Implementation and Calibration of a Viscoelastic Bonded Particle Model: from the Micromechanics to the Flow Properties

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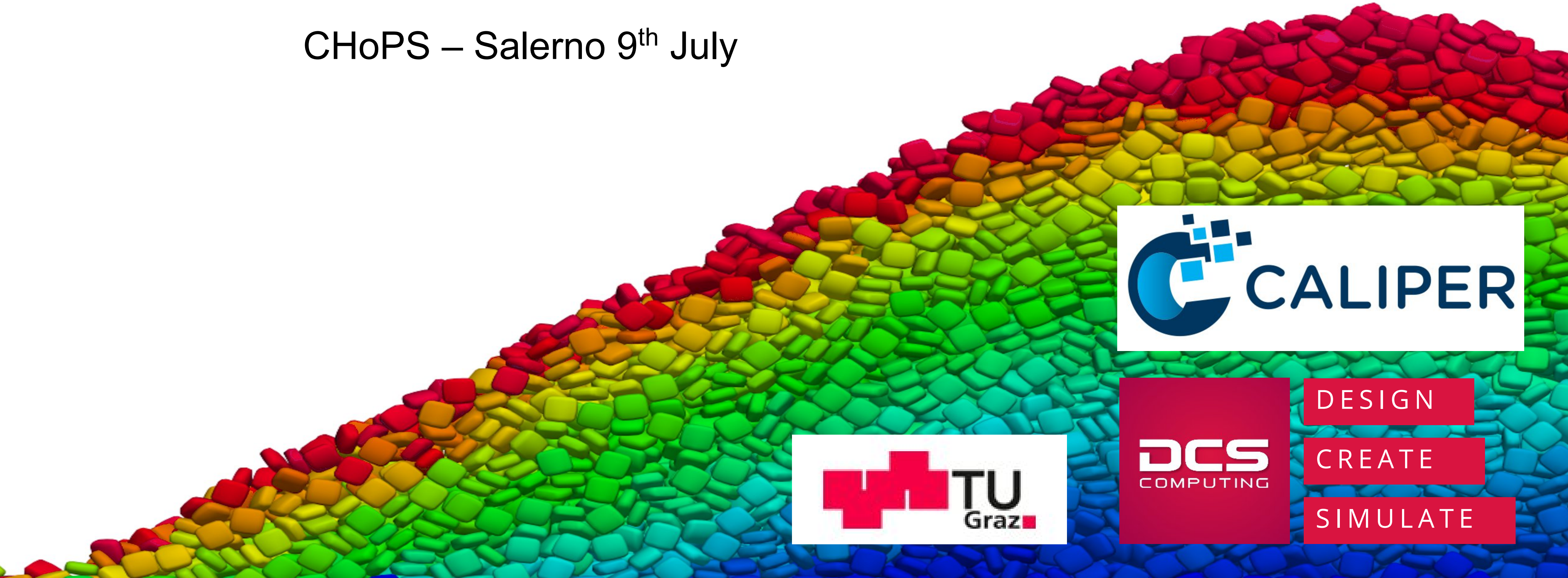


CALIPER

TU Graz

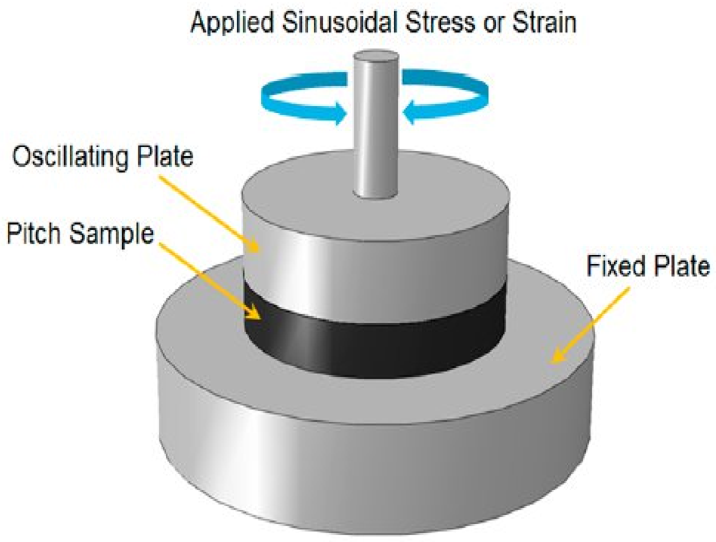
DCS COMPUTING

DESIGN

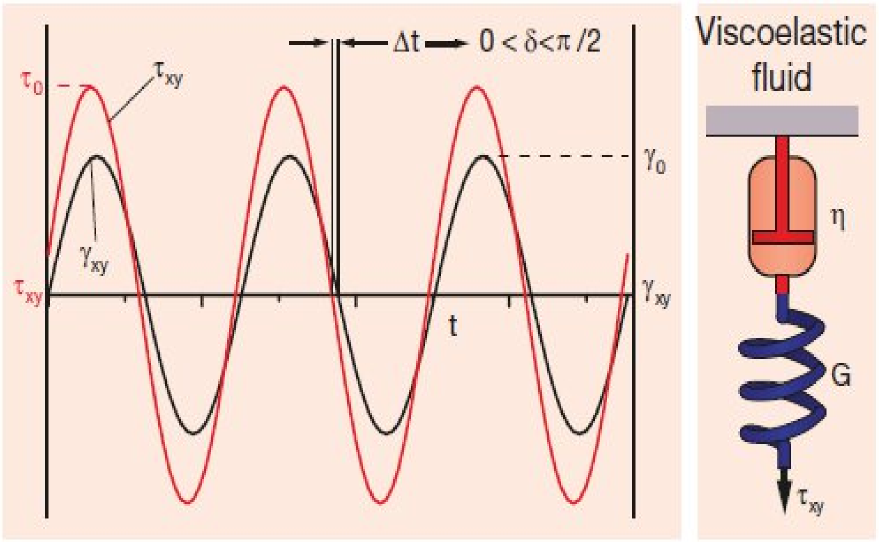
CREATE

SIMULATE

Introduction



source: https://www.mdpi.com/1996-1944/9/5/334

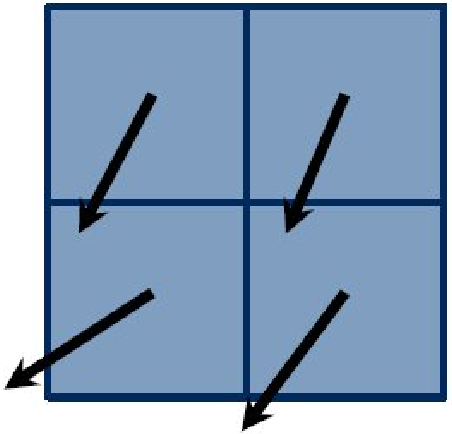


Source: T. Osswald & N. Rudolph, Polymer Rheology, 2014

- Experiments to measure rheological properties are not always enough to predict flow in a complex process
- Some materials are not "rheometer friendly"
- Experiments are limited in stress and applied frequency depending on the material

Introduction

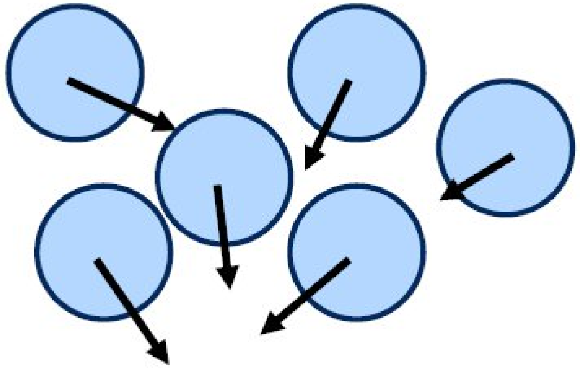
Mesh-based methods (Eulerian)



- Complex tensor-modified Navier-Stokes equations
- Tricky to apply in processes with rotating parts
- Challenging when describing granular matter

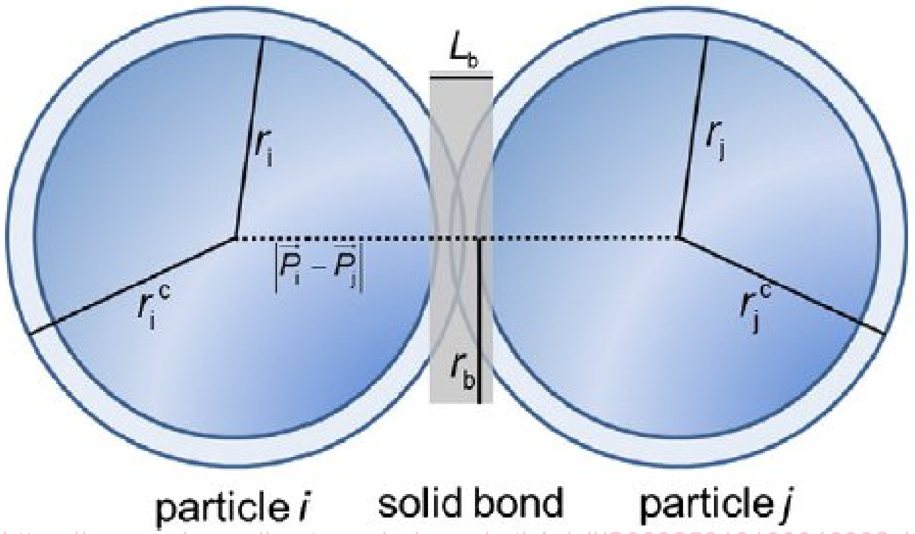
New "hybrid" model approach with bonded particles

Particle-based methods (Lagrangian)



- Strictly limited to granular or dispersed phases
- Particles size defined by ensemble to describe
- Need for calibration to match real physics

Bond Initialization



Source:https://www.sciencedirect.com/science/article/pii/S0032591013004683?via%3Dihub

- Particles are solid DEM spheres without overlap contact force
- Bond is formed at increased radii overlap
- Bond initialized with zero force
- At each bond, a visco-elastic constitutive equation is solved

Burgers model implementation

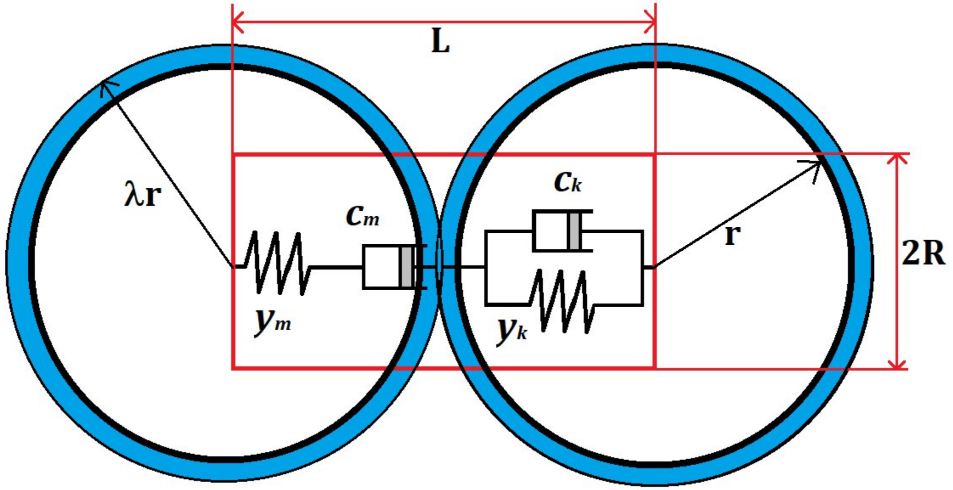
$$\sigma + \left[\frac{\mu_k}{k_k} + \mu_m\left(\frac{1}{k_k}+\frac{1}{k_m}\right)\right]\dot{\sigma} + \frac{\mu_k \mu_m}{k_k k_m}\ddot{\sigma} = \pm\ \mu_m \dot{\varepsilon} \pm \frac{\mu_k \mu_m}{k_k}\ddot{\varepsilon}$$

Solved new timestep dynamics and loaded old timestep values

$$\Delta u^{\{n+1\}}, f^{\{n\}}, u_k^{\{n\}}$$

$$f^{\{n+1\}} = -\frac{\Delta u^{\{n+1\}} + \left(1-\frac{B}{A}\right)u_k^{\{n\}} + D f^{\{n\}}}{C}$$

$$u_k^{\{n+1\}} = \frac{u_k^{\{n\}}B - \frac{0.5dt}{c_k}\left(f^{\{n+1\}} - f^{\{n\}}\right)}{A}$$



$$c_{m,k} = \frac{\mu_{m,k}\pi R^2}{L}, \quad y_{m,k} = \frac{k_{m,k}\pi R^2}{L}$$

$$A,B,C,D = f(c_m, c_k, y_m, y_k, \Delta t)$$

Generalized Maxwell model

Solved new timestep dynamics and loaded old timestep values

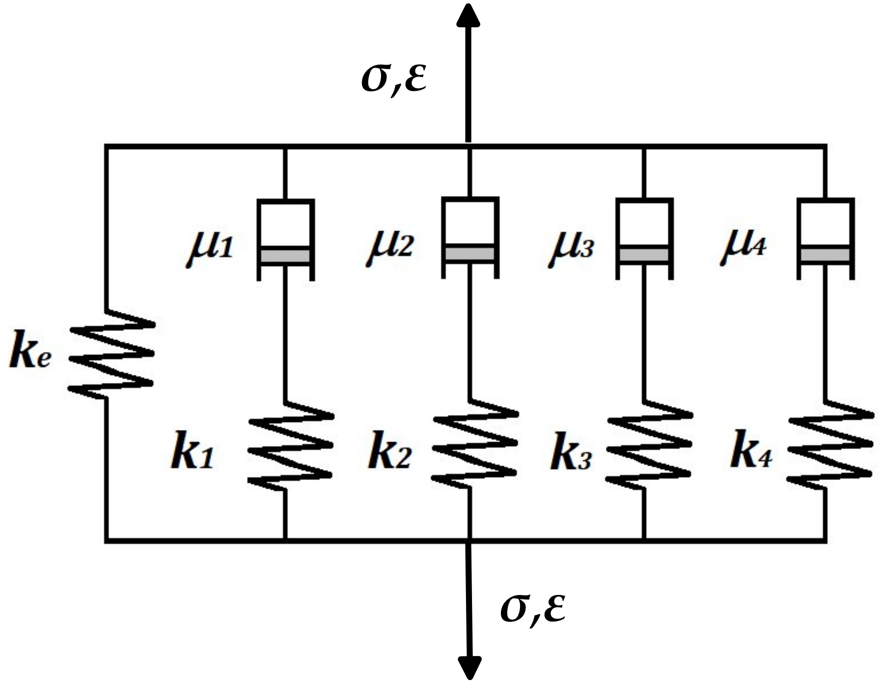
$$\Delta u^{\{n+1\}}, f^{\{n\}}$$

$$f_i^{\{n+1\}} = \frac{\Delta u^{\{n+1\}} + f_i^{\{n\}}\left(\frac{1}{y_i} - \frac{\Delta t}{2c_i}\right)}{\frac{1}{y_i} + \frac{\Delta t}{2c_i}}$$

$$f_e^{\{n+1\}} = y_e\left(u^{\{n+1\}} - u^{\{n_0\}}\right)$$

$$f^{\{n+1\}} = \sum_{i=1}^{4} f_i^{\{n+1\}} + f_e^{\{n+1\}}$$

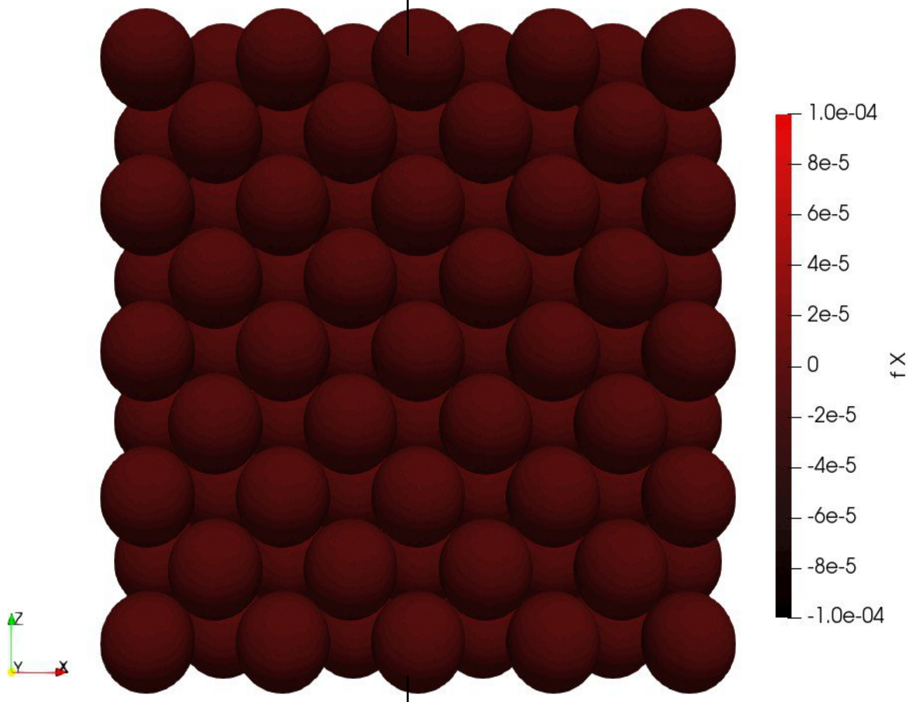
$$\dot{\varepsilon} = \frac{\dot{\sigma}_i}{k_i} + \frac{\sigma_i}{\mu_i}, \quad \sigma_e = k_e \varepsilon$$



$$y_{i,e} = \frac{k_{i,e}\pi R^2}{L} \qquad c_i = \frac{\mu_i \pi R^2}{L}$$

Test case and post-processing

$$x(t) = x_0 + A_0 \sin(\omega t)$$

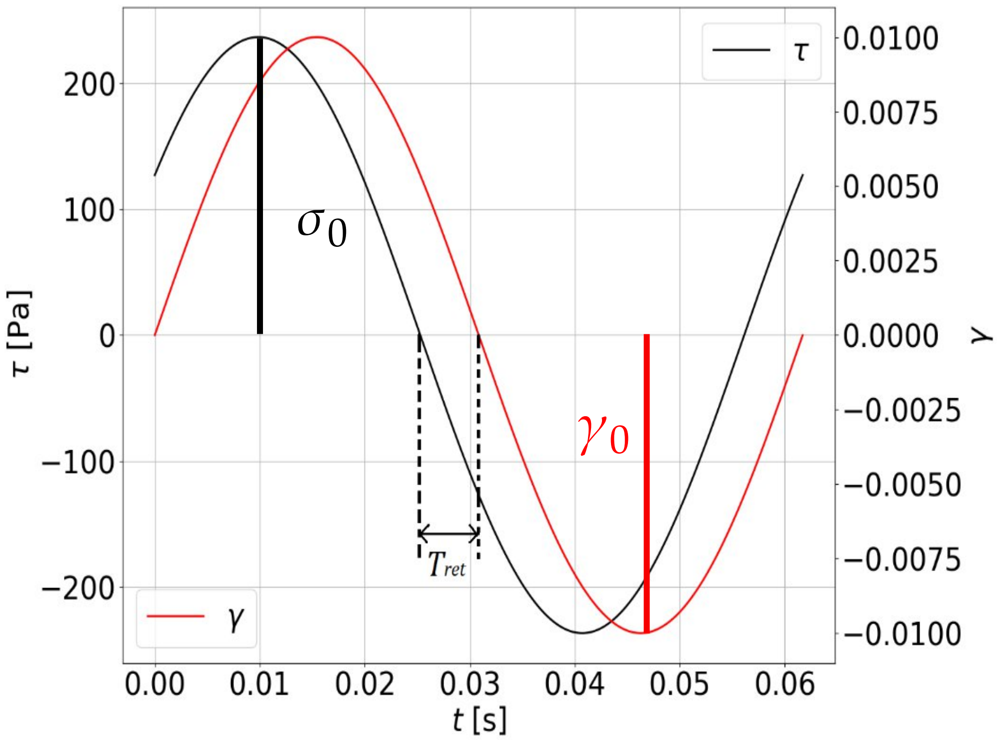


$$v(t) = 0$$

$$\sigma = \frac{1}{n_{top} A_{top}} \sum_{i}^{n_{top}} f_i$$

$$\phi = \omega \cdot T_{ret}$$

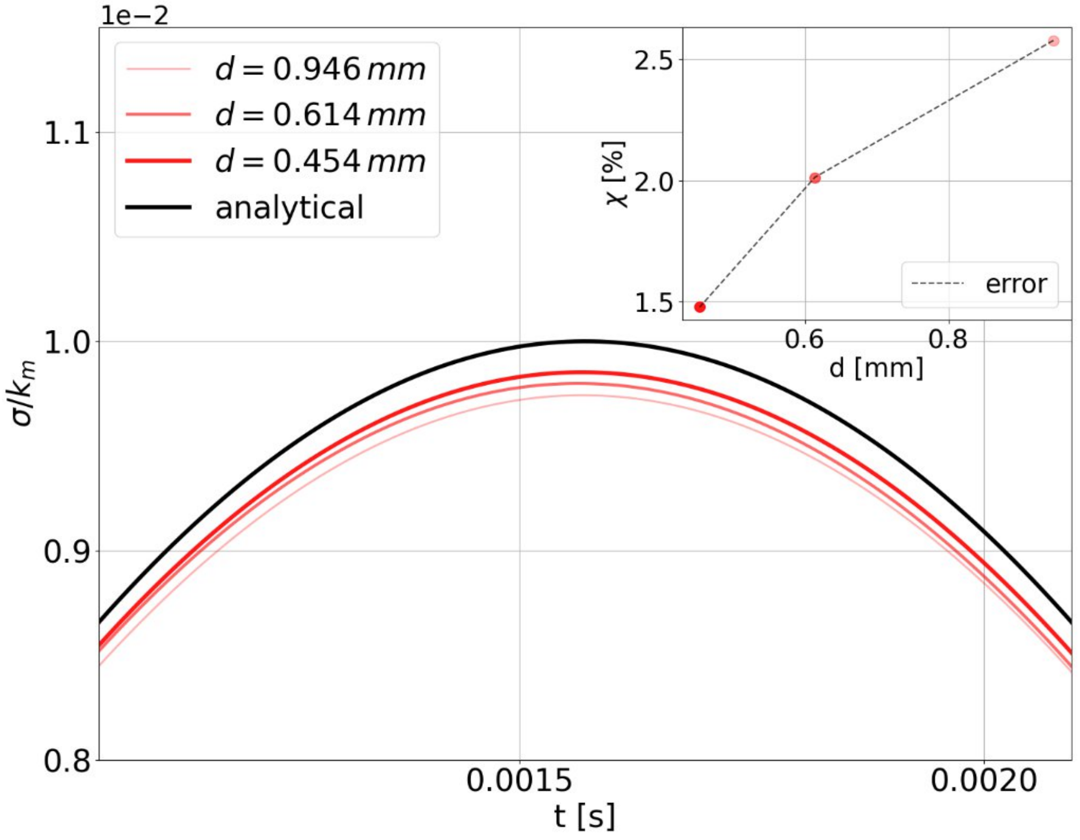
$$G' = \frac{\sigma_0}{\gamma_0} \cos\phi, \quad G'' = \frac{\sigma_0}{\gamma_0} \sin\phi$$



Particles size effect

Constant volume oscillating compression test at decreasing particles size to check for solution convergence

type	N	d
coarse	172	$0.946\,mm$
medium	666	$0.614\,mm$
fine	1688	$0.454\,mm$



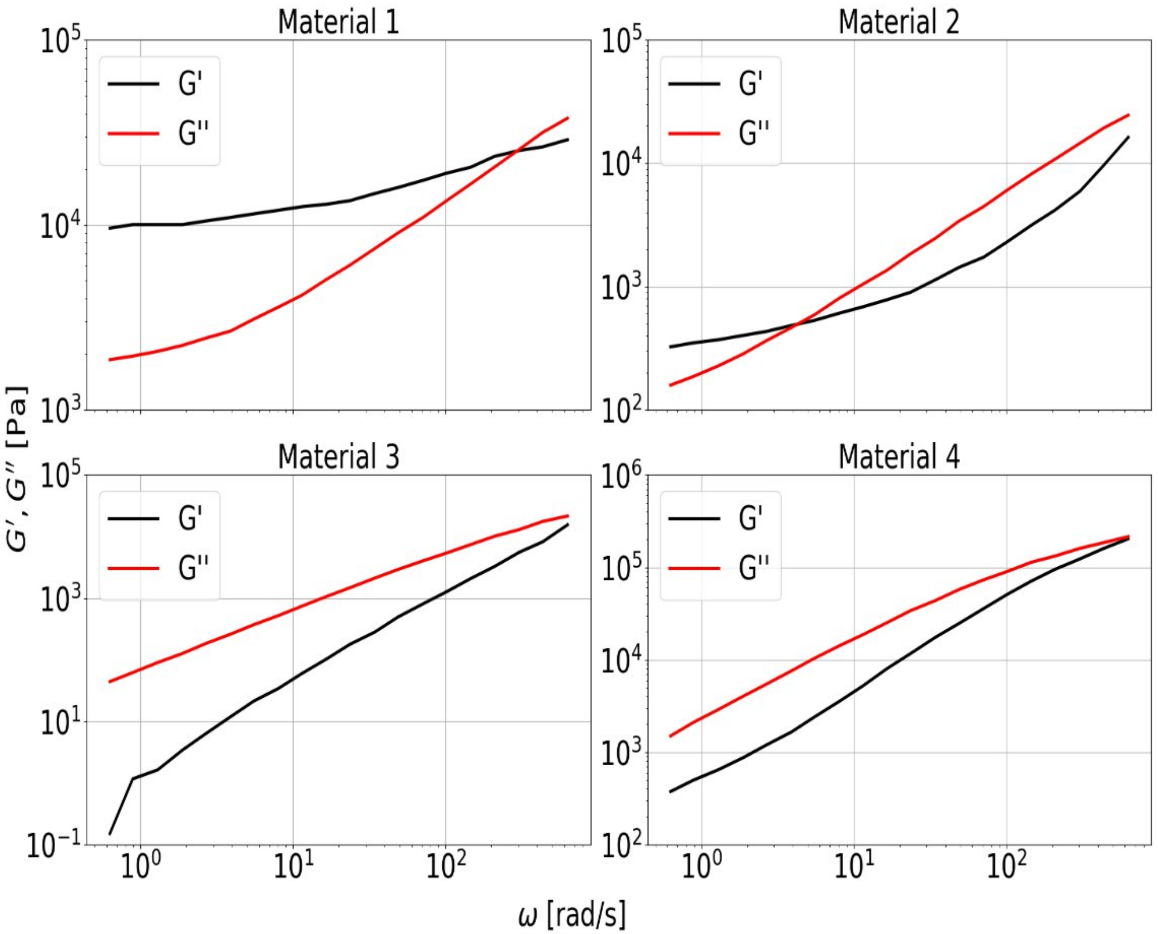
Analytical: $\sigma = E\varepsilon$

Elastic Burgers:

- Divide constitutive relation by $\mu_m \mu_k$
- Let $\mu_m, \mu_k \to \infty$
- Integrate twice in time

$$\sigma = k_m \varepsilon$$

Calibration strategy



1. **Read experimental data from oscillatory rheometer test**

2. **Compute G_0', G_0'' from:**

$$J' = \frac{1}{k_m} + \frac{k_k}{k_k^2 + (\omega\mu_k)^2}$$

$$J'' = \frac{1}{\omega\mu_m} + \frac{\omega\mu_k}{k_k^2 + (\omega\mu_k)^2}$$

$$G_0' = \frac{J'}{J'^2 + J''^2}, \quad G_0'' = \frac{J''}{J'^2 + J''^2}$$

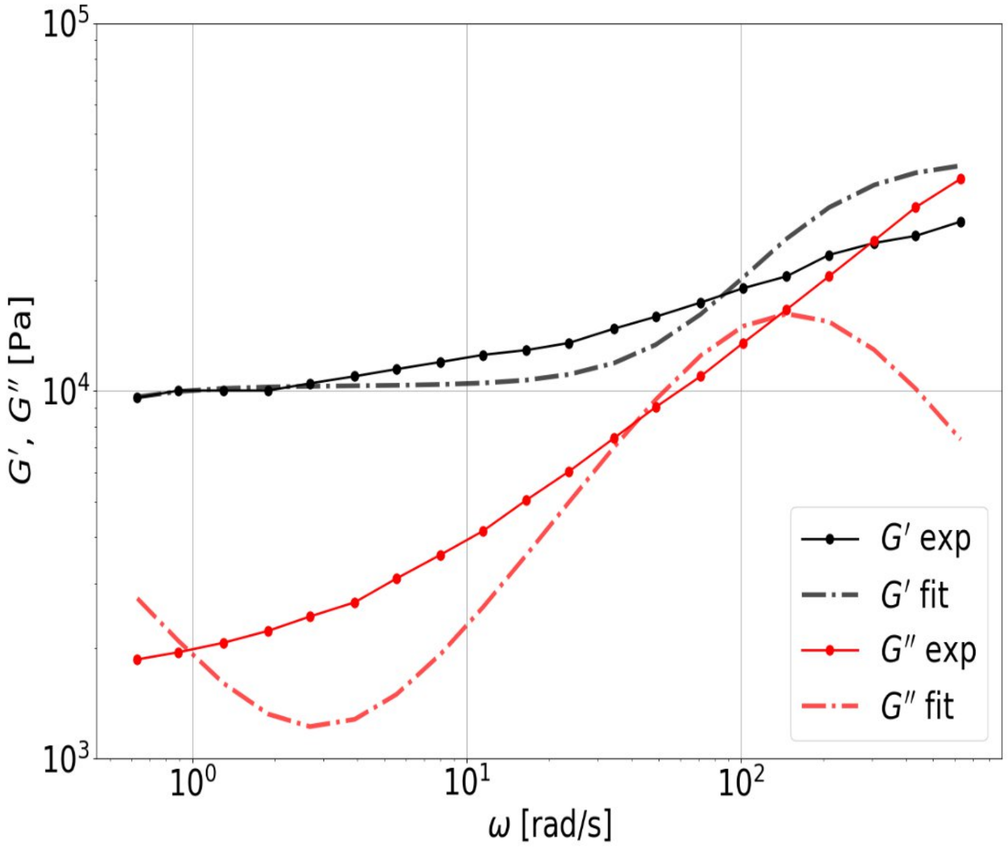
3. **Minimize cost function:**

$$f_{cost} = \sum_i^m \left[\left(\frac{G_0'}{G'} - 1 \right)^2 + \left(\frac{G_0''}{G''} - 1 \right)^2 \right]$$

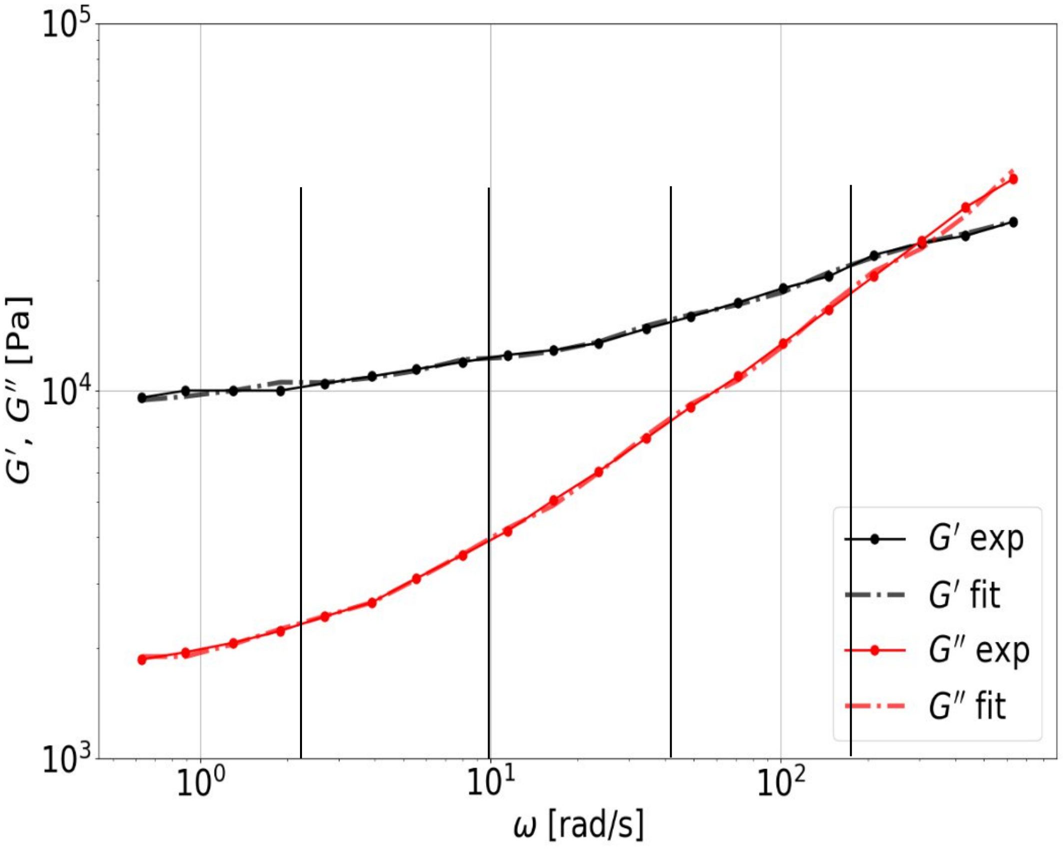
μ_m, μ_k, k_m, k_k

Burgers model analytical fitting

Full frequency range fitting



Sub-set frequency fitting

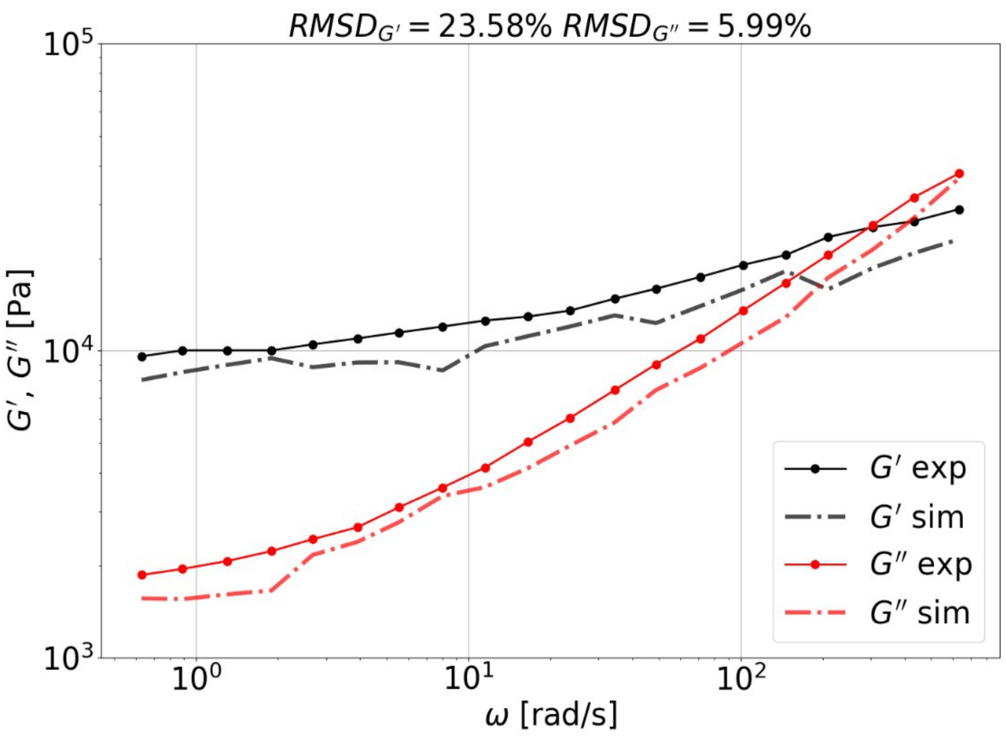


Burgers model not suited for large dataset

Burgers model calibration limits

Limit 1:

Non constant parameters through the dataset



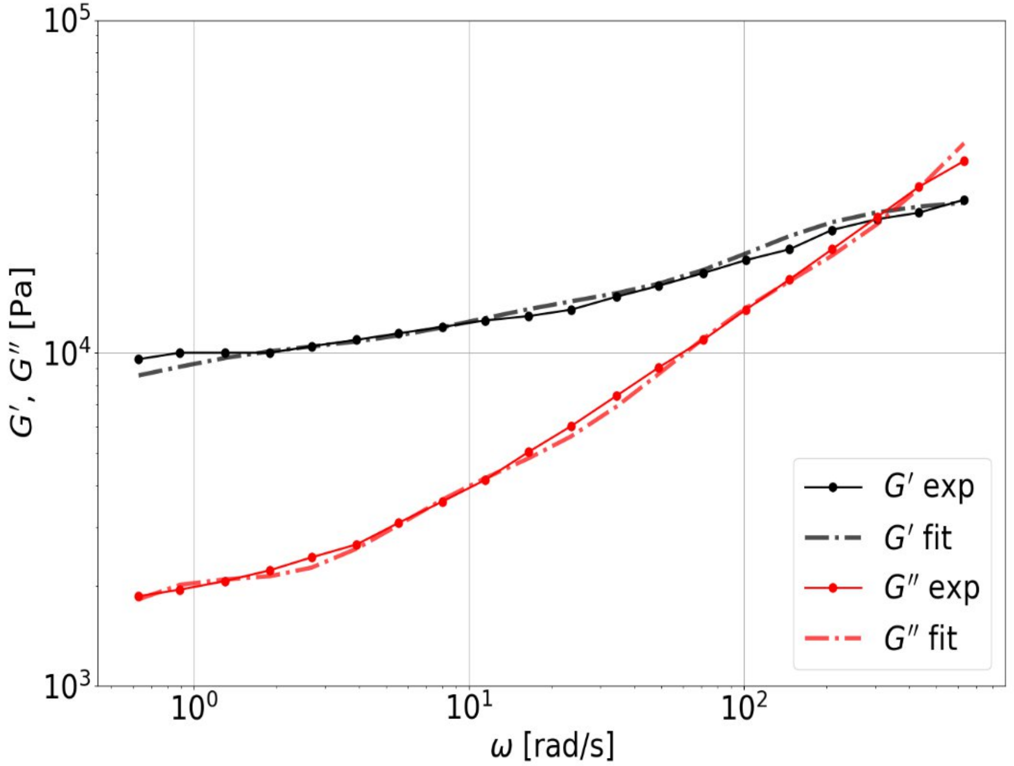
ω range $[\frac{rad}{s}]$	$\mu_m\,[Pas]$	$\mu_k\,[Pas]$	$k_m\,[Pa]$	$k_k\,[Pa]$
0.6-1.9	$1.325 \cdot 10^5$	$1.55 \cdot 10^4$	$1.36 \cdot 10^4$	$3.24 \cdot 10^4$
2.7-8.1	$3.76 \cdot 10^4$	$0.31 \cdot 10^4$	$1.8 \cdot 10^4$	$2.62 \cdot 10^4$
11.5-34.1	$0.85 \cdot 10^4$	658.1	$3.22 \cdot 10^4$	$2.14 \cdot 10^4$
48.8-146.5	$0.16 \cdot 10^4$	220.2	$7.33 \cdot 10^4$	$2.56 \cdot 10^4$
209.3-632.4	$3.75 \cdot 10^2$	77.86	$5.03 \cdot 10^5$	$3.98 \cdot 10^4$

Limit 2:

Jumps in simulated data due to sudden change in parameters

Generalized Maxwell calibration

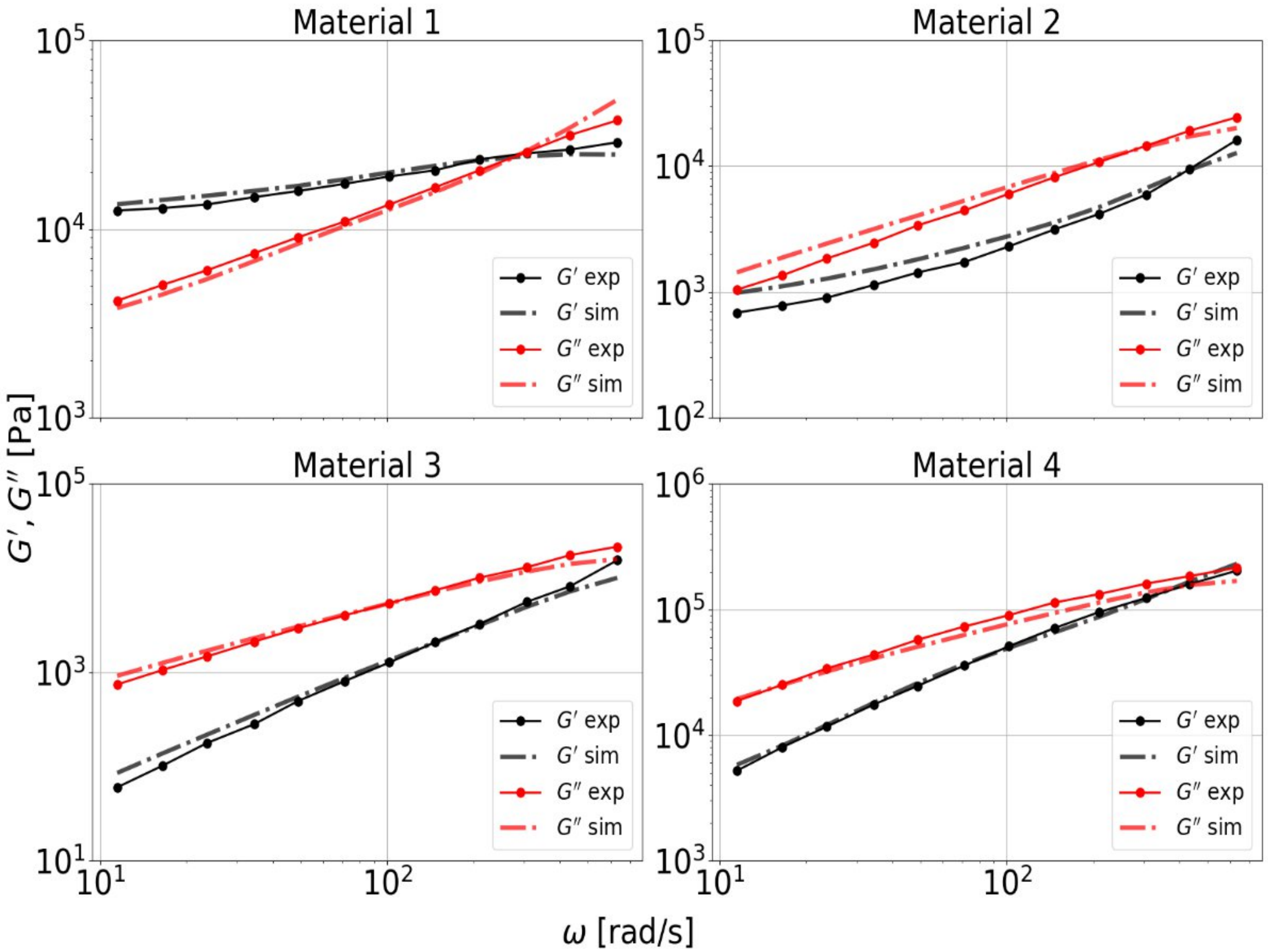
$$G' = \sum_i \frac{k_i \omega^2 \tau_i^2}{1 + \omega^2 \tau_i^2} + k_e \quad G'' = \sum_i \frac{k_i \omega \tau_i}{1 + \omega^2 \tau_i^2}$$



Generalized Maxwell maintains accuracy through the whole dataset

material	$\mu_1\,[Pas]$	$\mu_2\,[Pas]$	$\mu_3\,[Pas]$	$\mu_4\,[Pas]$	$k_1\,[Pa]$	$k_2\,[Pa]$	$k_3\,[Pa]$	$k_4\,[Pa]$	$k_e\,[Pa]$
1	3711	108.7	63.1	373.4	3067	$1.389 \cdot 10^4$	$3.98 \cdot 10^6$	4065.6	7422.8

Generalized Maxwell calibration

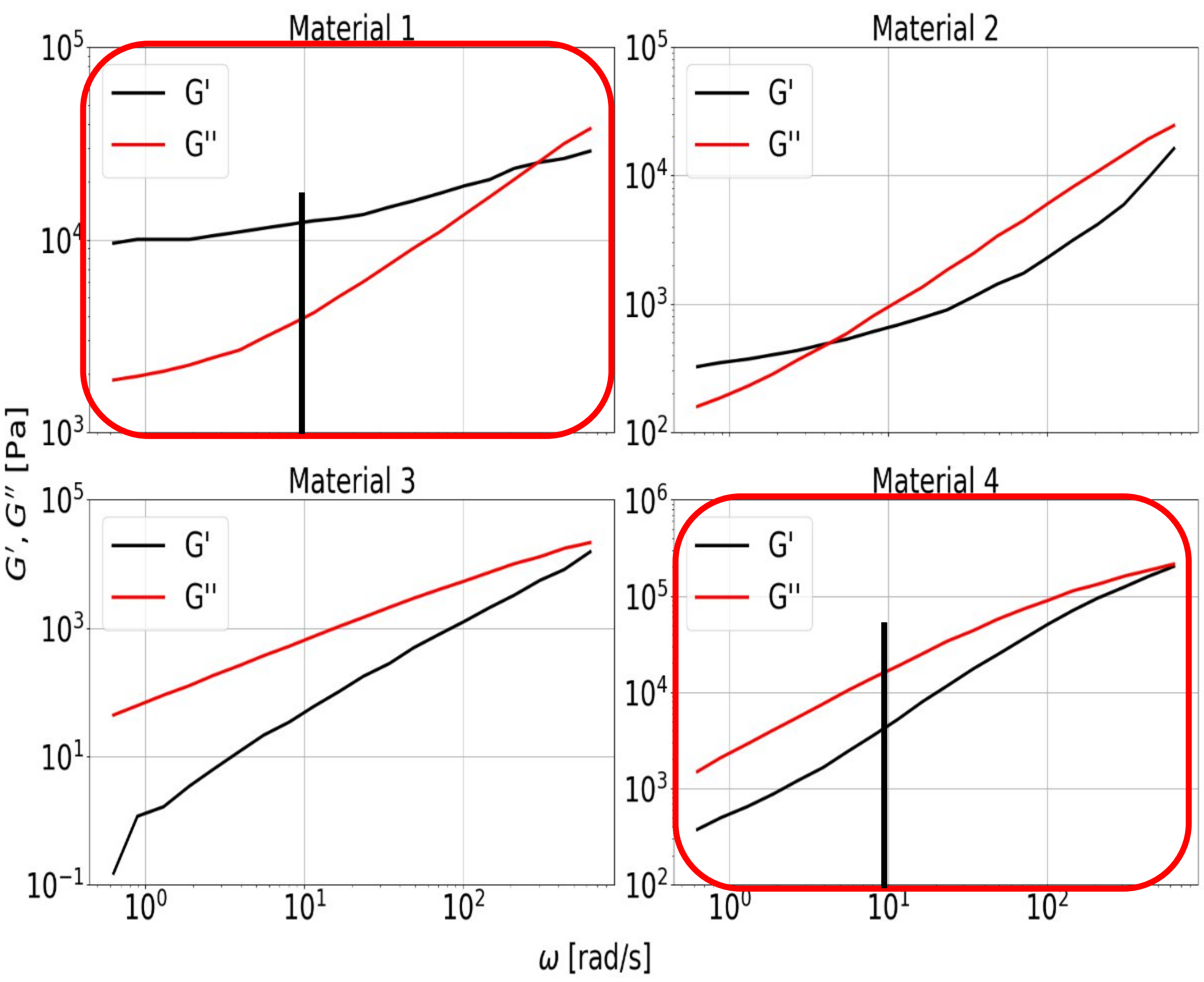


No more jumps in the rheometer simulations ☾ higher quality simulations

	material 1	material 2	material 3	material 4
$RMSD_{G'}$	9.65 %	7.01 %	10.39 %	4.38 %
$RMSD_{G''}$	9.82 %	6.36 %	9.43 %	9.94 %

Error drastically reduced over a variety of materials

Extrusion simulation setup

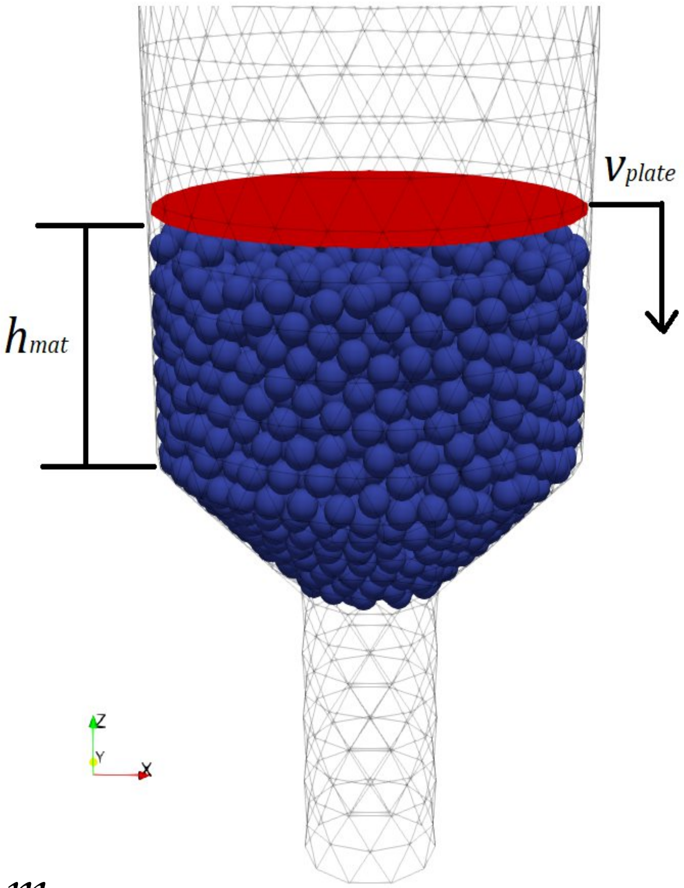


$$\omega = 10 \frac{rad}{s}$$

$$\dot{\varepsilon} = \frac{v_{plate}}{h_{mat}}$$

$$\omega \simeq 2\pi\dot{\varepsilon}$$

$$v_{plate} = \frac{\omega h_{mat}}{2\pi} \approx 0.012 \frac{m}{s}$$

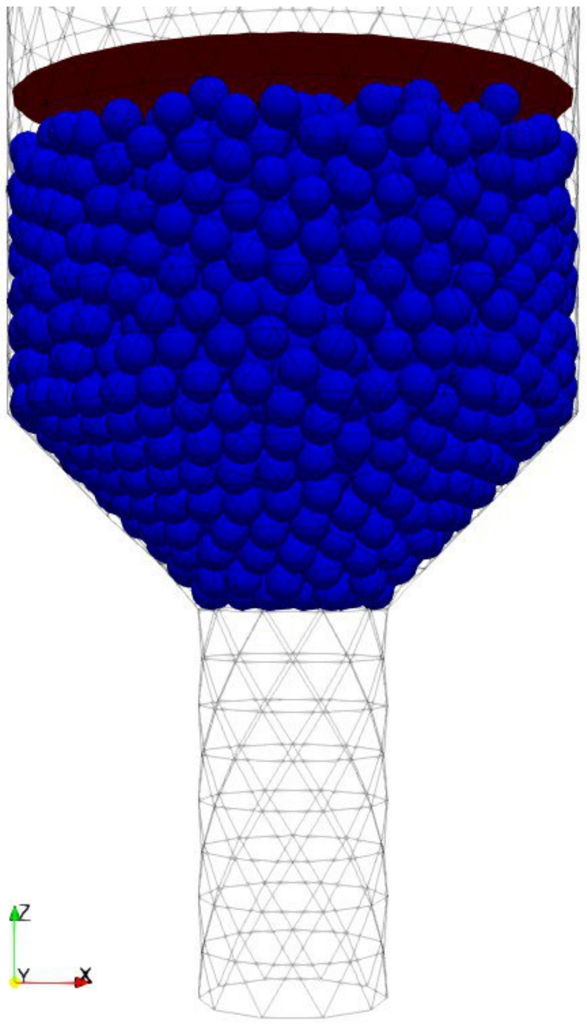


Extrusion simulation material 1

Compression phase: dynamic viscosity

$$\mu' = \frac{G''}{\omega} = \sum_{i=1}^{4} \frac{\mu_i}{1 + (\omega\tau_i)^2}$$

For material 1 ☾ $\mu_1' \;|_{\omega=10} = 399\ Pa\ s$



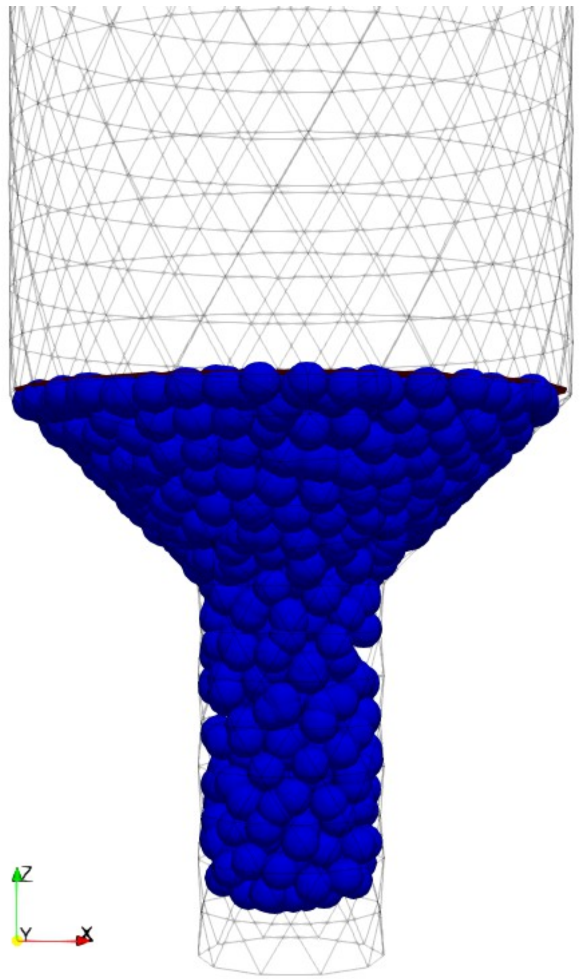
Extrusion simulation material 1

Relaxation phase: viscosity

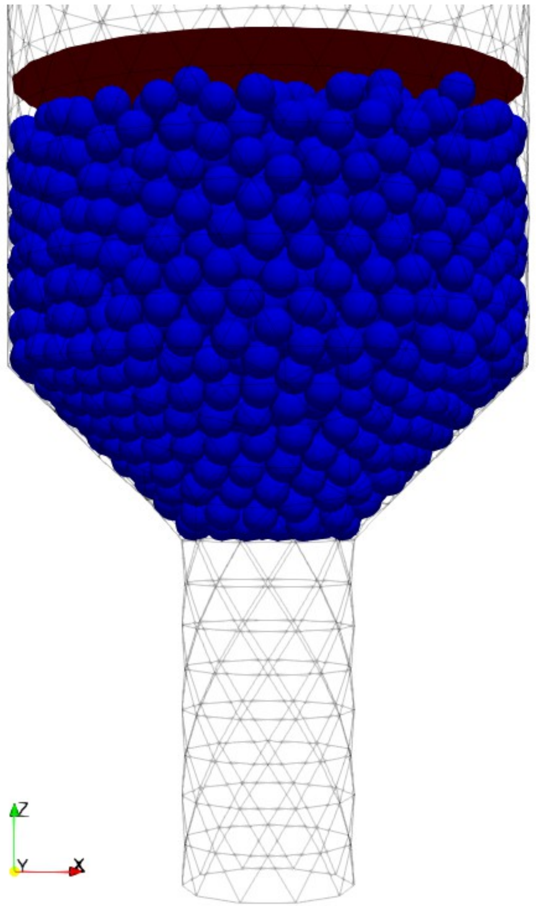
$$\mu(\dot{\gamma})\ |_{\dot{\gamma}\to 0} = \mu'(\omega)\ |_{\omega\to 0} = \sum_{i=1}^{4} \frac{\mu_i}{1+(\omega\tau_i)^2}$$

$$= \sum_{i}^{4} \mu_i$$

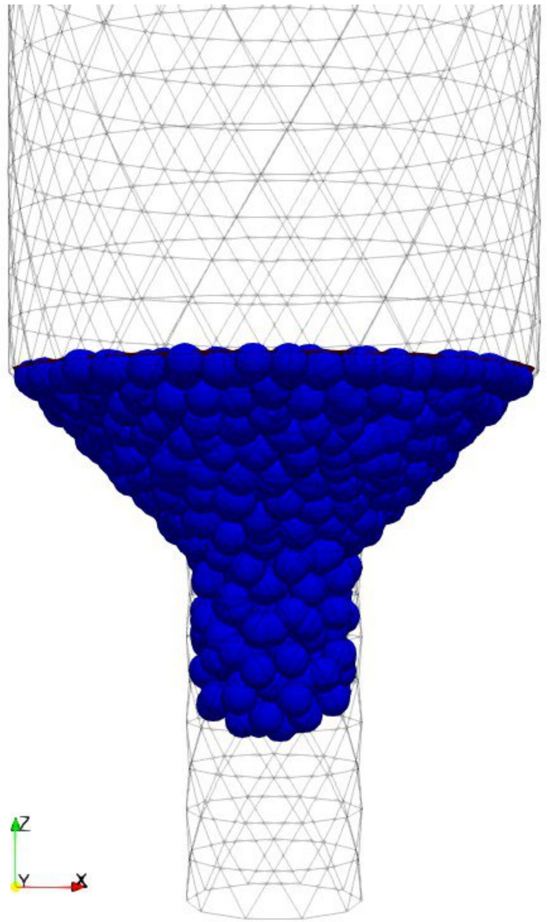
For material 1 $\quad \mu_1 = 4256\ Pa\ s$



Extrusion simulation material 4

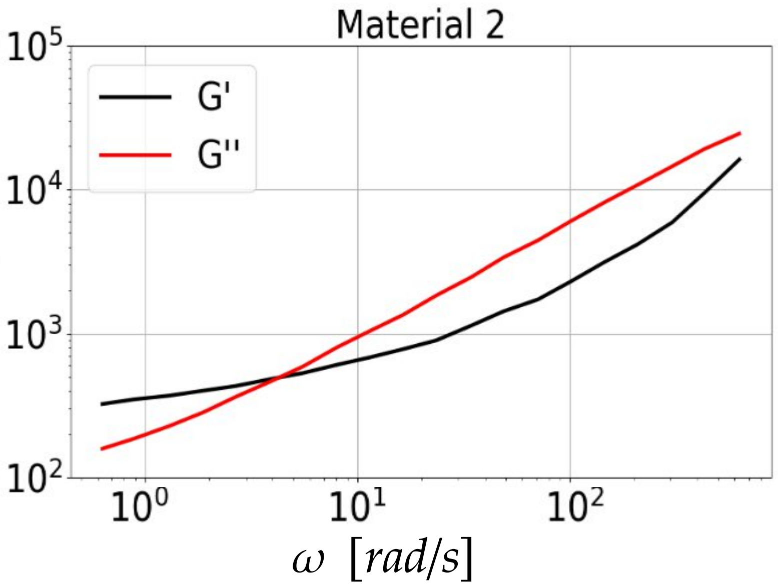


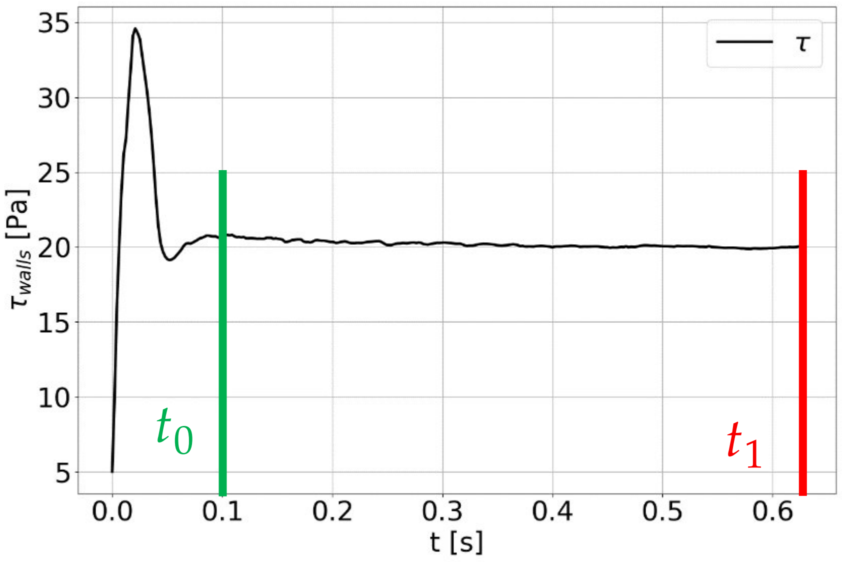
$\mu_4' \;|_{\omega=10} = 1606\ Pa\ s$

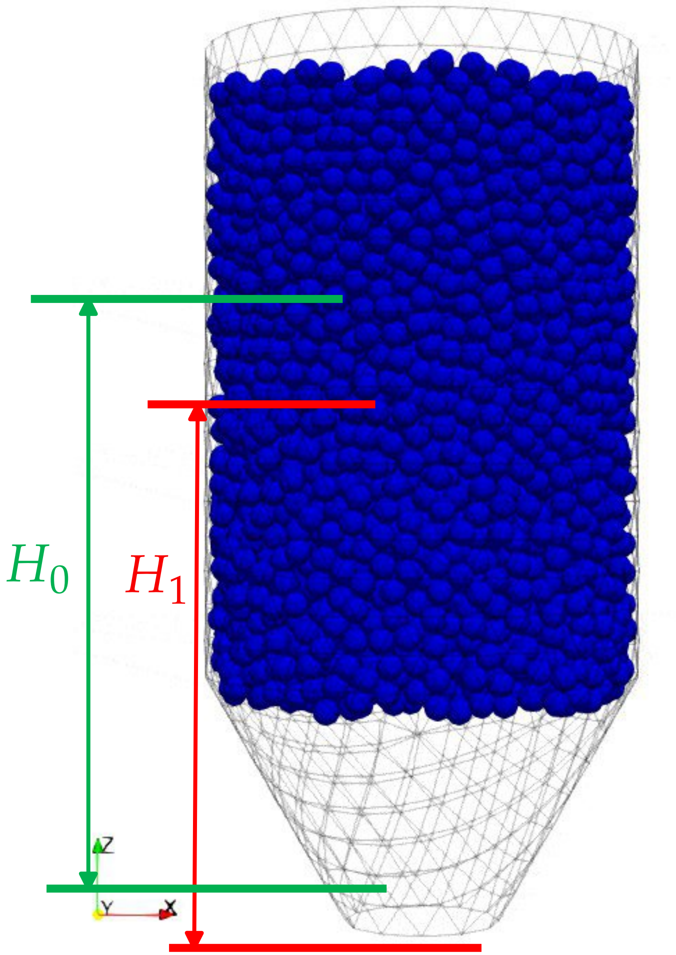


$\mu_4 = 2144\ Pa\ s$

Gravity driven flow material 2







Measured dynamic viscosity:

$$\mu'_{sim} = \frac{\tau_{walls}}{\dot{\varepsilon}} = 142.2\ Pa\ s, \quad \dot{\varepsilon} = \frac{|H_0 - H_1|}{H_0(t_1 - t_0)}$$

Predicted dynamic viscosity:

$$\mu' = \sum_{i=1}^{4} \frac{\mu_i}{1 + (\omega\tau_i)^2} = 107.9\ Pa\ s, \quad \omega = 2\pi\dot{\varepsilon}$$

Summary and future work

Obtained results:

- More robust Generalized Maxwell model to fit rheological properties
- Good agreement between simulation and rheometer experiment
- Material in process behaves according to predicted properties

To be improved:

- High compressibility of material
- Calibration for non-rheometer materials

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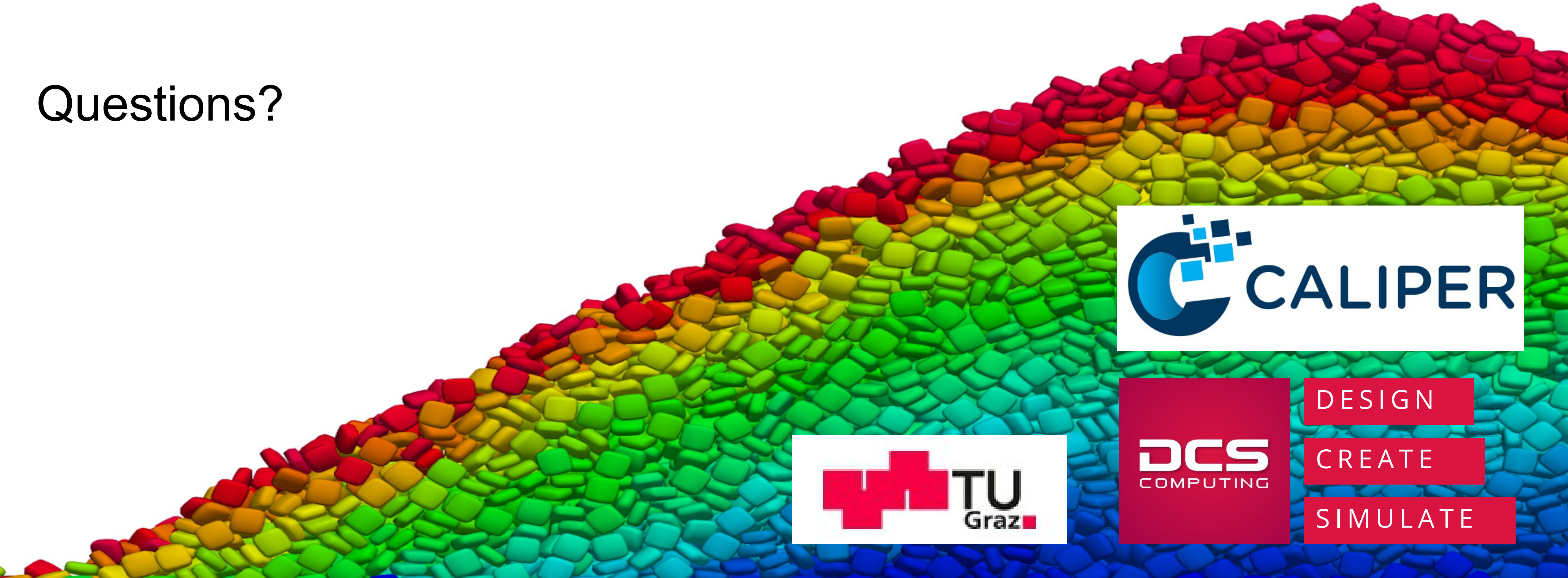
The end

Questions?



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