Sandia National Laboratories

Exceptional service in the national interest

Modeling Direct Ink Write for Filled Silicones

Presented by:

Rekha Rao

Team members:

Alec Kucala, Jess Kopatz, Adam Cook, Anne Grillet (SNL)
Melody Golobic (LLNL)
Weston Ortiz (UNM)

Society of Rheology Annual Meeting
Austin, Texas
October 13-17th, 2024

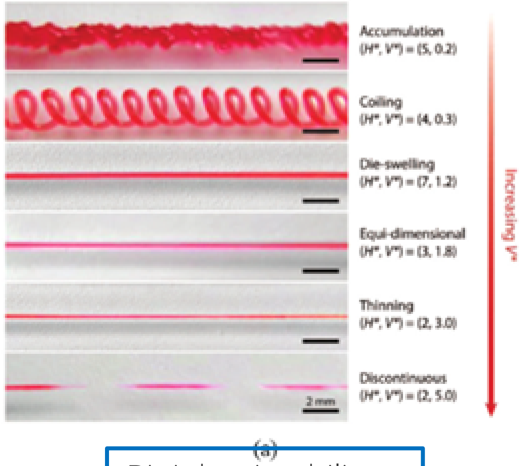
SAND2024-????

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

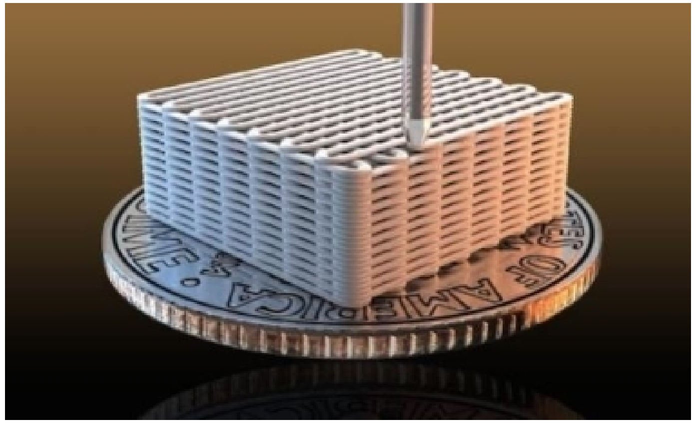
U.S. DEPARTMENT OF ENERGY

NNSA

Examples of Direct Ink Write

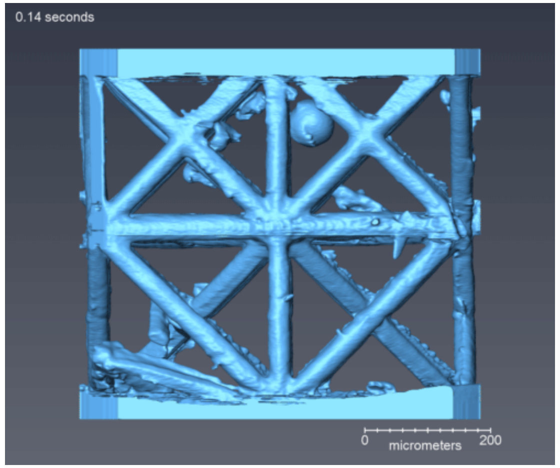


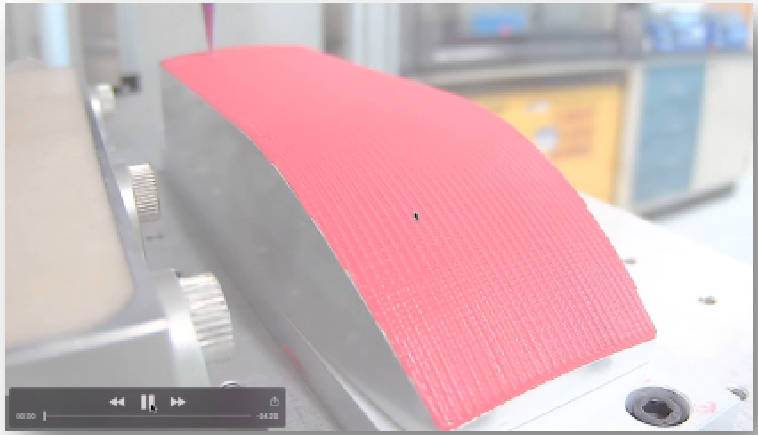
Bioink printability
Zhang et al, 2018



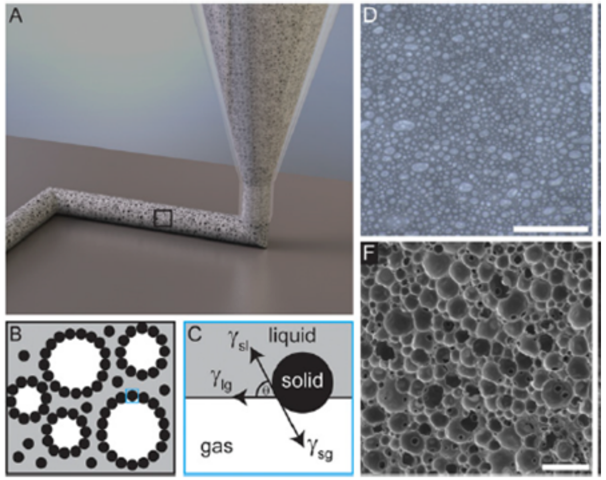
Graphene aerogel microlattices
Ryan Chen (LLNL)

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

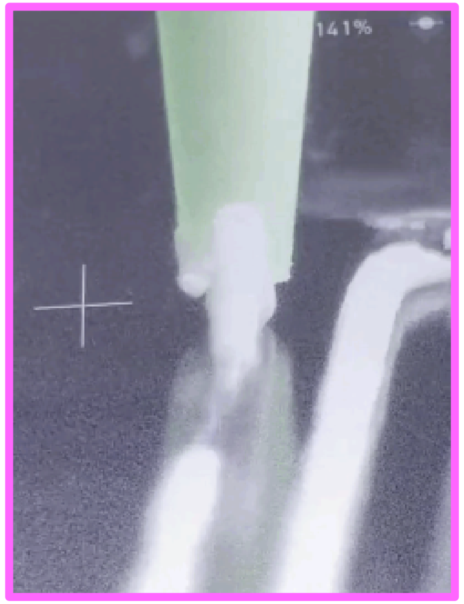
Possible Defects in 3D Printing

Manufacturing Defects can effect quality of printed parts

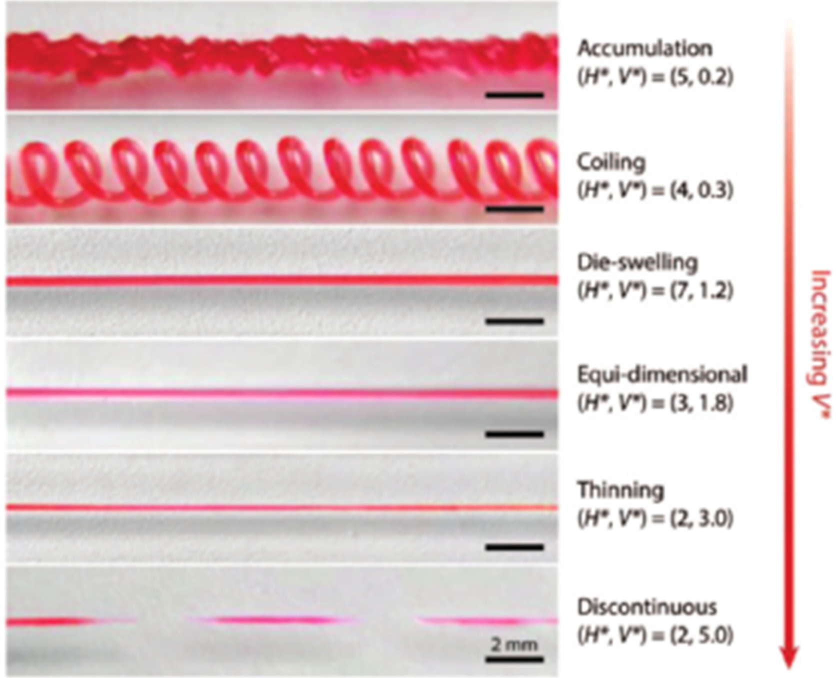
Examples include

- Coiling defects
- Line discontinuities
- Strut variability
- Clogging by aggregates
- Material sagging during or after printing

56vol% $CaCO_3$



56vol% Melamine

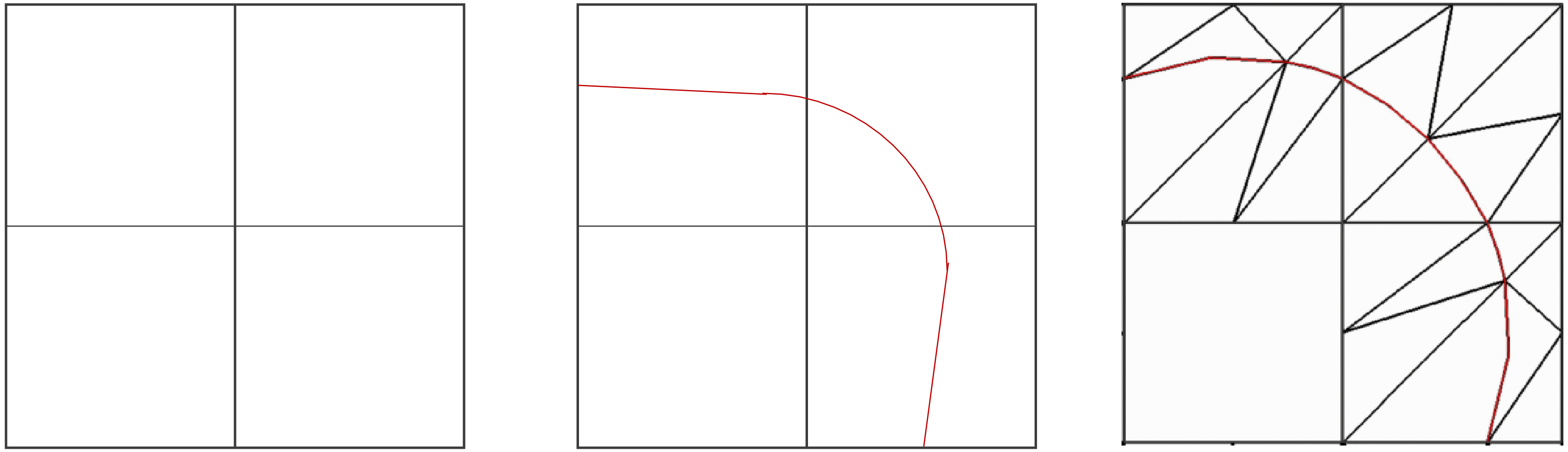


Bioink printability
Zhang et al, 2018

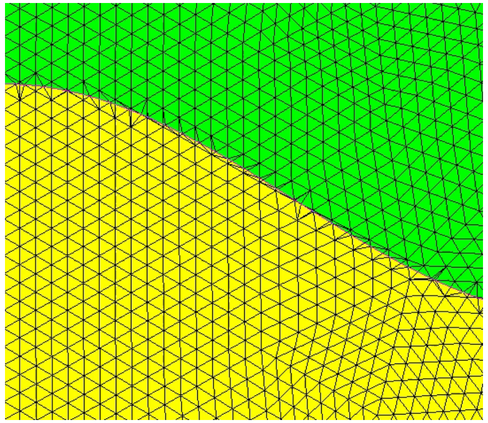
Modeling and simulation can be used to reduce defects in printed part, design/optimize/troubleshoot production problems, inform physics-based process controllers, and predict operating windows.

Level Set and CDFEM for Direct Ink Write

CDFEM Uses Ideas From XFEM, Level Set Methods, and ALE Moving Mesh



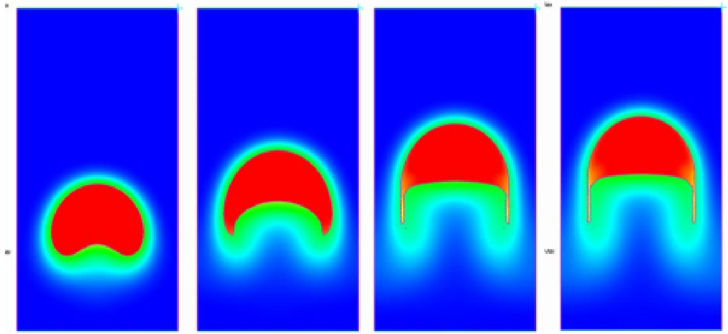
Base mesh | Level Set Function | CDFEM



Benefits: Meshed free surface allows for easy application of boundary conditions, discontinuous variables are straight forward, topological changes

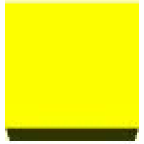
Drawbacks: Mass loss similar to diffuse interface methods, expensive, file bloat, solver issues

New Krino adaptive mesh capabilities allows for flexible load balancing across many processors in parallel, decreasing run times and memory usage, and improving robustness.



David Noble, Alec Kucala, Stephen Lin, and Dan Moser

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

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

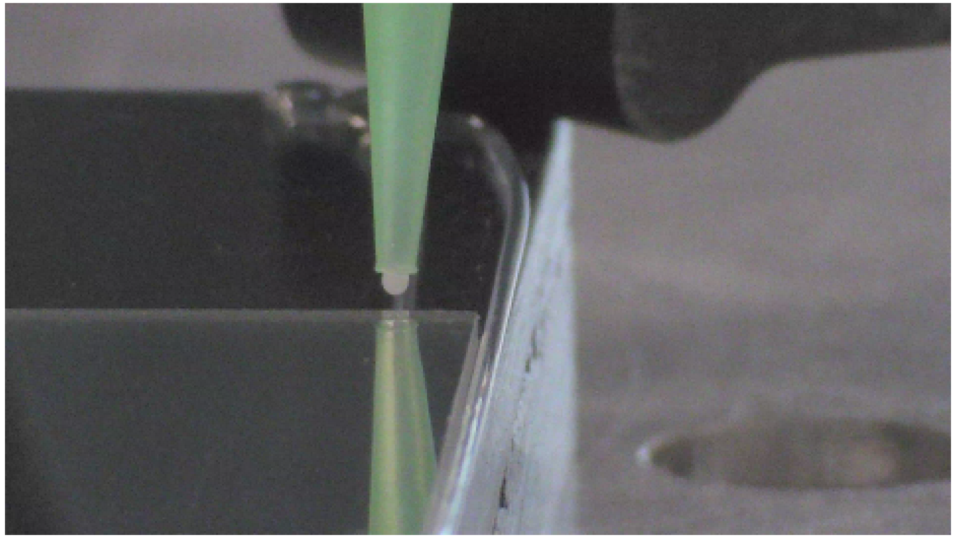
Interface Boundary Conditions

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

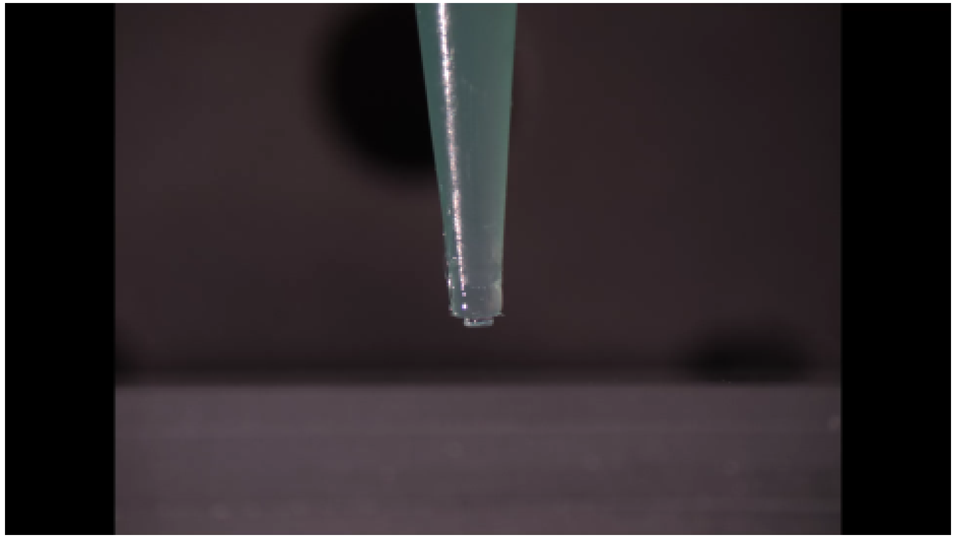
$$[-p\mathbf{I} + \mu(\mathbf{x})\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right)]_{\Delta}\cdot\hat{\mathbf{n}} = -\gamma\kappa\hat{\mathbf{n}}, \qquad \mathbf{x} \in \Gamma_{\mathrm{F}}$$

Validation Experiments

Serpentine Printing Pattern

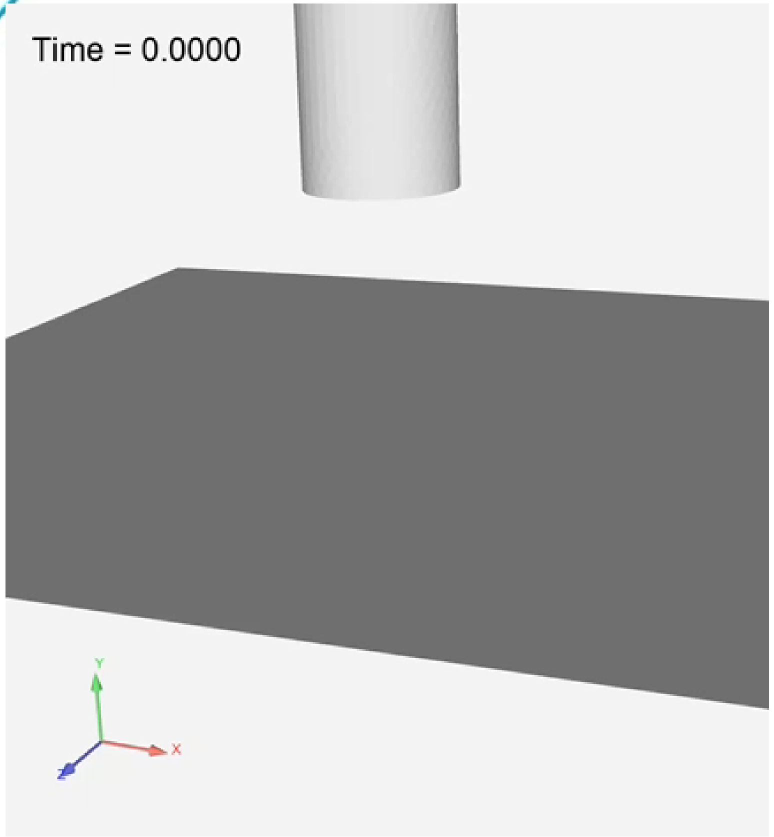


Stationary Drop

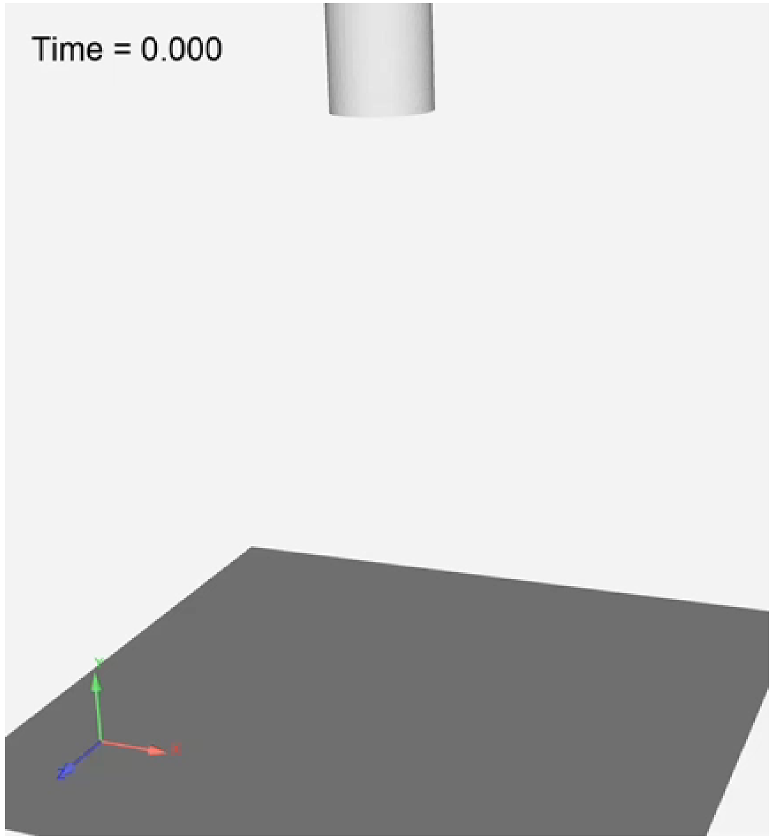


Printer designed by Adam Cook & Derek Reinholtz

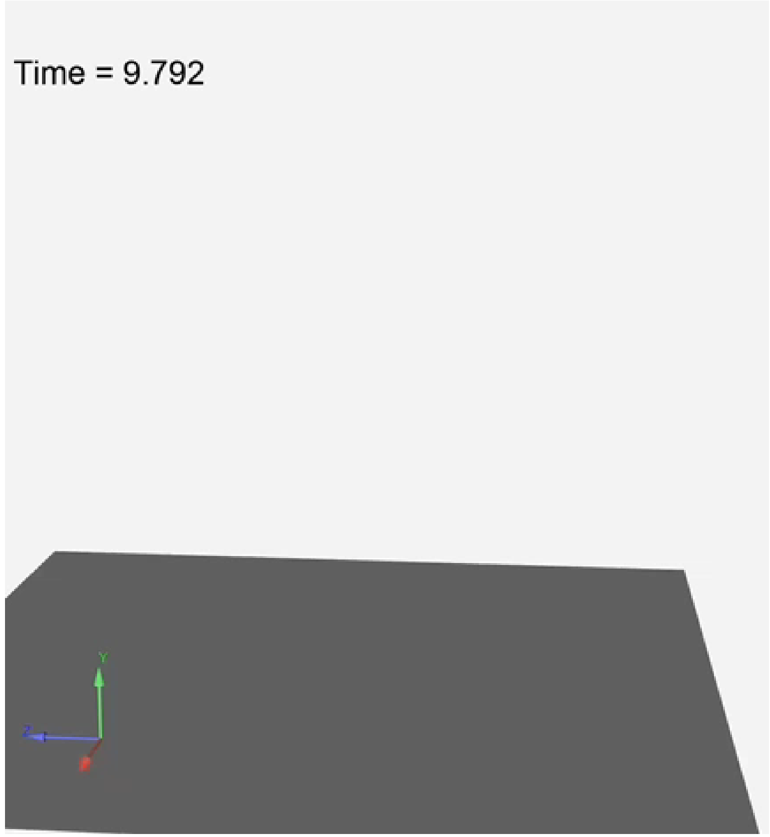
Stability of Print Related to Height of Nozzle: Stationary Plate



Newtonian with 1mm Nozzle Height



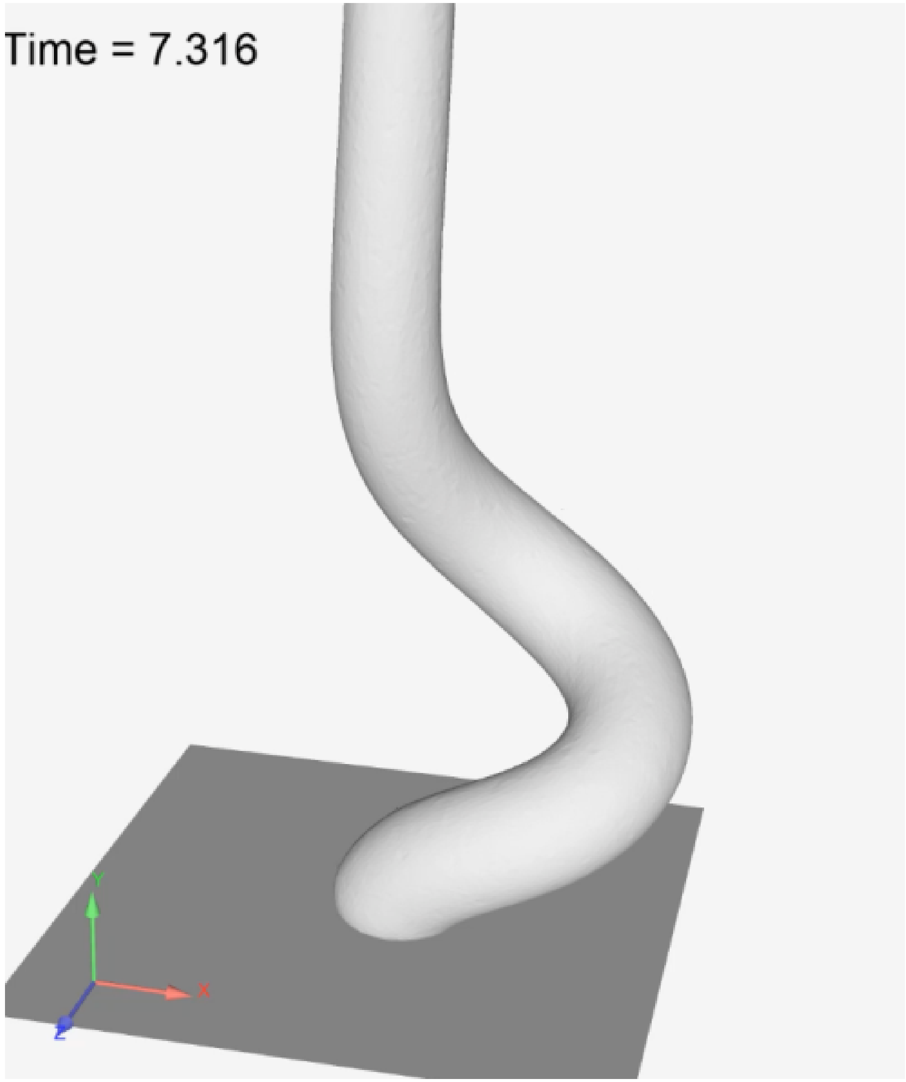
Newtonian with 5mm Nozzle Height



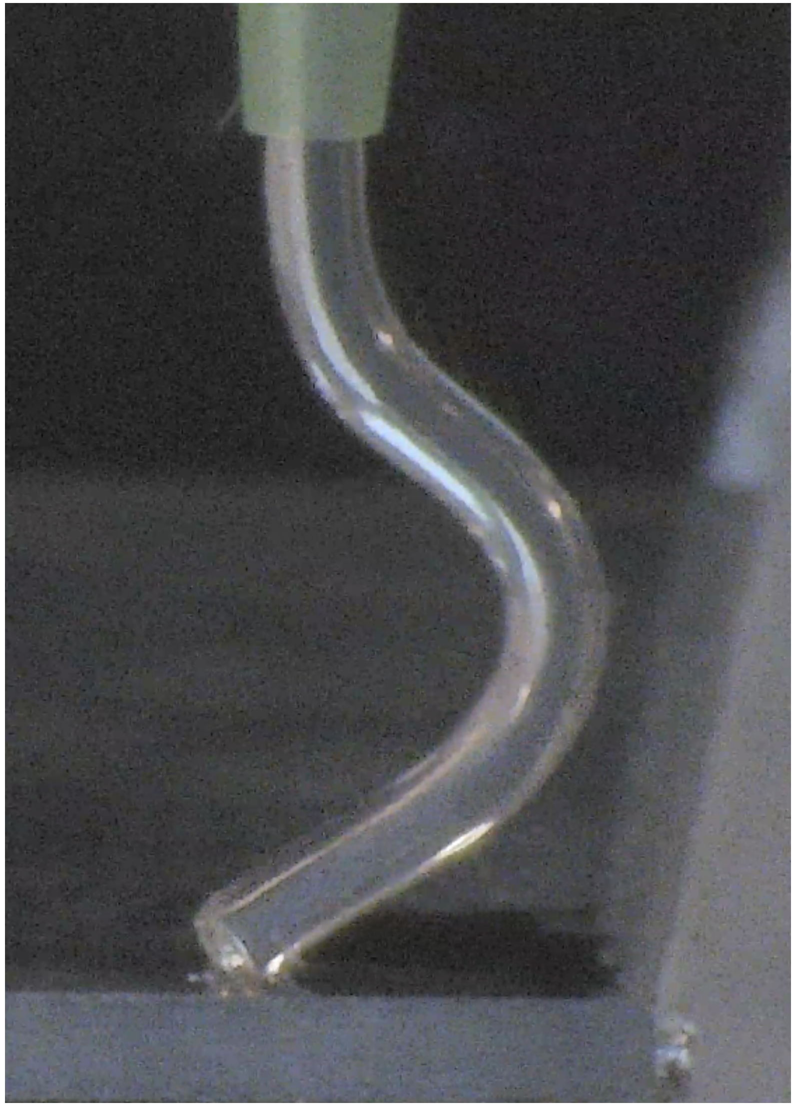
Newtonian with 10mm Nozzle Height

Alec Kucala, Jess Kopatz, Anne Grillet, Rekha Rao

Probability of Coiling Instability Increases with Nozzle Height

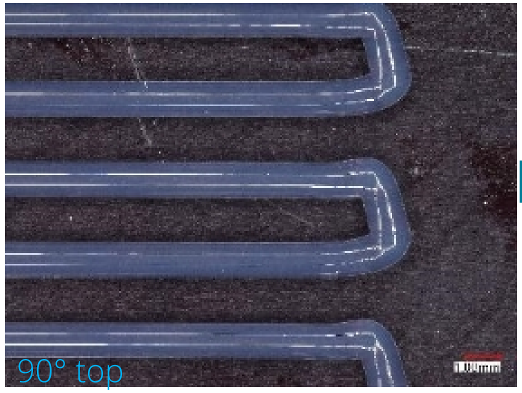


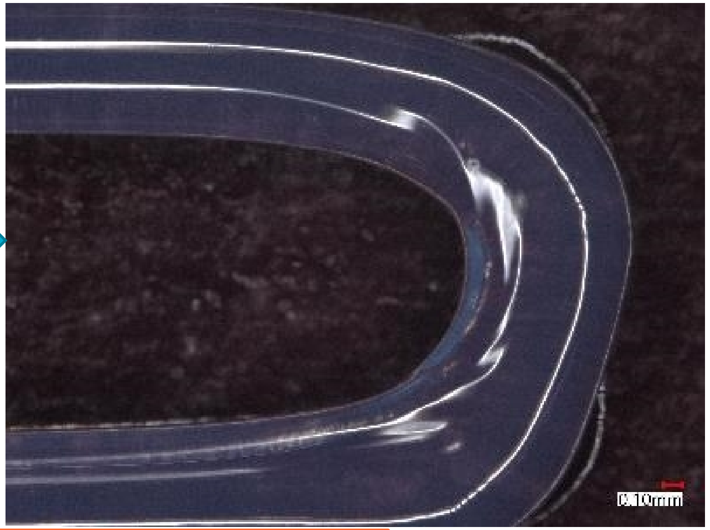
Newtonian with 10mm Nozzle Height



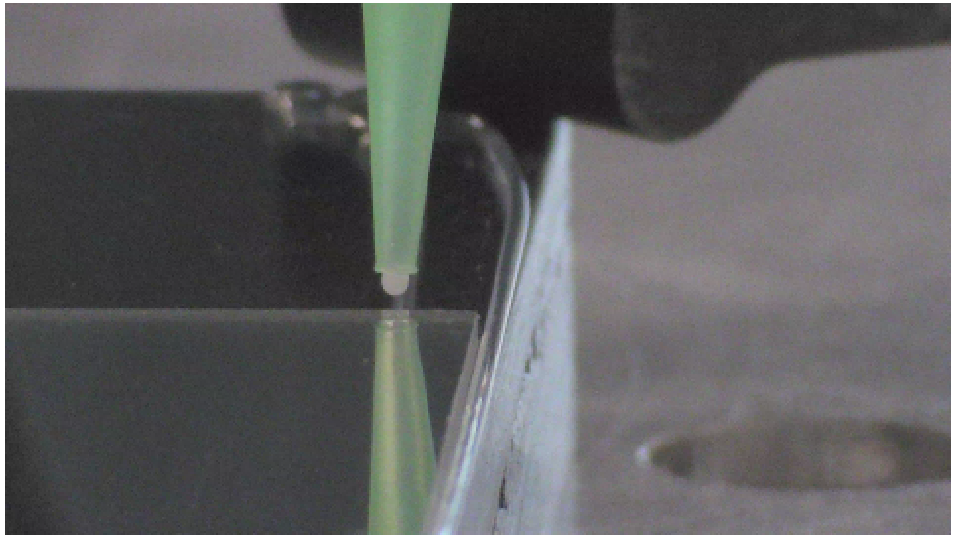
Alec Kucala, Jess Kopatz, Anne Grillet, Rekha Rao

CDFEM Model with Adaptive Refinement: Newtonian Model

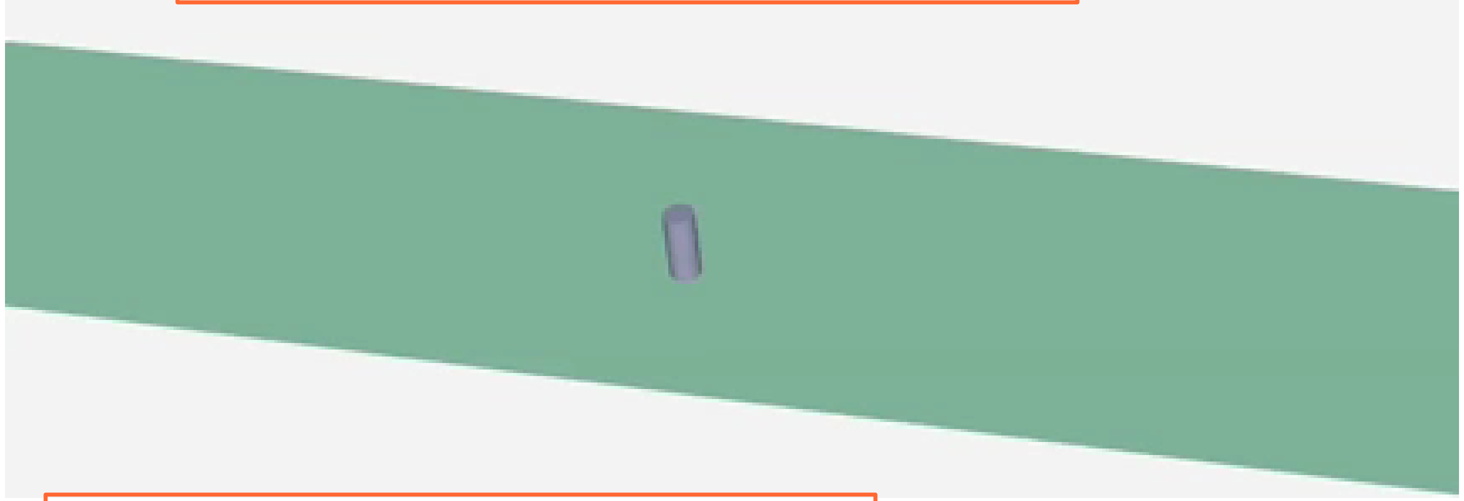


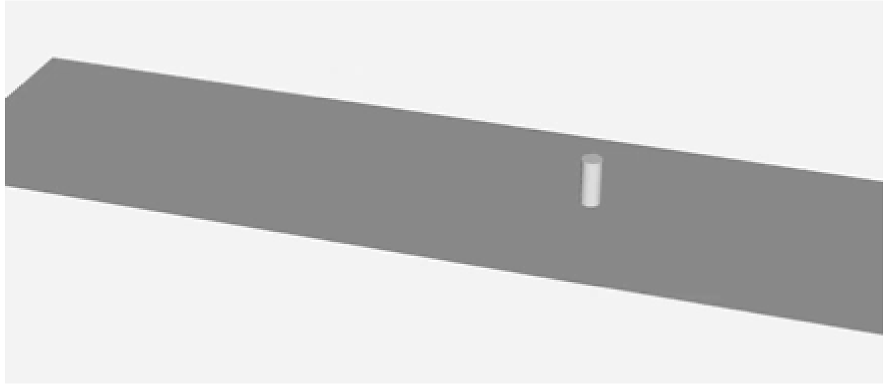


Serpentine Printing Pattern



CDFEM Model with adaptive mesh refinement shows good mass conservation

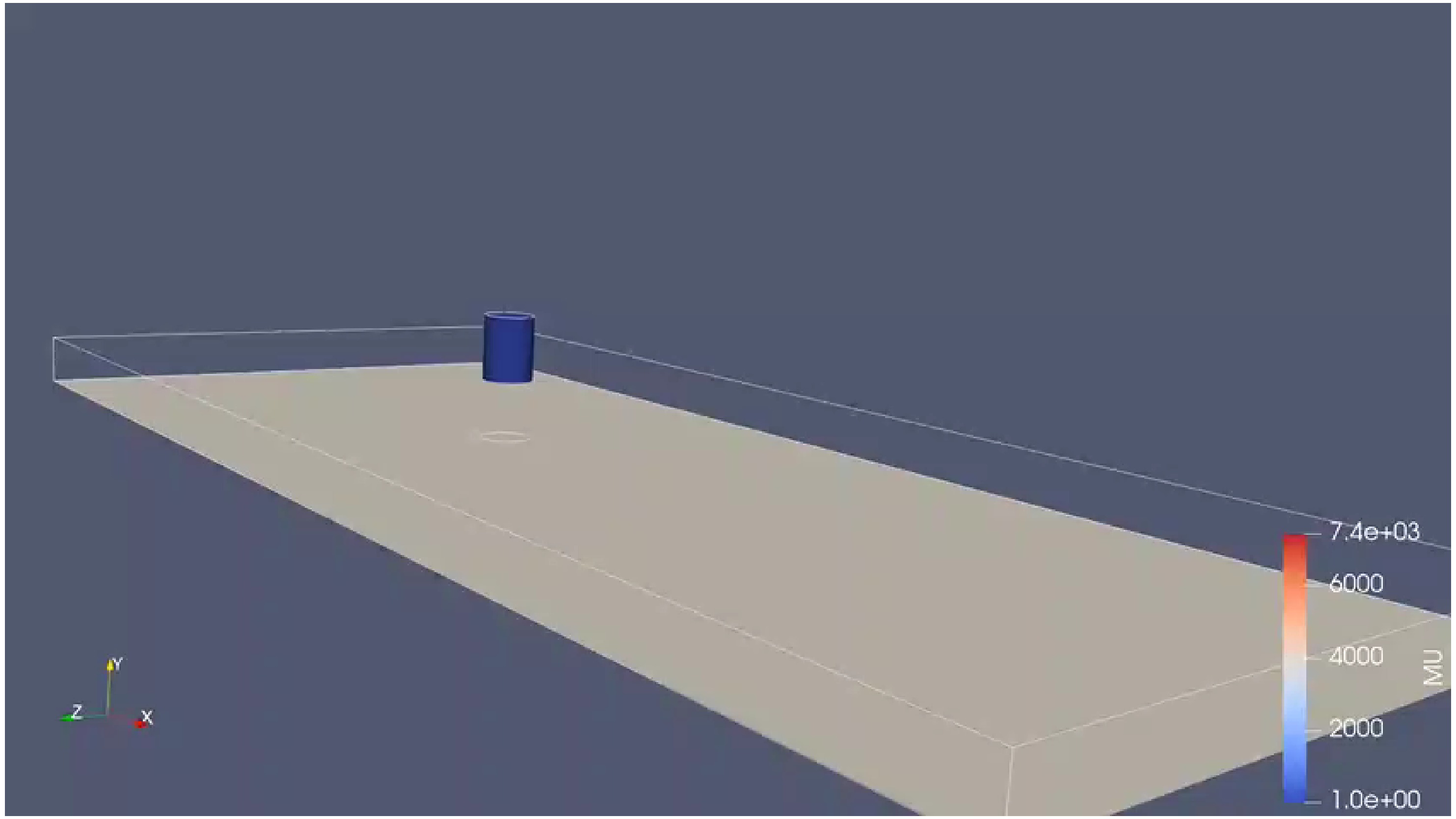


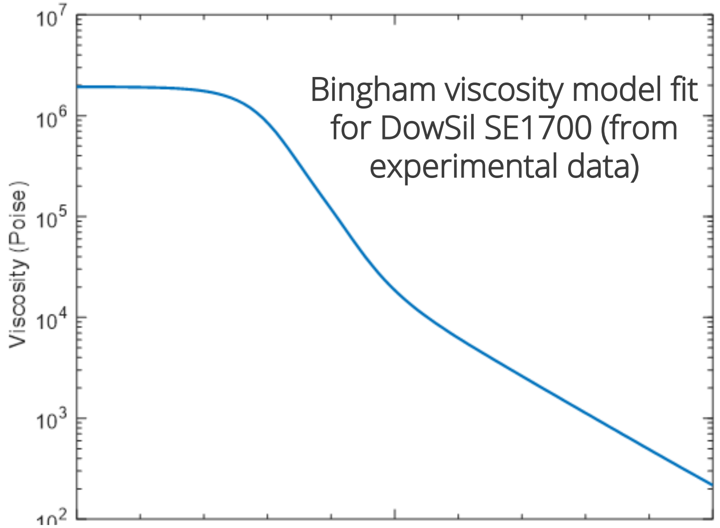


Increasing substrate speed can lead to defects

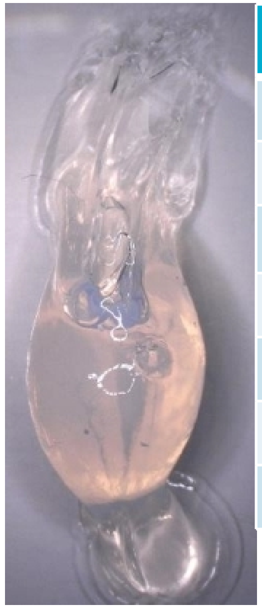
Alec Kucala, Jess Kopatz, Anne Grillet, Rekha Rao

Including Complex Rheology: Yield Stress Models





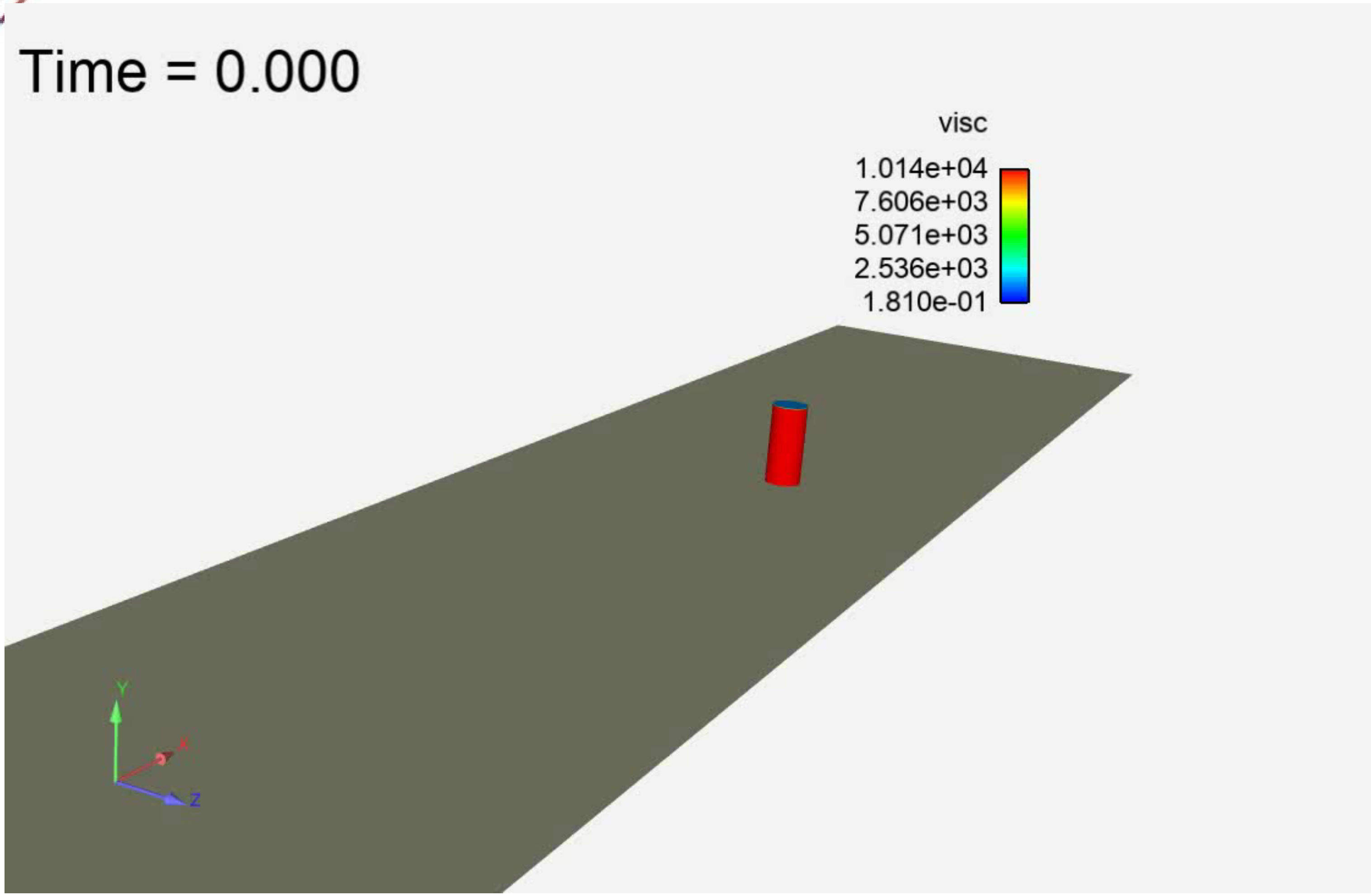
$$\mu(\dot{\gamma}) = \mu_\infty + \left(\mu_\circ - \mu_\infty + \tau_y \frac{1 - e^{-\dot{\gamma}F}}{\dot{\gamma}}\right)\left(1 + (\lambda\dot{\gamma})^a\right)^{\frac{n-1}{a}}$$



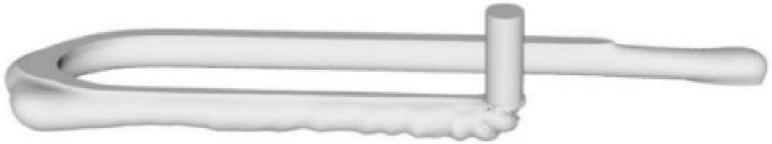
Variable	Value
μ_0	29740 Poise
μ_∞	10 Poise
τ_y	9520 Barye
λ	7.542
F	200
α	2.764
n	0.633586

Weston Ortiz, Rekha Rao, Anne Grillet, Helen Cleaves

Casson Model Including Yield Stress



Level set method with Casson Model and realistic viscosity model but less yield stress



Level set method with higher viscosity shows instability after the corner

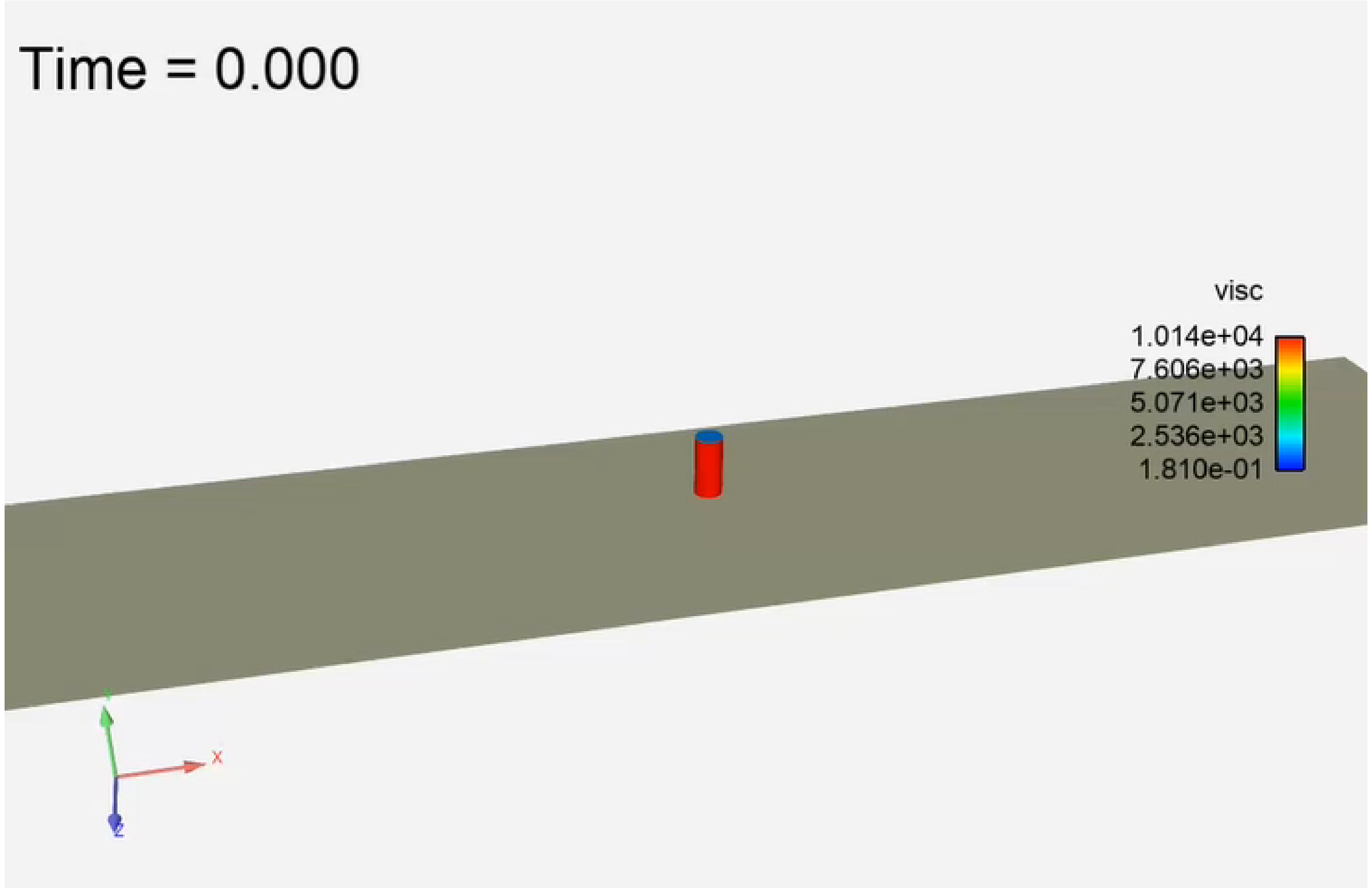
$$\mu(\dot{\gamma}) = \left[\sqrt{\mu_0} + \sqrt{\frac{\tau_y}{\dot{\gamma}}\left(1 - e^{-\sqrt{\frac{m\dot{\gamma}}{\dot{\gamma}_{ref}}}}\right)} \right]^2$$

Casson Model		
mu_0	136.4	Pa-s
tau_y	926.4	Pa
shear_ref	1	1/s
m	20	
m/shear_ref	20	

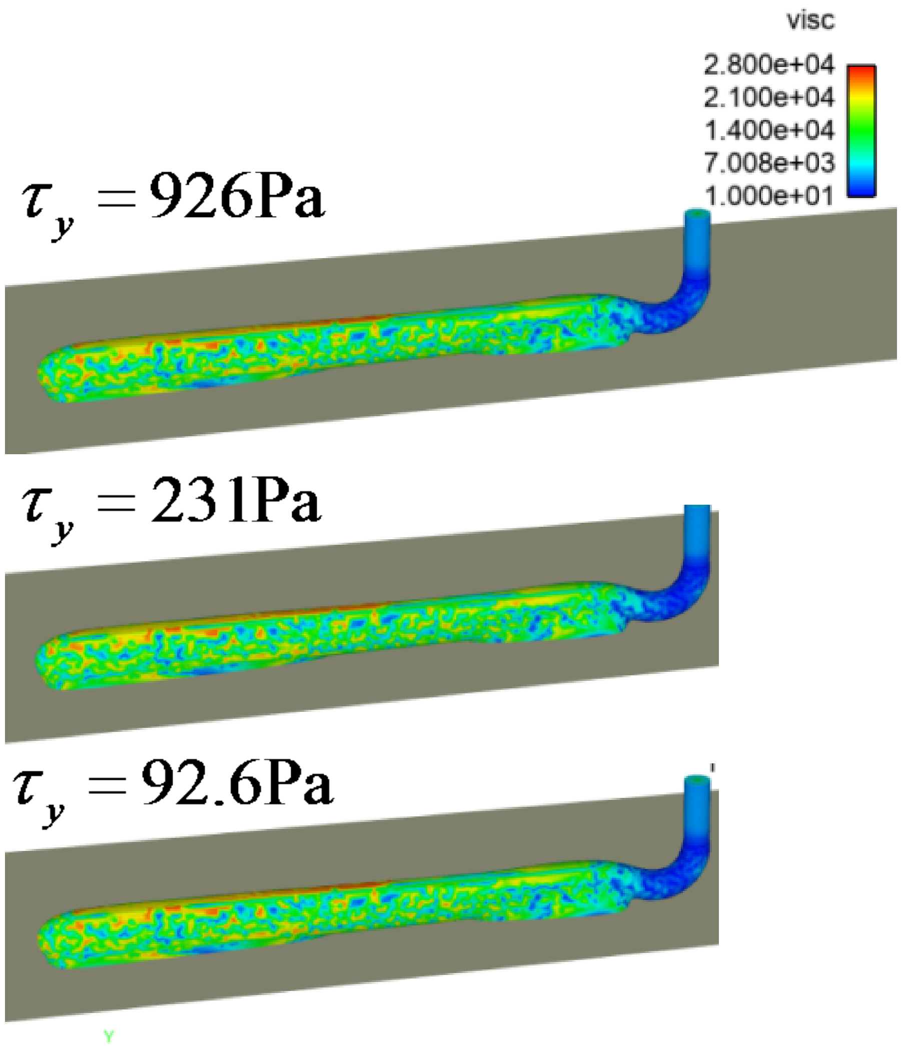
Two-Layer Study of Casson Yield Stress

Movie showing multi-layer deposition of a yield stress material in DIW printing.

- Rheology is presented as a Casson model which incorporates a yield stress and also shear thinning viscosity.
- The colors represent the viscosity of the fluid which drops when sheared (blue) and then resolidifies in the bead (red).



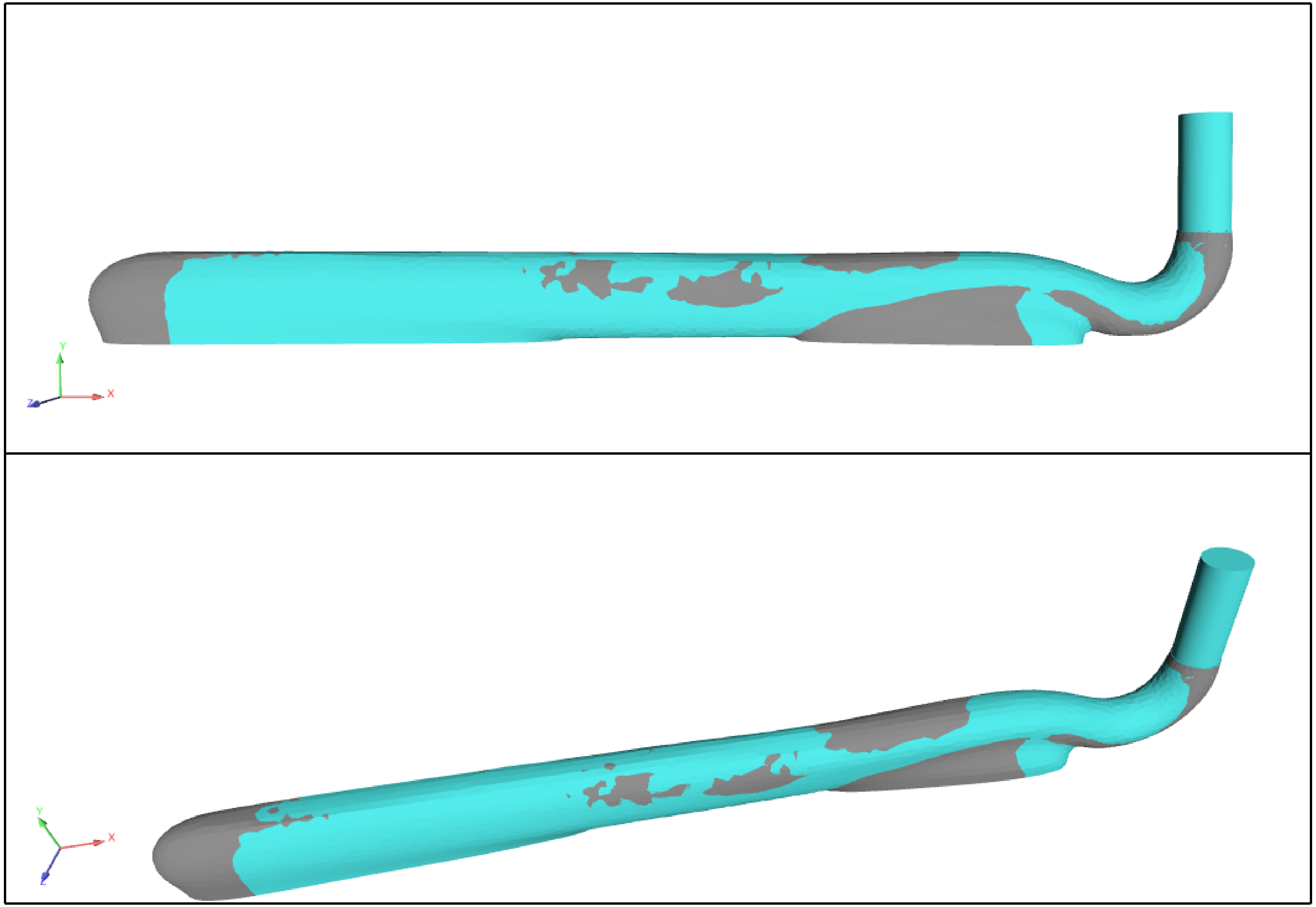
Sensitivity study for Casson Yield Stress



Casson Model		
mu_0	136.4	Pa-s
tau_y	926.4	Pa
shear_ref	1	1/s
m	20	
m/shear_ref	20	

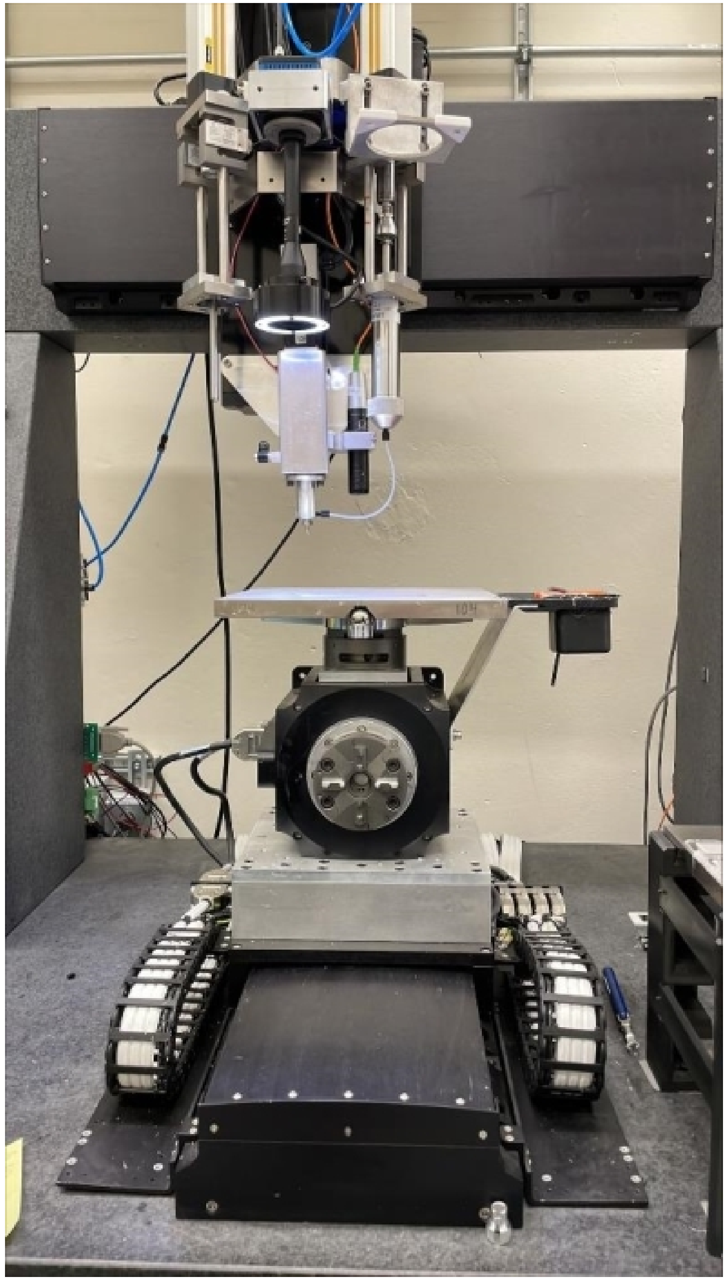
$$\mu(\dot{\gamma}) = \left[\sqrt{\mu_0} + \sqrt{\frac{\tau_y}{\dot{\gamma}}} \left(1 - e^{-\sqrt{\frac{m\dot{\gamma}}{\dot{\gamma}_{ref}}}}\right) \right]^2$$

Sensitivity study for Casson Yield Stress: Two Viewing Angles



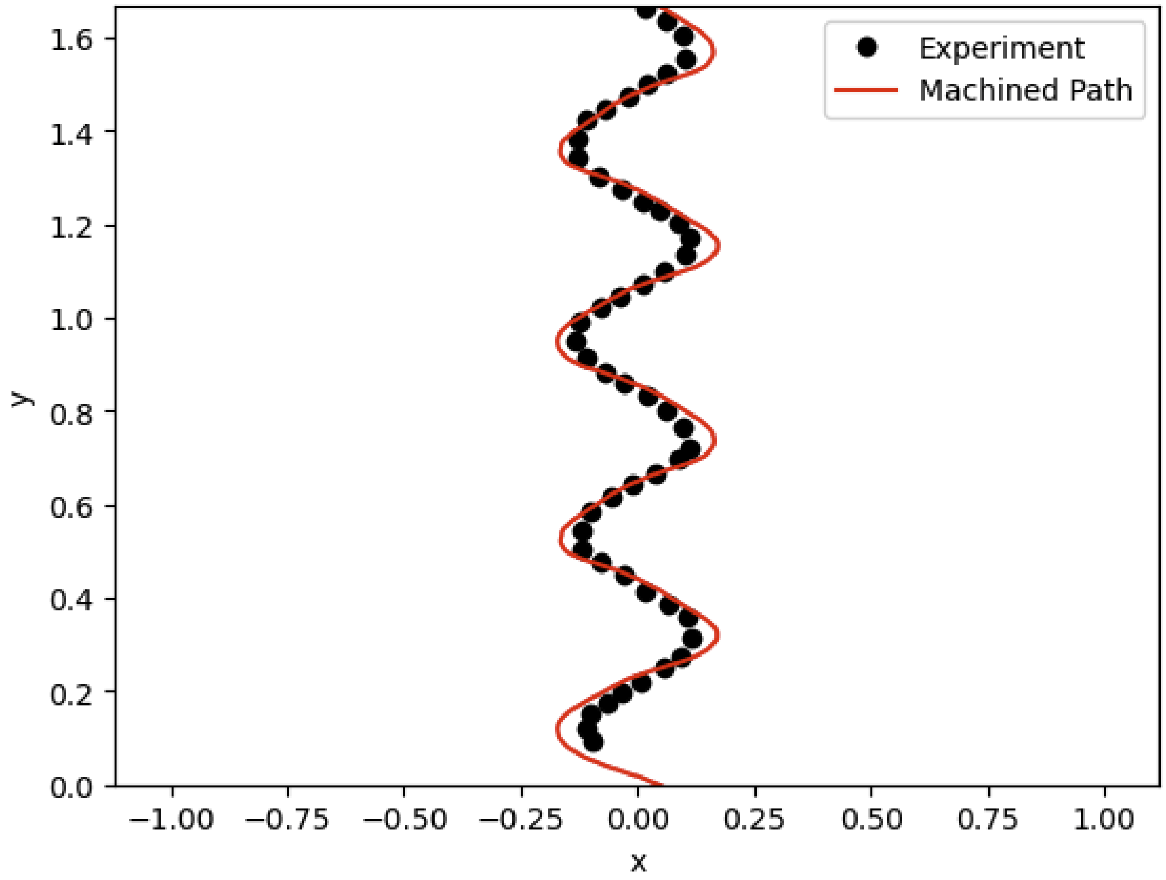
New work -Sinusoidal printing pattern

- 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

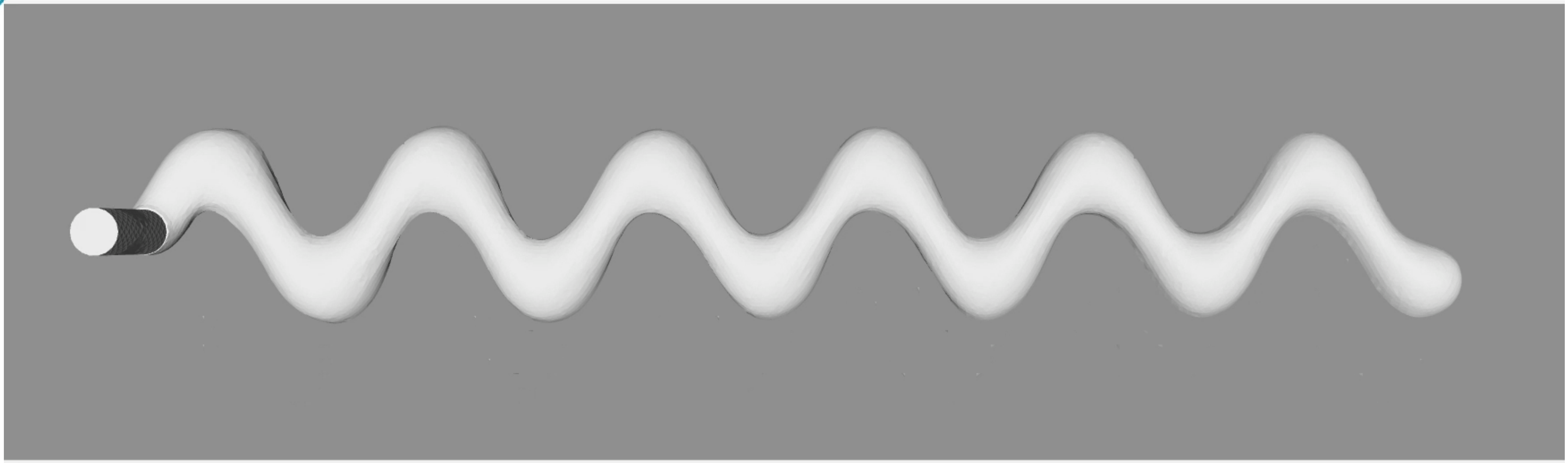


Experimental result

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



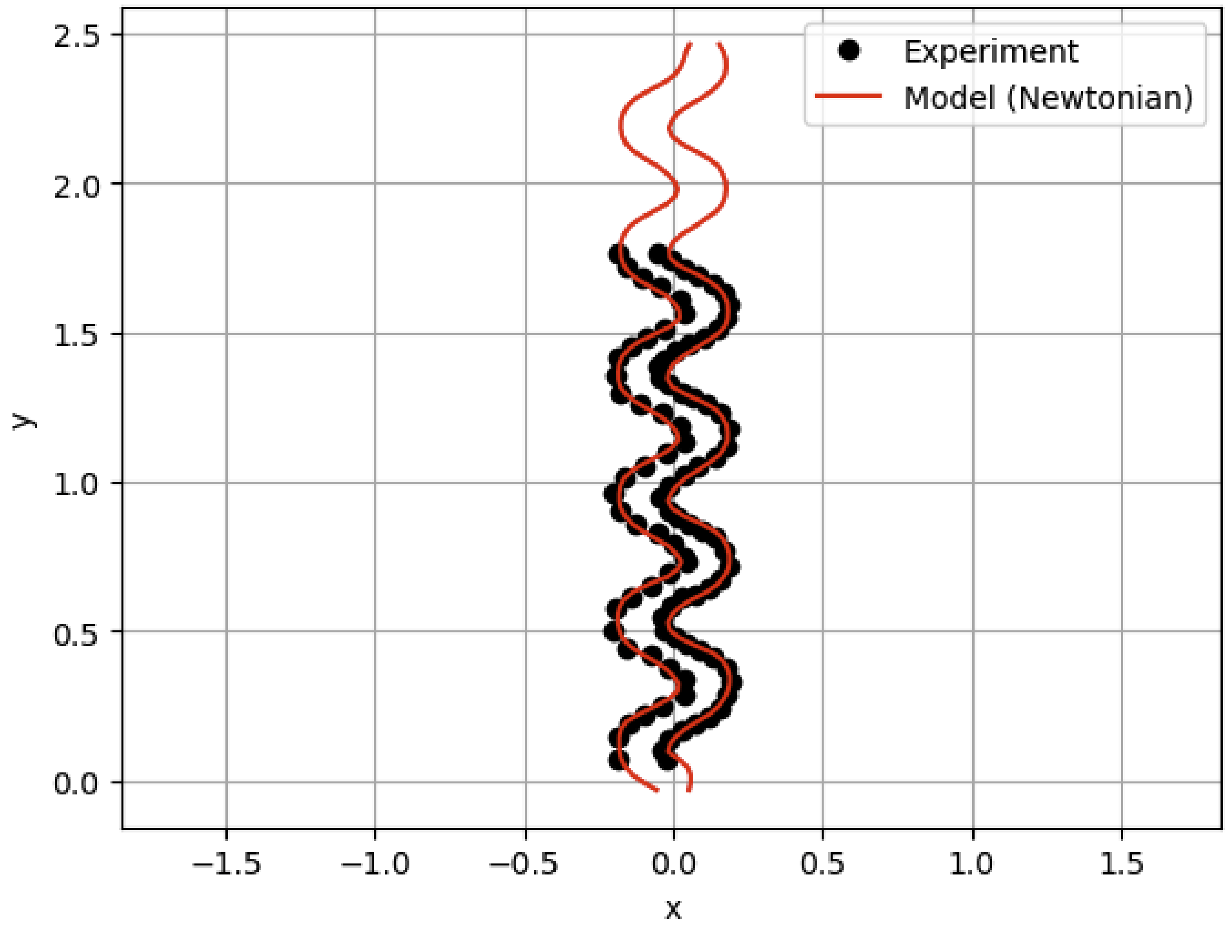
Model result - Newtonian fluid



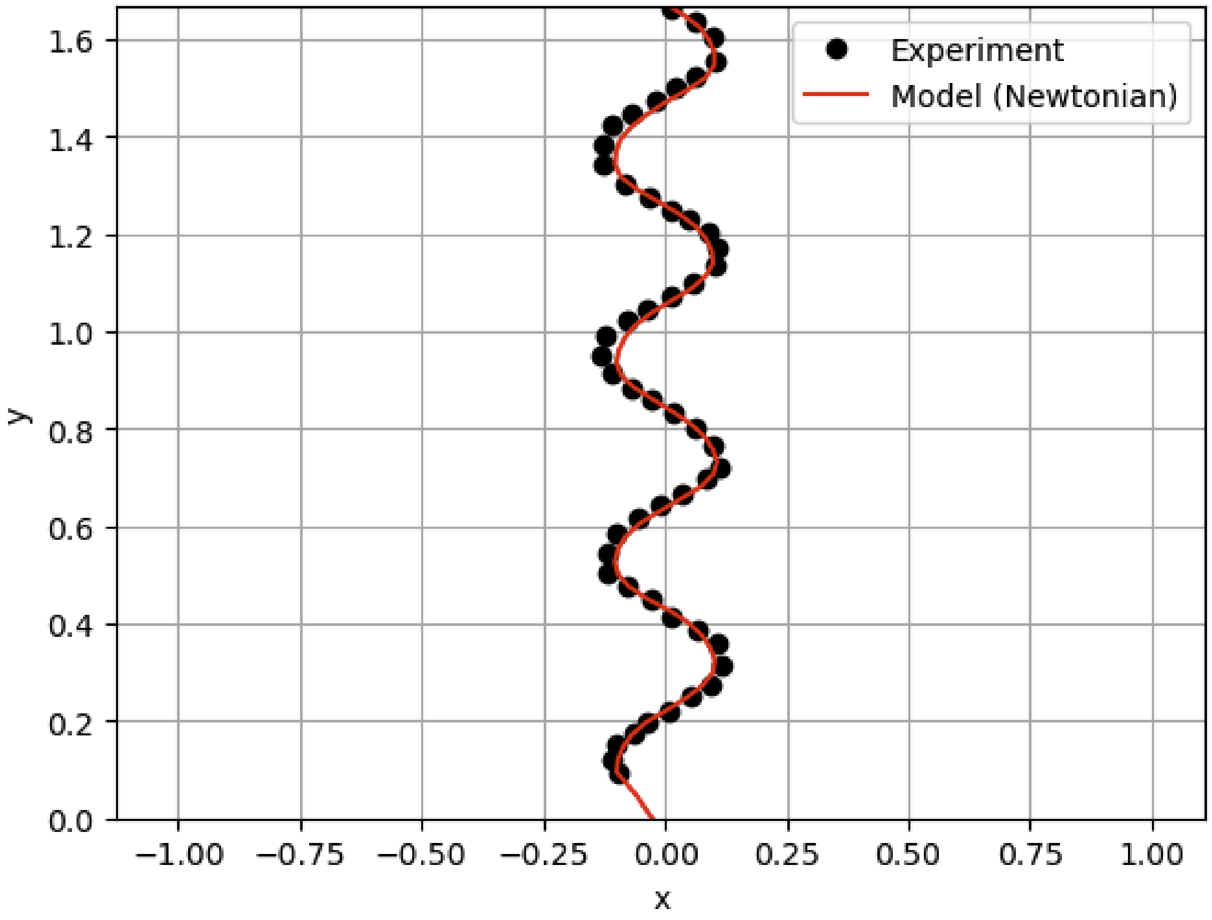
- Used the machine velocity data for substrate boundary conditions
- Printed sinusoidal pattern
- Newtonian fluid (mu = 1e5 poise)

Sinusoidal pattern comparison - Newtonian

Model vs Experiment Path

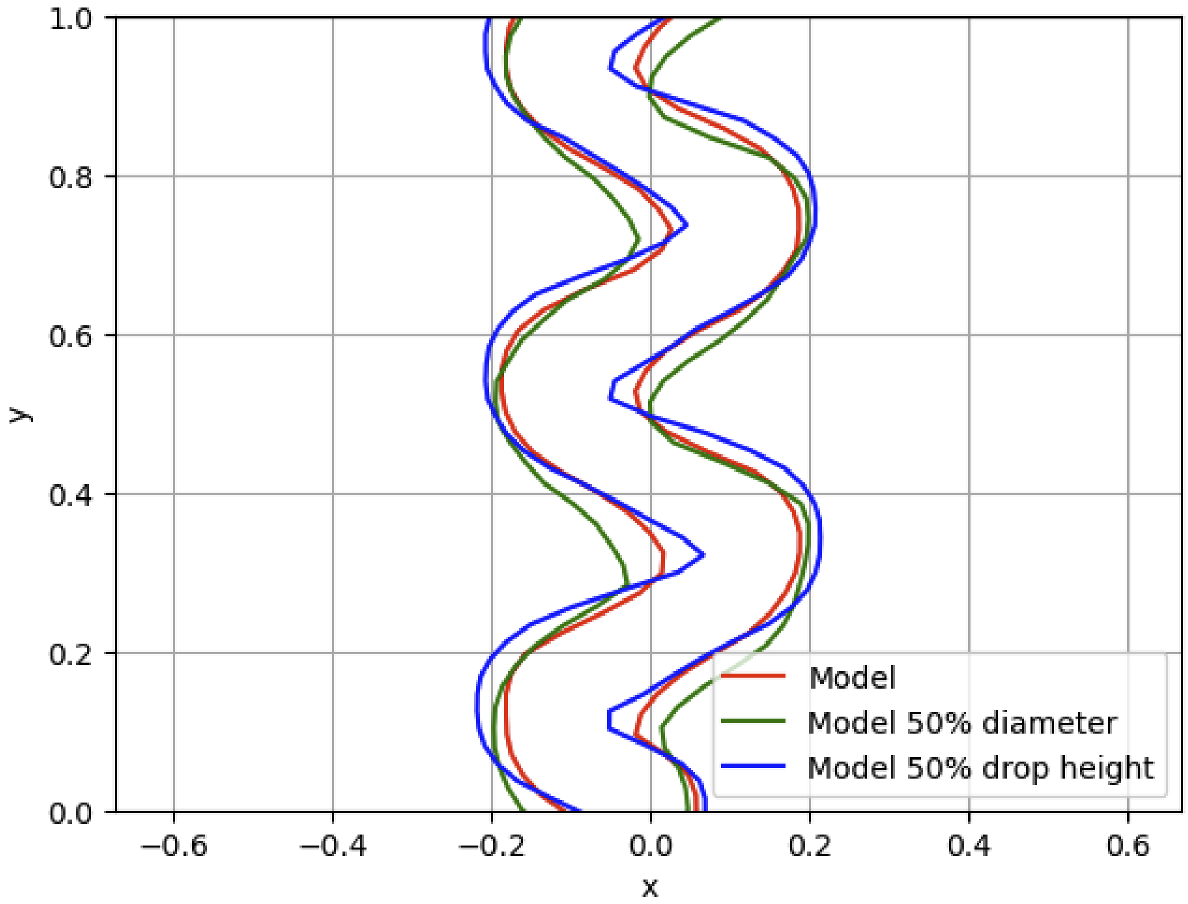


Model vs Experiment Mean Path

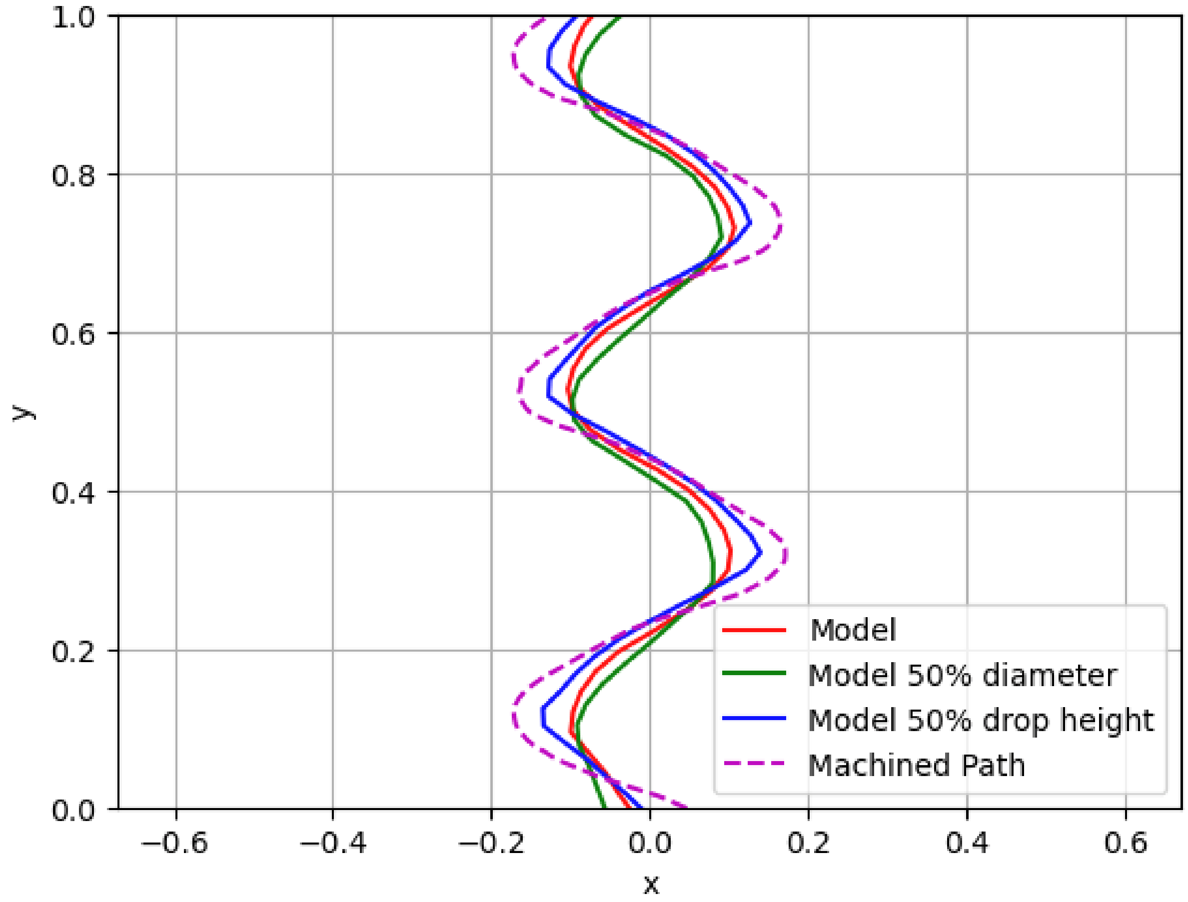


Parameterization of the drop height and diameter

- 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



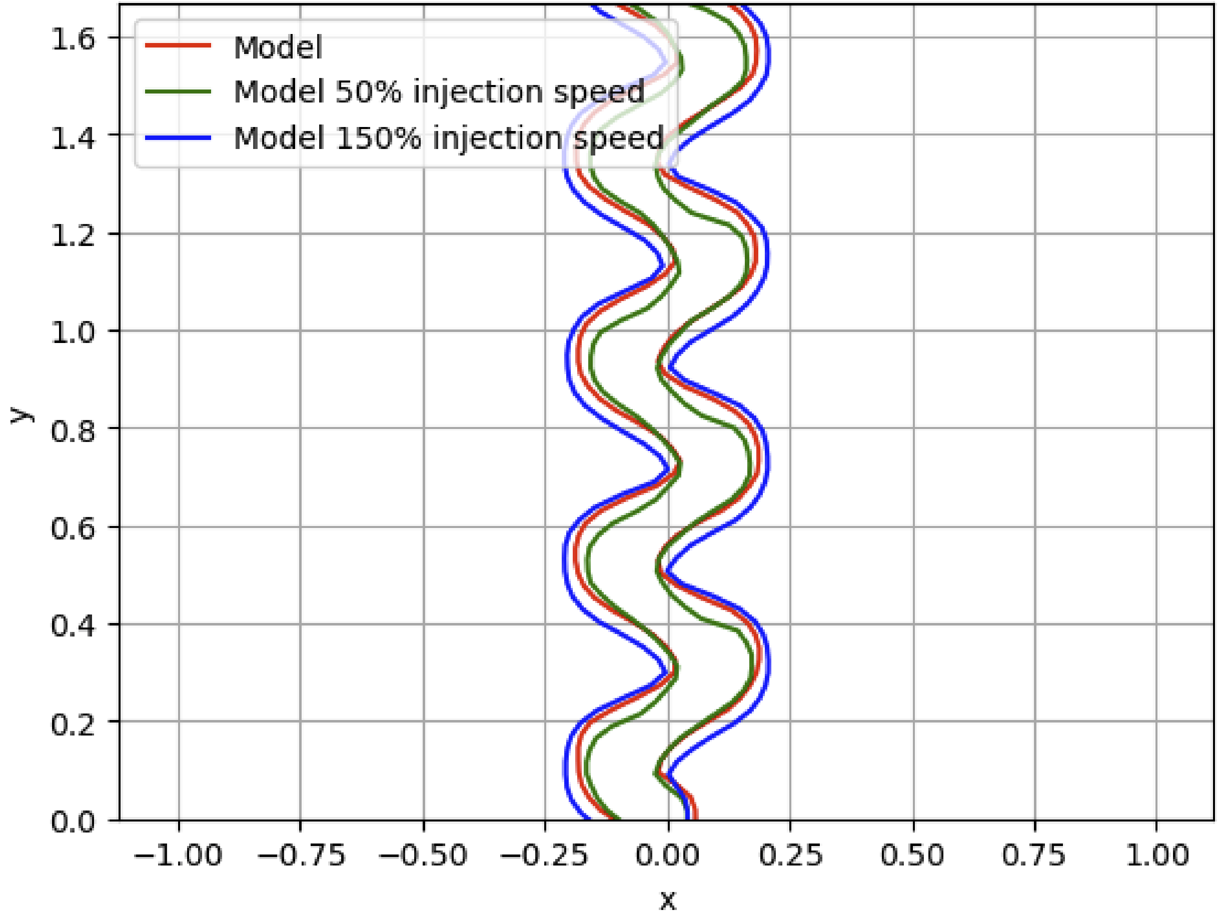
Topography (z-plane) projection



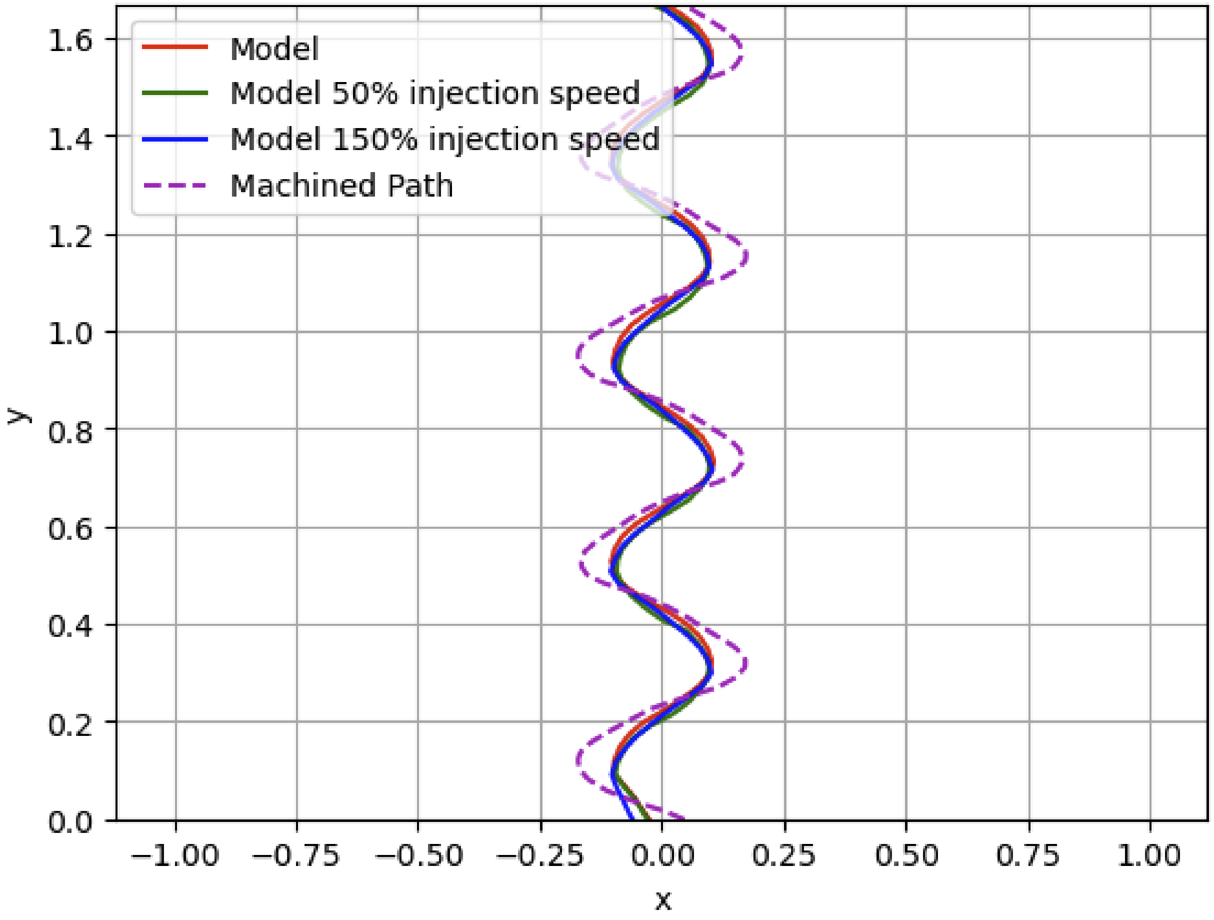
Mean path

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

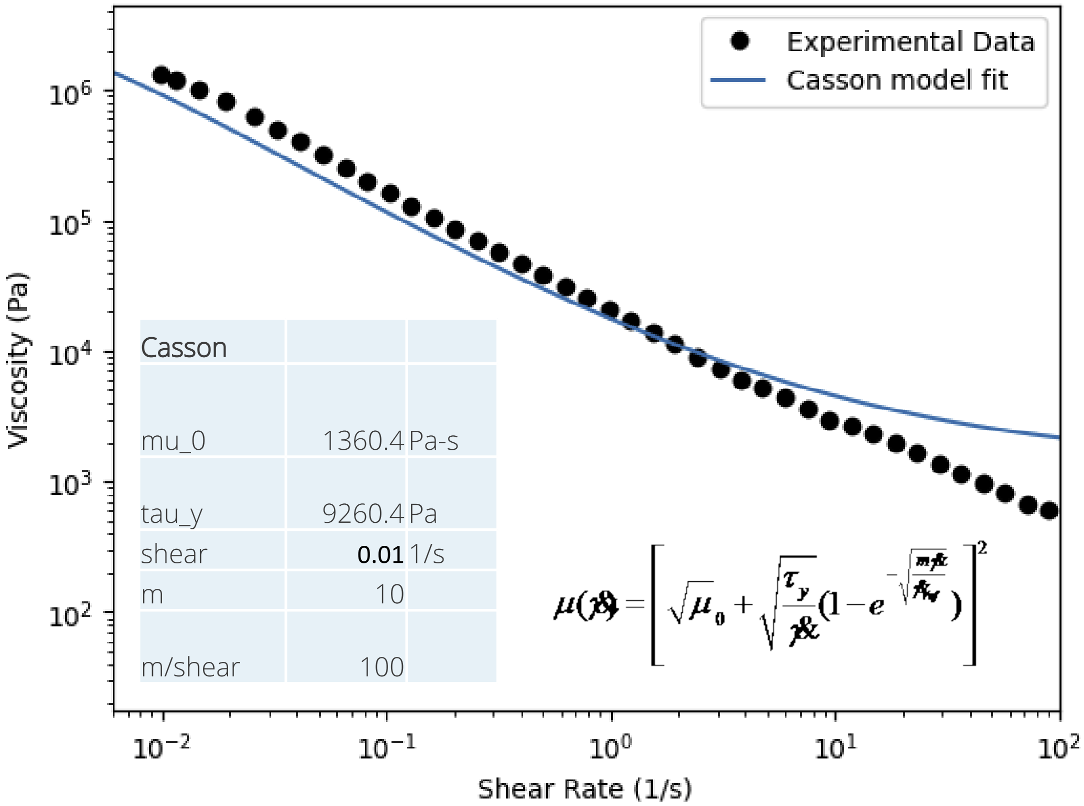


Topography (z-plane) projection

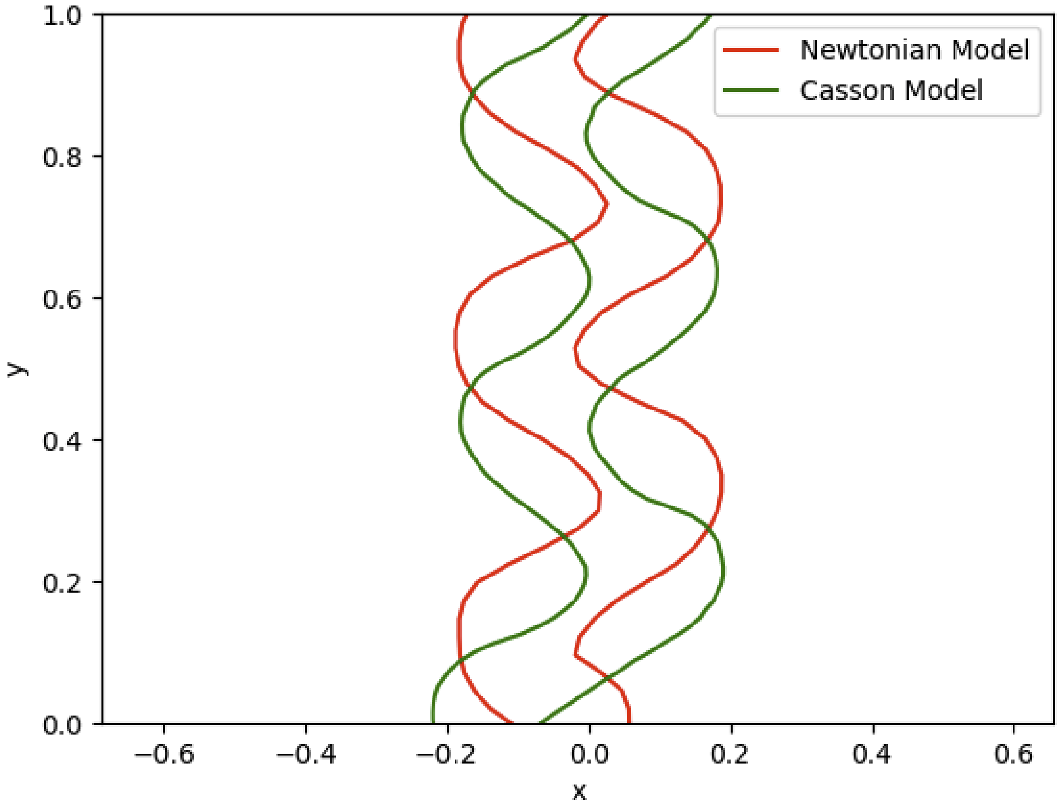


Mean path

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

Conclusions and Next Steps

- Presented a model for DIW using CDFEM to capture material interfaces
- CDFEM is a promising method for capturing material interfaces
  - Good conditioning of the resulting matrix
  - Potential issues with coarser mesh resulting in mass loss ameliorated with adaptive mesh refinement
- Bingham-Carreau-Yasuda and Casson viscosity models were used to incorporate the Non-Newtonian physics of the DIW inks material
  - Difficult to converge in 3D for fully-implicit FEM
- Other exciting Sandia work
  - Artificial Neural Nets and Computer Vision for 3D Printing
  - Digital Twin for lattice performance
- Future Work:
  - PiNNs models for experimental understanding and process control
  - NeRFs for solid model of real geometry

Incorporate elastoviscoplastic material models in work flow