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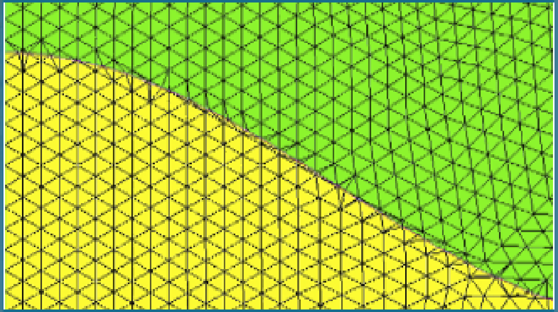
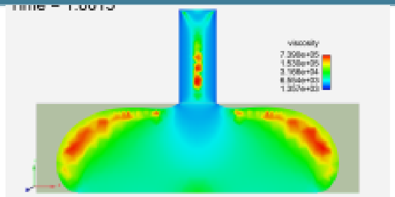
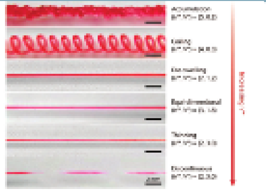
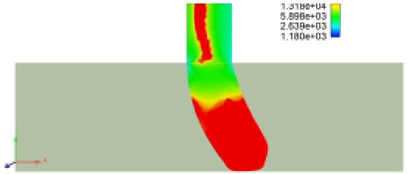


Modeling the Direct Ink Write process using a sharp interface finite-element method







Presented By:

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WCCM 2024 – Vancouver, CA

U.S. DEPARTMENT OF ENERGY NNSA

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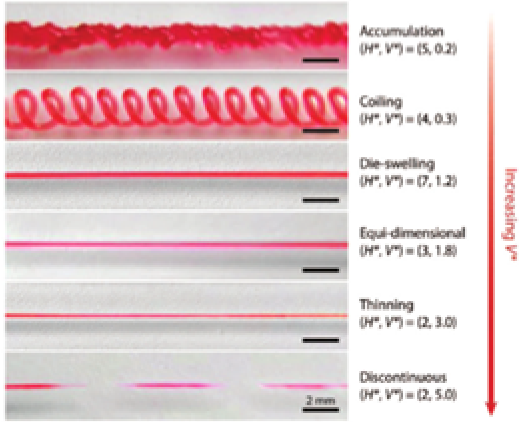
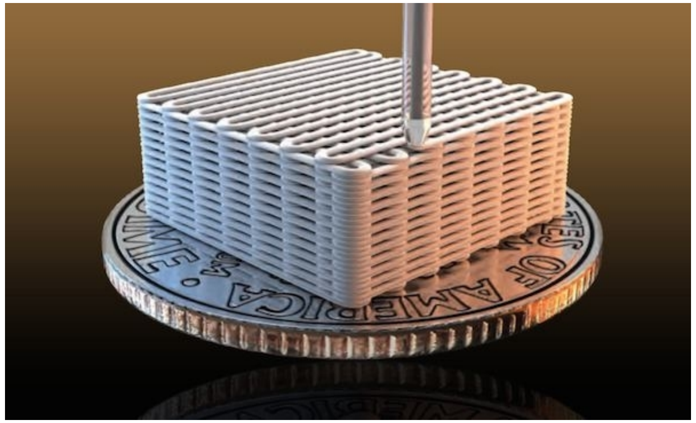
Direct Ink Write Process

- 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
- CDFEM – a sharp-interface capturing method in the Krino library is used

Examples of Direct Ink Write

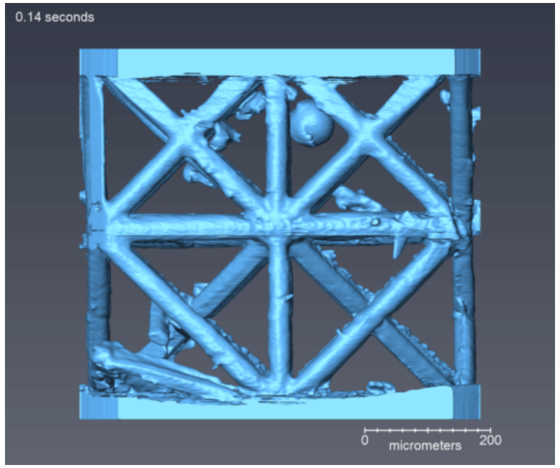


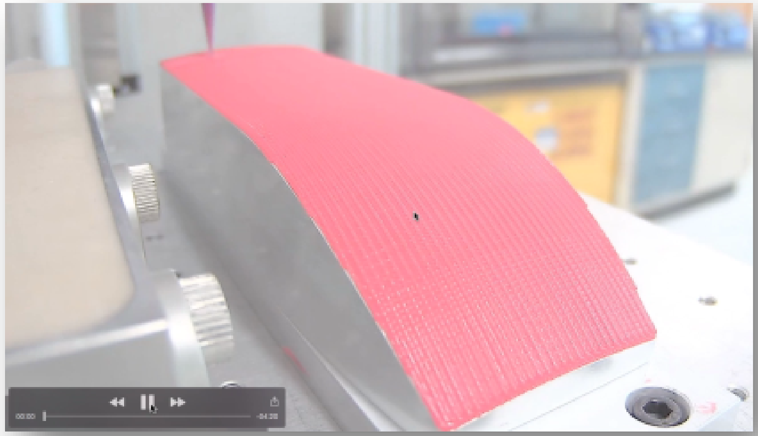
Bioink printability
Zhang et al, 2018



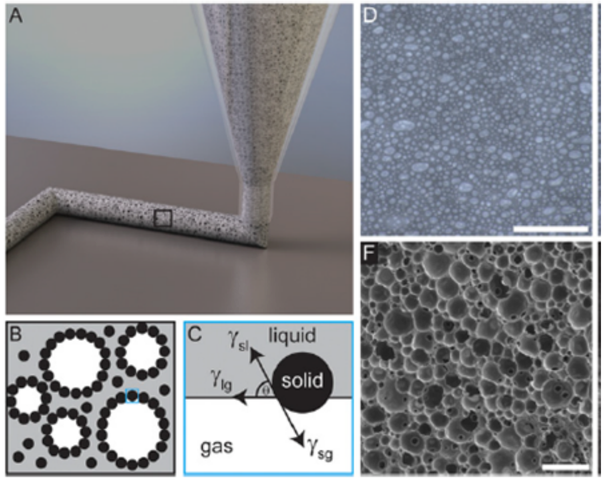
Graphene aerogel
microlattices
Ryan Chen (LLNL)

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



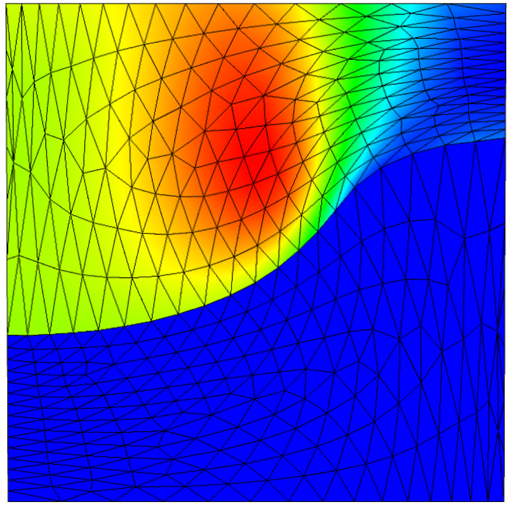
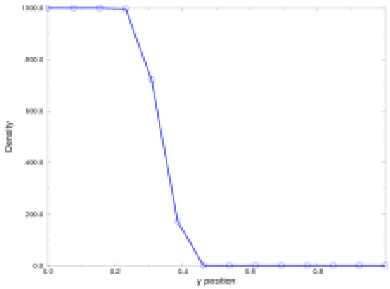
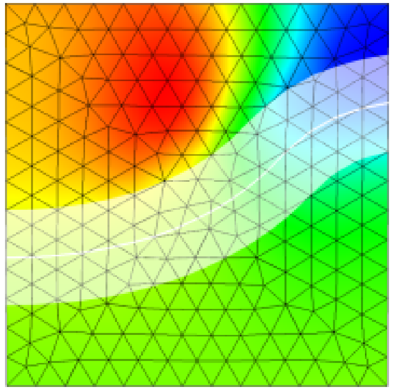
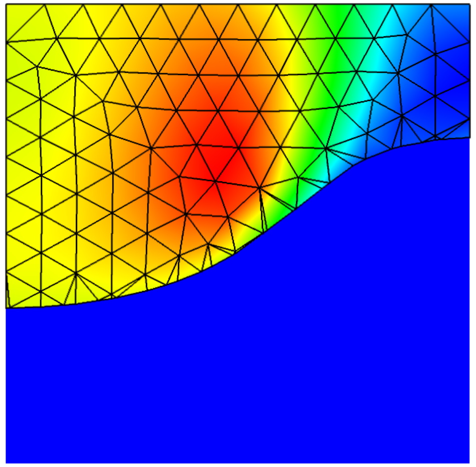


Silicone Engineered Foam
Adam Cook (SNL)



Direct Foam Writing
Muth et al., 2017

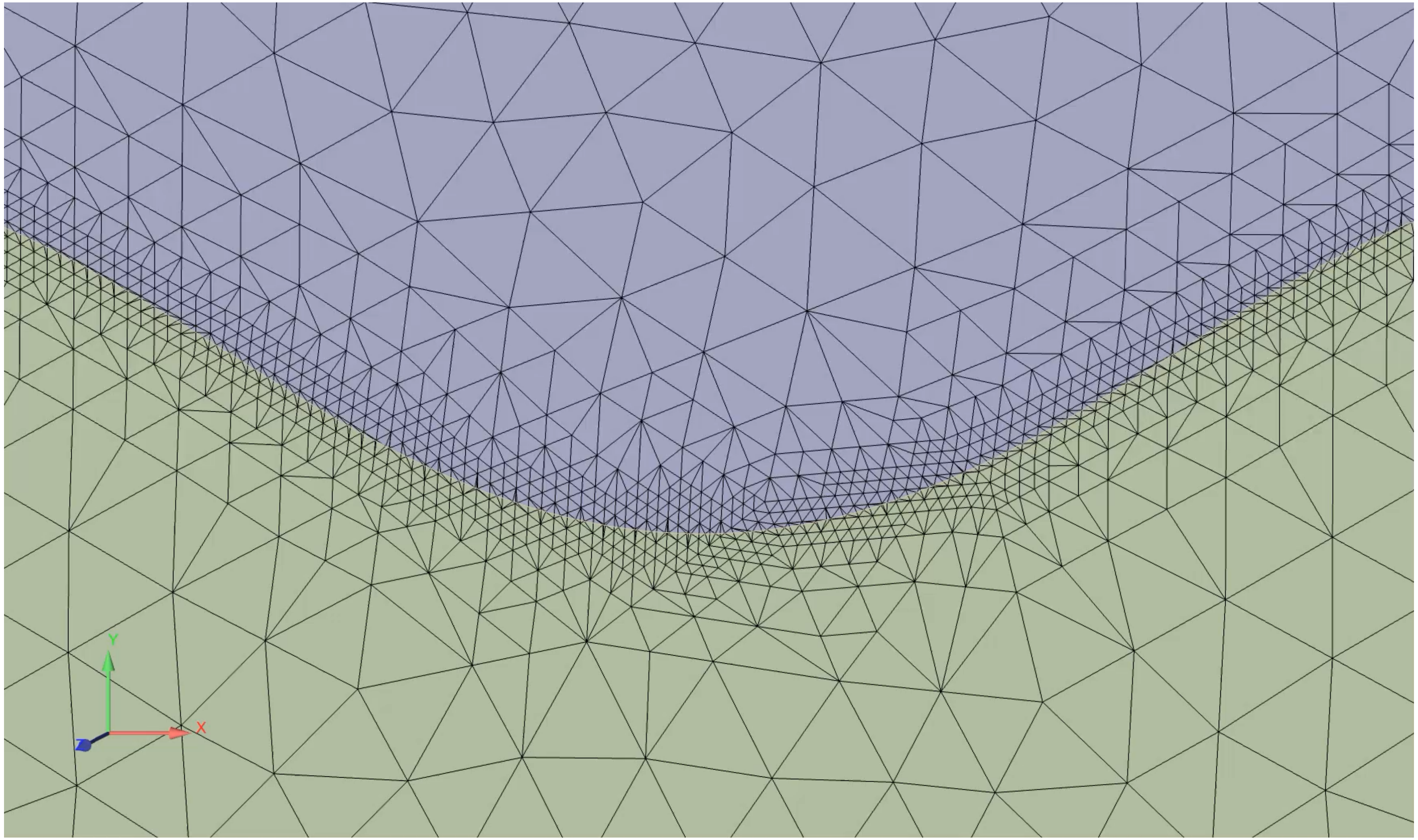
Finite Element Methods for Interfaces in Fluid/Thermal Applications

ALE	Diffuse LS	XFEM	CDFEM
• Separate, static blocks for air and water phases • Static discretization 	• Single block with smooth transition between air and water phases • Static discretization  	• Single block with sharply enriched elements spanning air and water phases • Interfacial elements are dynamically enriched to describe phases	• Separate, dynamic blocks for air and water phases • Interfacial elements are dynamically decomposed into elements that conform to phases 

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
- Interface refinement
  - Locally refining mesh around the interface seems to relieve some of these sliver elements and keeps the matrix well-posed
  - Increases accuracy of interface gradients
  - More performant, less mesh cost

Capillary wave decay problem using CDFEM and refinement



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
- BDF2 time discretization
- Adaptive mesh refinement at the interface will be used to lower computational cost and increase solution accuracy at the interface
- Compare to experiments
  - Static printing patterns (straight drop)
  - Serpentine printing patterns
  - Sinusoidal printing patterns

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

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

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

Slip condition

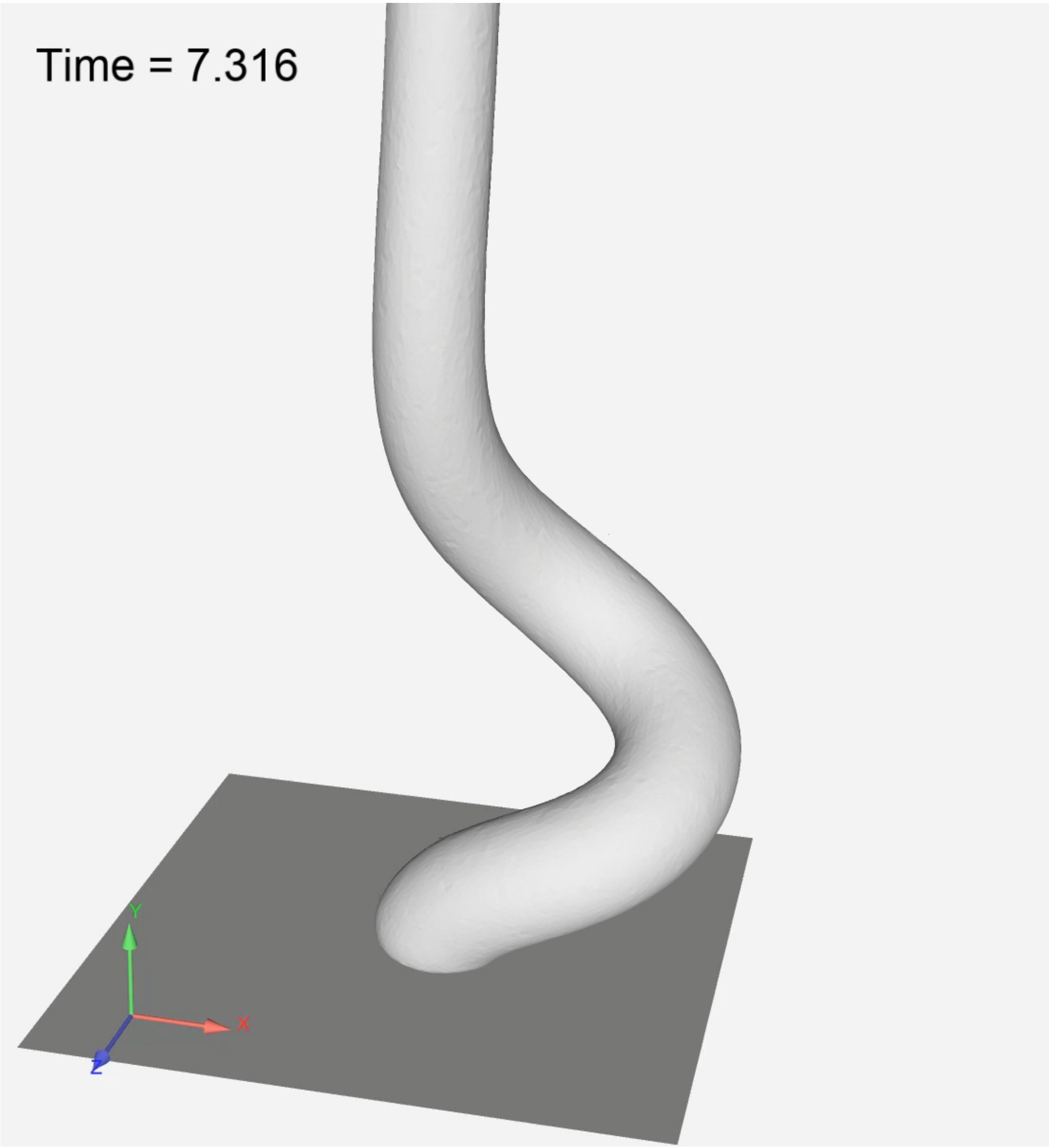
- In order to model the movement of the interface through the syringe "tip", a slip model must be used in lieu of a no-slip model
  - This allows the contact line between the syringe wall, air, and ink material interface to advect along the surface wall
- The Navier-slip condition is used to model the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

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

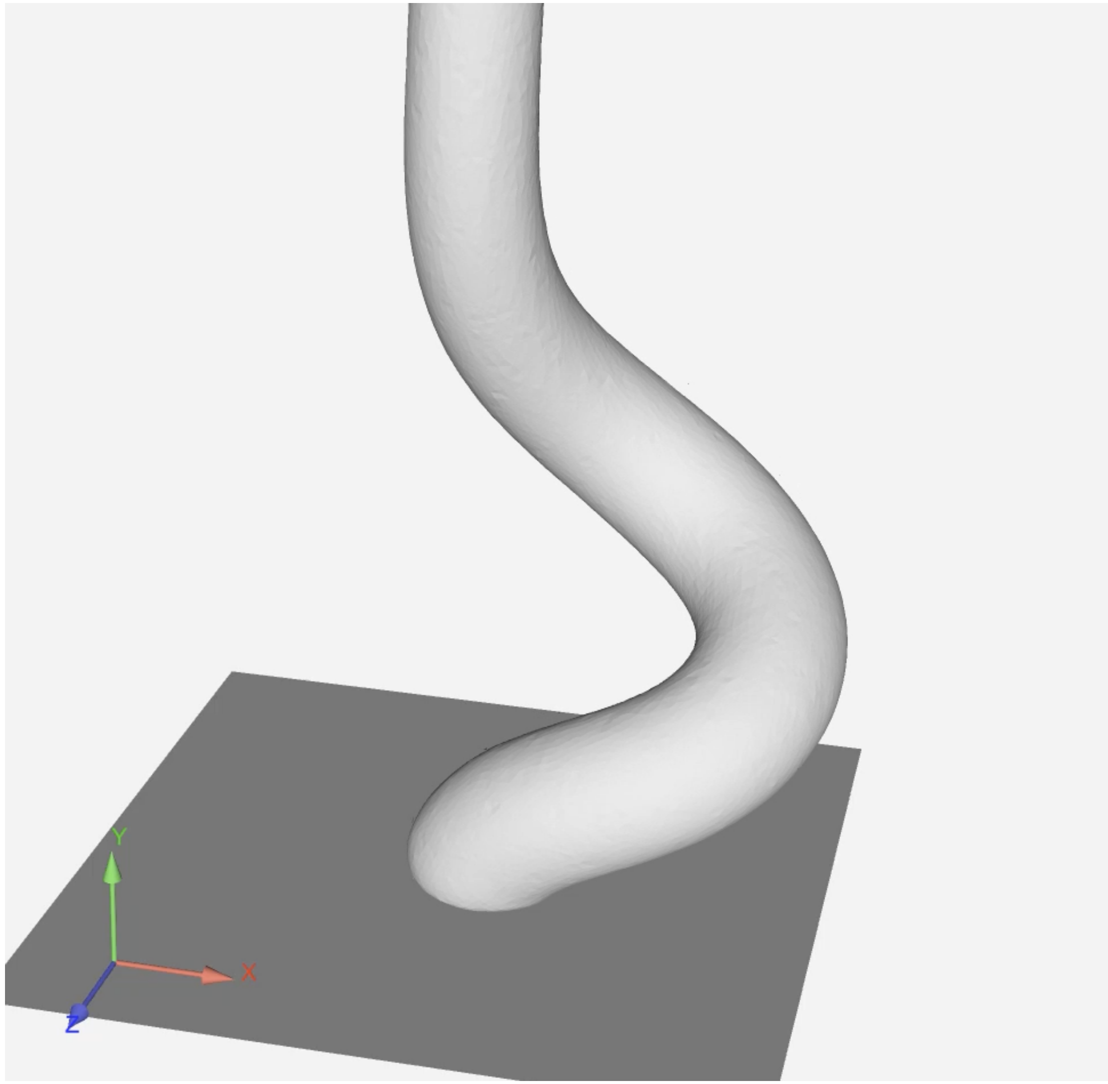
- Can recover the no-slip condition as $\beta \to 0$

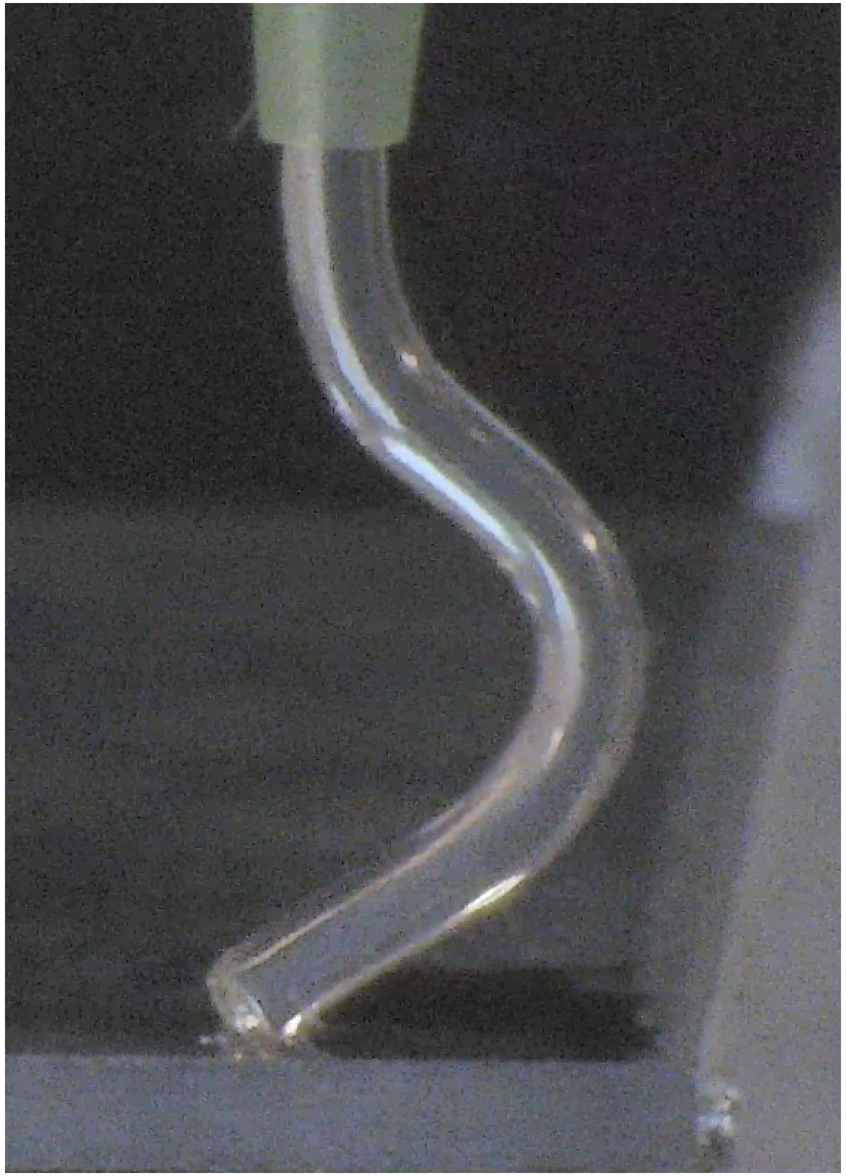
Previous work - Using CDFEM and DIW

- Stationary drop experiment (10mm)
- As the drop height is increased, we see a coiling instability after the first of the material comes in contact with the substrate
- The coiling instability is well known, and has been seen in our experiments
- Able to capture coiling using a (very viscous) Newtonian fluid
- Good qualitative agreement with the experimental videos

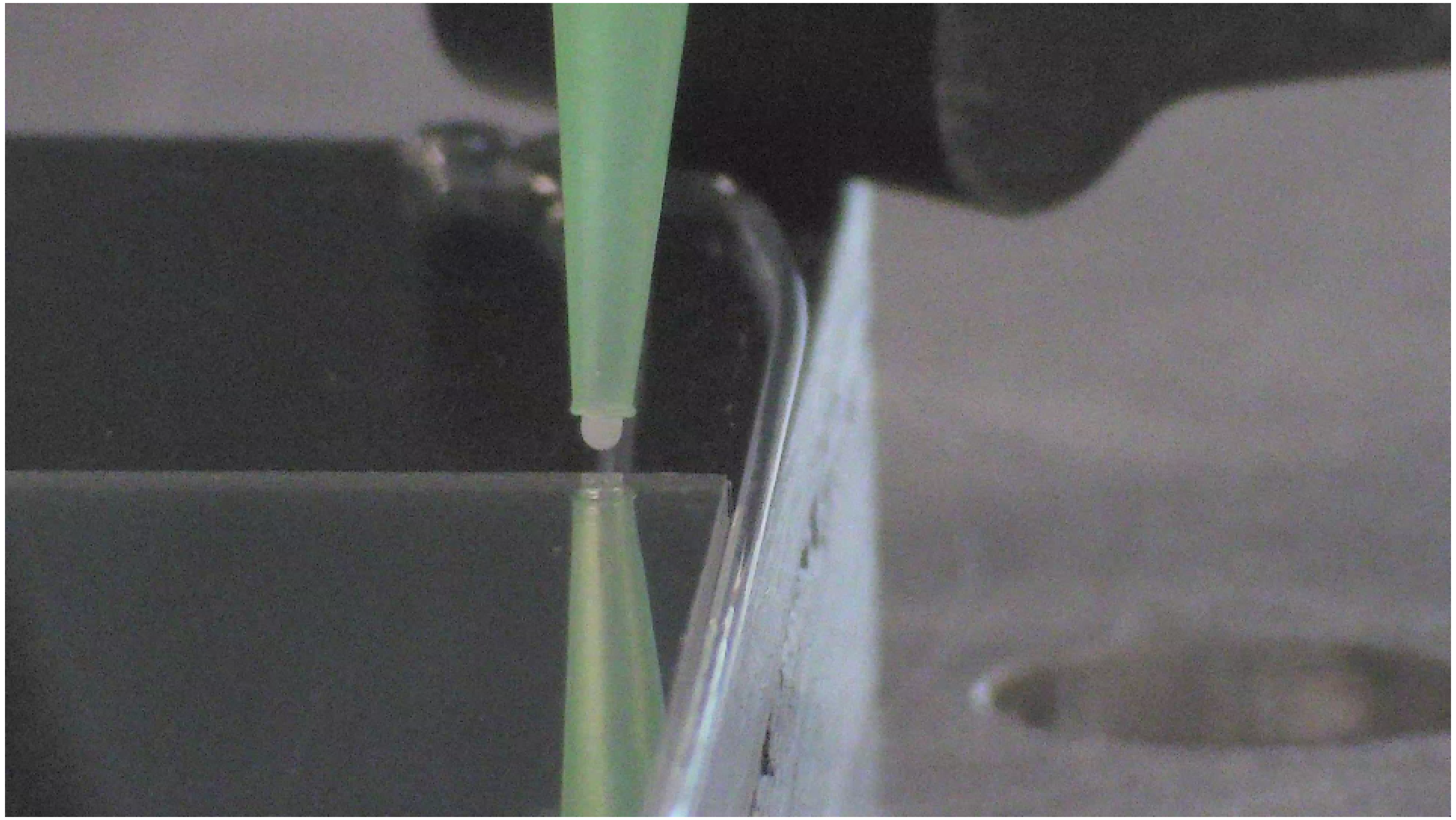


Stationary Drop 3D – 10mm drop height



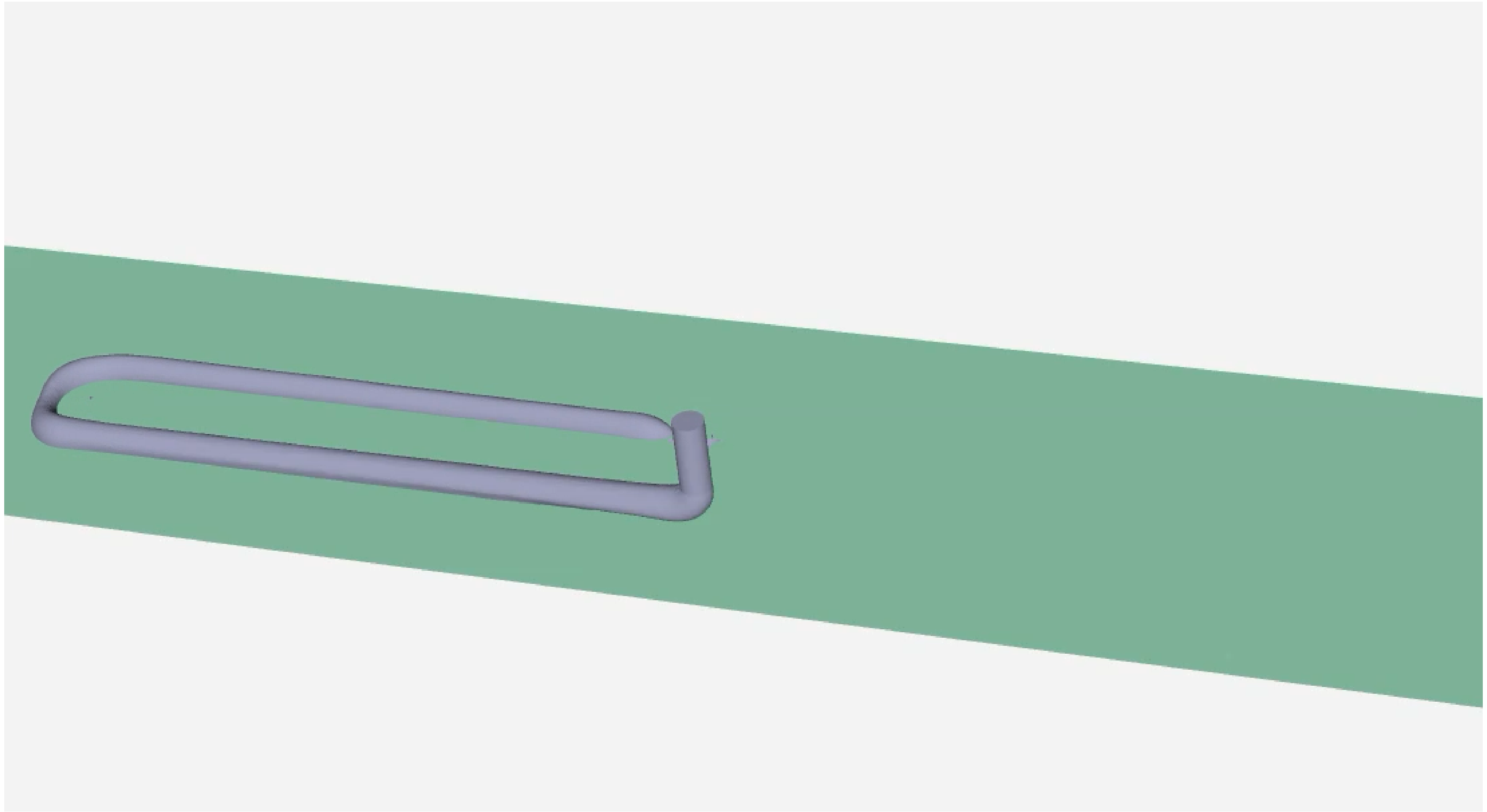


DIW printing of serpentine patterns



- Serpentine patterns are desired in our use cases
- Modeled using CDFEM
- Moving substrate (fixed nozzle position)
- Newtonian fluid

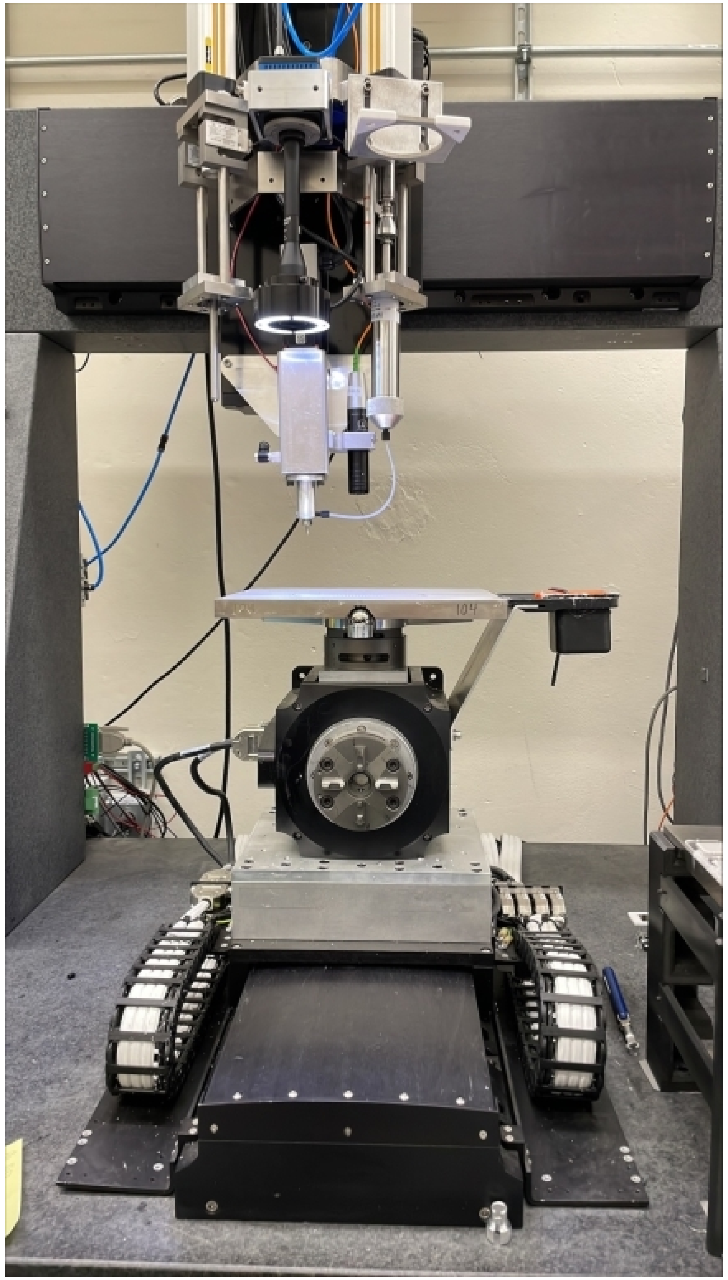
Serpentine model– 3D (Newtonian)



- Able to model the serpentine printing pattern in 3D for a Newtonian fluid
- Potential manufacturing defect shown in the “curve” of the serpentine.

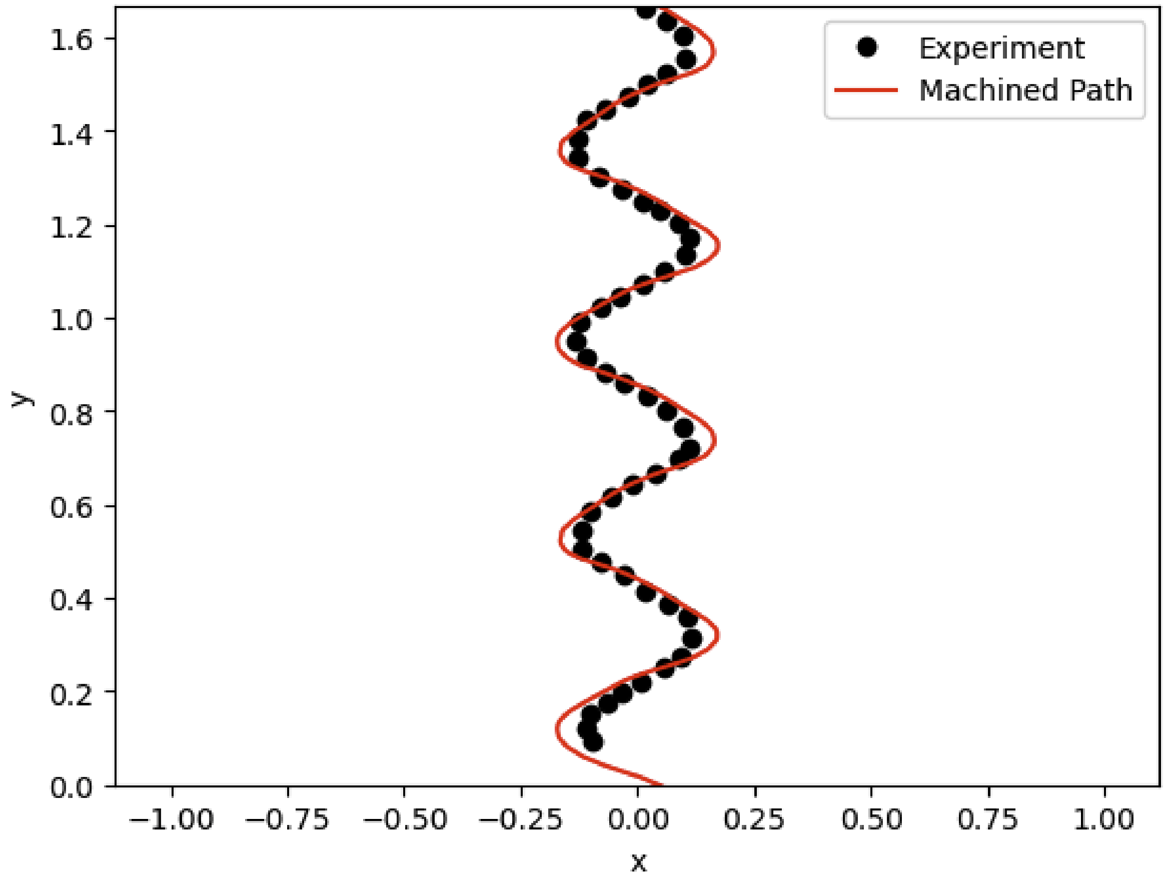
New work -Sinusoidal printing pattern

- Print sinusoidal pattern on substrate at specified amplitude and period
- Nozzle moves in the x-z (in-plane) direction
- Substrate can move in y-direction (normal to syringe movement plane)
- Uses silicone as the printing material
- Desirable to match amplitude and period of machined path
- Currently, errors in the printing amplitude are present



Experimental result

- Top-down view of experimental printing pattern
- Amplitude mismatch between experiment and machined path.



Model setup

- Inject material at a constant flow rate through cylindrical "nozzle"
- Move substrate at specified velocity (given from experimental machine data)
- Test Newtonian and non-Newtonian model
- Test how injection speed, drop height, nozzle diameter affect printing pattern

Figure 1. 3D isometric view of geometry (without CDFEM interfaces)

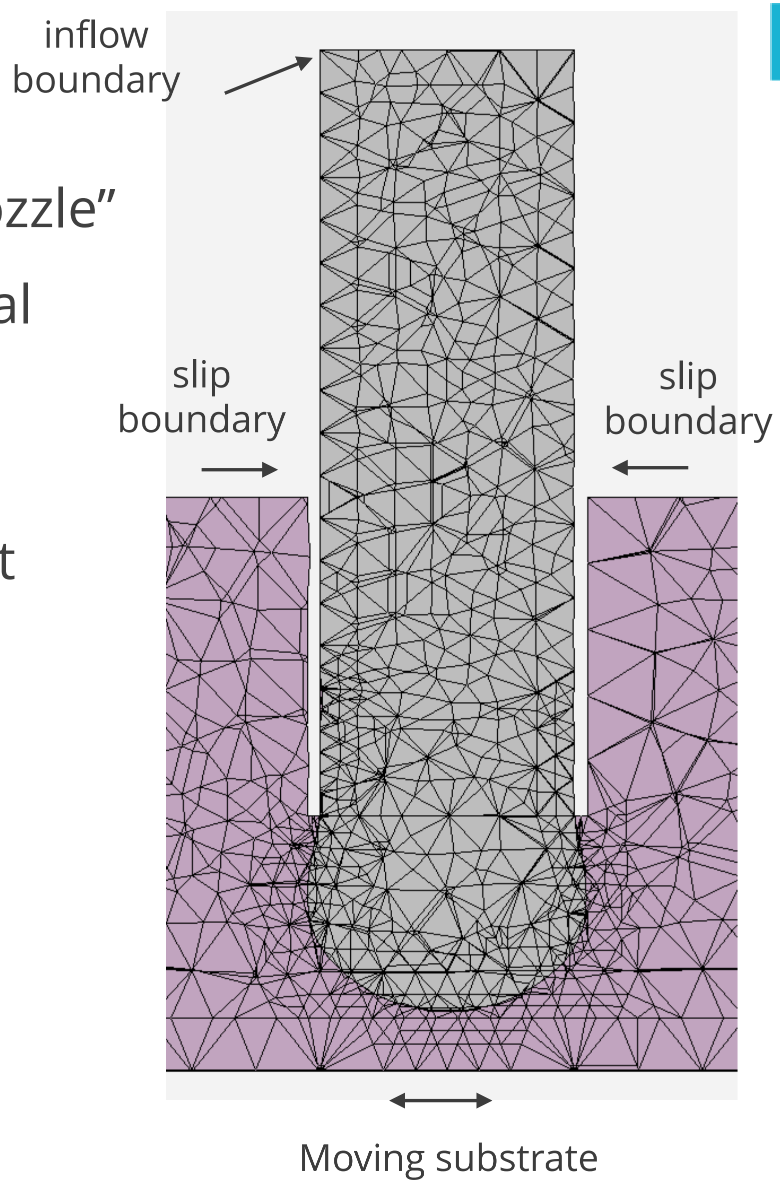
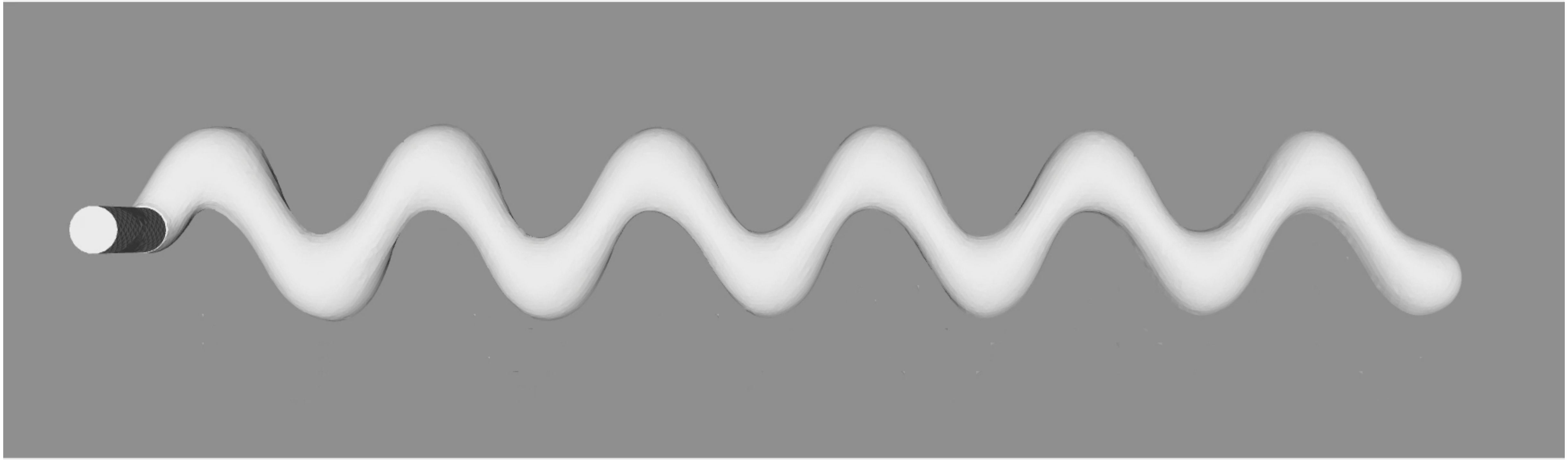


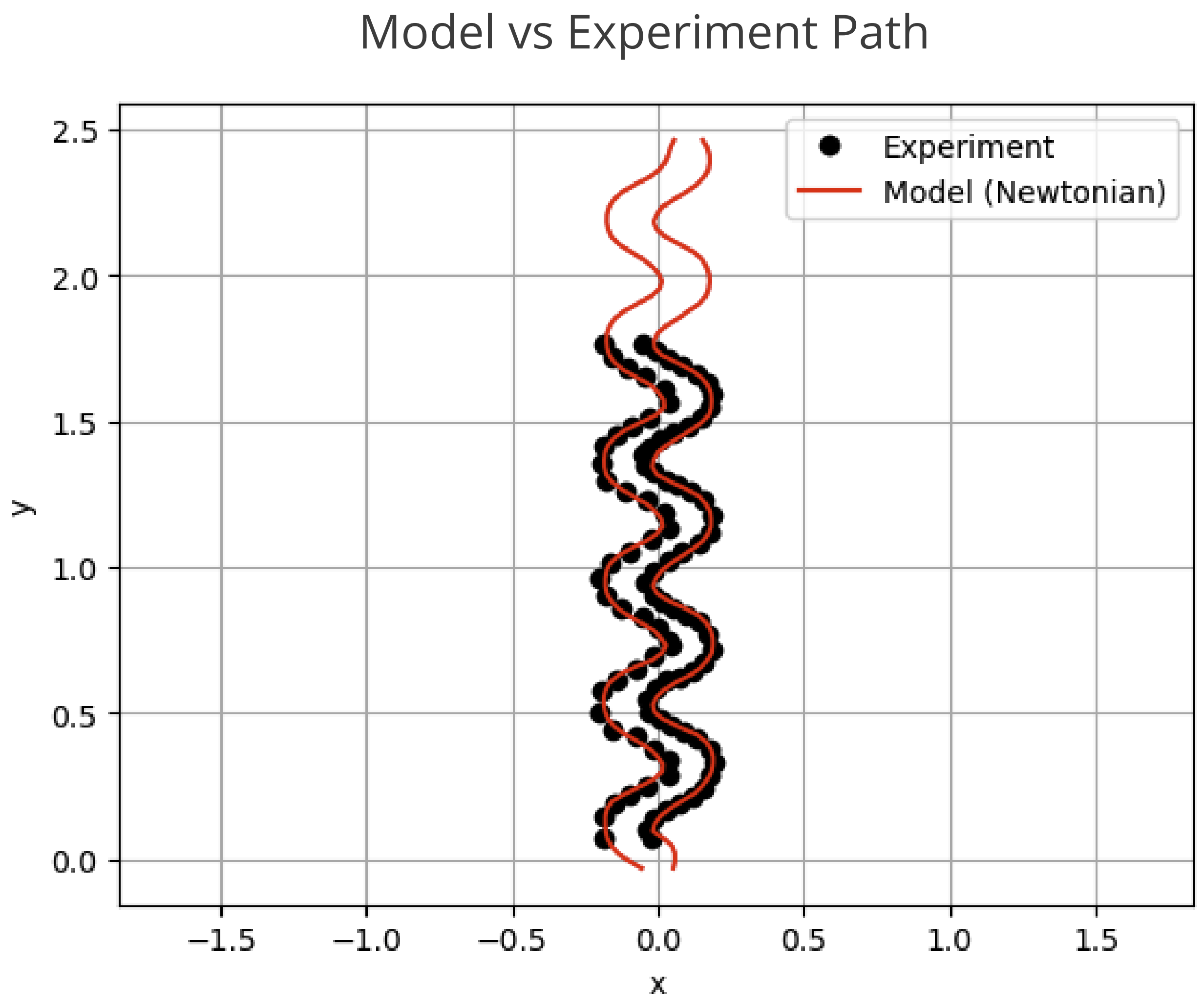
Figure 2. 2D cross section of nozzle inflow boundary and substrate (with mesh). Gray is the ink material

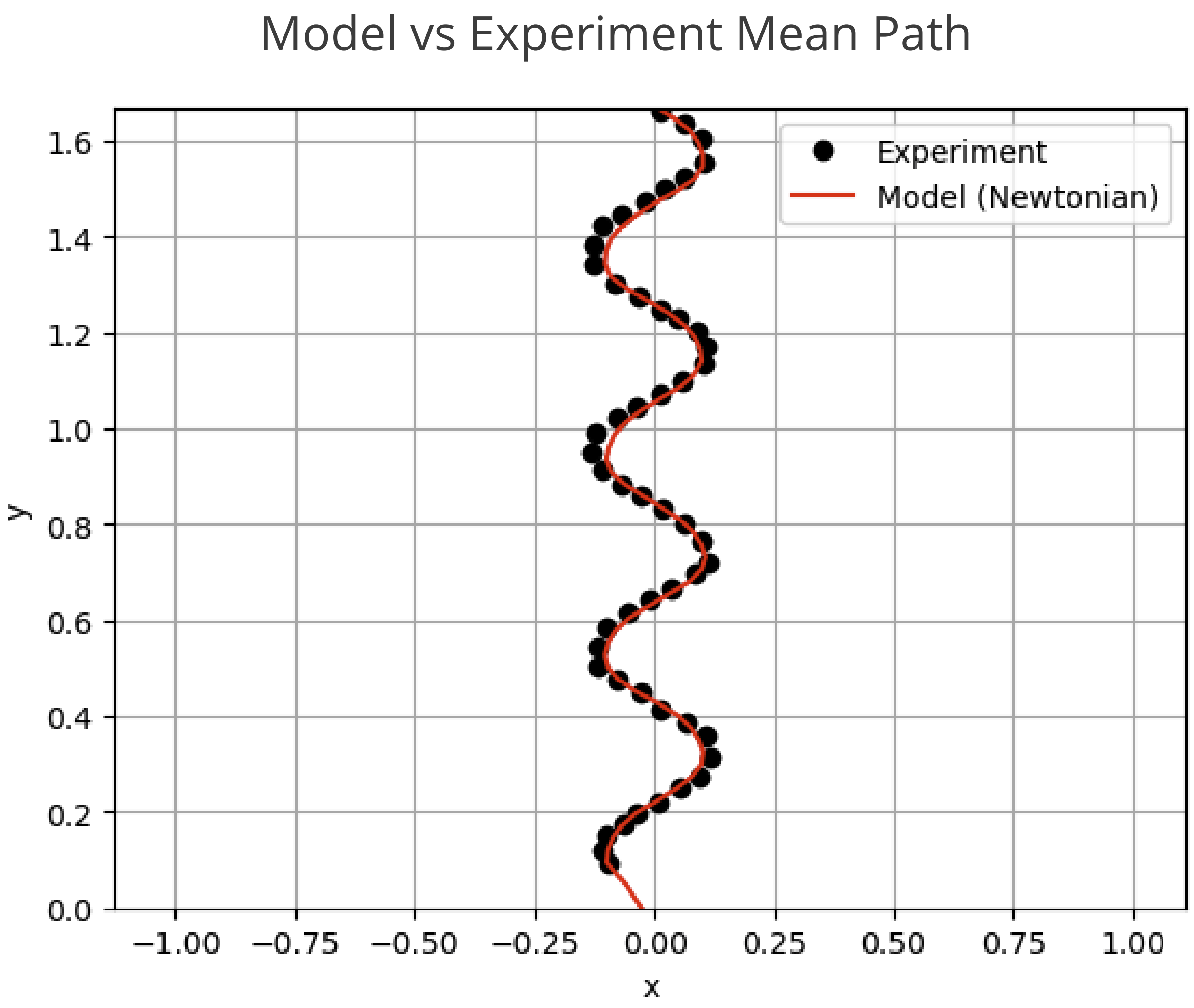
Model result - Newtonian fluid



- Used the machine velocity data for substrate boundary conditions
- Printed sinusoidal pattern
- Newtonian fluid (mu = 1e5 poise)

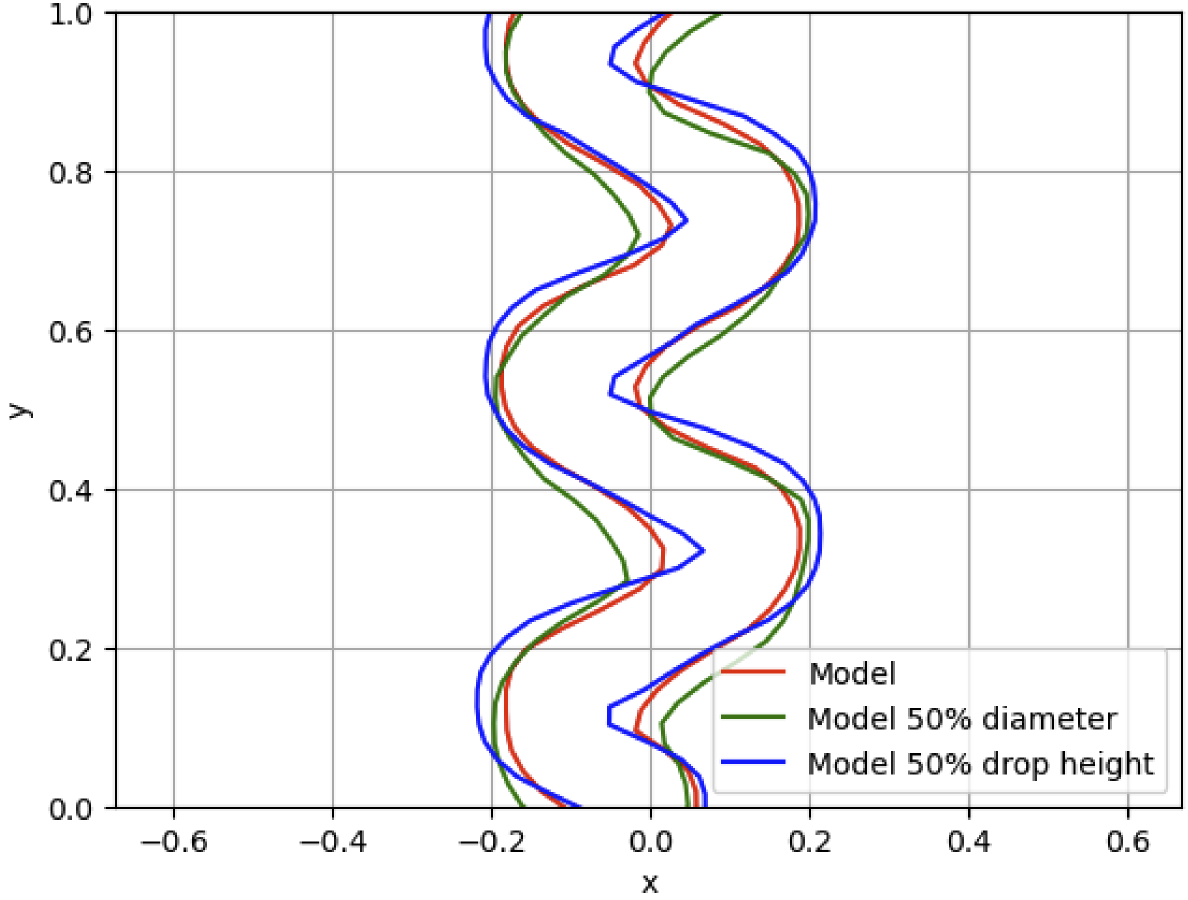
Sinusoidal pattern comparison - Newtonian



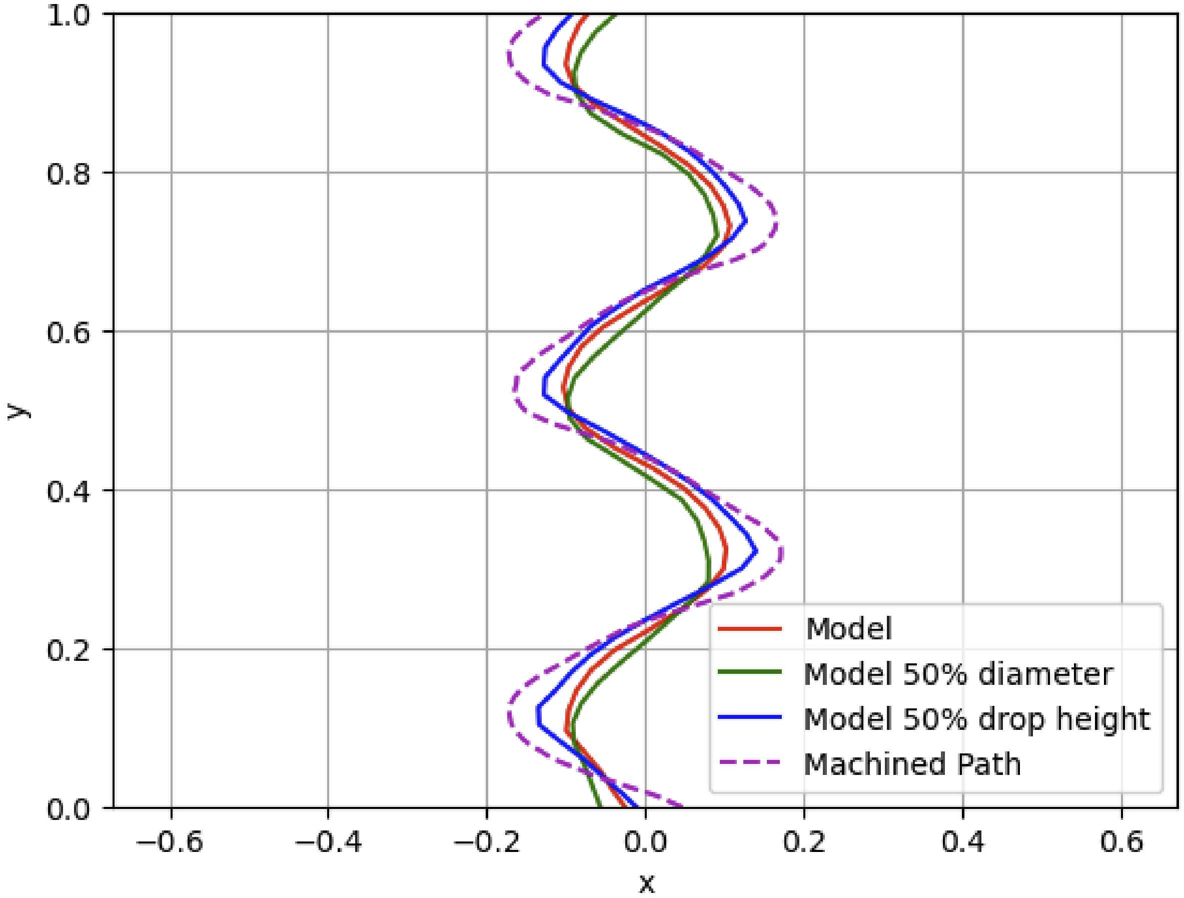


Parameterization of the drop height and diameter

- Alter the diameter of the nozzle and drop height
- **Decreasing the drop height appears to increase the mean path amplitude closer to the machined path**
- Decreasing nozzle diameter (while keeping flow rate constant) shrinks amplitude, but increases thickness of printed material



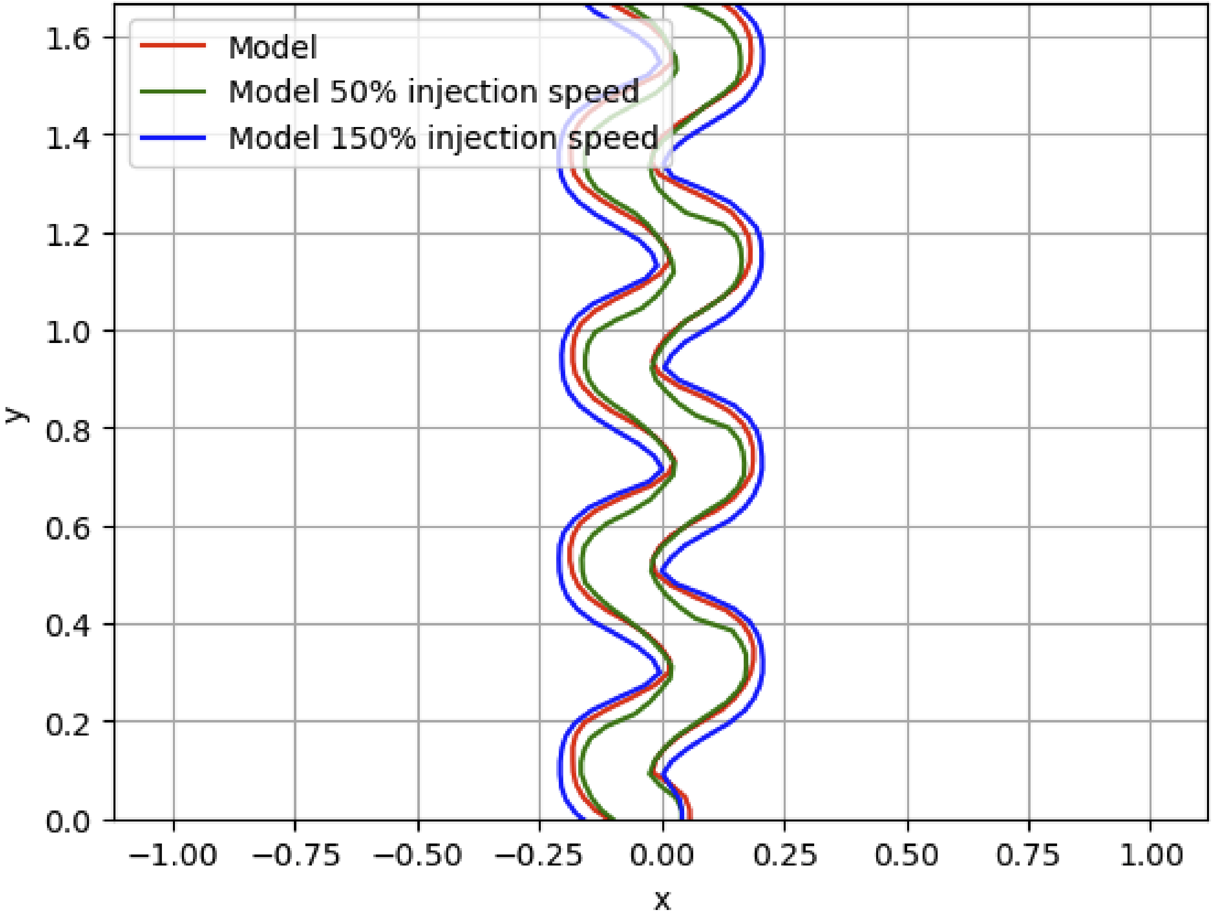
Topography (z-plane) projection



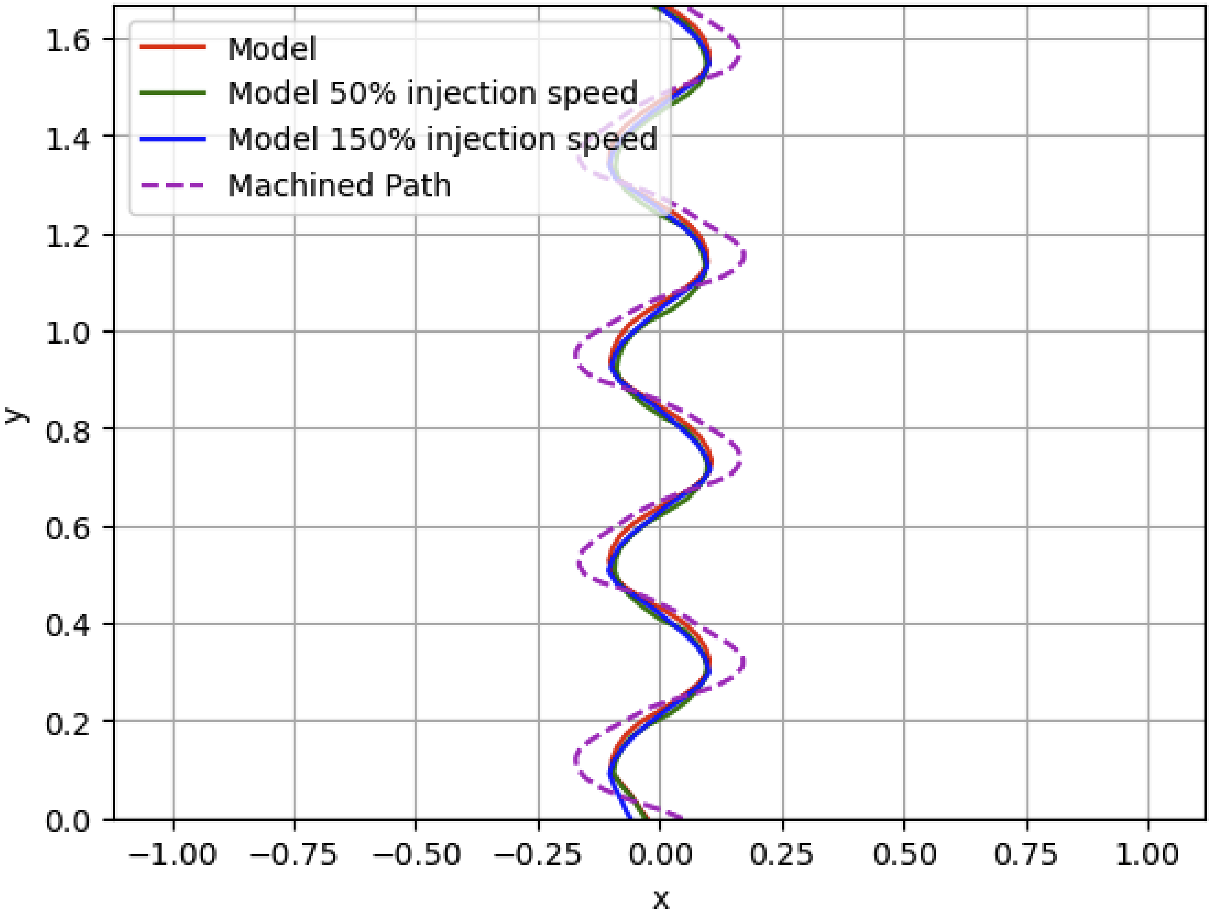
Mean path

Parameterization of injection speed

- Alter the injection speed of the material
- Decreasing the injection speed leads to a thinner sinusoidal pattern, while increasing injection speed thickens the pattern
- **Injection speed does not seem to change the mean-path amplitude of the pattern**



Topography (z-plane) projection

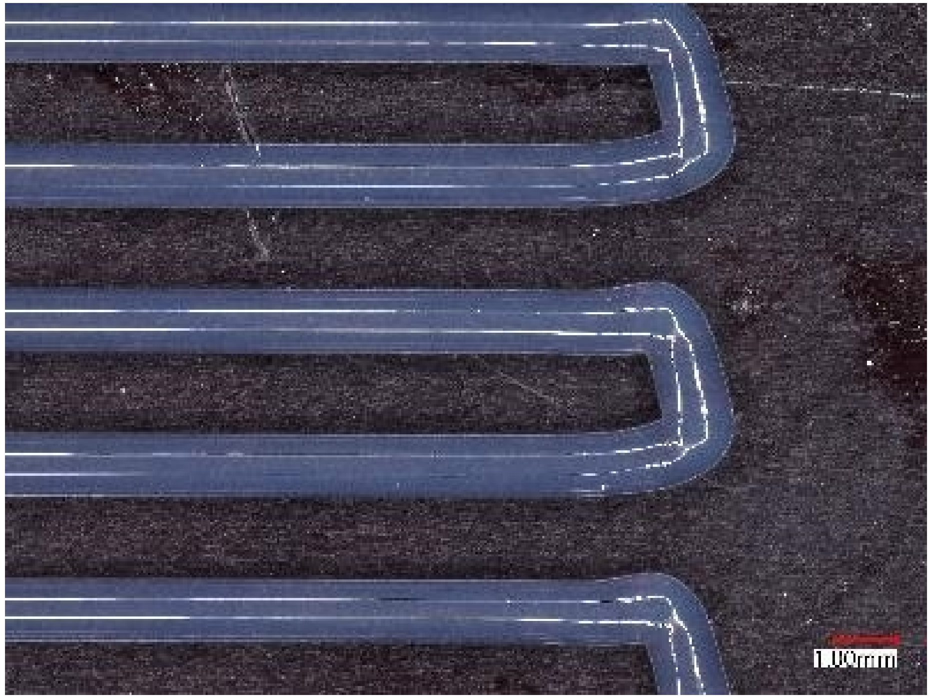


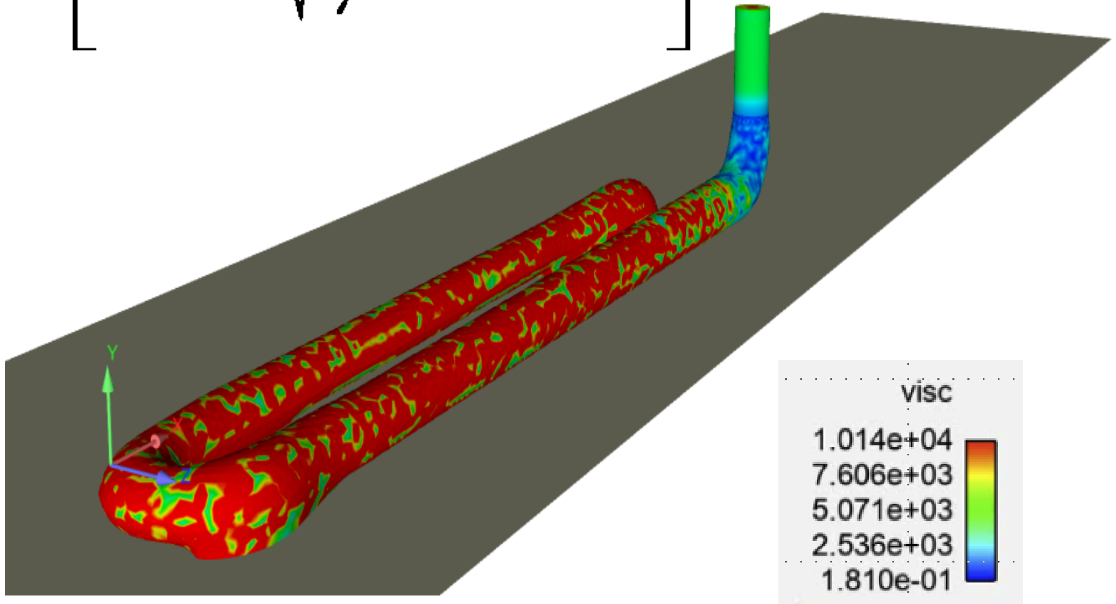
Mean path

Non-Newtonian casson model for viscosity

Yield stress

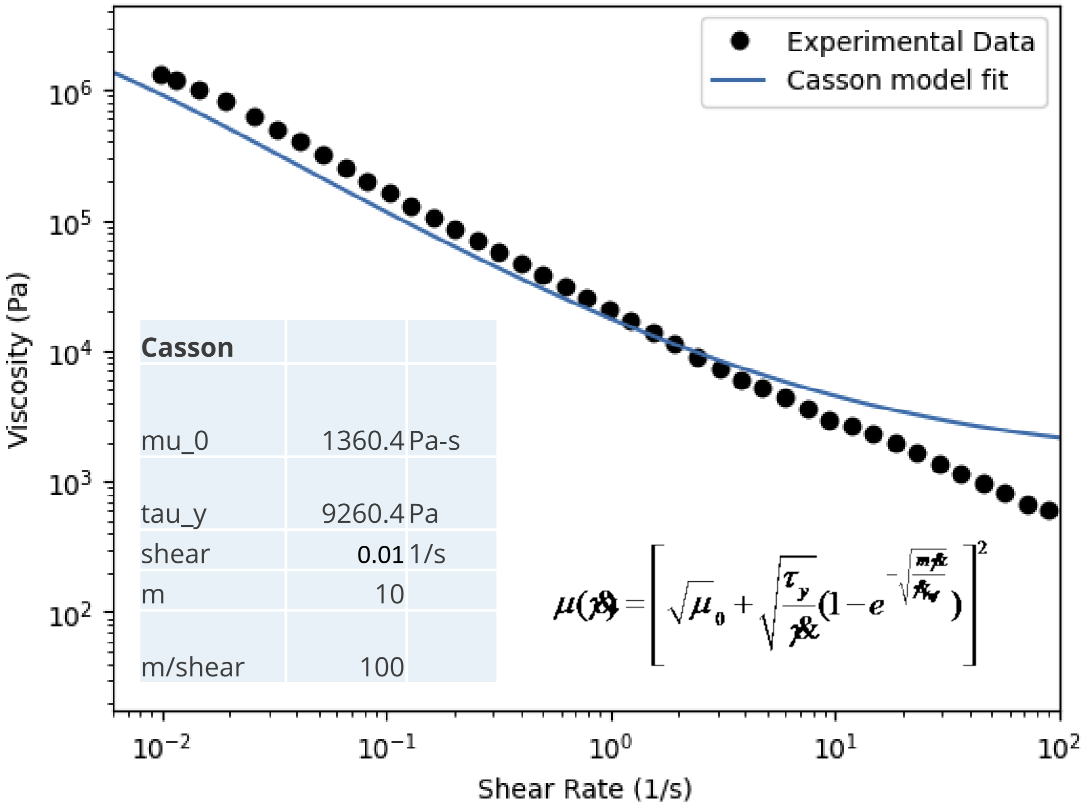
$$\mu(\dot{\gamma}) = \left[\sqrt{\mu_0} + \sqrt{\frac{\tau_y}{\dot{\gamma}}\left(1 - e^{-\sqrt{\frac{m\dot{\gamma}}{\dot{\gamma}_{ref}}}}\right)} \right]^2$$



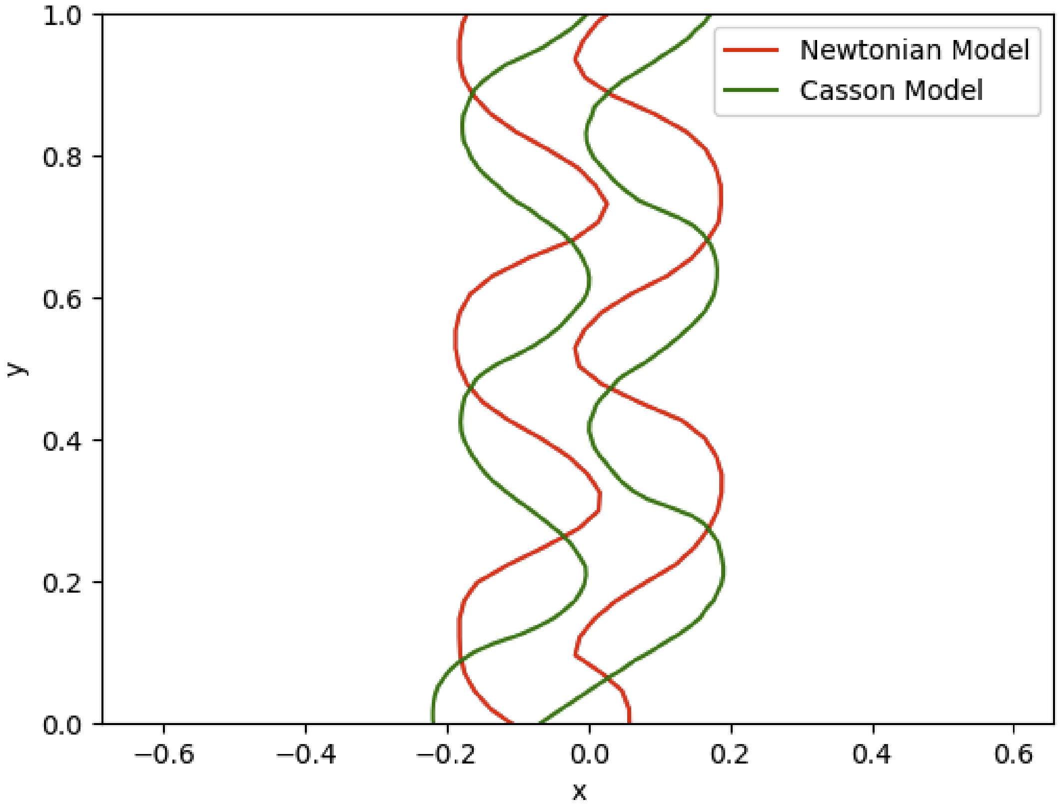


- Casson model is a shear-thinning non-Newtonian viscosity model
- Fit constants to match experimental measurements (viscosity vs shear rate)
- Ran with diffuse level sets on serpentine problem
- Careful to pick constants to match experimental data
  - Regularization (exponential term) gives smooth transition between yielded and un-yielded flow

Newtonian vs non-Newtonian (NN) model



Viscosity vs. shear rate for silicone printing material



Topography (z-plane) projection

- Fit the Casson shear-thinning viscosity model to provided experimental data for the silicone material
- Compare to Newtonian
- Phase shifted the printing pattern, but did not affect amplitude or thickness of printed pattern

Summary and conclusions

- Demonstrated the ability of CDFEM to model the direct ink-write process
  - Static drops
  - Serpentine printing patterns
  - Sinusoidal printing patterns
- Newtonian fluid seems to capture the printing pattern physics well
  - Mean-line and topographical projections match well with the experiment
- Print defect in the experiment (too low of amplitude compared to machined function)
  - Mean-line amplitude can be increased by decreasing the drop height
  - Thickness of the printing pattern can change based on
    - Injection speed
    - Drop height
- Fit the Casson shear-thinning viscosity model to provided experimental data for the silicone material
  - Comparable to Newtonian result, phase-shifts the sine-wave
  - No impact on mean-line amplitude/period or thickness
- Next steps involve taking 2D cross-sections and comparing to experiment
- Any questions?