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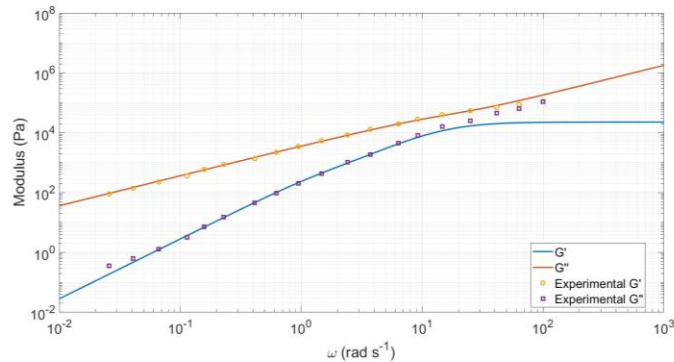
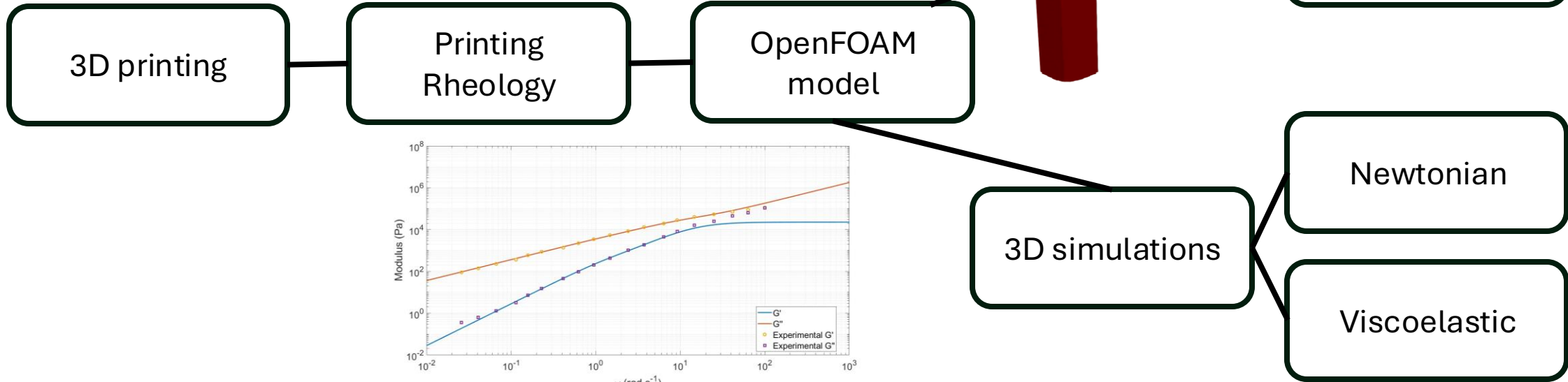
# Modelling 3D printing of rheologically complex materials using OpenFOAM

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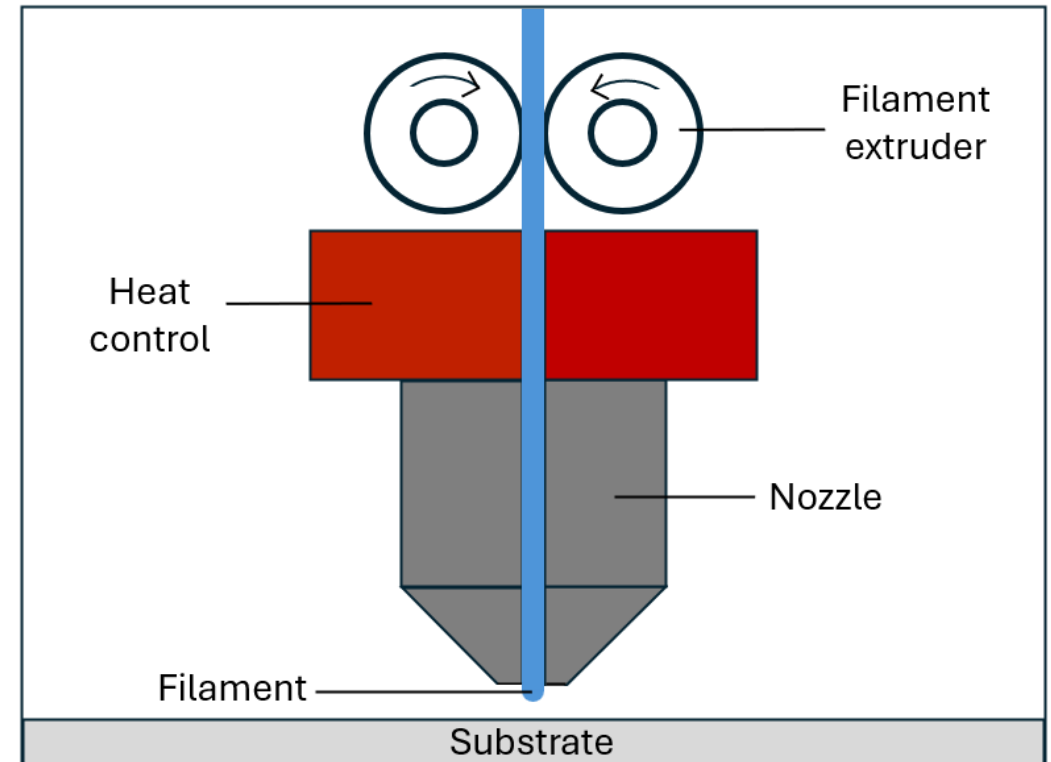
EPSRC Centre for Doctoral Training in Fluid Dynamics

# Outline

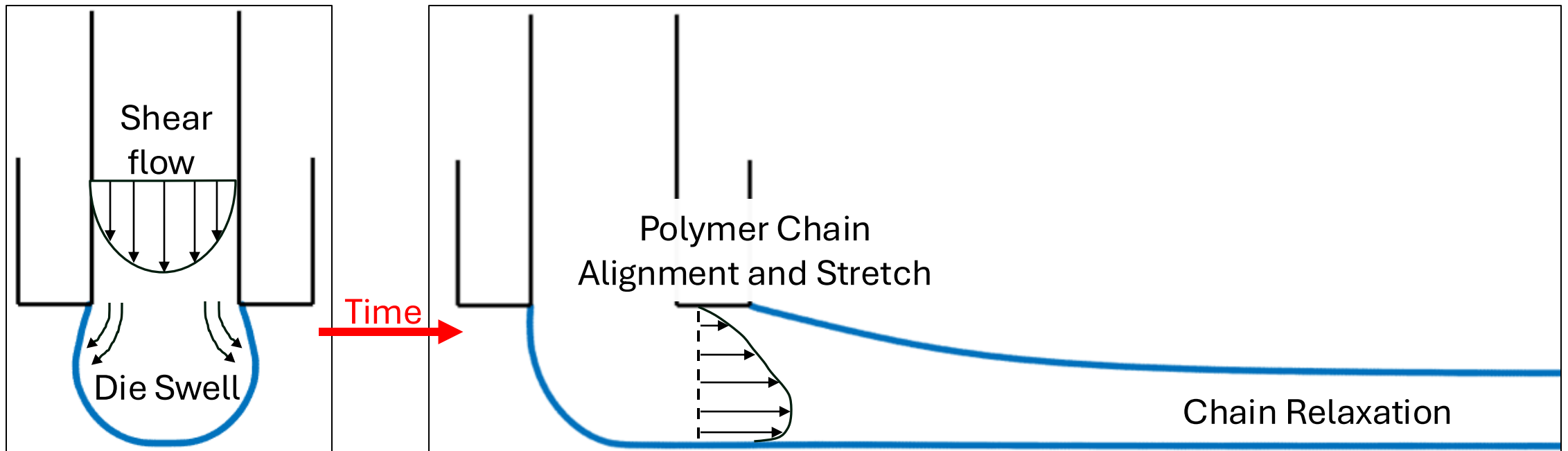


# 3D Printing Setup

- This project focuses on Fused Deposition Modelling (FDM).
- Produces objects through layer-by-layer material deposition
- The Reynolds number is low due to:
  - Small nozzles
  - High viscosity
  - Low speeds.
- Viscoelastic effects are significant, with Weissenberg numbers  $Wi \approx 1$ .



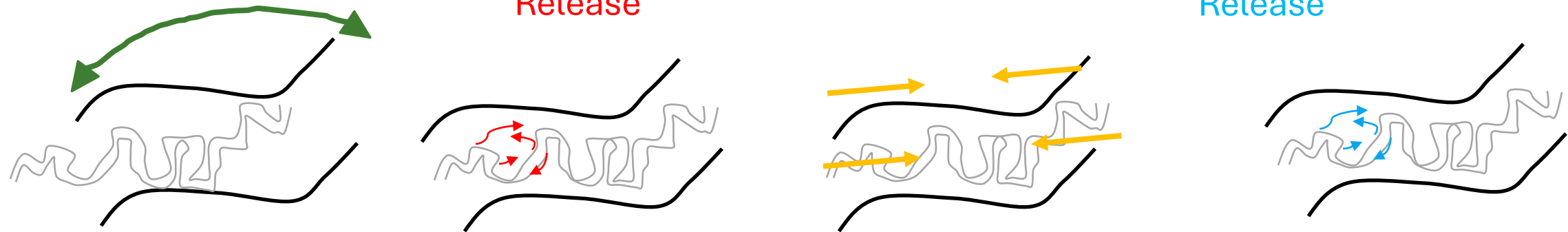
# Fluid Dynamics of 3D Printing



# Polydisperse Entangled Linear Polymers

$$\sigma_p = G_N^0 \sum_{I=1}^N \sum_{J=1}^N \phi_I \phi_J f_E(\lambda_I) A_{IJ}$$

$$\overset{\nabla}{A}_{IJ} = \underbrace{-\frac{1}{\tau_{d,I}} (A_{IJ} - I)}_{\text{Reptation}} - \underbrace{\frac{\beta_{th}}{\tau_{d,J}} (A_{IJ} - I)}_{\text{Constraint Release}} - \underbrace{\frac{2(1 - \lambda_I^{-1})}{\tau_{s,I}} f_E(\lambda_I) A_{IJ}}_{\text{Retraction}} - \underbrace{2\beta_{cca} \frac{(1 - \lambda_J^{-1})}{\tau_{s,I}} f_E(\lambda_J) \lambda_I^{2\delta} (A_{IJ} - I)}_{\text{Convective Constraint Release}}$$



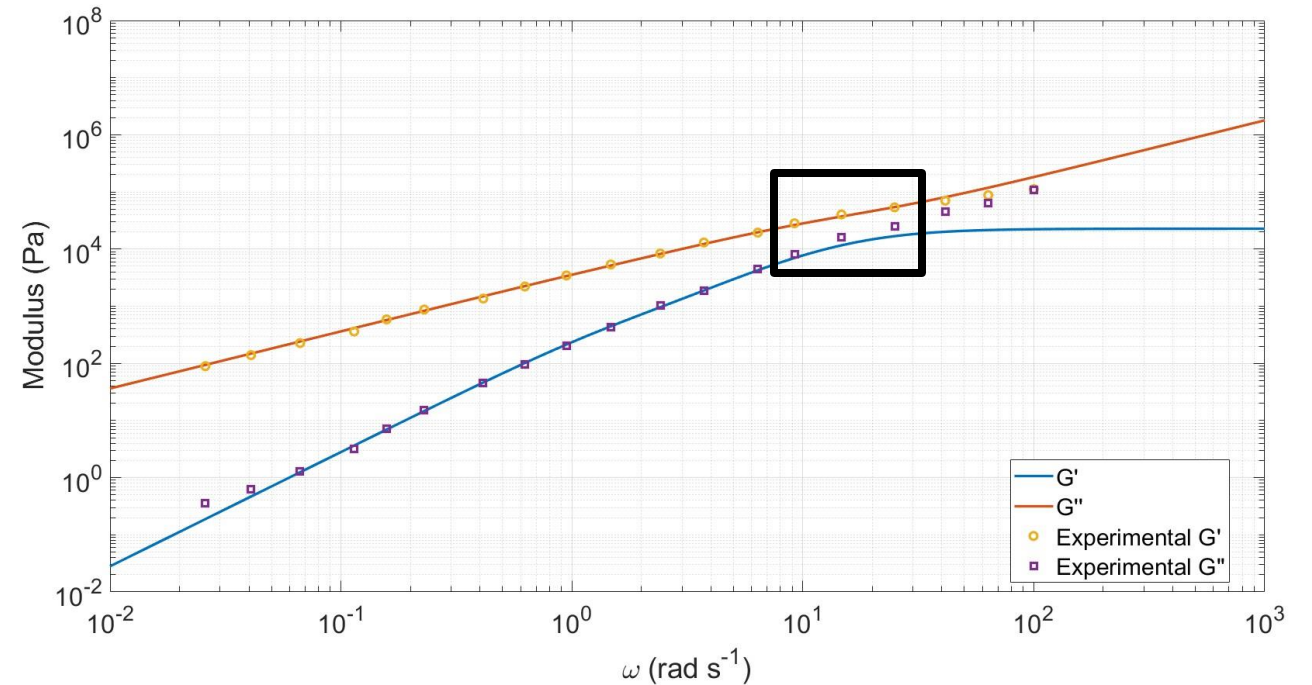
# Linear Rheology of PLA Filament

Chain Species	Volume Fraction	Relaxation Time
Chain 1	0.13	1.28
Chain 2	0.87	0.12

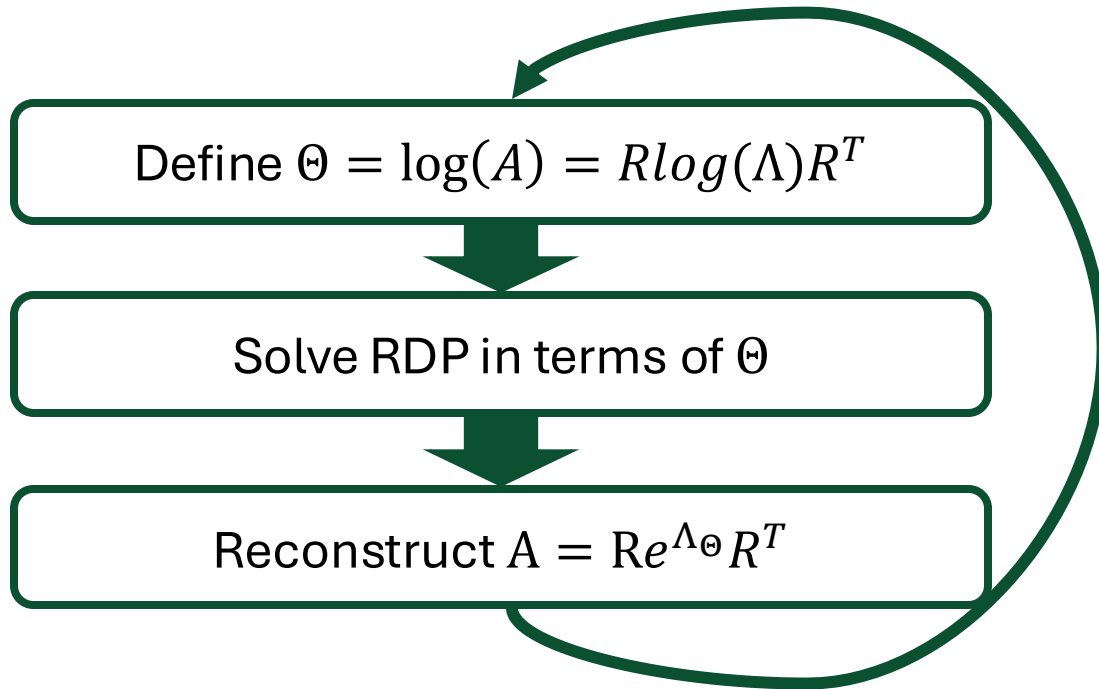
$G_0 = 22736 \text{ Pa}$

Solvent Viscosity =  $1790 \text{ Pa}\cdot\text{s}$

$$G(t) = \mu_s \delta(t) + G_0 \sum_{i,j=1}^2 \phi_i \phi_j e^{-t/\tau_i} e^{-t/\tau_j}$$

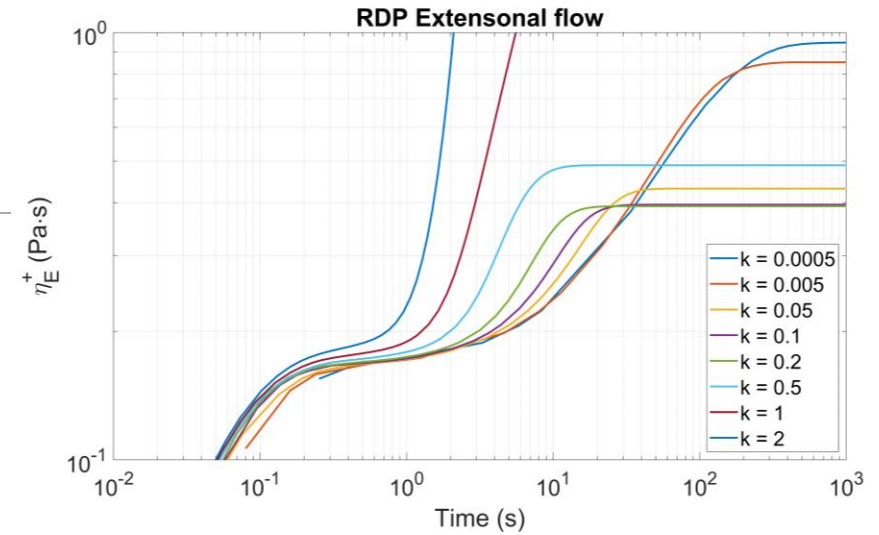


# Log Conformation Tensor

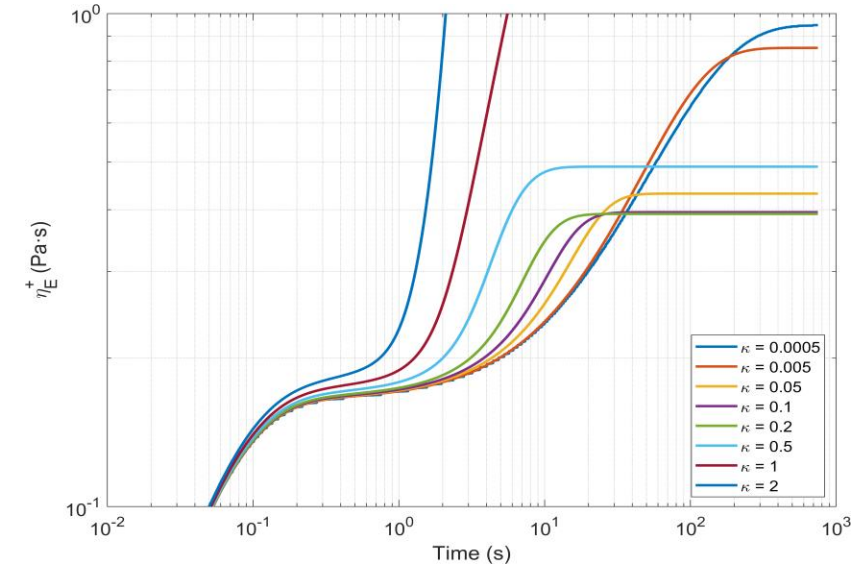


- This loop is applied to each  $A_{ij}$  component
- Stabilises the simulation and ensures  $A$  is positive definite

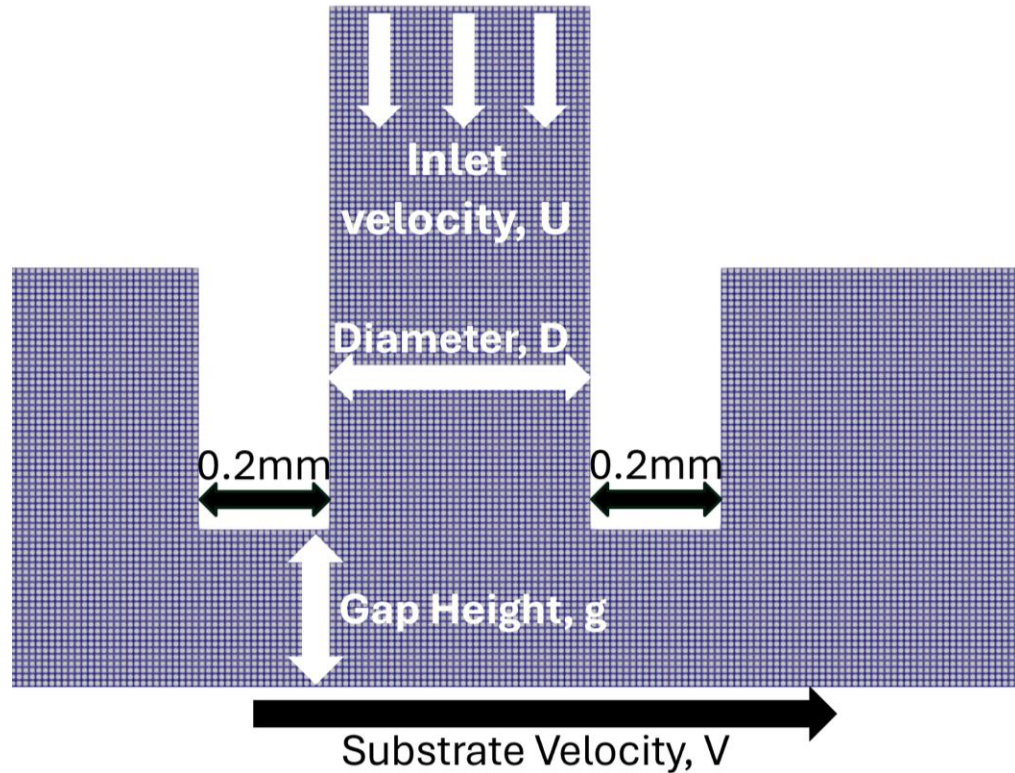
(Boudara et al 2019)



Log Conformation Tensor



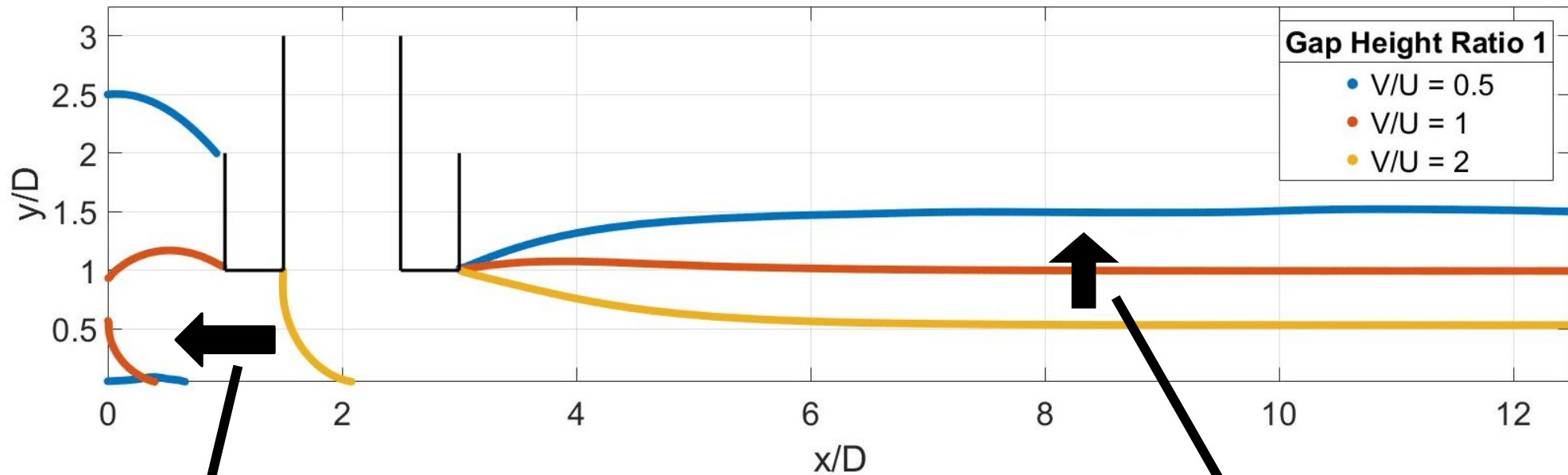
# 2D Geometry and Mesh



Parameter	Value
Inlet Speed $U$	20 mm/s
Substrate speed $V$	10, 20, 40 mm/s
Velocity Ratio $V/U$	0.5, 1, 2
Nozzle Diameter $D$	0.4 mm
Gap Height $g$	0.24, 0.32, 0.4 mm
Gap Height Ratio $g/D$	0.6, 0.8, 1

- OpenFOAM using the RheoTool toolbox
- Volume of Fluid (VOF) method
- Finite Volume Method

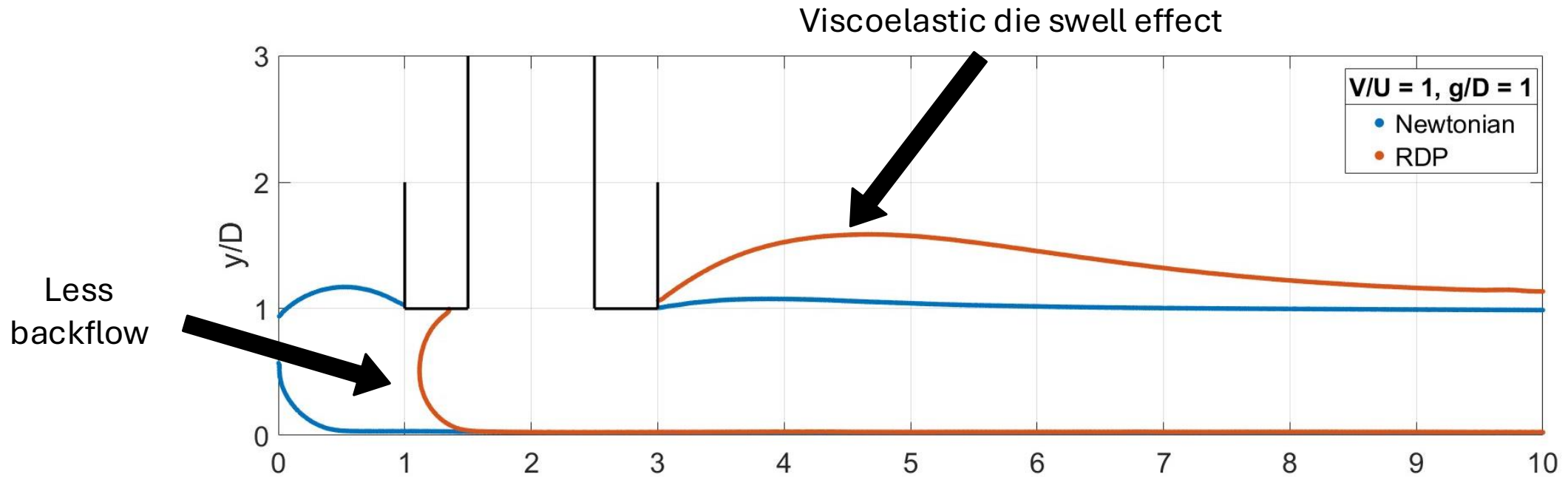
# 2D Newtonian Simulation



Fluid is forced backwards against the flow

Increase in strand height due to conservation of mass

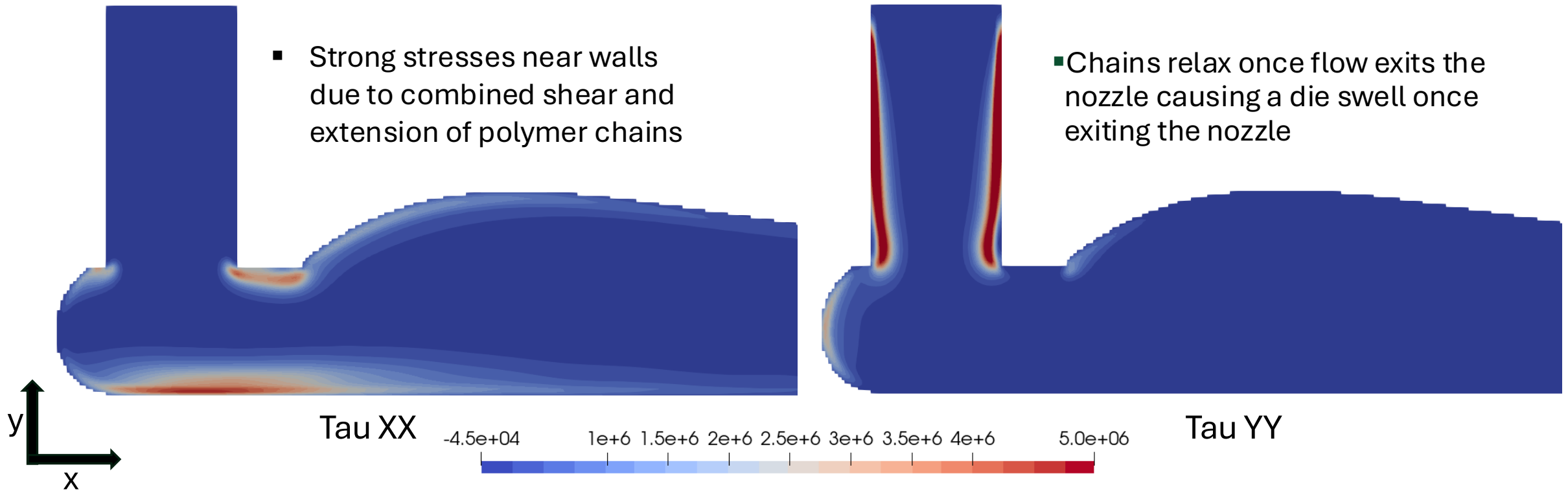
# 2D Newtonian vs RDP



$$Wi = \frac{\text{Relaxation Time} * \text{Gap height}}{\text{Substrate Speed}}$$

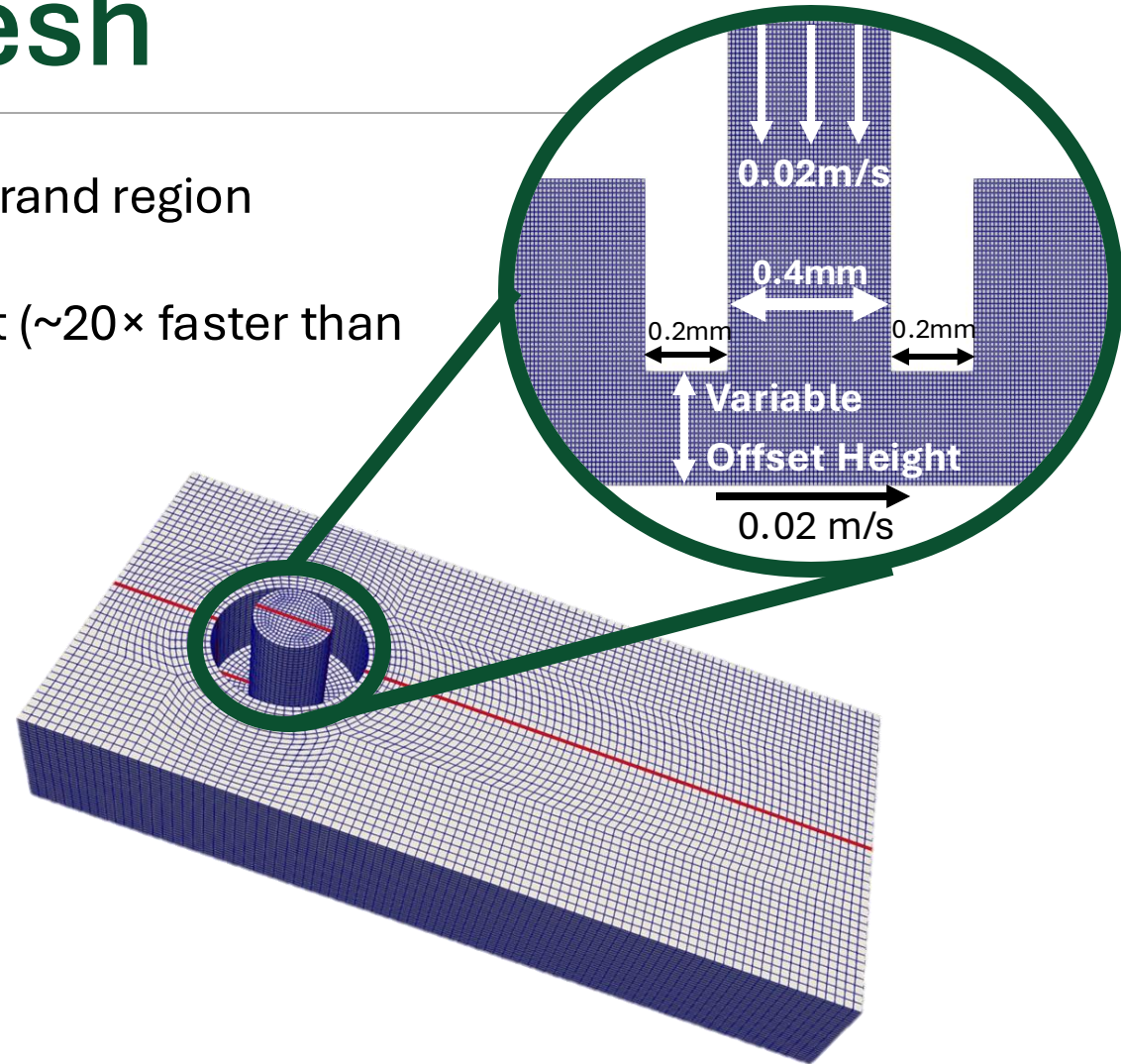
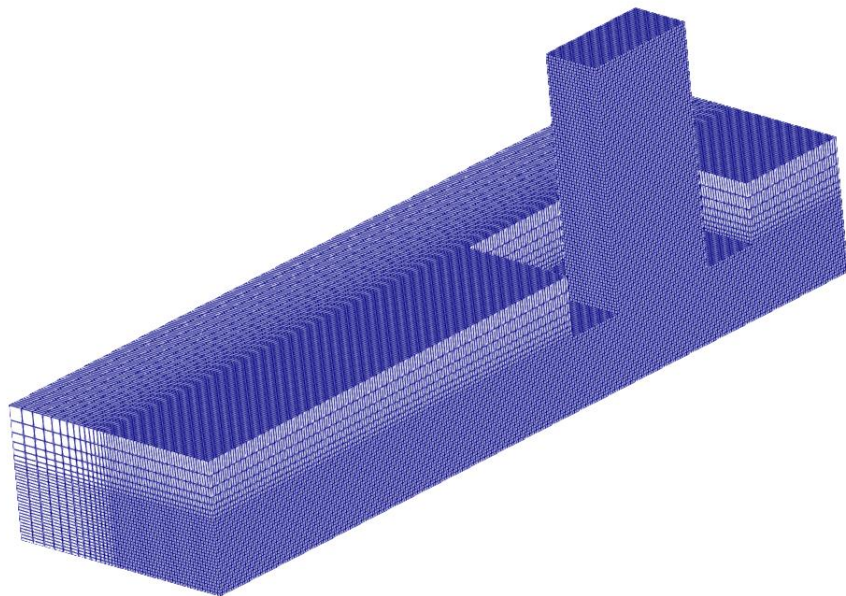
$$Wi_{chain 1} = 0.64, Wi_{chain 2} = 0.06$$

# 2D RDP Stress Field



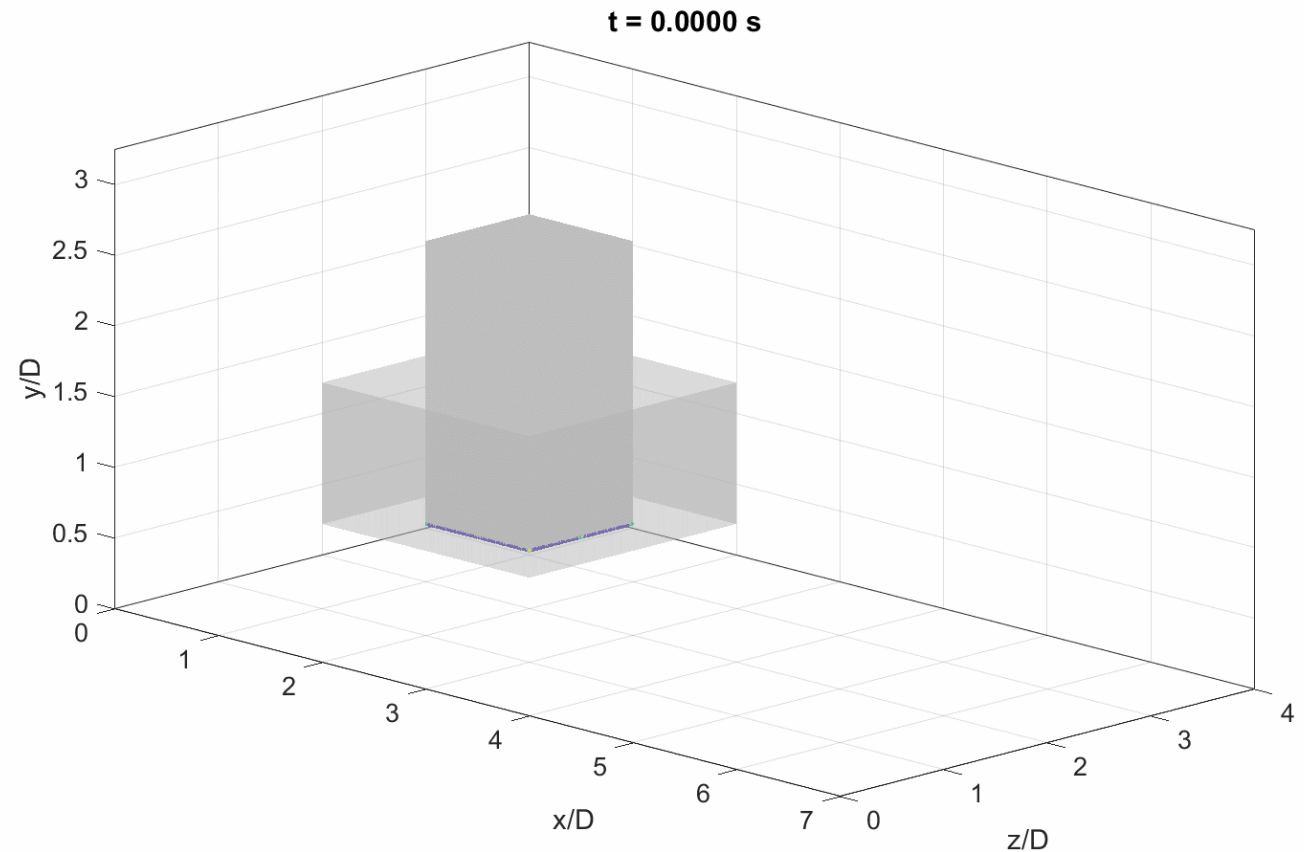
# 3D Geometry and Mesh

- Cells are refined (biased) towards the printed strand region
- Simplified nozzle geometry with no taper
- Rectangular nozzle reduces computational cost ( $\sim 20\times$  faster than cylindrical geometry)



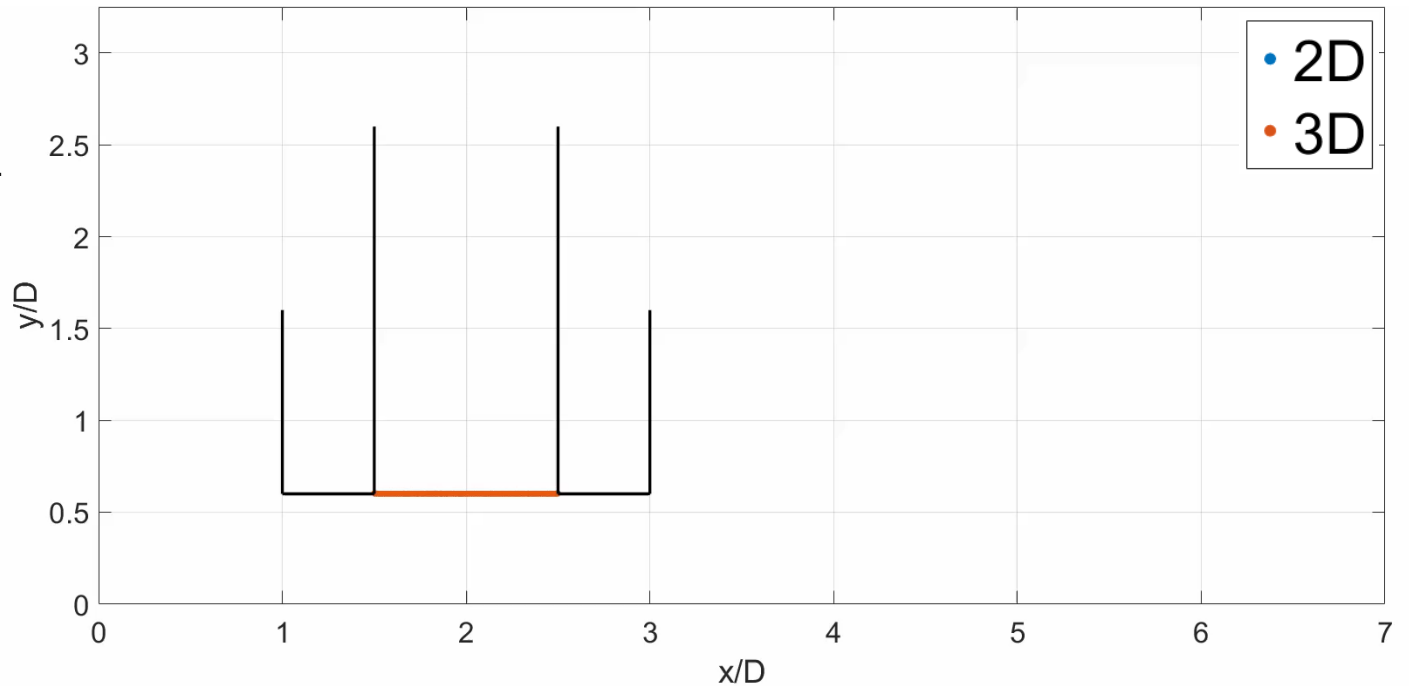
# 3D Newtonian Simulation

- Gap height ratio = 0.6, speed ratio = 2
- Gap height ratio set to 0.6 to better match printing parameters
- Contour visualisation used to determine strand height
- Concave upper surface
  - Consistent with (Comminial et al., 2018)



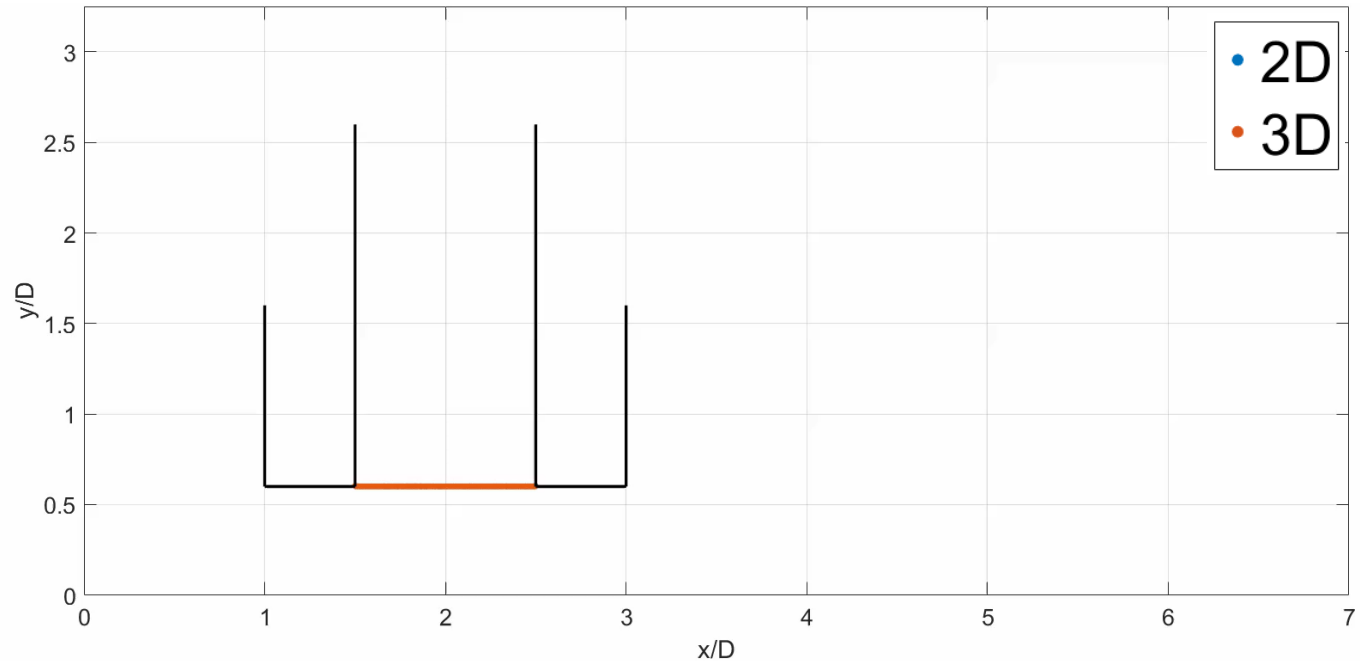
# 2D vs 3D Newtonian

- Gap height ratio = 0.6, speed ratio = 1
- 2D simulations over-predict die swell and material accumulation
- 3D flow enables lateral spreading, reducing build-up
- 2D: 7 hours (16 cores)
- 3D: 14 hours (64 cores)



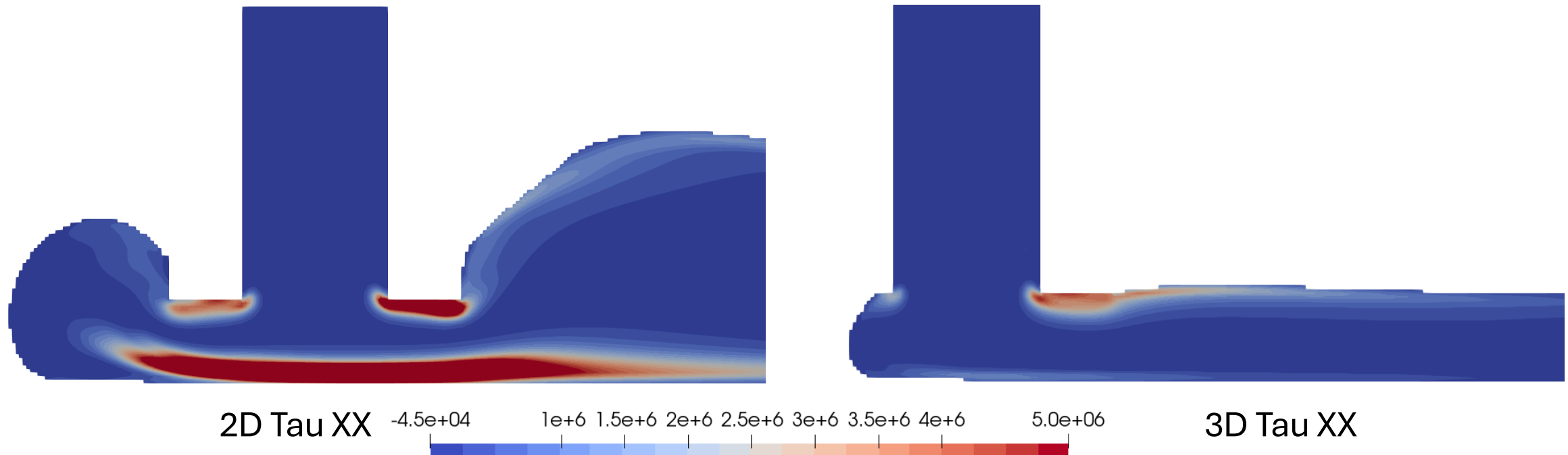
# 2D vs 3D RDP

- Gap height ratio 0.6, Speed ratio 1
- Exaggerated die swell and buildup in 2D
- 3D spreads the material laterally, reducing accumulation.
- 2D 28 hrs (16cores)
- 3D 96 hrs (64cores)



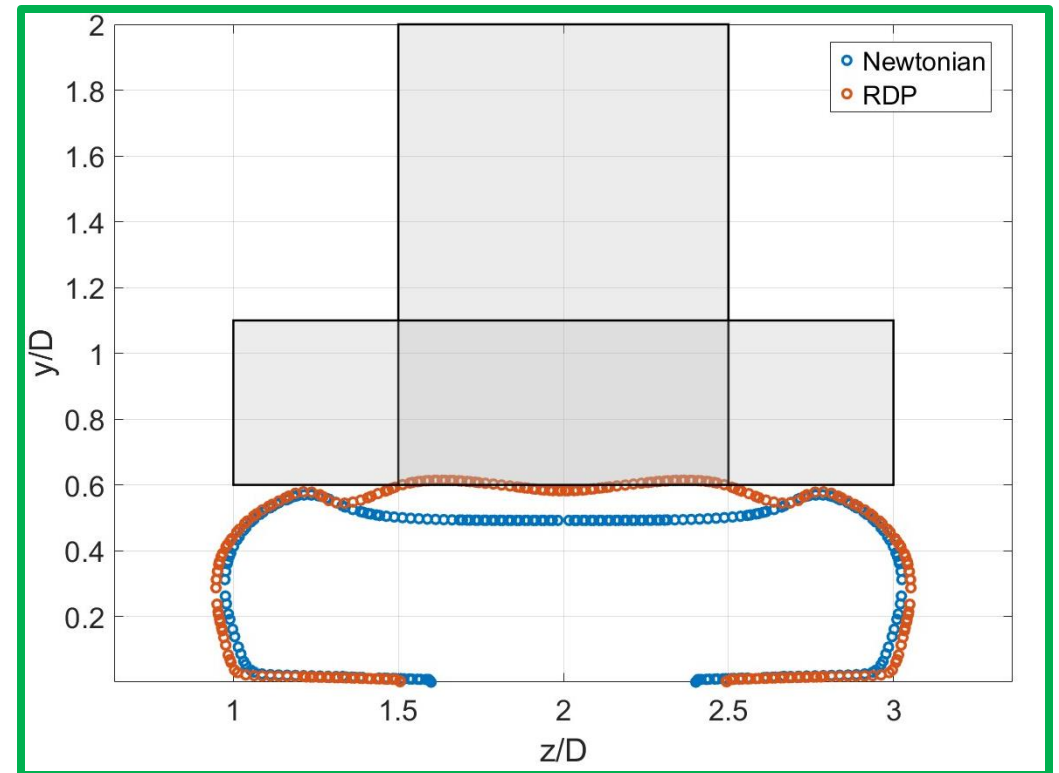
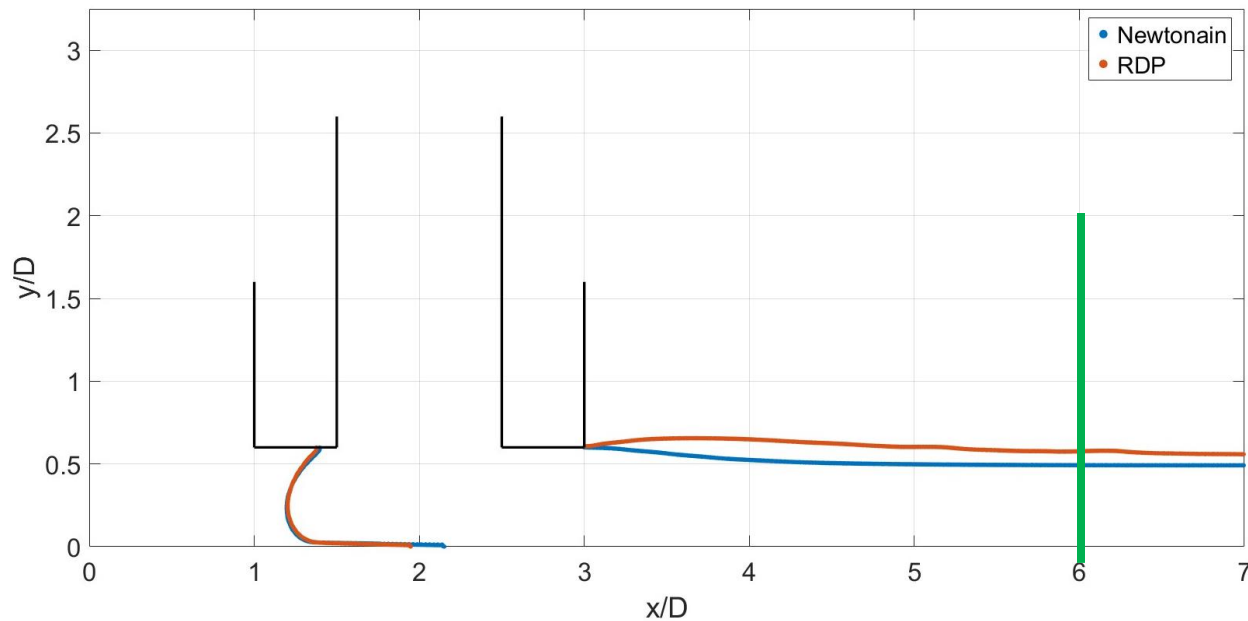
# 2D vs 3D RDP

- 2D over predicts  $Tau_{xx}$  compared to 3D
- 3D flow enables lateral spreading lowering the stress in  $x$ -direction
- 3D flow introduces chain alignment in the  $z$ -direction
- Significantly reduced die swell in the 3D case



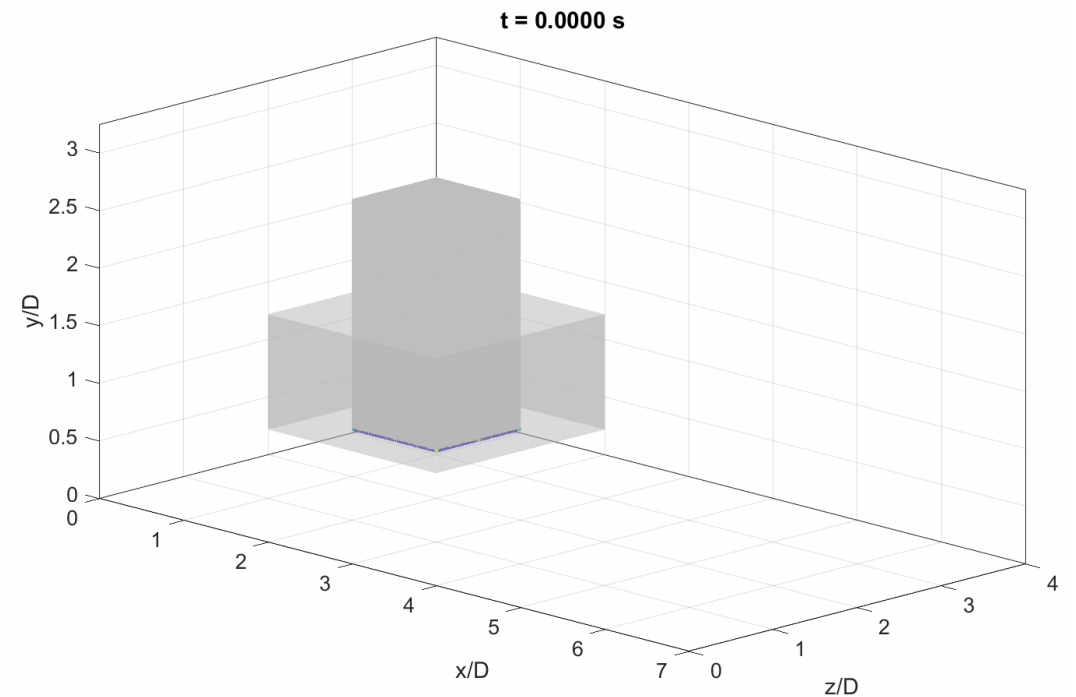
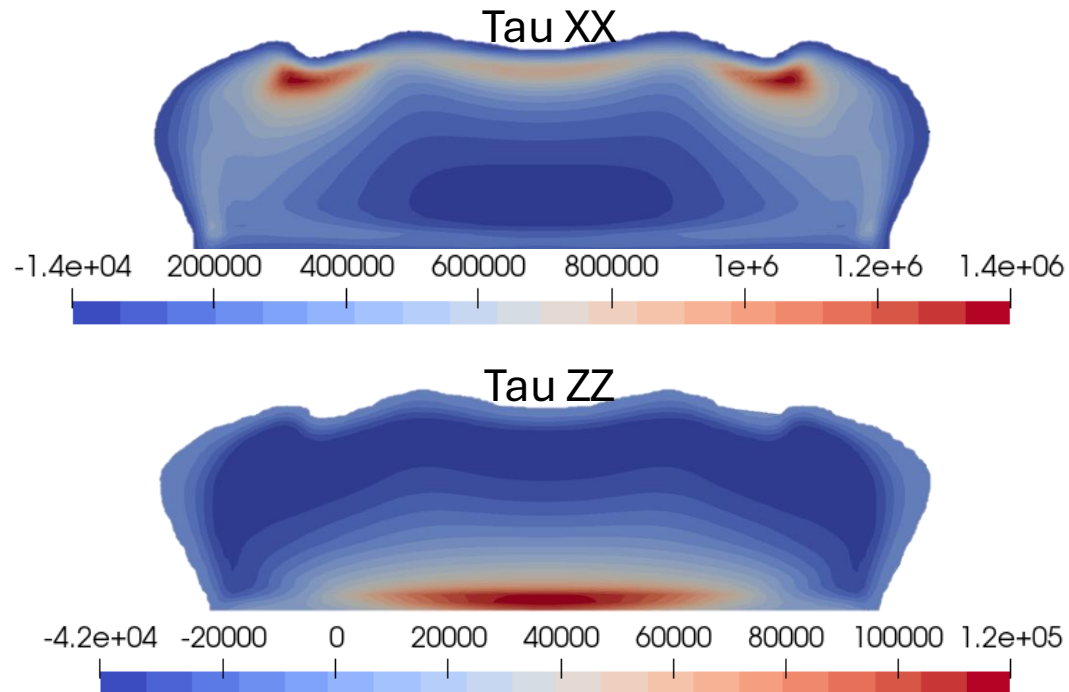
# 3D Newtonian vs RDP

- Cross-section at  $x/D = 6$ , highlighted by the green line
- RDP exhibits slight die swell
- Side strand shape remains similar between models



# Cross Section Stress Distribution

- Cross-section at  $x/D = 6$  downstream of the nozzle
- Stresses remain significant away from the nozzle
- Residual stresses are likely to be frozen in as the polymer cools



# Conclusion and Future Work

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- 2D and 3D simulations exhibit fundamentally different flow behaviour
  - 2D exhibits unphysical backflow behind the nozzle
  - 2D over-predicts die swell due to confinement at small gap heights
  - 3D flow enables biaxial stretching in the  $x$ - $z$  plane
- Stresses are highest near the free surface, where rapid cooling may lead to frozen-in residual stresses
- Future work:
  - Validate a coupled heat transfer model for multiphase flow
  - Investigate frozen-in residual stresses in the deposited strand
  - Perform experimental validation
  - Investigate the influence of nozzle geometry