Determination of material coefficients for a non-linear viscous fluid by a numerical inverse analysis and its verification with a finite element simulation

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Goals of our research

- How to model and compute non-linear materials?
- How to measure and determine the necessary material parameters?

Outline

- Experimental setup
- Two material models
- Inverse analysis
- Computation

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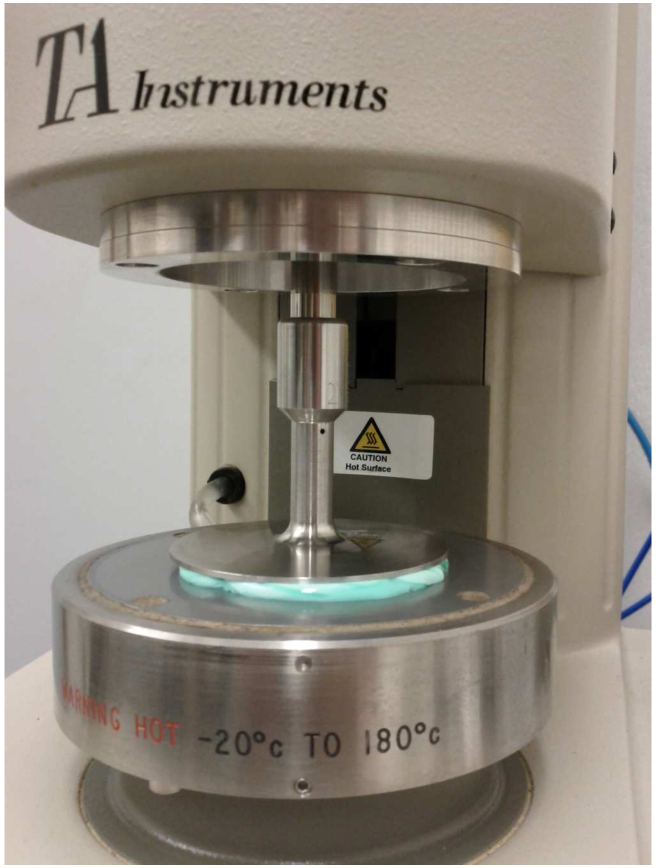
Experimental setup - I

- Rotary viscometer

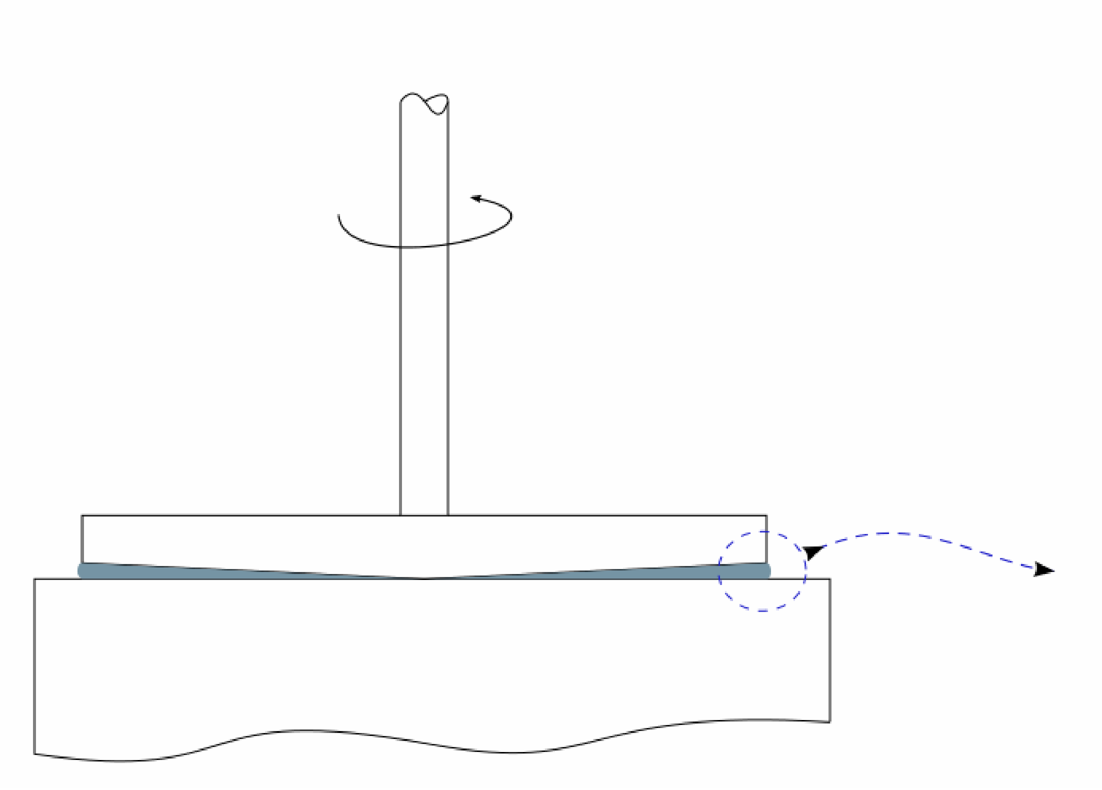
Experimental setup - II

- Rotary viscometer
- Toothpaste



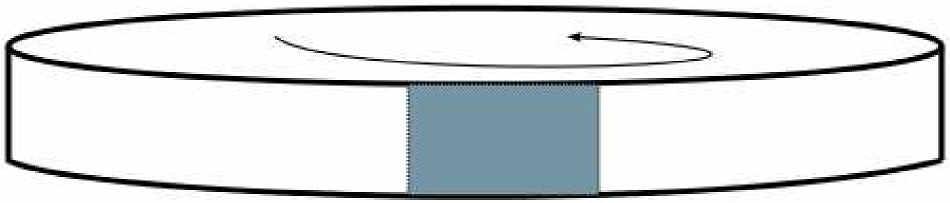
Experimental setup - III

- Rotary viscometer
- Toothpaste
- Cone-plate



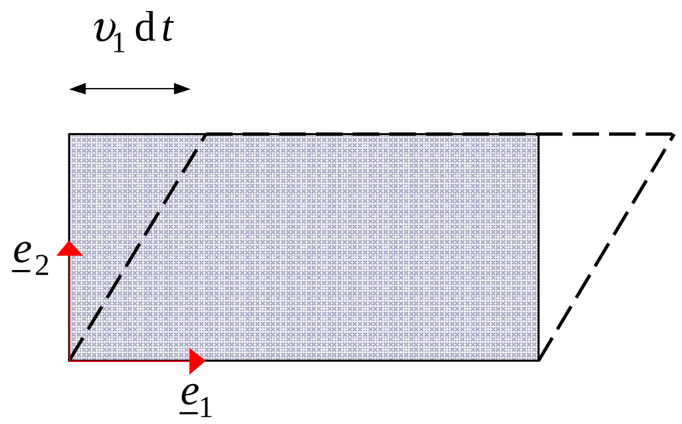
Experimental setup - IV

- Rotary viscometer
- Toothpaste
- Cone-plate
- Outer shell



Experimental setup - V

- Rotary viscometer
- Toothpaste
- Cone-plate
- Outer shell
- Velocity gradients - Stress



$$d_{ij} = \frac{\partial \upsilon_{(i}}{\partial x_{j)}} = \frac{1}{2}\left(\frac{\partial \upsilon_i}{\partial x_j} + \frac{\partial \upsilon_j}{\partial x_i}\right) = \begin{pmatrix} 0 & \frac{\partial \upsilon_1}{\partial x_2} \\ \frac{\partial \upsilon_1}{\partial x_2} & 0 \end{pmatrix}, \qquad \sigma_{ij} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$$

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Material models - I

- Balance law for mass and linear momentum:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \frac{\partial \upsilon_i}{\partial x_i} = 0 \qquad \rho \frac{\mathrm{d}\upsilon_i}{\mathrm{d}t} - \frac{\partial \sigma_{ji}}{\partial x_j} = \rho f_i \qquad \text{(assume } f_i \text{ is given)}$$

mass density $\rho(\underline{x},t)$
velocity $\upsilon_i(\underline{x},t)$

- How to find $\sigma_{ij}(\rho,\upsilon_i)$?

Material models - II

- Balance law for mass and linear momentum:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \frac{\partial \upsilon_i}{\partial x_i} = 0 \qquad \rho \frac{\mathrm{d}\upsilon_i}{\mathrm{d}t} - \frac{\partial \sigma_{ji}}{\partial x_j} = \rho f_i$$

(assume f_i is given)

mass density $\rho(\underline{x}, t)$

velocity $\upsilon_i(\underline{x}, t)$

- How to find $\sigma_{ij}(\rho, \upsilon_i)$?
  - Herschel Bulkley model: $$\sigma_{ij} = \left(\mu \frac{(II_{\underline{d}})^{n/2}}{\sqrt{II_{\underline{d}}}} + \frac{\tau}{\sqrt{II_{\underline{d}}}} \right) d_{ij}, \quad II_{\underline{d}} = \frac{1}{2} d_{ij} d_{ij},$$
  - Ziegler model: $$\sigma_{ij} = \mu' d_{ij} + \frac{2\tau'}{\pi \sqrt{II_{\underline{d}}}} \arctan\left(\frac{\sqrt{II_{\underline{d}}}}{n'} \right) d_{ij},$$

Material models - III

- for the experimental state:

$$d_{ij} = \begin{pmatrix} 0 & d_{12} = \dfrac{\partial v_1}{\partial x_2} \\ d_{12} = \dfrac{\partial v_1}{\partial x_2} & 0 \end{pmatrix}, \quad II_{\underline{d}} = (d_{12})^2 ,$$

  – Herschel Bulkley model:

$$\sigma_{12} = \mu (d_{12})^n + \tau ,$$
$$\mu = ? \quad n = ? \quad \tau = ?$$

  – Ziegler model:

$$\sigma_{12} = \mu' d_{12} + \frac{2\tau'}{\pi} \arctan\left(\frac{d_{12}}{n'} \right),$$
$$\mu' = ? \quad n' = ? \quad \tau' = ?$$

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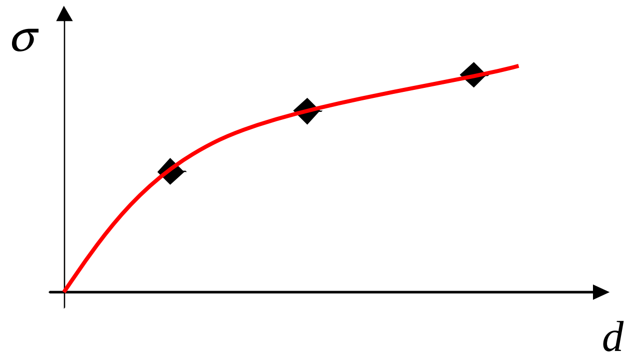
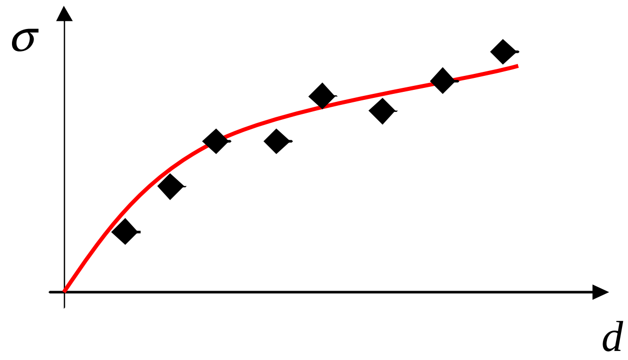
Inverse analysis - I

- Experiment: {input , output} $\Rightarrow \{\sigma^N, d^N\}$



Inverse analysis - II

- Experiment: {input , output} $\Rightarrow \{\sigma^N, d^N\}$



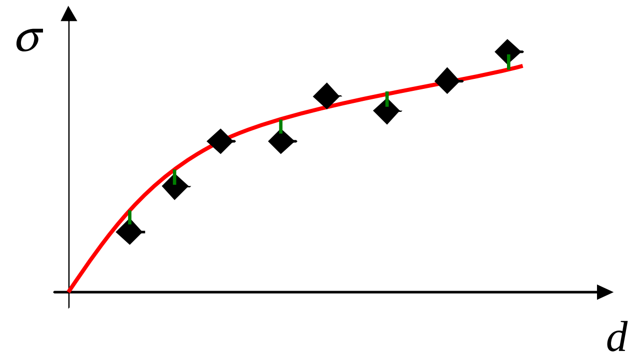
Inverse analysis - III

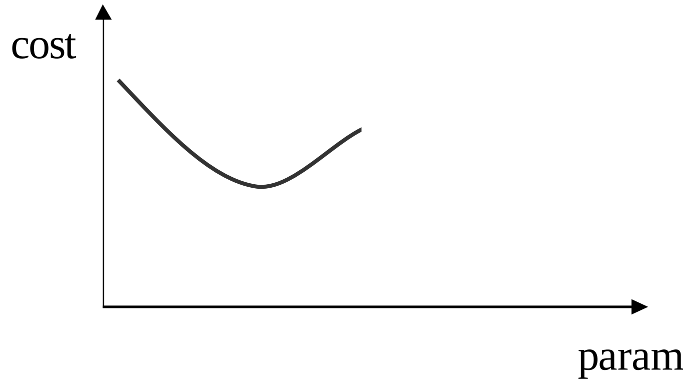
- Experiment: {input , output} $\Rightarrow \{\sigma^N, d^N\}$
- Levenberg-Marquardt:

$$\text{cost}\left(\sigma^N, d^N, \text{param}\right) = \sum_N \left(\sigma^N - \sigma_{12}\left(d^N, \text{param}\right)\right)^2 ,$$

$$\text{param}_{\text{init}} = \{\mu_0, n_0, \tau_0\},$$

$$\text{param} = \arg\min\left(\text{cost}\left(\sigma^N, d^N, \text{param}_{\text{init}}\right)\right)$$





Inverse analysis - IV

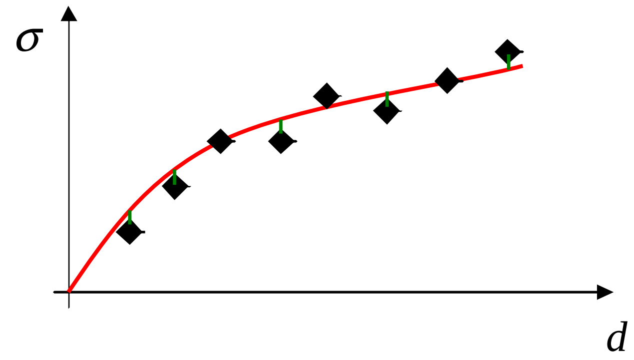
- Experiment: {input , output} $\Rightarrow \{\sigma^N, d^N\}$
- Levenberg-Marquardt:

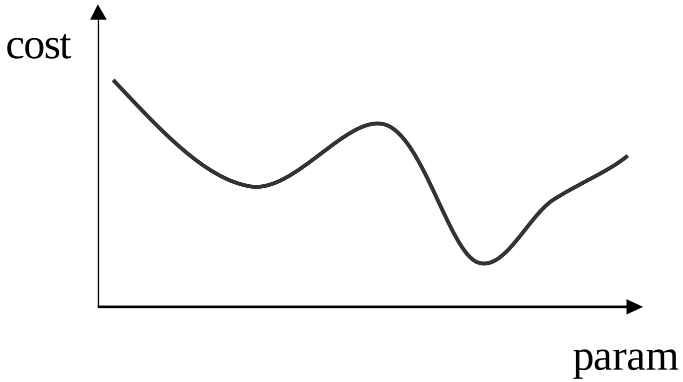
$$\mathrm{cost}\left(\sigma^N, d^N, \mathrm{param}\right) = \sum_N \left(\sigma^N - \sigma_{12}\left(d^N, \mathrm{param}\right)\right)^2 ,$$

$$\mathrm{param}_{\mathrm{init}} = \{\mu_0, n_0, \tau_0\},$$

$$\mathrm{param} = \arg\min\left(\mathrm{cost}\left(\sigma^N, d^N, \mathrm{param}_{\mathrm{init}}\right)\right)$$

- Monte Carlo:
  - choose random $\mathrm{param}_{\mathrm{init}} = \{\mu_0, n_0, \tau_0\},$





Inverse analysis - V

– Herschel Bulkley model:

$$\sigma_{12} = \mu (d_{12})^n + \tau ,$$

$$\mu = 220.056 \text{ Pa s} \quad n = 0.599 \quad \tau = 5.420 \text{ Pa}$$

– Ziegler model:

$$\sigma_{12} = \mu' d_{12} + \frac{2\tau'}{\pi} \arctan\left(\frac{d_{12}}{n'}\right),$$

$$\mu' = 61.446 \text{ Pa s} \quad n' = 0.267 \quad \tau' = 190.217 \text{ Pa}$$

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Finite element method - I

- Residuals are tested arbitrarily

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \frac{\partial \upsilon_i}{\partial x_i} = 0 \qquad \rho \frac{\mathrm{d}\upsilon_i}{\mathrm{d}t} - \frac{\partial \sigma_{ji}}{\partial x_j} = 0$$

- Time discretized in finite difference scheme

$$\frac{\mathrm{d}}{\mathrm{d}t}(\cdot) = \frac{\partial}{\partial t}(\cdot) + \frac{\mathrm{d}x_i}{\mathrm{d}t}\frac{\partial}{\partial x_i}(\cdot) = \frac{(\cdot)-(\cdot)^0}{t-t^0} + \upsilon_i \frac{\partial}{\partial x_i}(\cdot)$$

- Integration by parts to get first-order in space

$$\sum_{\text{elements}} \int_{\Omega^{\text{ele}}} \left(\frac{\rho-\rho^0}{t-t^0}\delta\rho + \upsilon_i \frac{\partial \rho}{\partial x_i}\delta\rho + \rho \frac{\partial \upsilon_i}{\partial x_i}\delta\rho + \rho \frac{\upsilon_i - \upsilon_i^0}{t-t^0}\delta\upsilon_i + \rho\upsilon_j \frac{\partial \upsilon_i}{\partial x_j}\delta\upsilon_i + \sigma_{ji}\frac{\partial \delta\upsilon_i}{\partial x_j} \right) \mathrm{d}v -$$
$$- \oint_{\partial\Omega} \sigma_{ji}\delta\upsilon_i n_j \,\mathrm{d}a$$

- Coded and computed in FEniCS

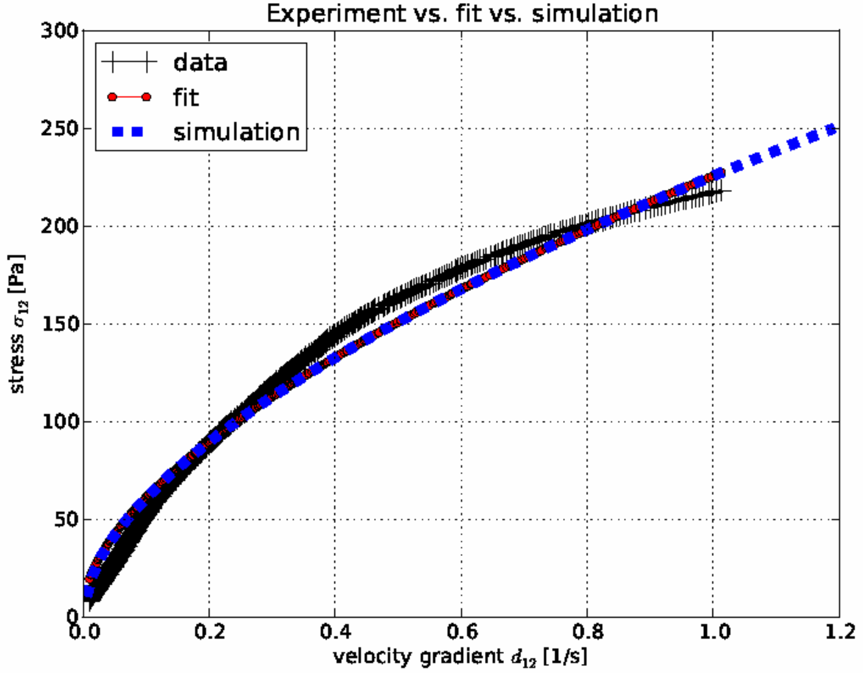
Results

- Experimental data, inverse analysis (SciPy) and finite element (FEniCS) code in:

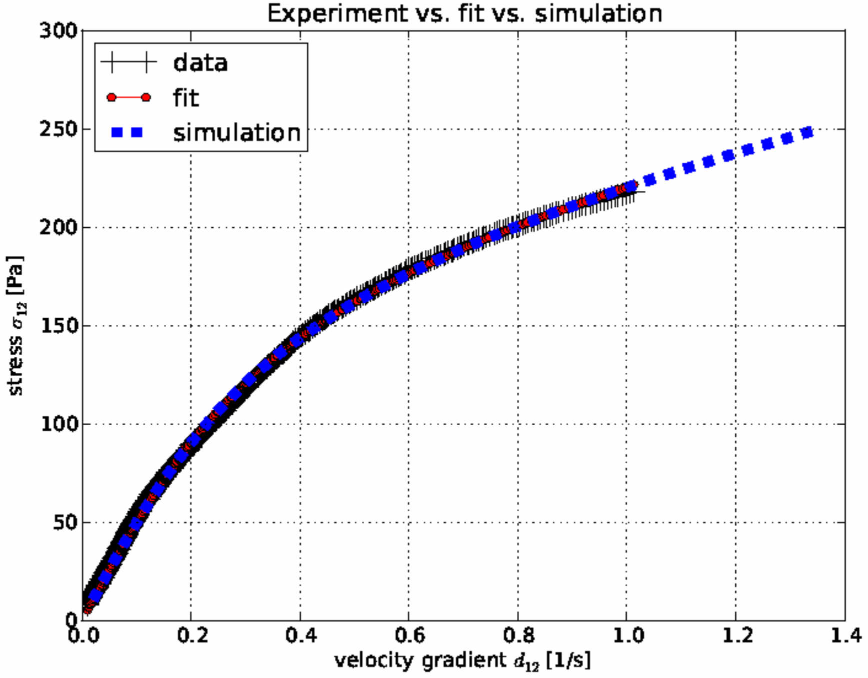
  www.lkm.tu-berlin.de/ComputationalReality

  under GNU Public license.

Herschel-Bulkley:



Ziegler model:



Summary

- Two non-linear material models with three parameters,
- Determination of the parameter by rotary viscometer and inverse analysis,
- Validation by finite element approximation.

Thanks a lot for your attention!

Questions?