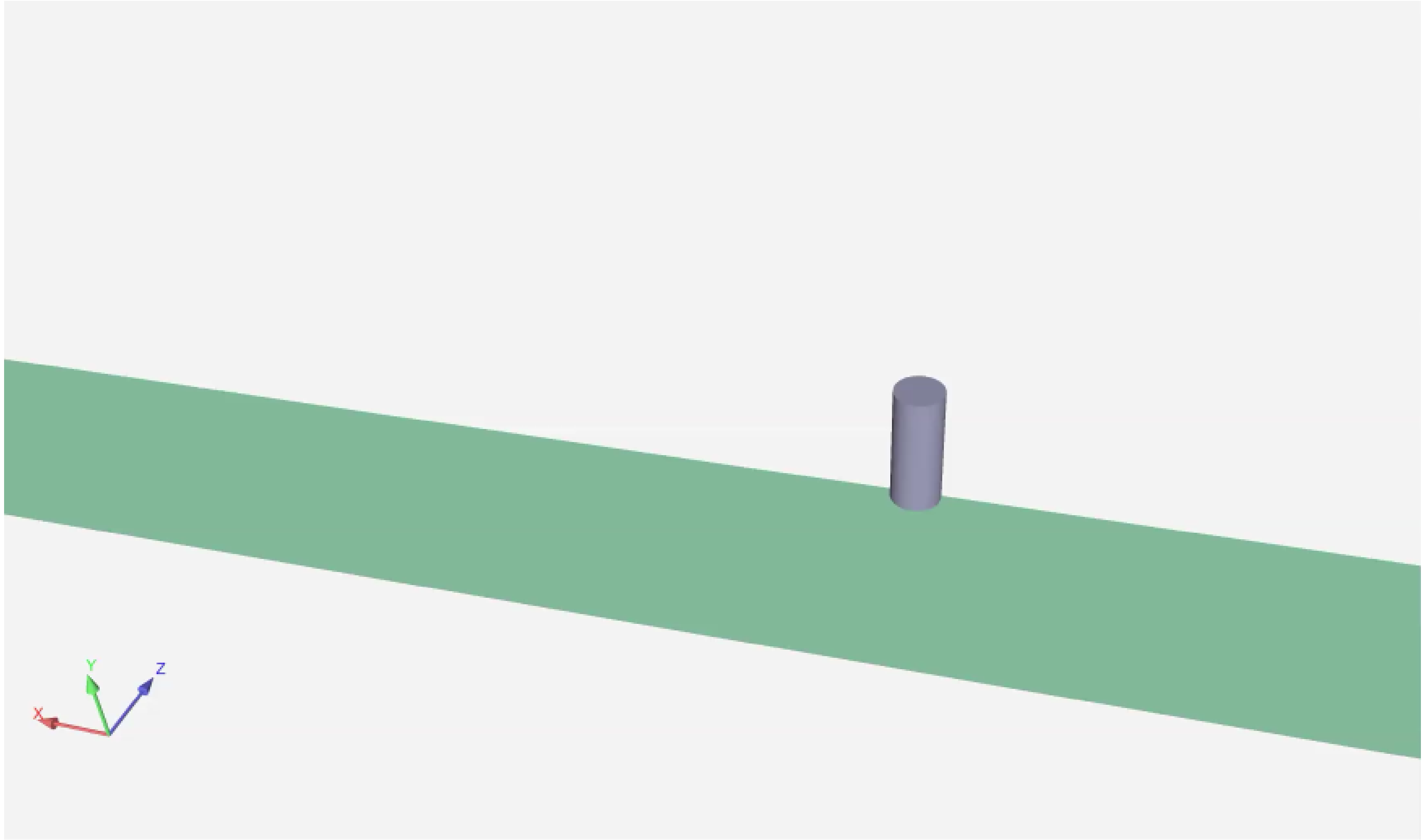
2D moving substrate cont.

Newtonian

Non-Newtonian (BWLF)

- Final state shows some small qualitative differences
- Appears that Newtonian captures the physics well-enough
  - May not be true for 3D

Moving substrate – 3D



Summary and conclusions

- Presented a model for DIW using cThruAMR to capture material interfaces
- cThruAMR is a promising method for capturing material interfaces
  - Good conditioning of the resulting matrix
  - Potential issues with coarser mesh resulting in mass loss
- Bingham-Carreau-Yasuda viscosity model was used to model the non-Newtonian physics of the DowSil ink material
  - Difficult to converge in 3D for fully-implicit FEM
- Asymmetry of the ink material deposition can potentially be explained by enhanced slip on parts of the syringe wall
  - Qualitatively invariant to Newtonian/non-Newtonian fluids
- Future Work:
  - Full 3D models using the non-Newtonian BCY (or other Non-Newtonian models with yield stress such as Casson or Herschel-Bulkley)
- Questions?