Spring, 2022

ME 597 – Solid Mechanics II

Lecture 12
Material parameter estimation

PURDUE UNIVERSITY | Mechanical Engineering

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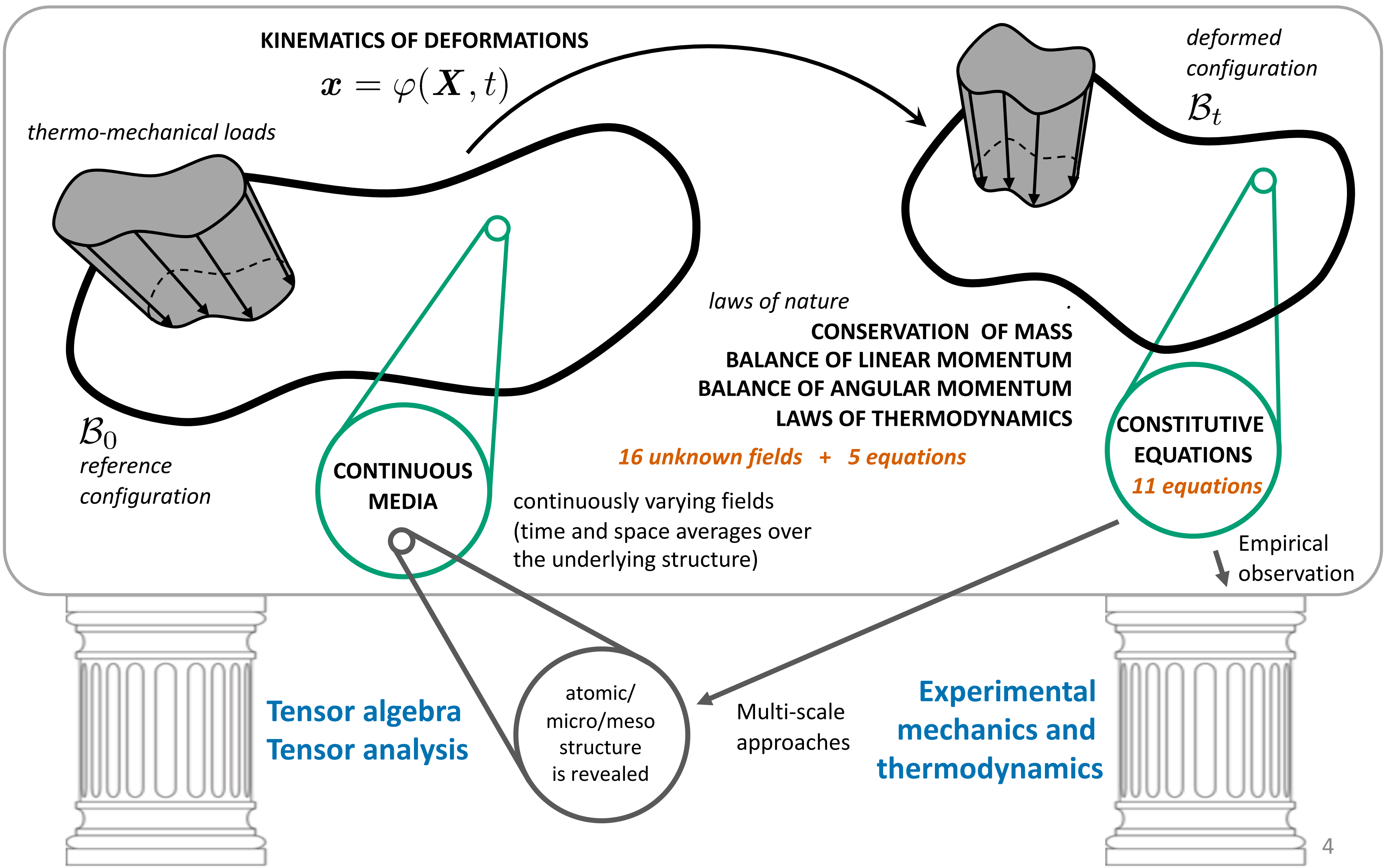
Last modified: 2/22/22 8:47:15 AM

Lecture 12 – Material parameter estimation

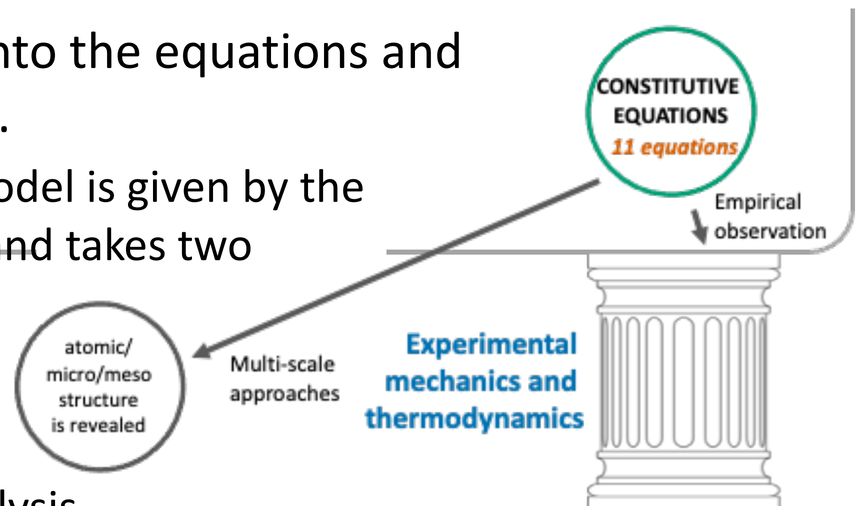


Material parameter estimation

Material model selection and parameter estimation

- Every computational solid mechanics model/software (e.g., FEM/Abaqus) requires a calibrated material model for each material to be simulated.
- Each material model, in turn, consists of two parts:
  + a constitutive model specifying the equations that govern the material response, and
  + a set of parameters that go into the equations and are specific for each material.

  Example: a linear elastic material model is given by the generalized Hooke's law equations and takes two material parameters: E and ν .
- Experimental data sets required!



Alternative paradigm: multiscale analysis

Material parameter estimation

Material model selection and parameter estimation

Material parameter estimation (as well as material model selection) is a topic that traditionally hasn't been well covered in the literature.

Aim: to find those parameters for which the predictions obtained from a model best match measurements or observations in the actual physical system.

- Deterministic (traditional) approach: to find the *best* set of material parameters, i.e., those values for which the predicted behavior best matches actual measurements (there are different, competing ways to define what constitutes the best parameters).
  Note: any approach that only produces a single best value does not consider the fact that measurements contain measurement noise or that the exact model is not known.
- Statistical approach (Bayesian method): it accounts for information about the measurement process and the measured data, as well as any prior knowledge about the material parameters.

Material parameter estimation

Material model selection and parameter estimation

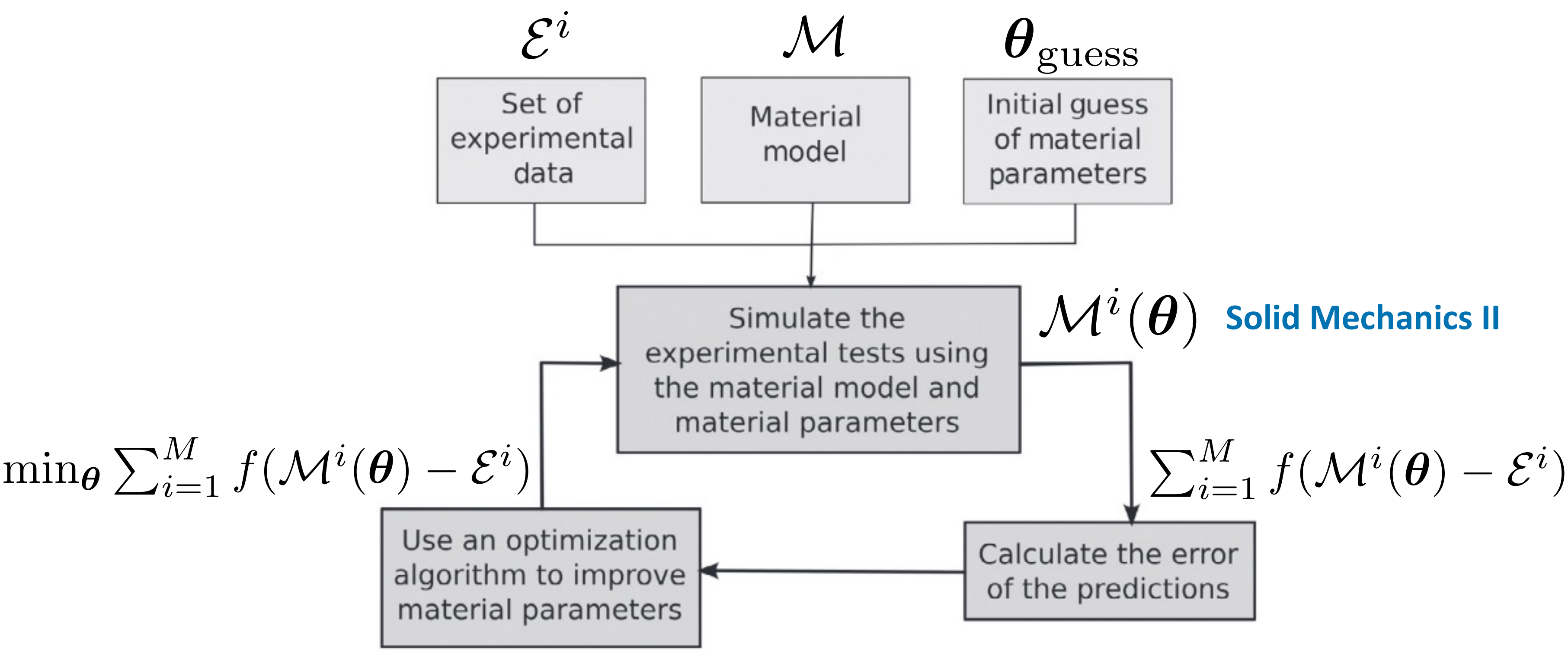
Aim: to find those parameters for which the predictions obtained from a model best match measurements or observations in the actual physical system.

- Material model and type of experimental data
- Initial guess of the material parameters
- Error measurement functions
- Algorithm for finding optimal material parameters

Material parameter estimation

Material model and type of experimental data

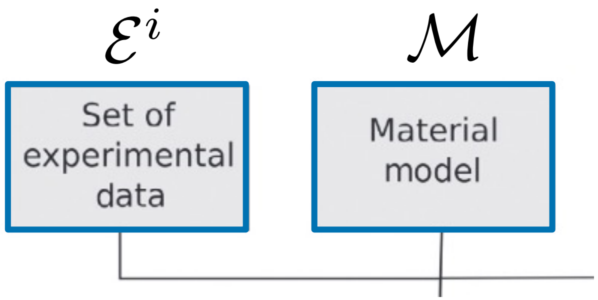
estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$



Material parameter estimation

Material model and type of experimental data

estimated material parameters $$\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$$



Note: different constitutive models need different types of experimental data for the purpose of calibration.

Examples:

- Hyperelastic isotropic solid: monotonic loading in one or more loading modes to a final finite strain; no need of experimental data at different strain rates.
- Viscoelastic isotropic solid: monotonic loading in one or more loading modes and at different strain-rates.

Material parameter estimation

Initial guess of the material parameters

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

- Finding a good initial guess of the material parameters is important in order to ensure that the material parameters that are determined by the minimization algorithm are close to the global optimum.
- A poor initial guess can cause the minimization algorithm to get stuck at an undesirable local minimum, and it can also significantly slow down the parameter extraction procedure.
- Most common approaches for finding a good initial guess:
    - *The Monte Carlo method*: each material parameter is first restricted to be in a certain pre-defined interval, and then for each parameter a random value in the specified range is generated.
    - *Prior knowledge of similar materials.*

Material parameter estimation

Error measurement functions

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

- Normalized root-mean square difference

$$\sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i) = \frac{\frac{1}{M}\sqrt{\sum(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)^2}}{\frac{1}{M}\sqrt{\sum(\mathcal{E}^i)^2}}$$

- Normalized mean absolute difference

$$\sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i) = \frac{\frac{1}{M}\sum|\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i|}{\frac{1}{M}\sum|\mathcal{E}^i|}$$

- Coefficient of determination

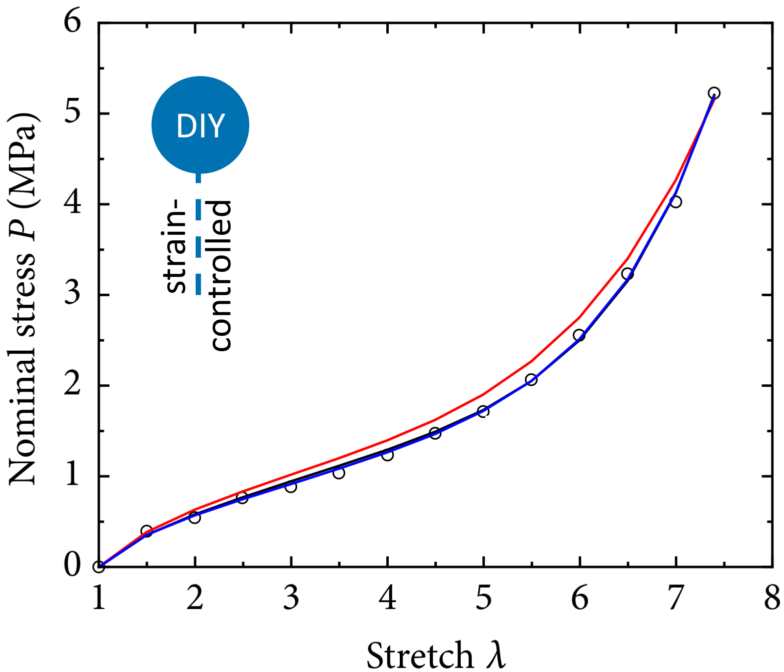
$$\sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i) = 1 - \sum \frac{(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)^2}{\sum(\mathcal{E}^i - \frac{1}{M}\sum\mathcal{E}^i)^2}$$

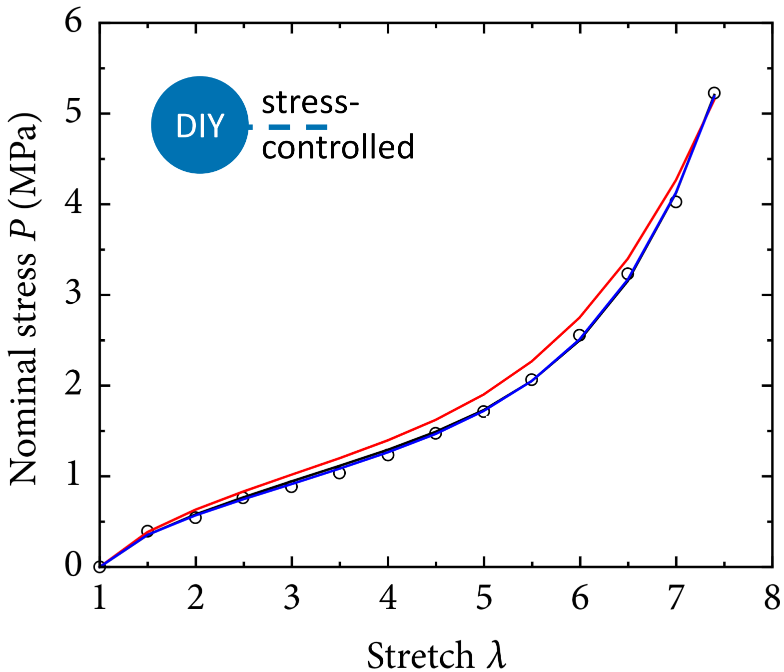
Material parameter estimation

Error measurement functions

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

- Strain-control vs stress-control || Stress-time || Strain-time



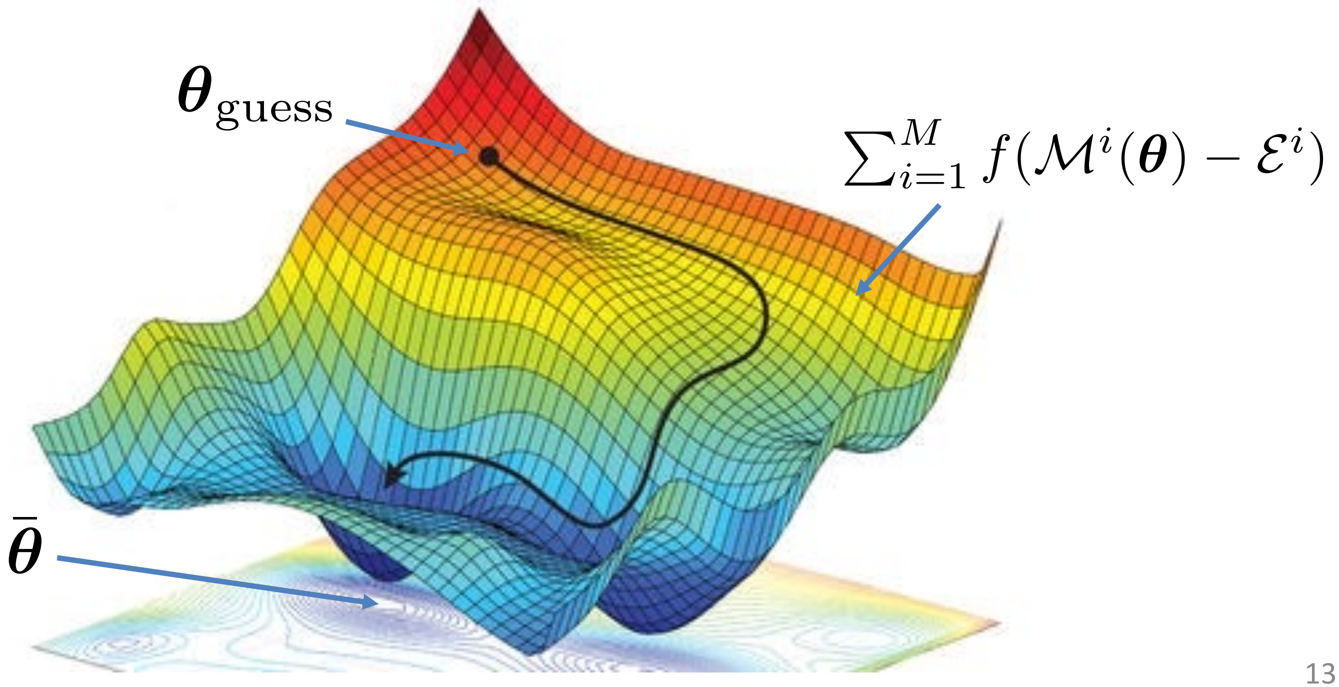


Material parameter estimation

Error measurement functions

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

- Algorithm for finding optimal material parameters (gradient descent algorithms)

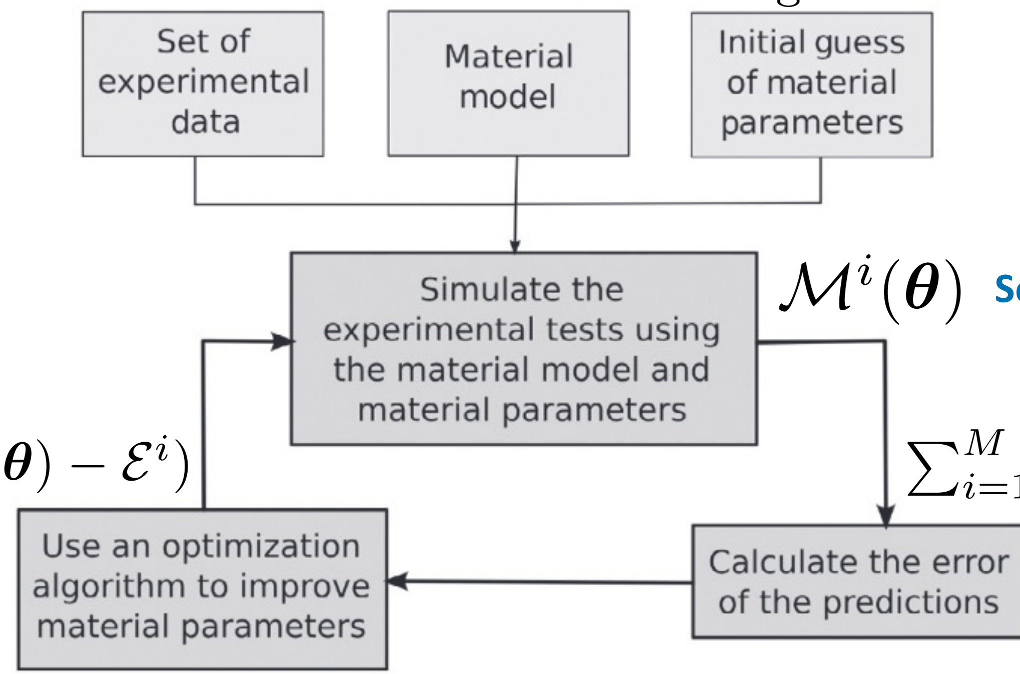


Material parameter estimation

Summary

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

$\mathcal{E}^i$ $\mathcal{M}$ $\boldsymbol{\theta}_{\text{guess}}$



$\mathcal{M}^i(\boldsymbol{\theta})$ **Solid Mechanics II**

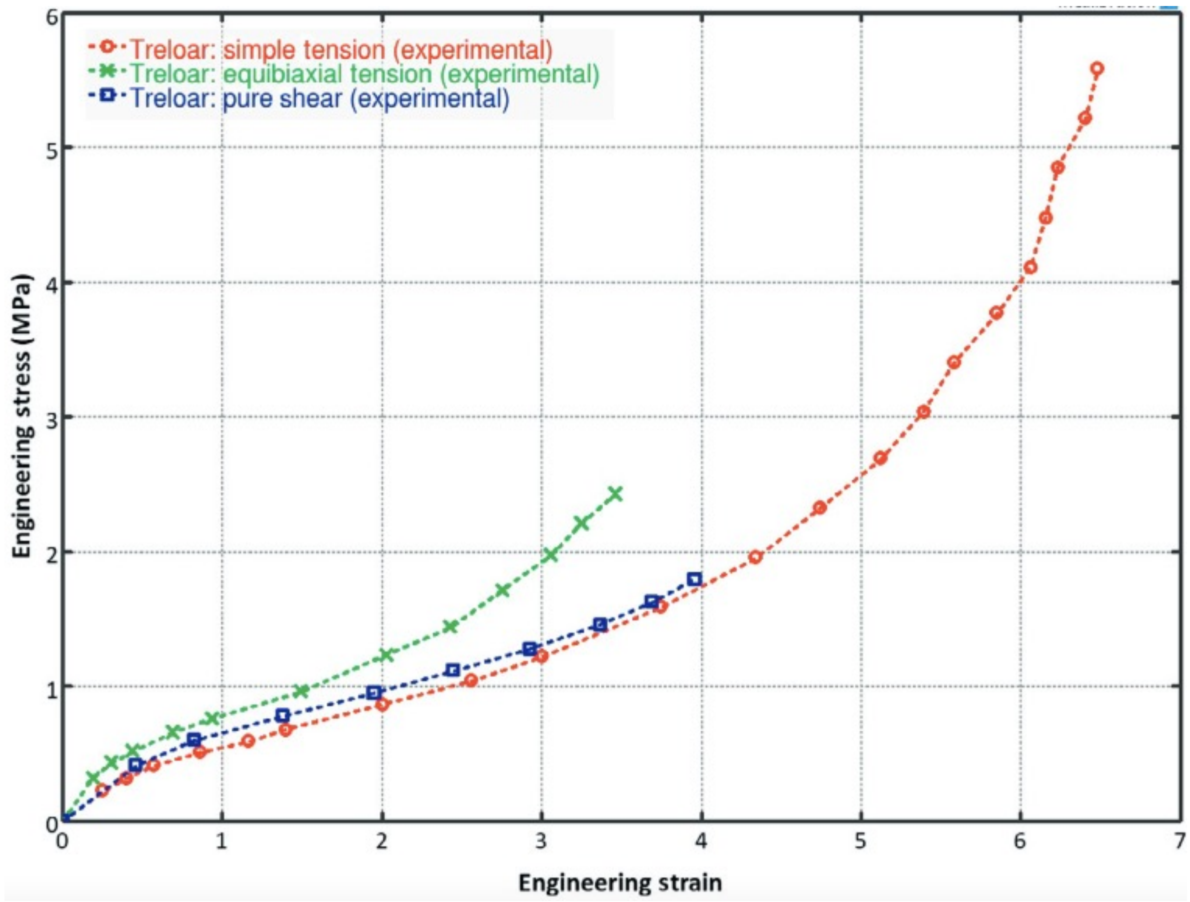
$\sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

$\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

Material parameter estimation

Homework Assignment #3

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$



Material parameter estimation

Material model selection

estimated material parameters $\bar{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{M} f(\mathcal{M}^i(\boldsymbol{\theta}) - \mathcal{E}^i)$

Two models with different number of parameters

$$\mathcal{M}_{(1)} \qquad \boldsymbol{\theta}_{\text{guess}} \in \mathbb{R}^{n_{(1)}} \qquad \bar{\boldsymbol{\theta}}_{(1)}$$

$$\mathcal{M}_{(2)} \qquad \boldsymbol{\theta}_{\text{guess}} \in \mathbb{R}^{n_{(2)}} \qquad \bar{\boldsymbol{\theta}}_{(2)}$$

Akaike information criterion (AIC): balance between minimization of goodness of the fit and number of parameters (or complexity of the model)

$$\text{AIC}_{1,2} = (n_{(2)} - n_{(1)}) - M \ln(\text{SSE}_{(1)}/\text{SSE}_{(2)})$$

with $\text{SSE}_{(1)} = \sum(\mathcal{M}^i_{(1)}(\boldsymbol{\theta}) - \mathcal{E}^i)^2$. If $\text{AIC}_{1,2} < 0$ then model 2 is a better option than model 1.

Material parameter estimation

Any questions?