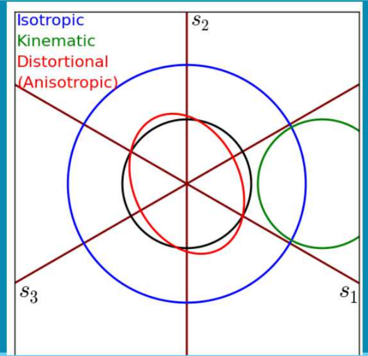
SAND2019-13623PE

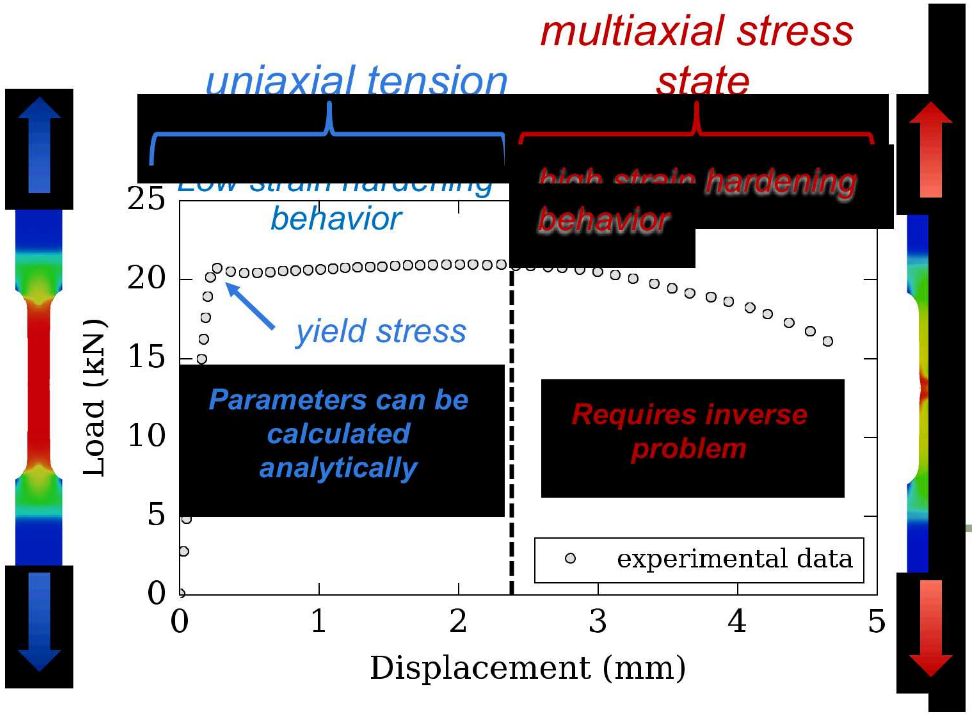
Material Model Exemplars – Sandia National Laboratories



Brian Lester

Elizabeth Jones

Matt Kury



NSE CROSS-SITE MEETING ON CALIBRATED MATERIAL MODELS

Constitutive Modeling Introduction

Brian Lester, Sandia National Laboratories

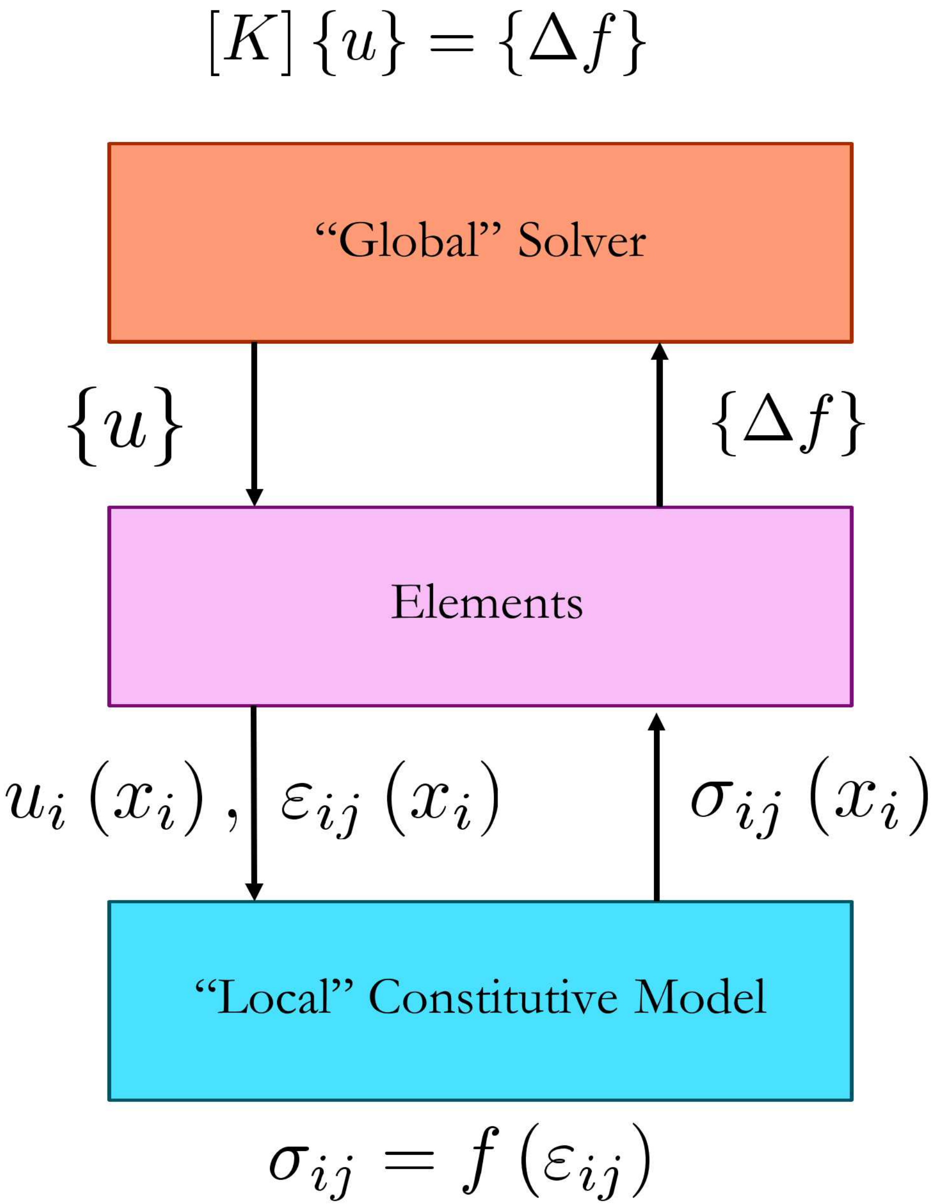
NSE CROSS-SITE MEETING ON CALIBRATED
MATERIAL MODELS

Constitutive Model

- "A constitutive equation demonstrates a relation between two physical quantities that is specific to a material or substance and does not follow directly from physical laws" (J. Fish, 2014, *Practical Multiscaling*, Wiley)

- Essential for the solution of structural boundary value problems

- Provides closure relations
  - Mathematically
  - Introduces material physics



$$[K]\{u\} = \{\Delta f\}$$

"Global" Solver

$\{u\}$

$\{\Delta f\}$

Elements

$u_i(x_i), \varepsilon_{ij}(x_i)$

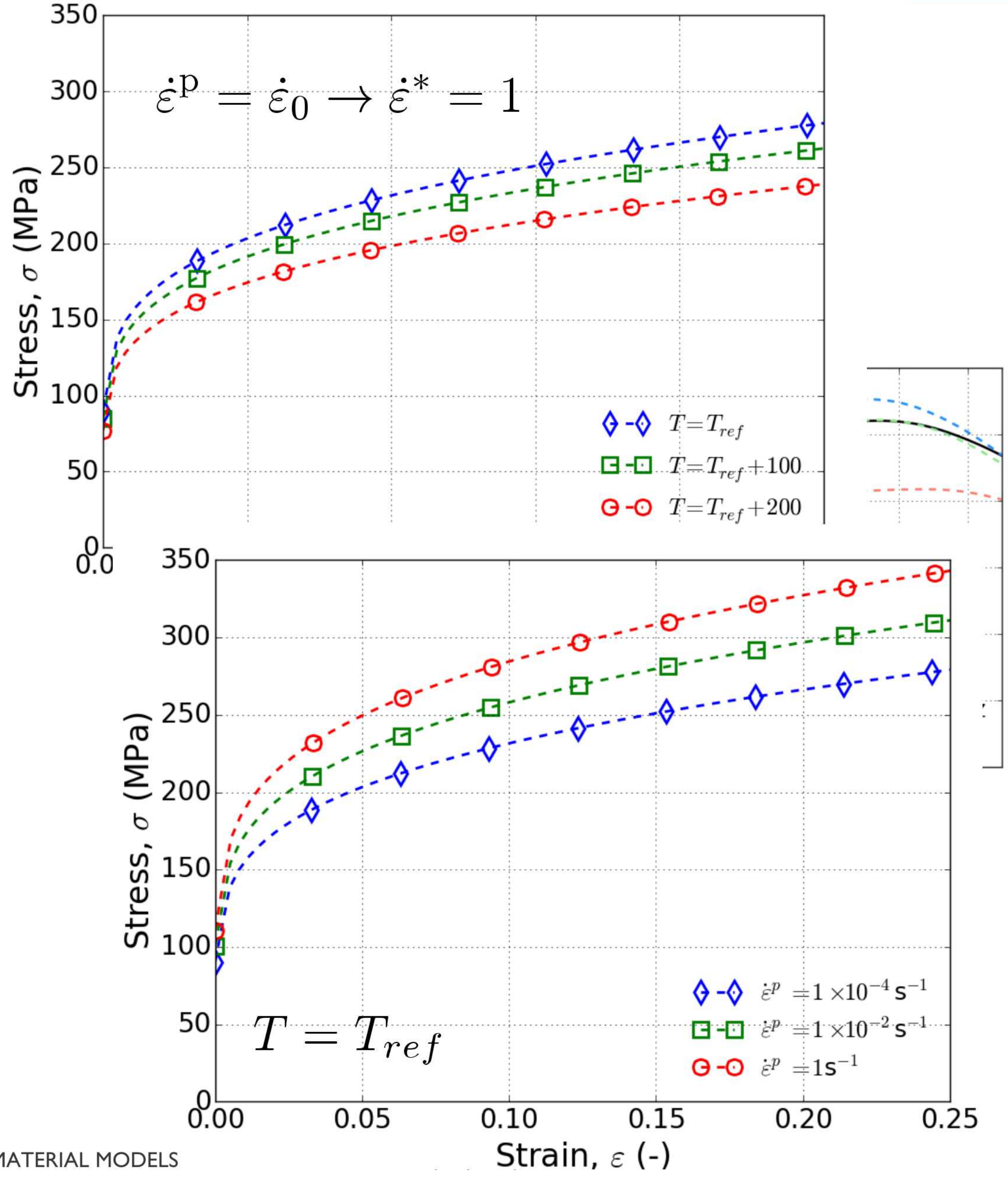
$\sigma_{ij}(x_i)$

"Local" Constitutive Model

$$\sigma_{ij} = f(\varepsilon_{ij})$$

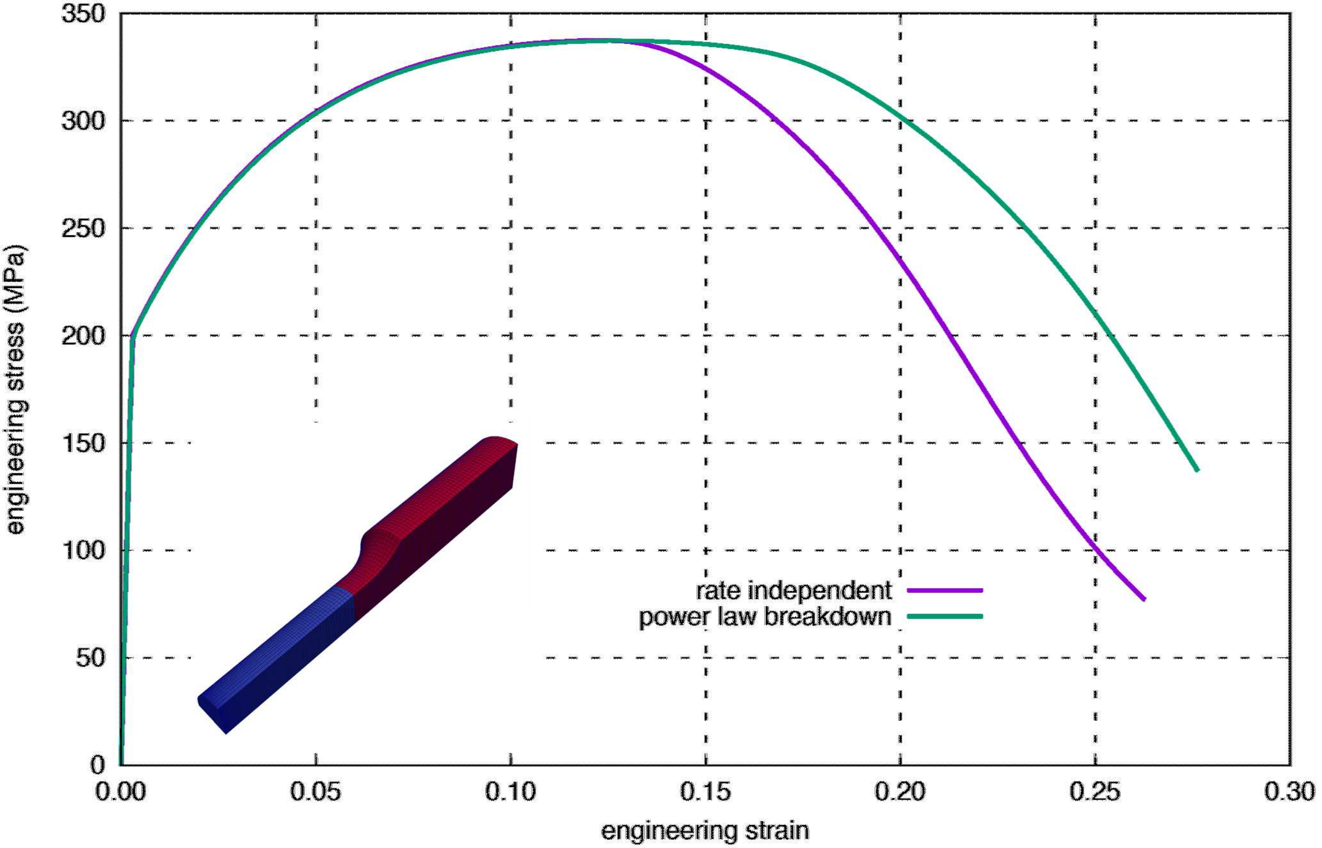
Constitutive Modeling in FEA

- Constitutive model implementation in Sierra/SolidMechanics via Library of Advanced Materials for Engineering (LAMÉ)
- LAMÉ consists of large set of models covering different responses, cost, and fidelity
- Require flexible, robust, and verified numerical implementation
- Models span:
    - Deformation mechanisms (e.g. plasticity, viscoelasticity,)
    - Dependencies (e.g. rate, temperature)



Constitutive Calibration

Model of Tensile Test w/ anisotropic plasticity model w/ and w/out rate-dependence



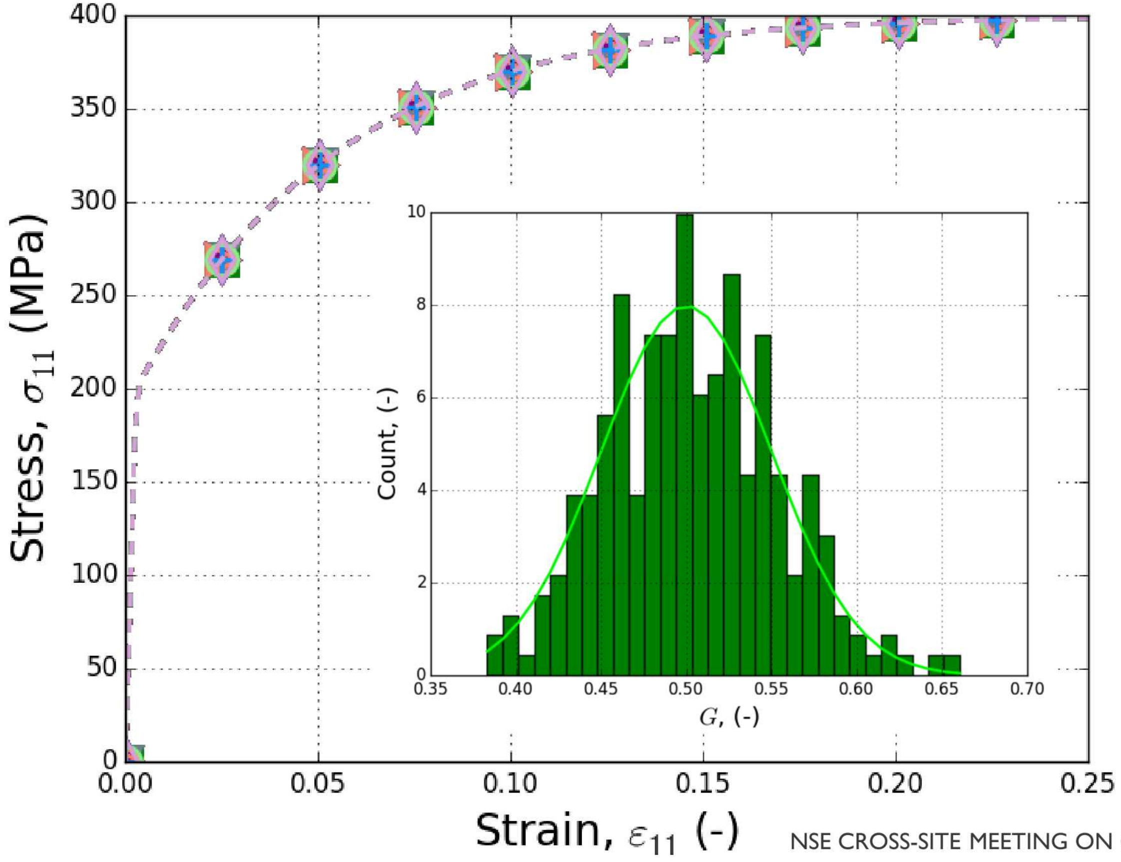
- Calibration is essential for constitutive model utilization
  - Different fits to same data can result from various choices
  - Increasing fidelity requires increased fit parameters
  - Efficient approaches represent enabling capability

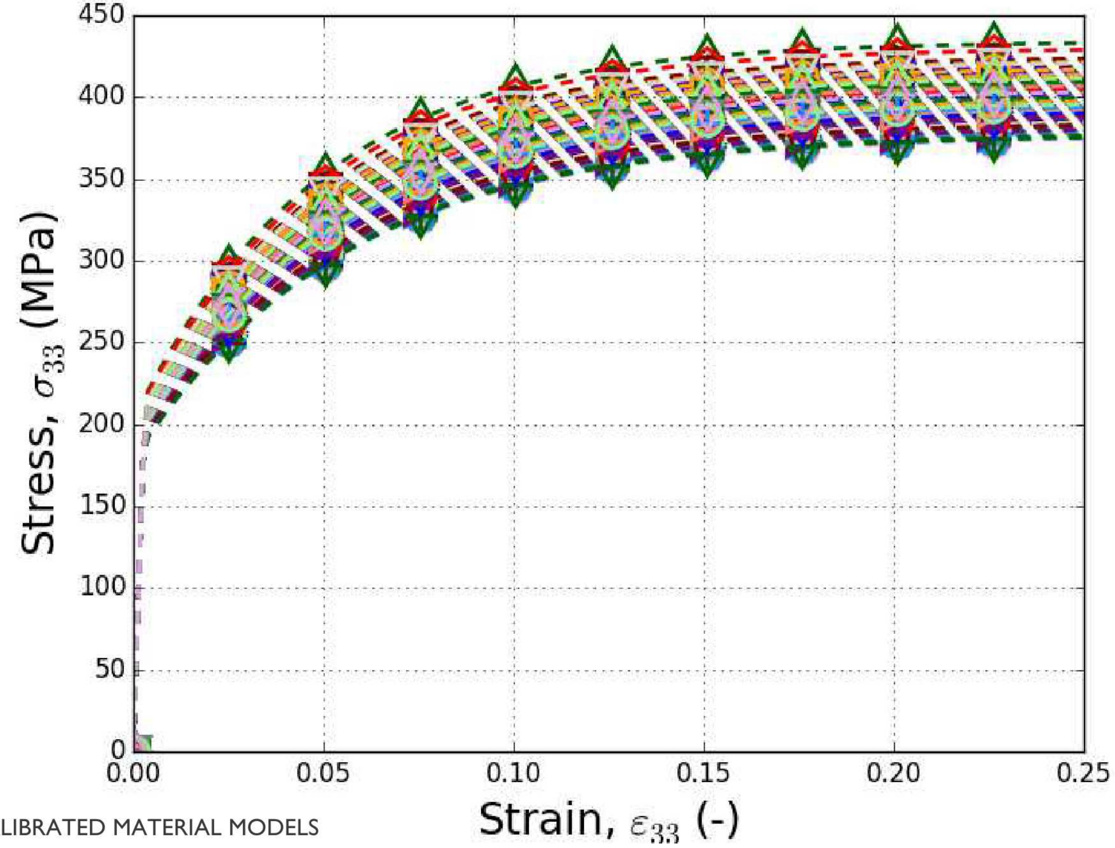
- Need to be able to parse different phenomenology
  - Model form selection
  - Some response characteristics can be produced via multiple fits

Model Form Issues

- Parsing impact of different model forms and appropriate identification important in calibration
  - “Under resolved” data to model form (AKA “non-unique” fits)
  - Correctly identifying these issues essential for structural prediction

$$\left(\phi^{(\mathrm{H})}\left(\sigma_{ij}\right)\right)^2 = F\left(\hat{\sigma}_{22}-\hat{\sigma}_{33}\right)^2 + G\left(\hat{\sigma}_{33}-\hat{\sigma}_{11}\right)^2 + H\left(\hat{\sigma}_{11}-\hat{\sigma}_{22}\right)^2 + 2L\hat{\sigma}_{23}^2 + 2M\hat{\sigma}_{31}^2 + 2N\hat{\sigma}_{12}^2$$



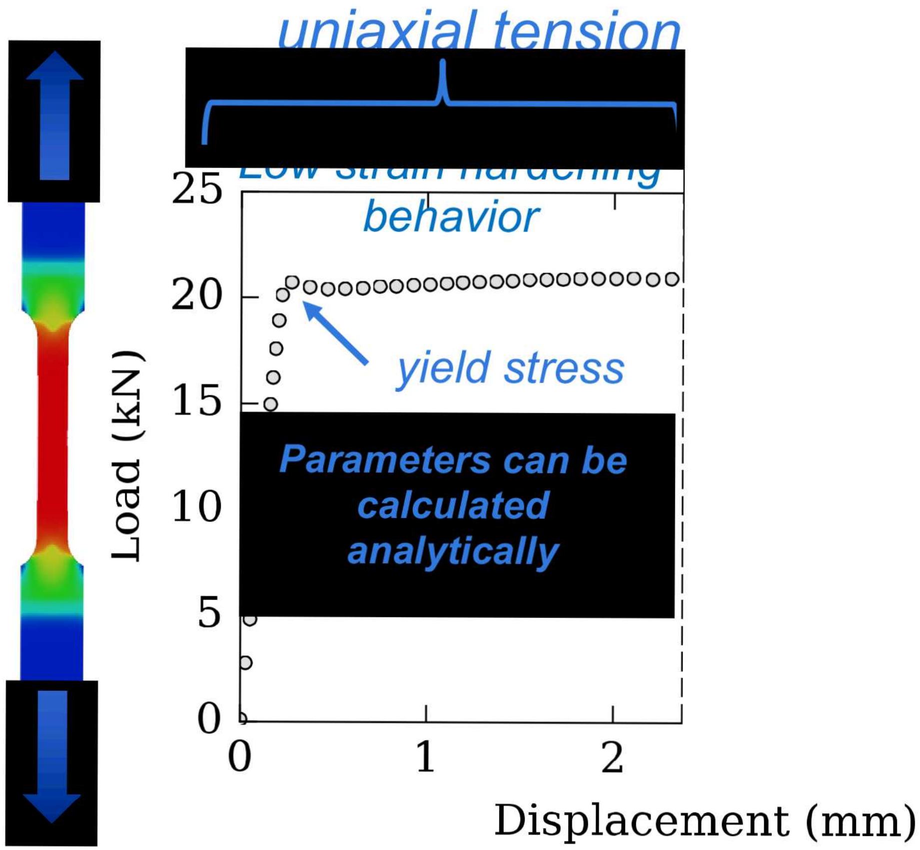


Calibration Workflow Overview

Matt Kury, Sandia National Laboratories

Material Model Calibration Process

$$\sigma = f(\nabla_s u\ , \nabla_s v; s_0, s_1, ..s_n; p_1, p_2, ..p_n)$$



uniaxial tension

[redacted]

behavior

yield stress

Parameters can be calculated analytically

Material Model Calibration Process

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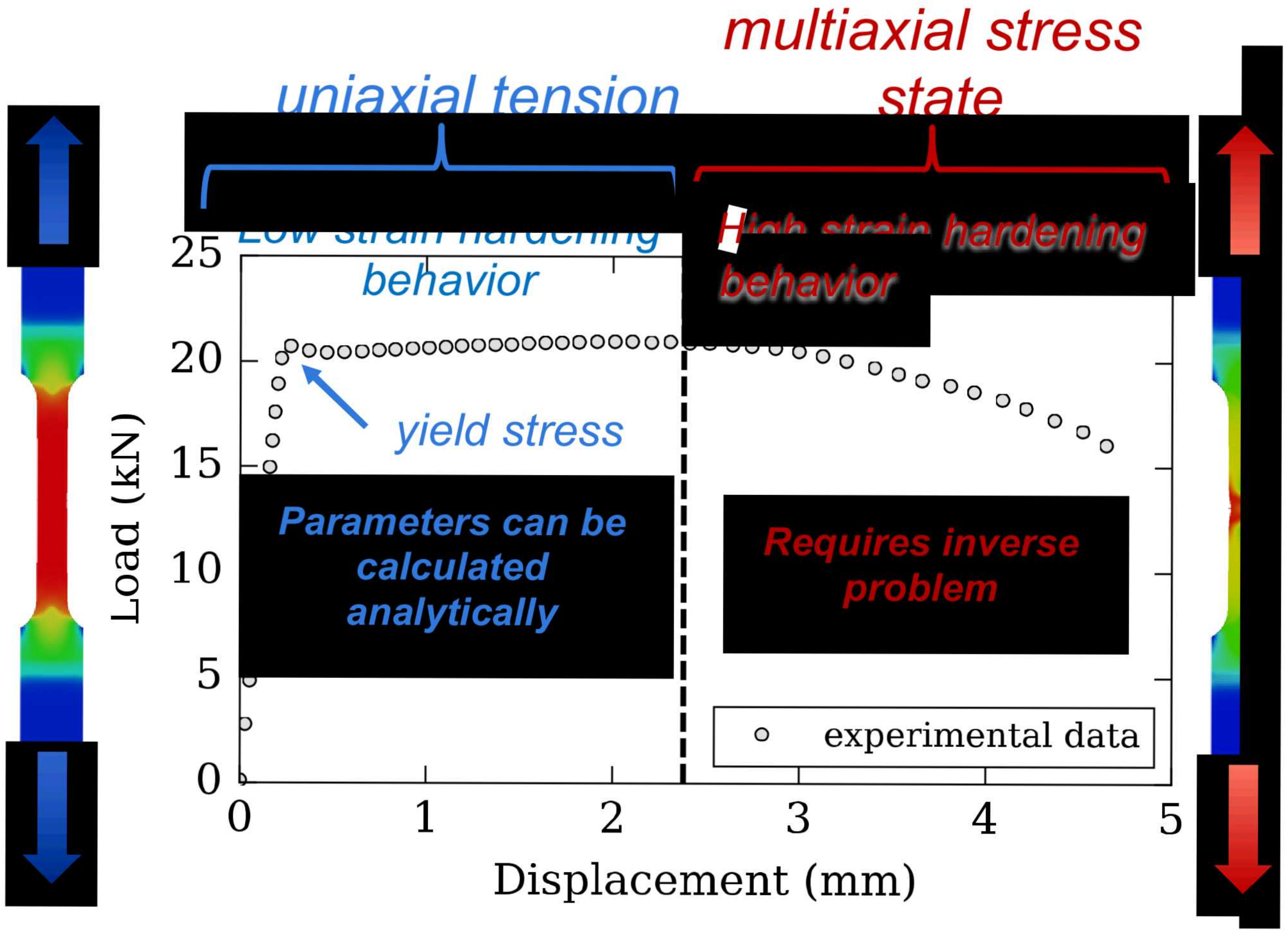
multiaxial stress state

uniaxial tension

Low strain hardening behavior

High strain hardening behavior

yield stress

Parameters can be calculated analytically

Requires inverse problem

Material Model Calibration Process

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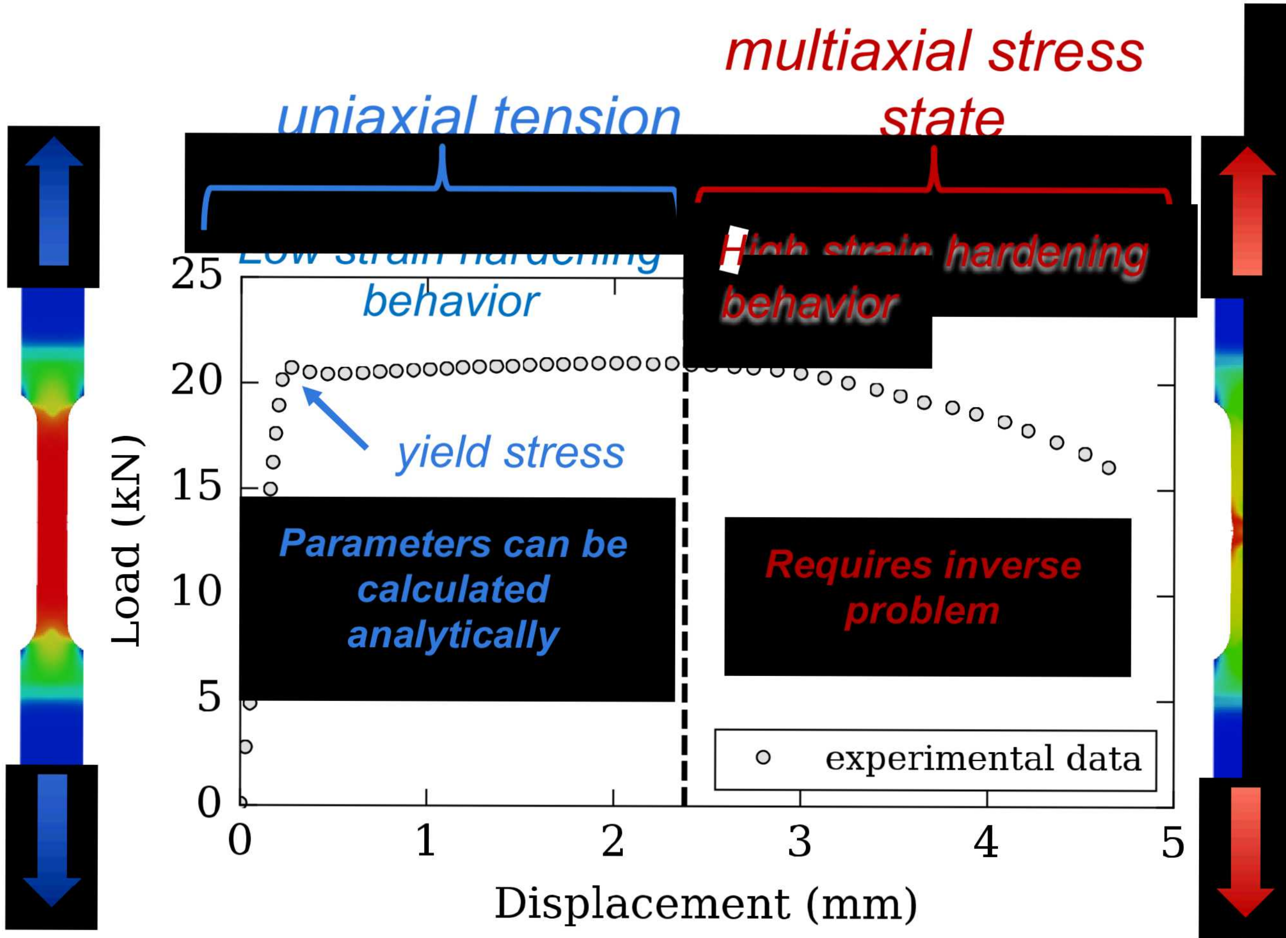

[redacted]

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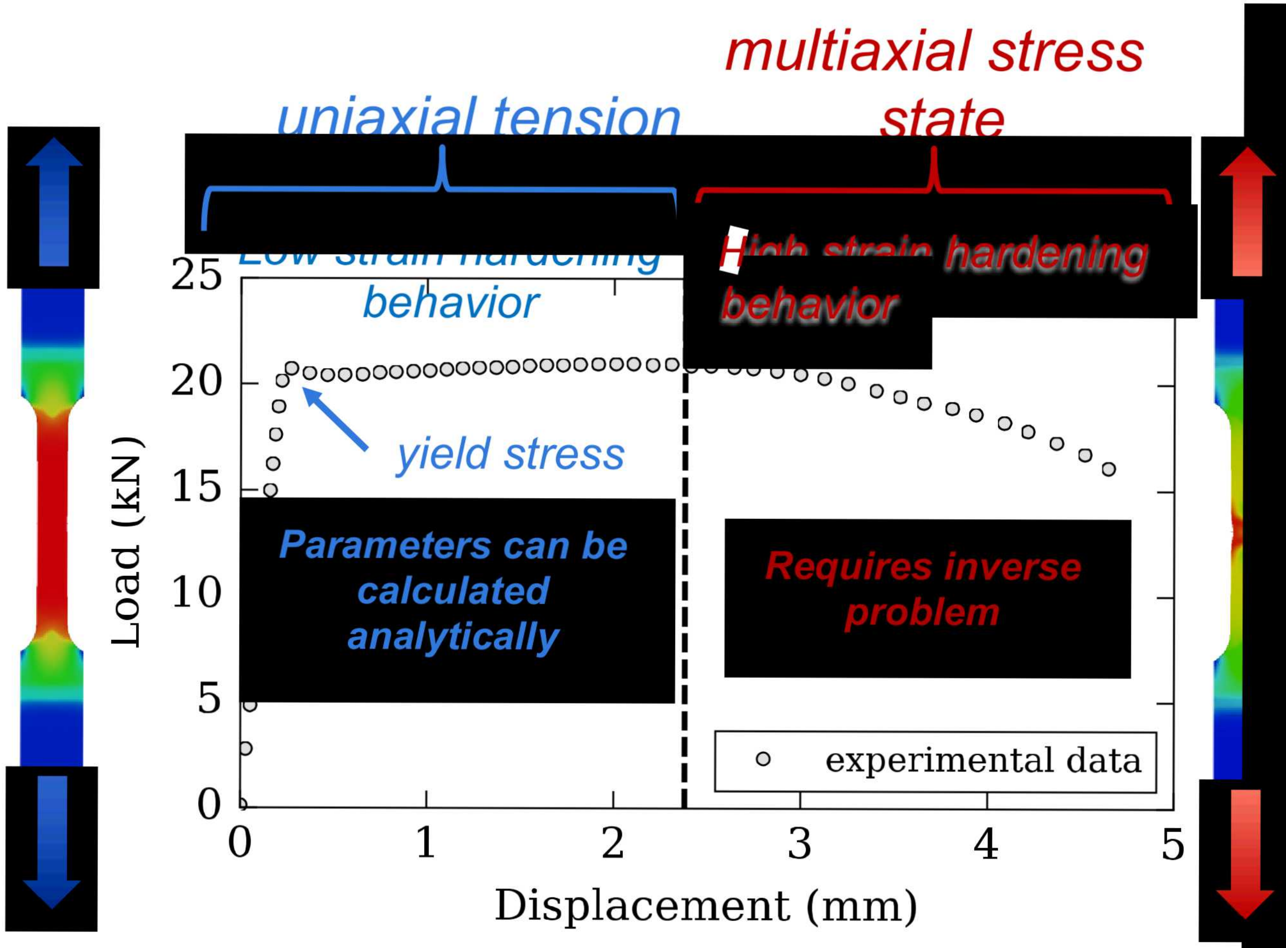
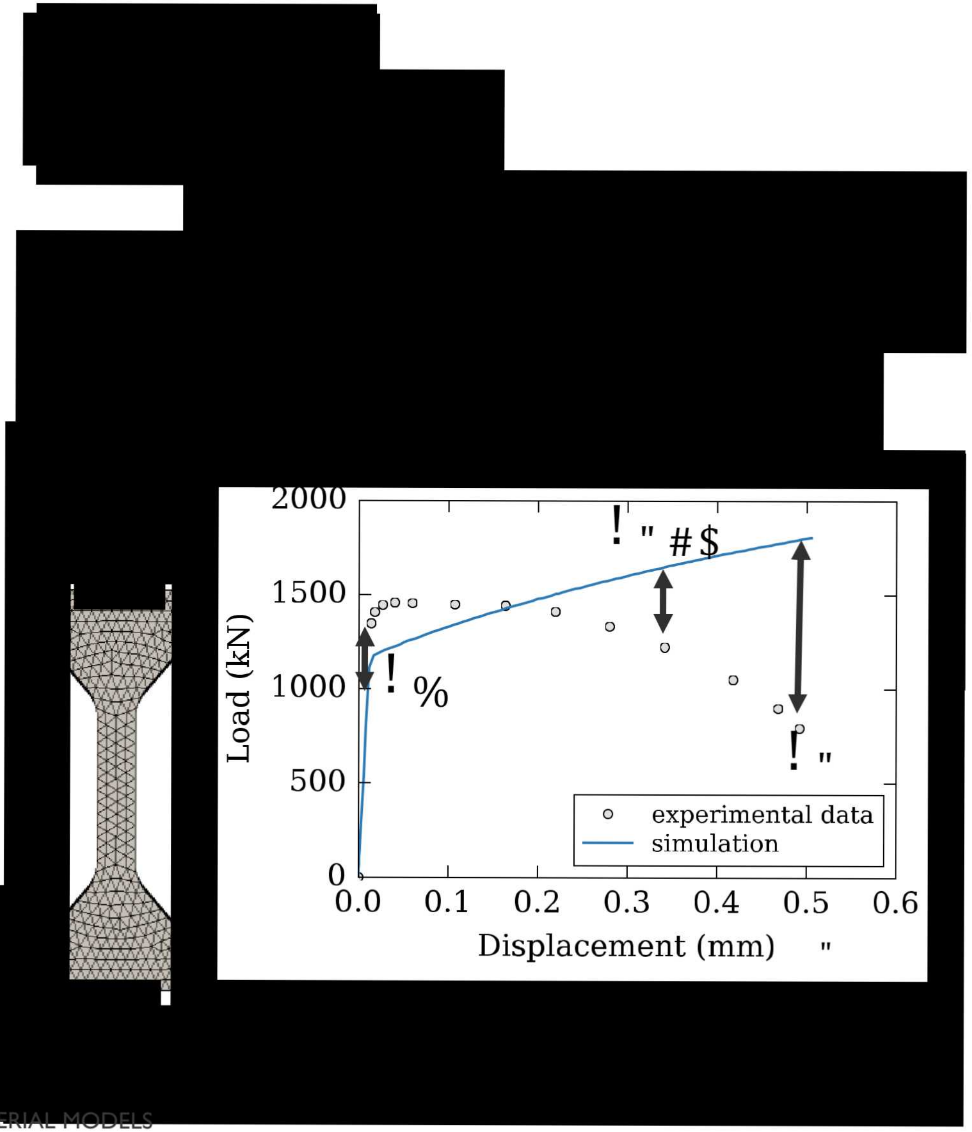
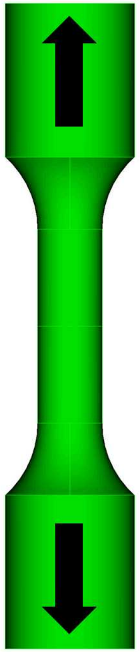




Workflow to get a Calibration Result



1. Gather and process experimental data
2. Decide on a material model form for calibration
3. Create my mesh & input deck to simulate each experiment
4. Create my input script for my optimization library
5. Create my analysis tool to translate my simulation results to a residual or objective function for my optimization library
6. Run my optimization
7. Debug errors I made somewhere along the way

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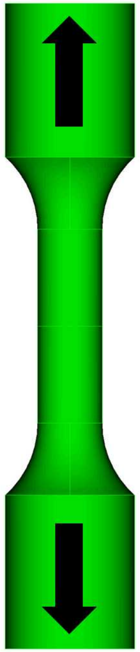

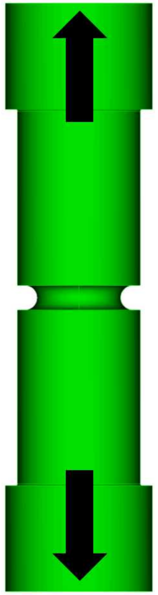

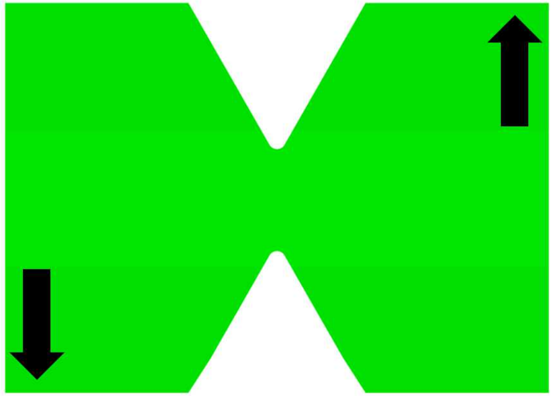

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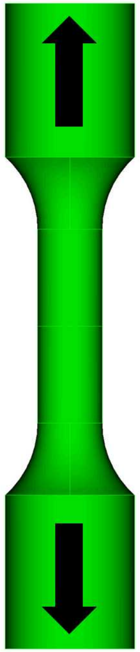

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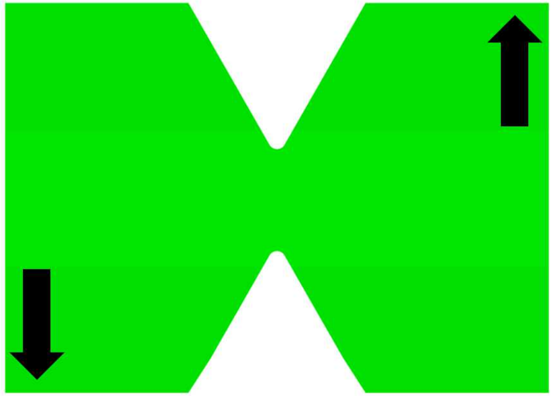
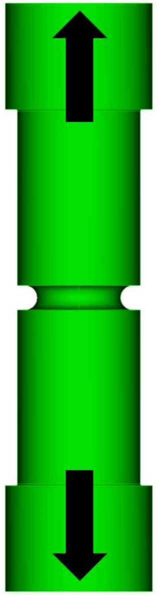
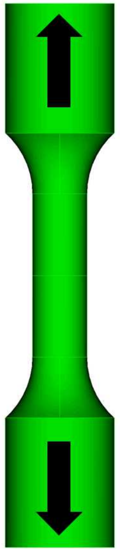




Workflow to get a Calibration Result with MatCal



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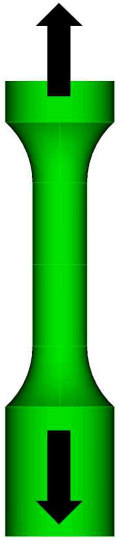

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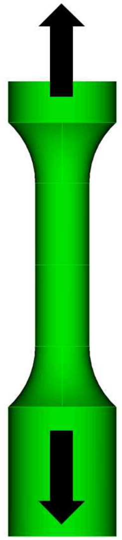
MatCal

Workflow to get a Calibration Result with MatCal



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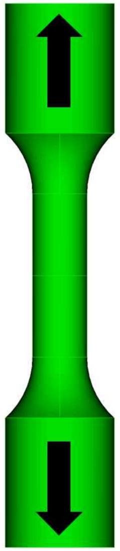

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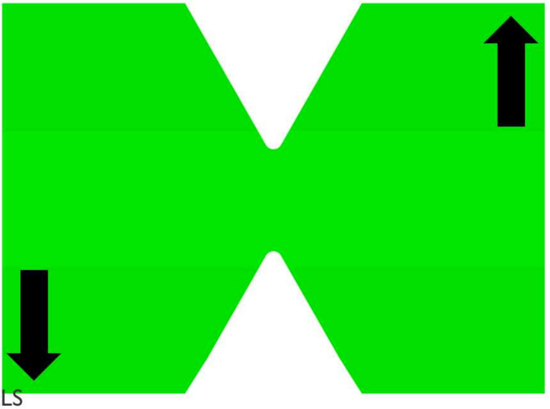

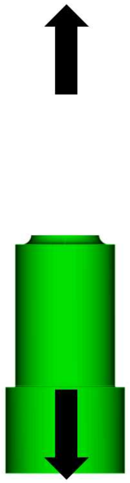

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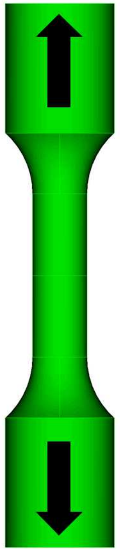

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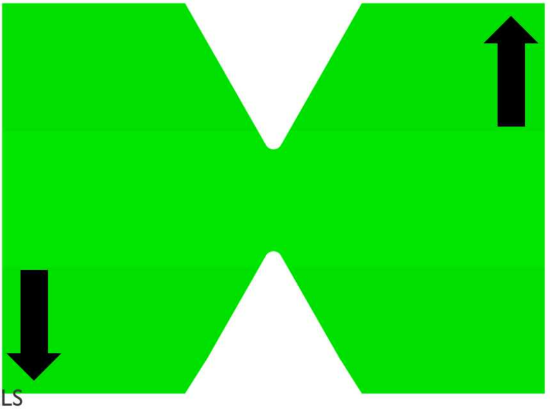
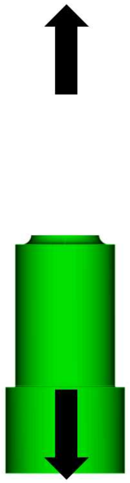




MatCal Features Overview

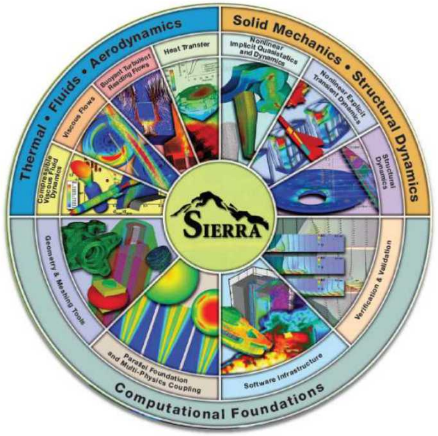
Matt Kury, Sandia National Laboratories

Simple and Powerful Unified Interface for Material Calibration

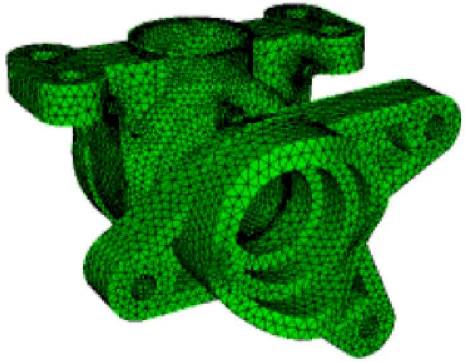
- Leverages various Sandia computing tools
- Written in Python
  - Leverage the power of scripting
- Verification testing suite to ensure correctness of methods
- Built in plotting tools to easily monitor the progression of calibrations
- Written with extensibility in mind

DAKOTA

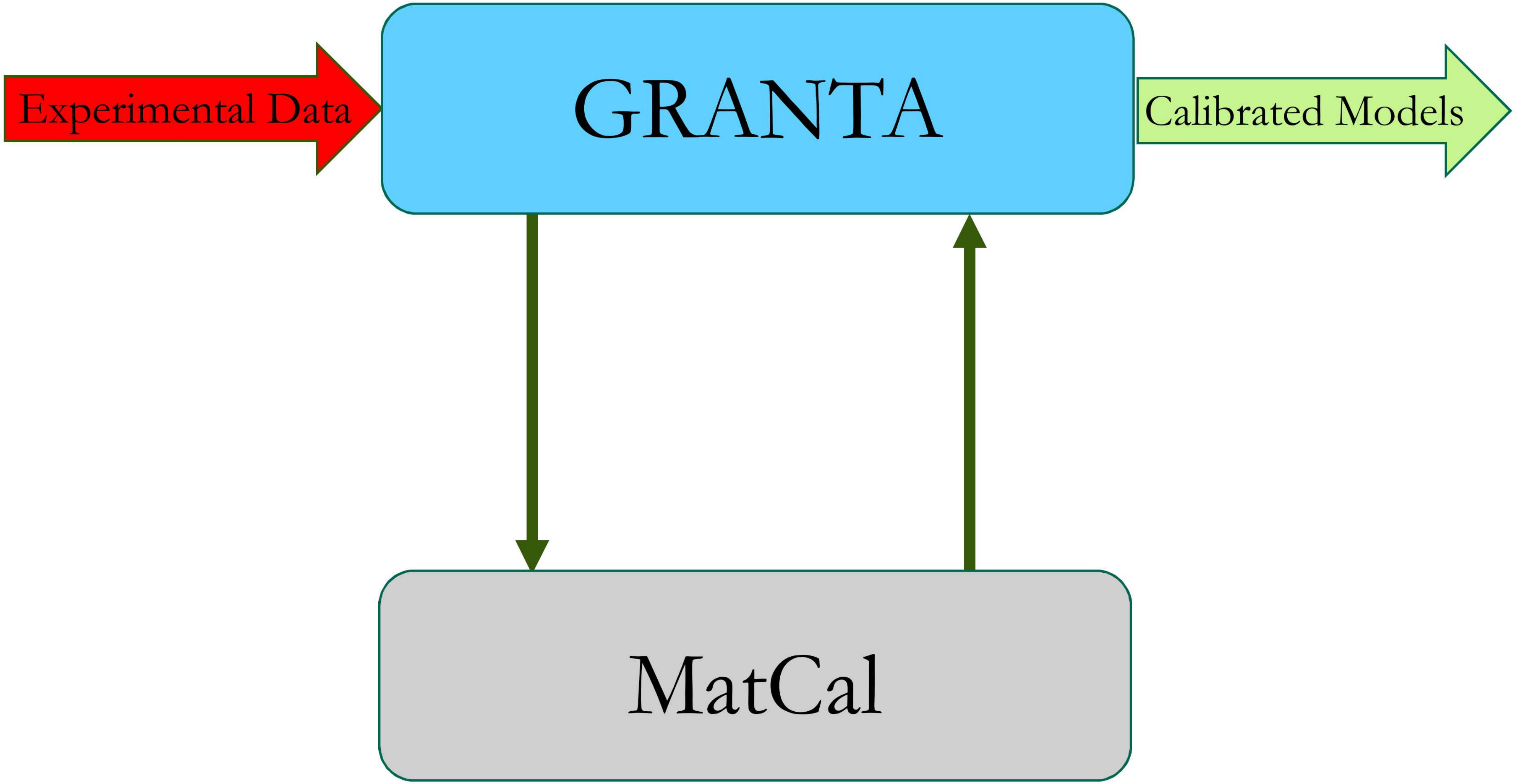
Explore and predict with confidence.



python™



Traceability Built Into The Workflow.



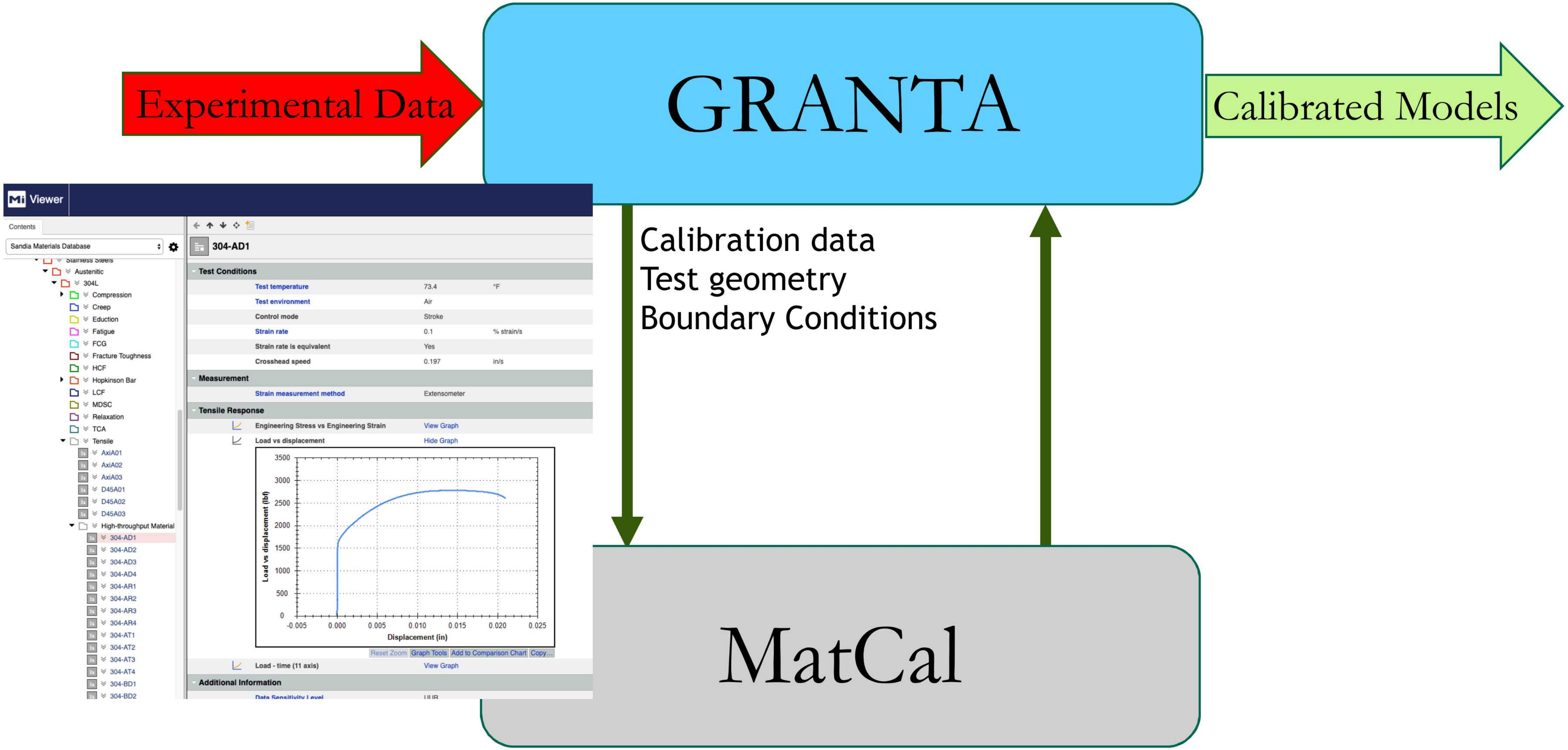
Experimental Data

GRANTA

Calibrated Models

MatCal

Traceability Built Into The Workflow.



Experimental Data

GRANTA

Calibrated Models

Calibration data
Test geometry
Boundary Conditions

MatCal

- Stainless Steels
  - Austenitic
    - 304L
      - Compression
      - Creep
      - Eduction
      - Fatigue
      - FCG
      - Fracture Toughness
      - HCF
      - Hopkinson Bar
      - LCF
      - MDSC
      - Relaxation
      - TCA
      - Tensile
        - AxiA01
        - AxiA02
        - AxiA03
        - D45A01
        - D45A02
        - D45A03
        - High-throughput Material
          - 304-AD1
          - 304-AD2
          - 304-AD3
          - 304-AD4
          - 304-AR1
          - 304-AR2
          - 304-AR3
          - 304-AR4
          - 304-AT1
          - 304-AT2
          - 304-AT3
          - 304-AT4
          - 304-BD1
          - 304-BD2

304-AD1

Test Conditions

Test temperature	73.4	°F
Test environment	Air	
Control mode	Stroke	
Strain rate	0.1	% strain/s
Strain rate is equivalent	Yes	
Crosshead speed	0.197	in/s

Measurement

Strain measurement method	Extensometer

Tensile Response

Engineering Stress vs Engineering Strain	View Graph
Load vs displacement	Hide Graph

Load - time (11 axis)	View Graph

Additional Information

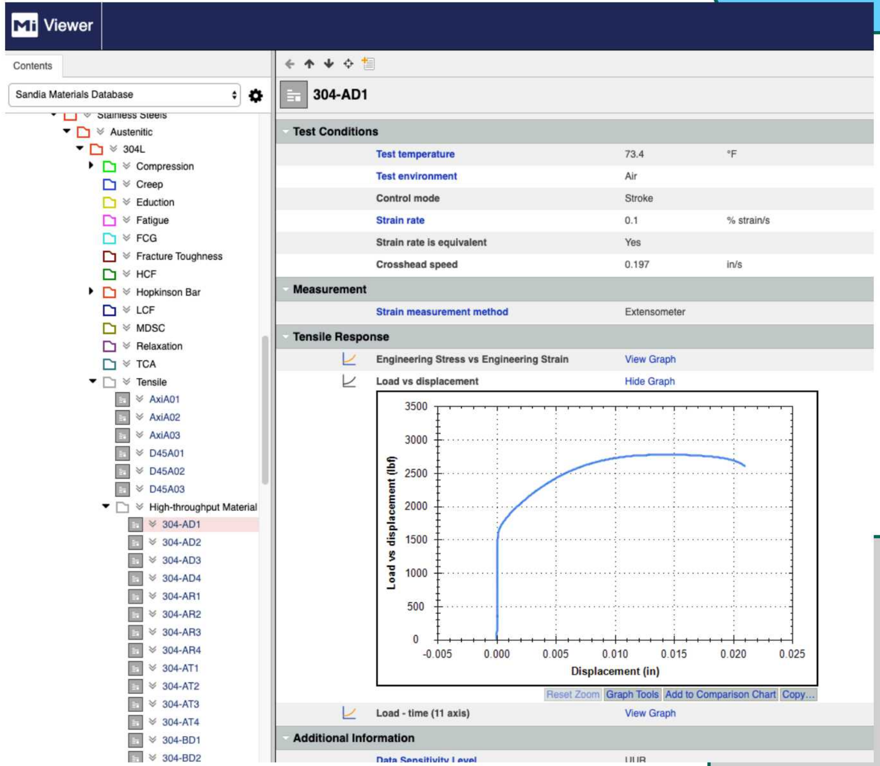
Data Sensitivity Level	UUR

Traceability Built Into The Workflow.

Experimental Data

GRANTA

Calibrated Models



304-AD1

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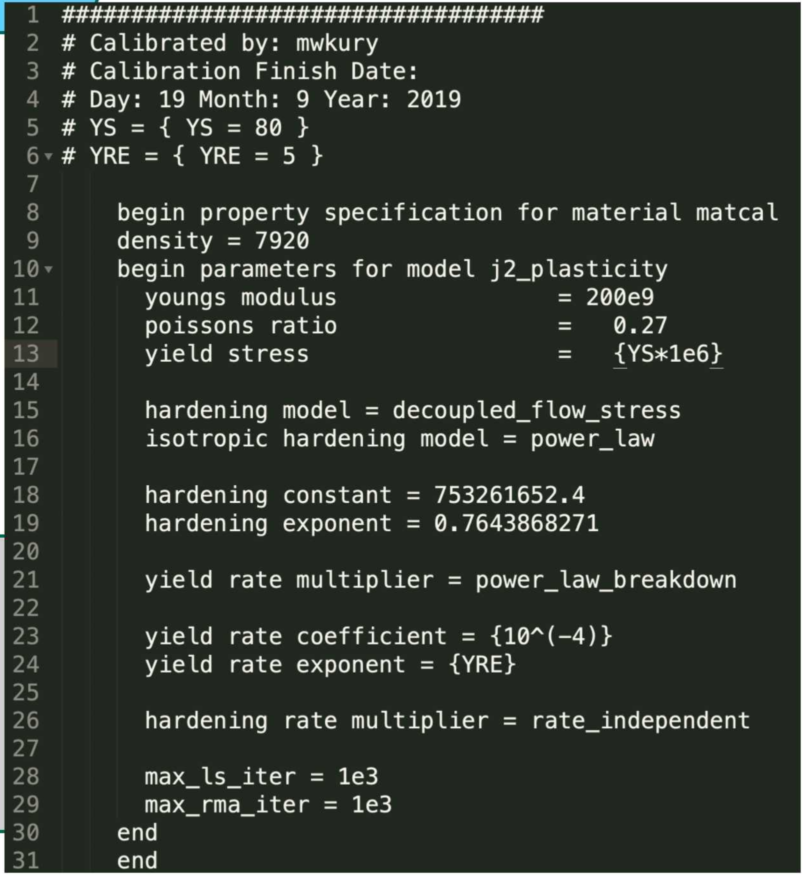
Calibration data
Test geometry
Boundary Conditions

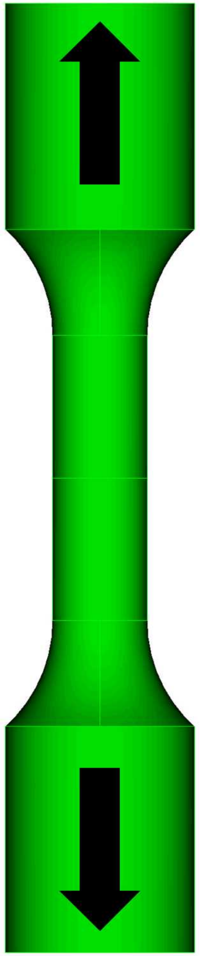
Parameters
Objective
function
Valid regime

MatCal



```
####################################
# Calibrated by: mwkury
# Calibration Finish Date:
# Day: 19 Month: 9 Year: 2019
# YS = { YS = 80 }
# YRE = { YRE = 5 }

    begin property specification for material matcal
    density = 7920
    begin parameters for model j2_plasticity
      youngs modulus                 = 200e9
      poissons ratio                 =   0.27
      yield stress                   =   {YS*1e6}

      hardening model = decoupled_flow_stress
      isotropic hardening model = power_law

      hardening constant = 753261652.4
      hardening exponent = 0.7643868271

      yield rate multiplier = power_law_breakdown

      yield rate coefficient = {10^(-4)}
      yield rate exponent = {YRE}

      hardening rate multiplier = rate_independent

      max_ls_iter = 1e3
      max_rma_iter = 1e3
    end
    end
```

Built-in Standardized Tests



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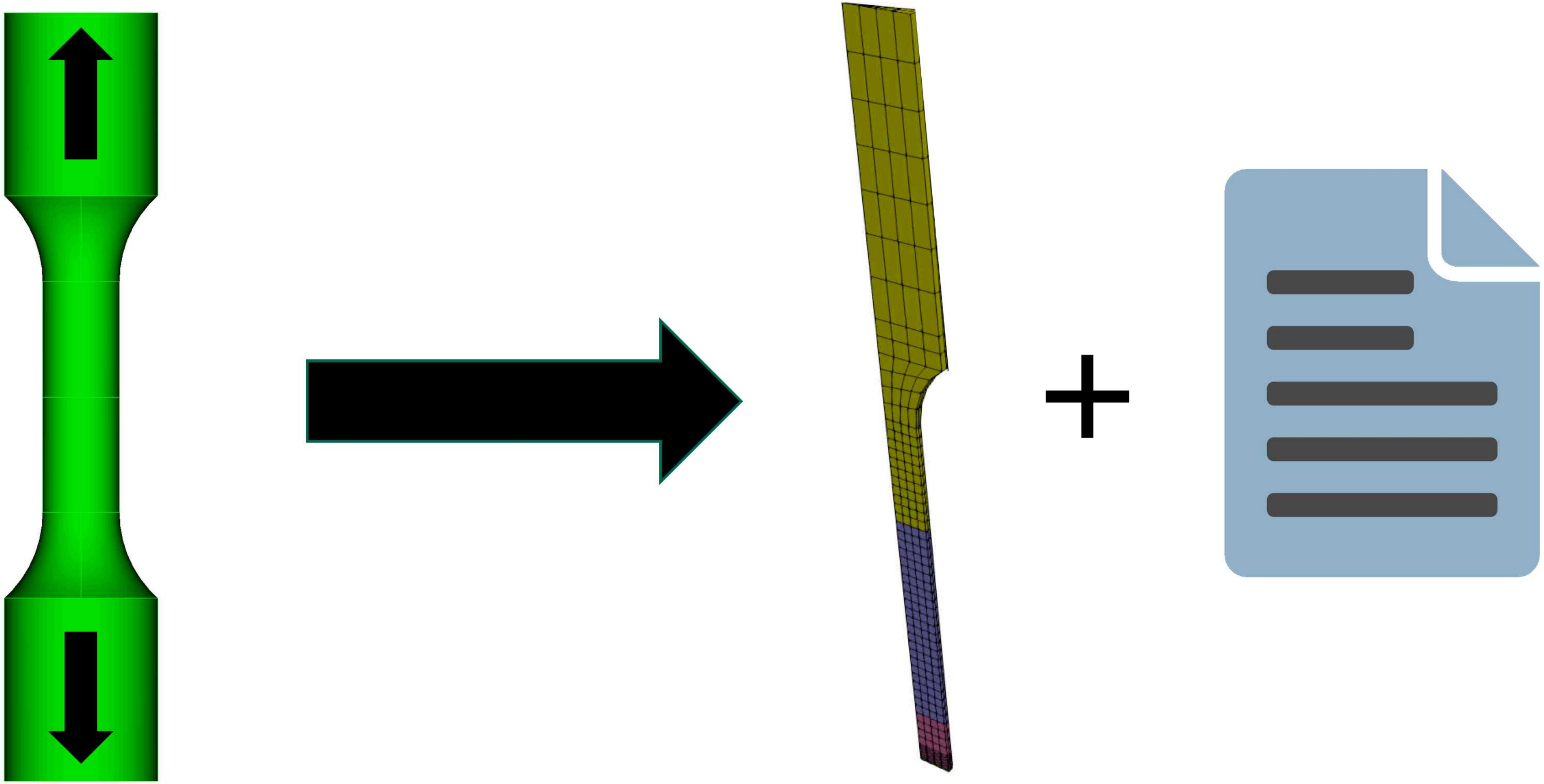
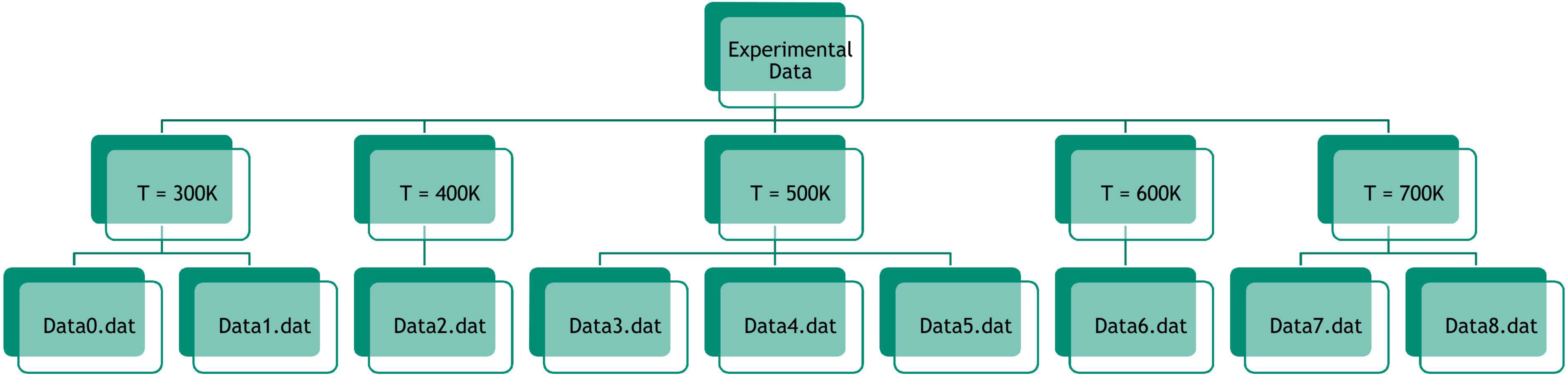


Built with Experimental States in Mind



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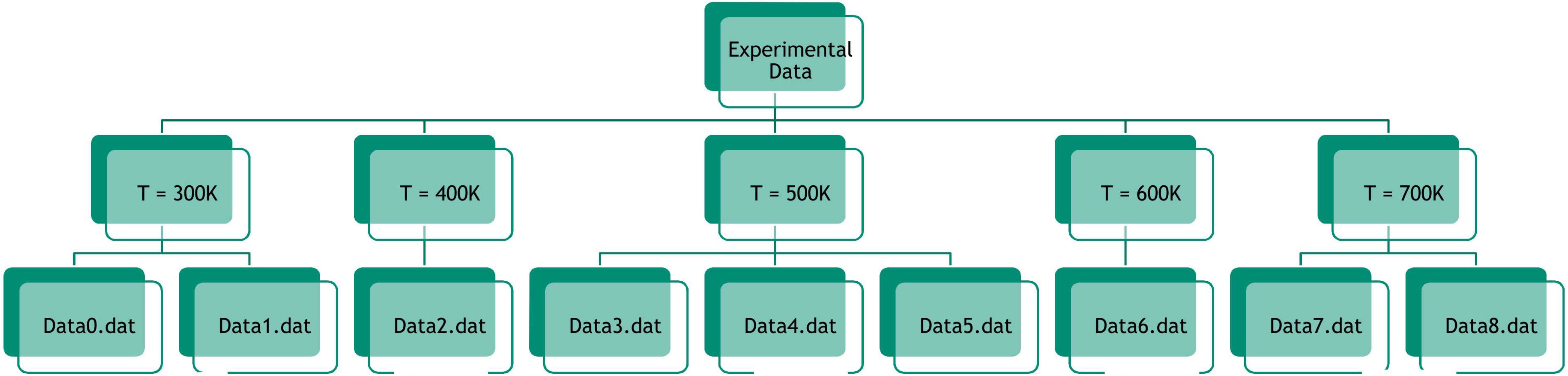
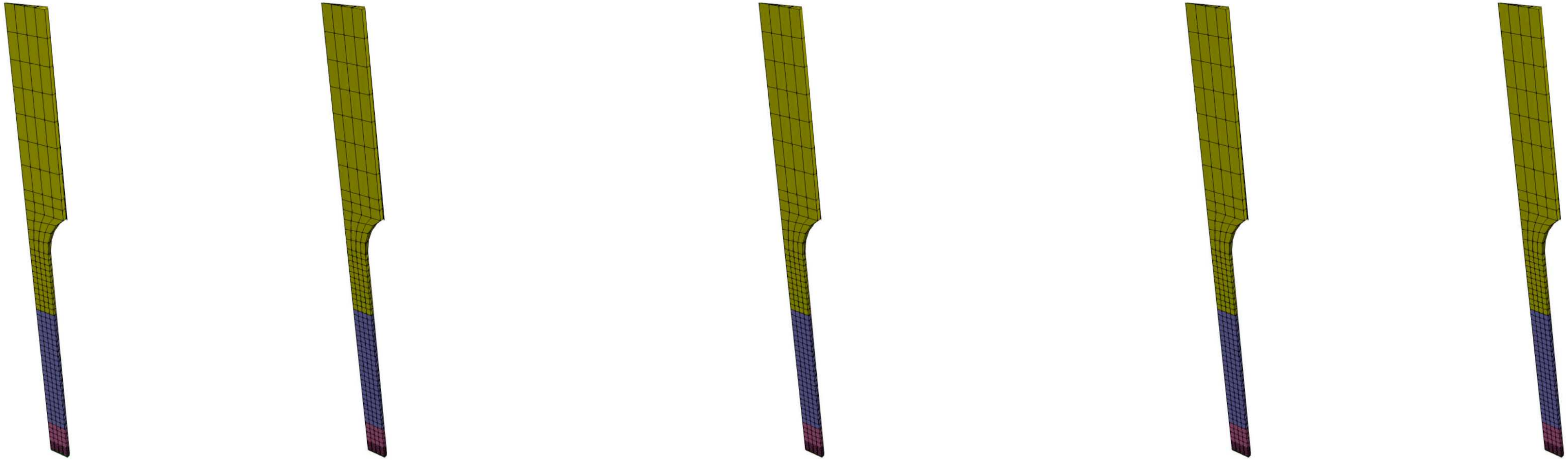


- Experimental Data
  - T = 300K
    - Data0.dat
    - Data1.dat
  - T = 400K
    - Data2.dat
  - T = 500K
    - Data3.dat
    - Data4.dat
    - Data5.dat
  - T = 600K
    - Data6.dat
  - T = 700K
    - Data7.dat
    - Data8.dat

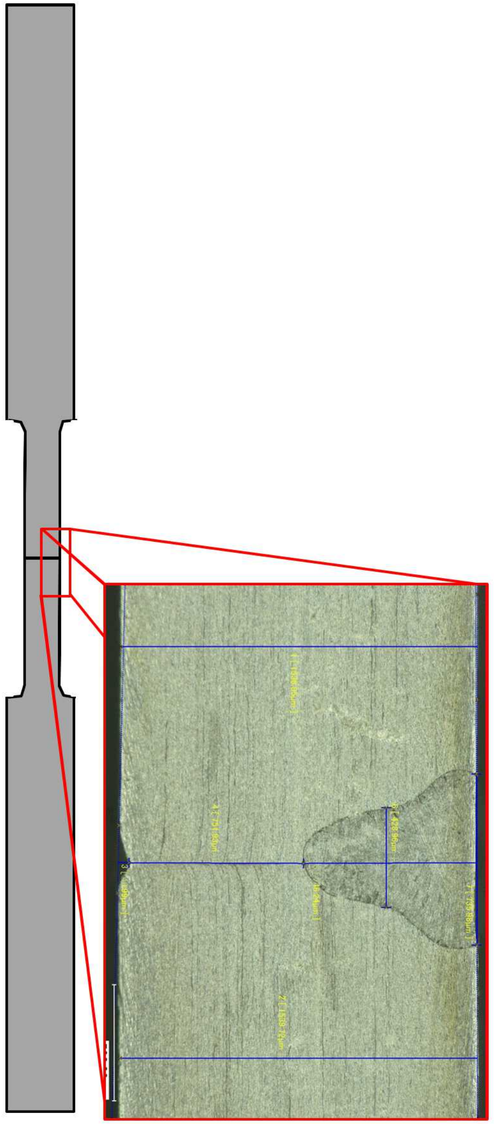


MatCal Stories

Matt Kury, Sandia National Laboratories

Determining Cause of Laser Weld Mechanical Variability

Experimental Setup



Experimental data provided by John Madison, Helena Jin

Determining Cause of Laser Weld Mechanical Variability

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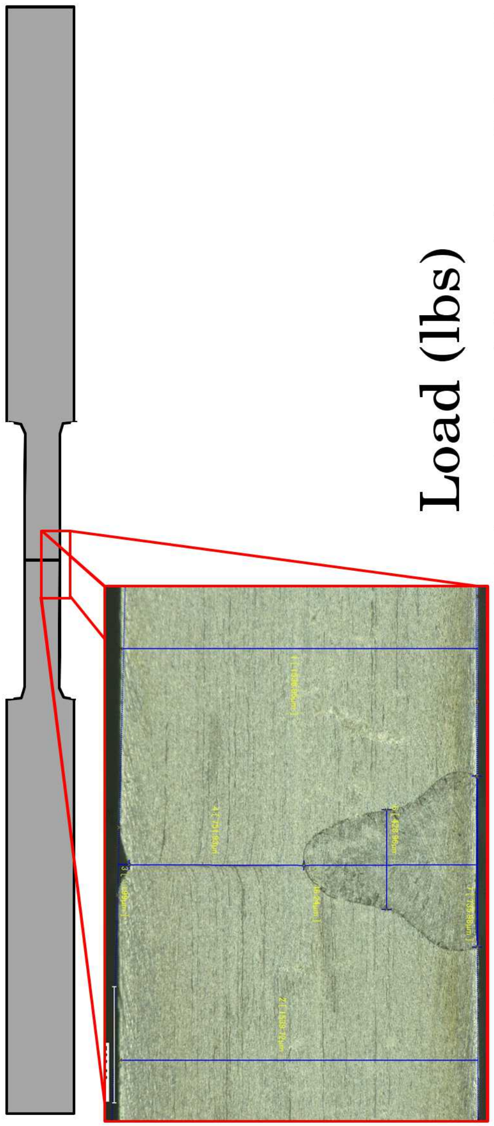

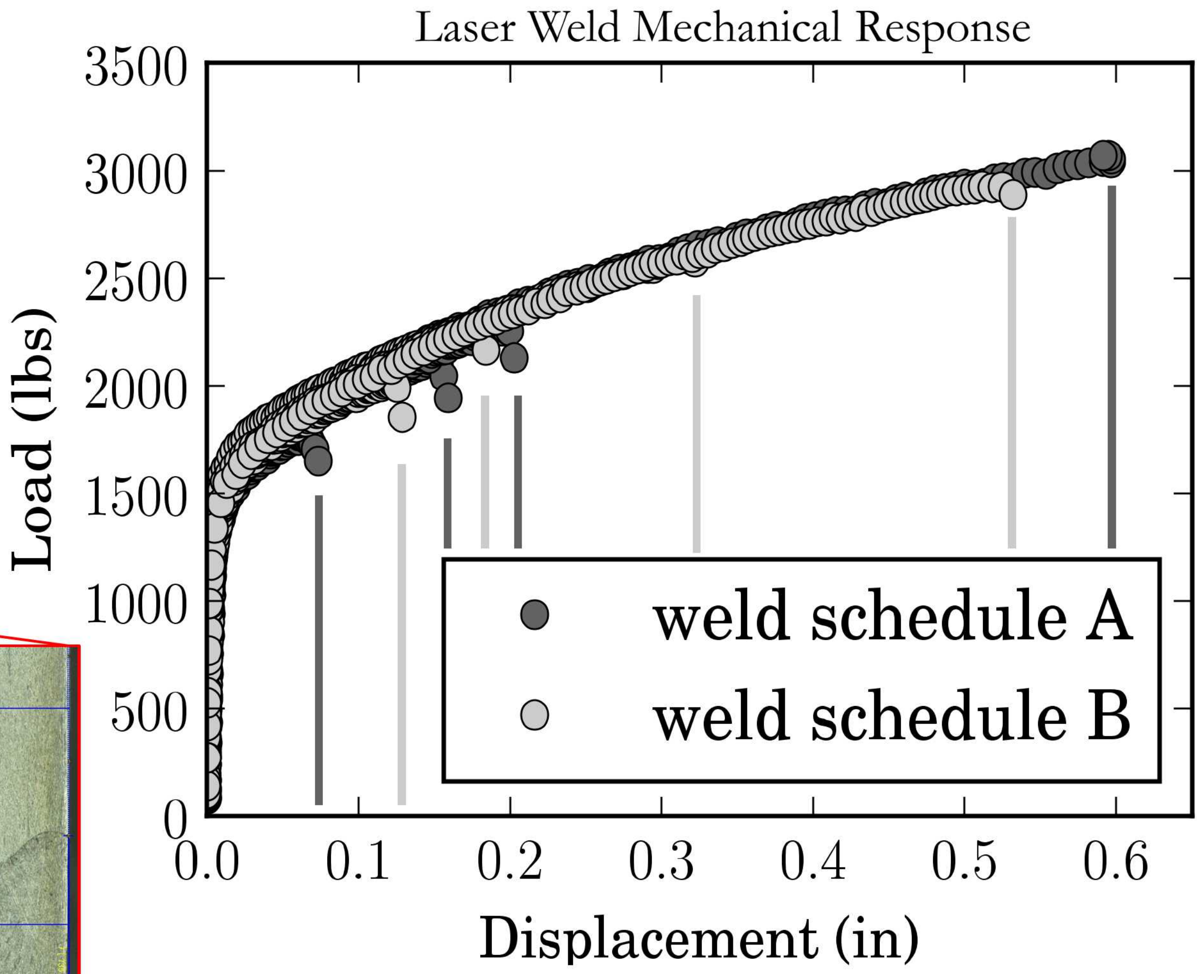

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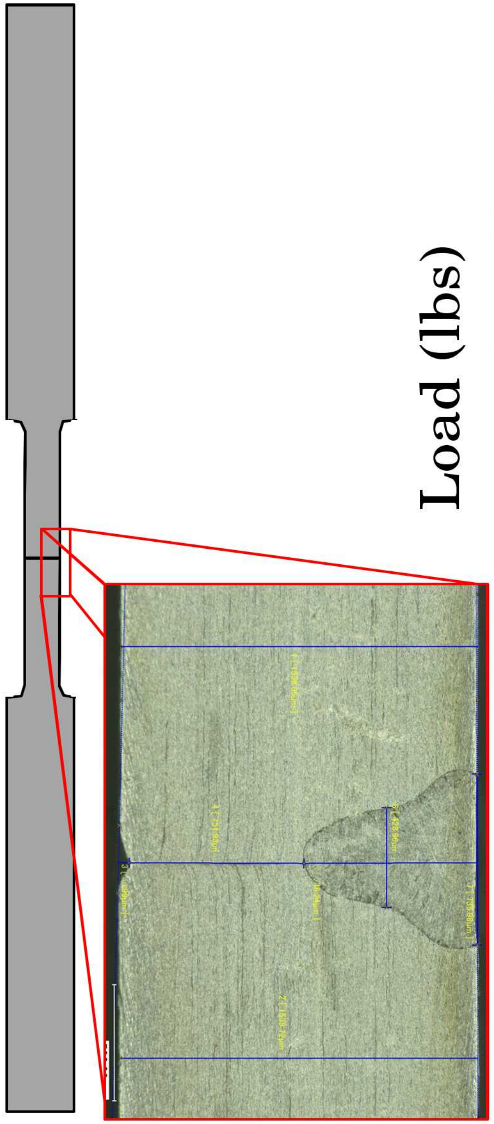
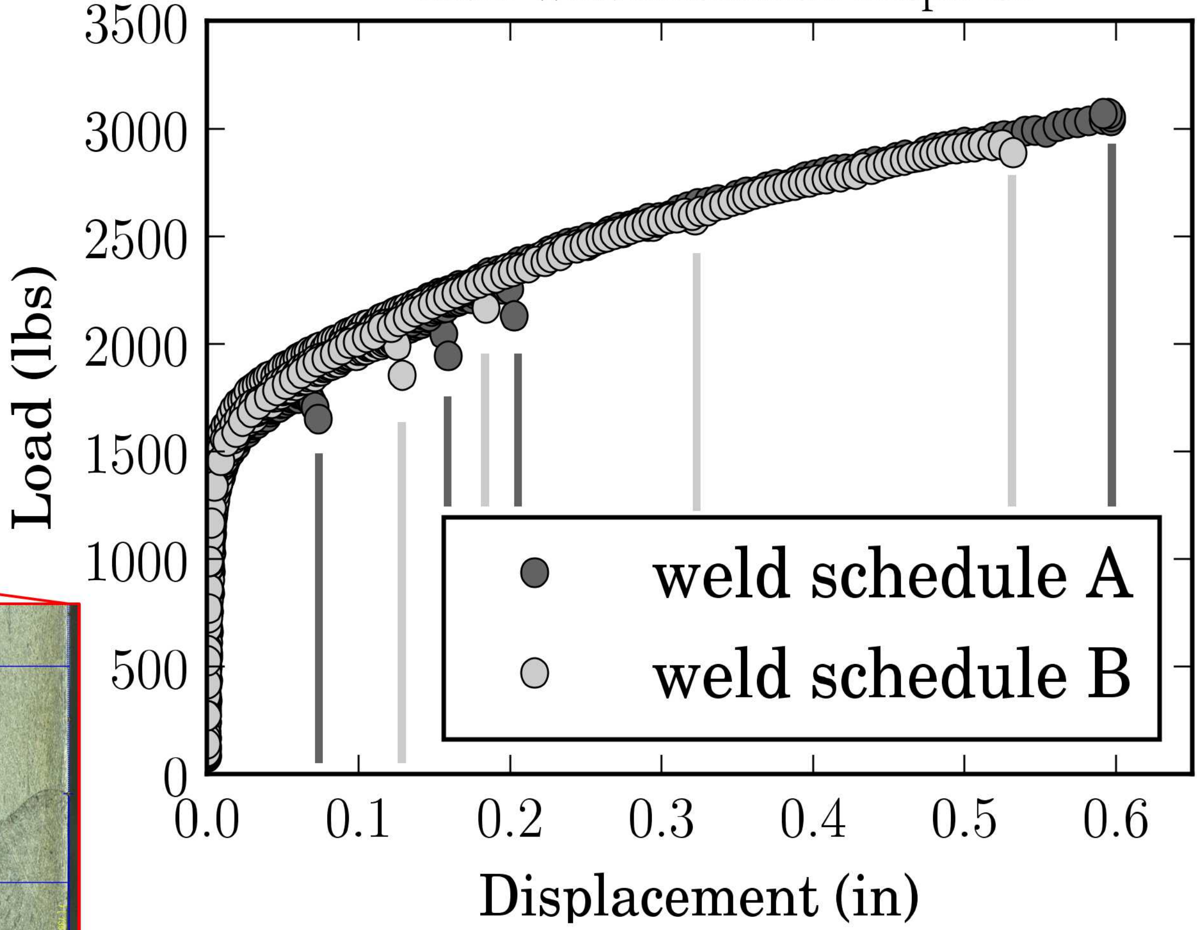
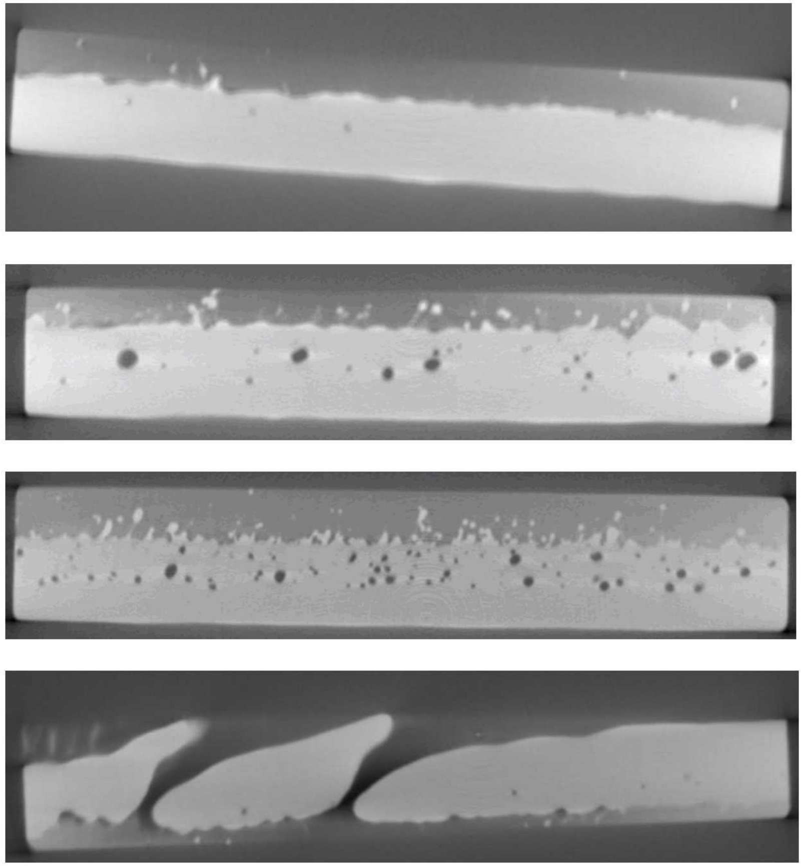


Laser Weld Mechanical Response



Images of Weld Substructure



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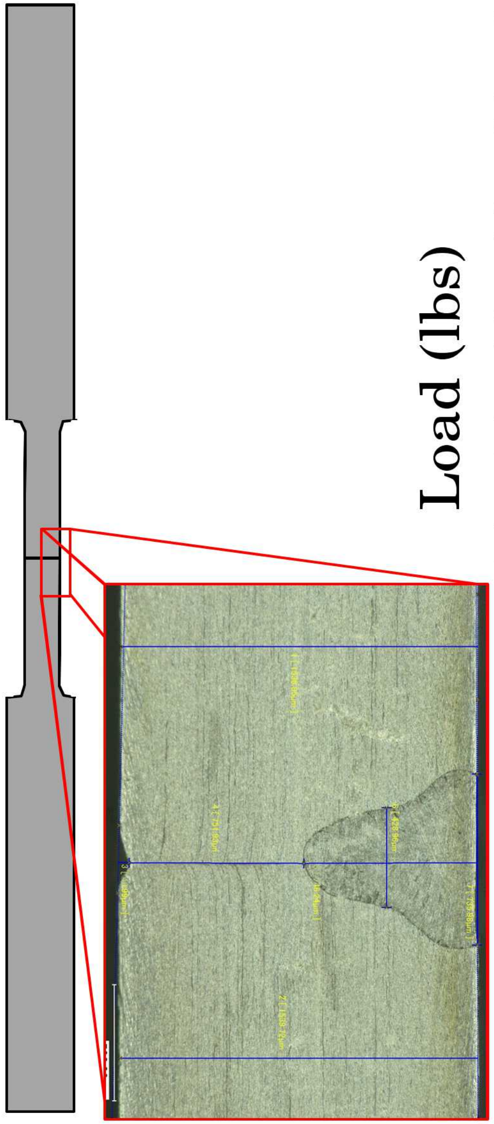

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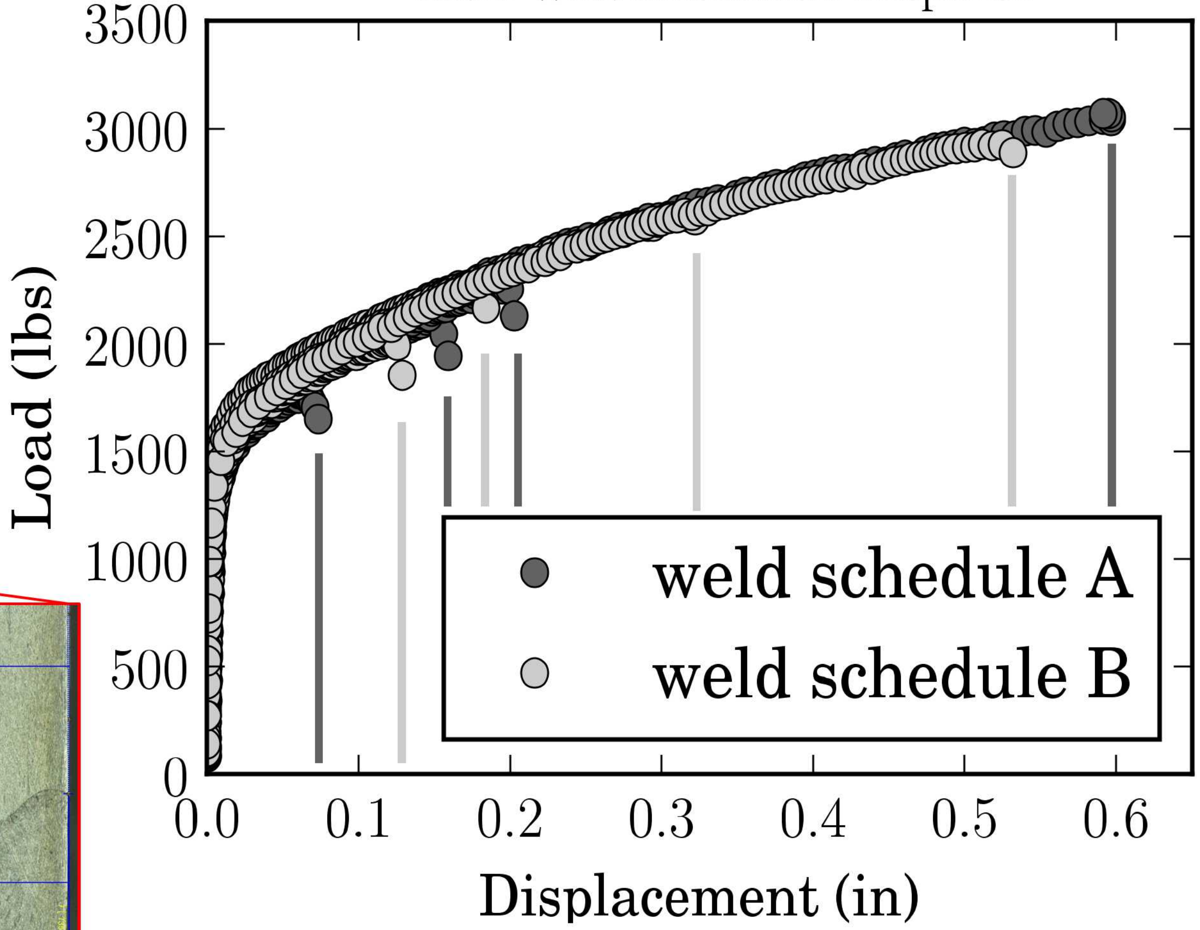
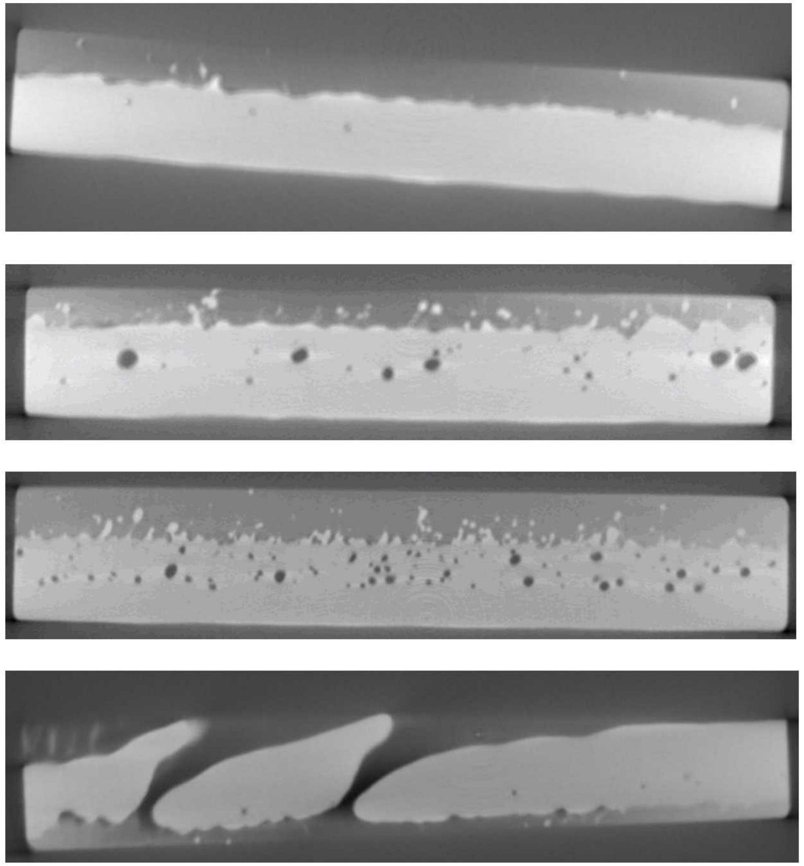


Images of Weld Substructure

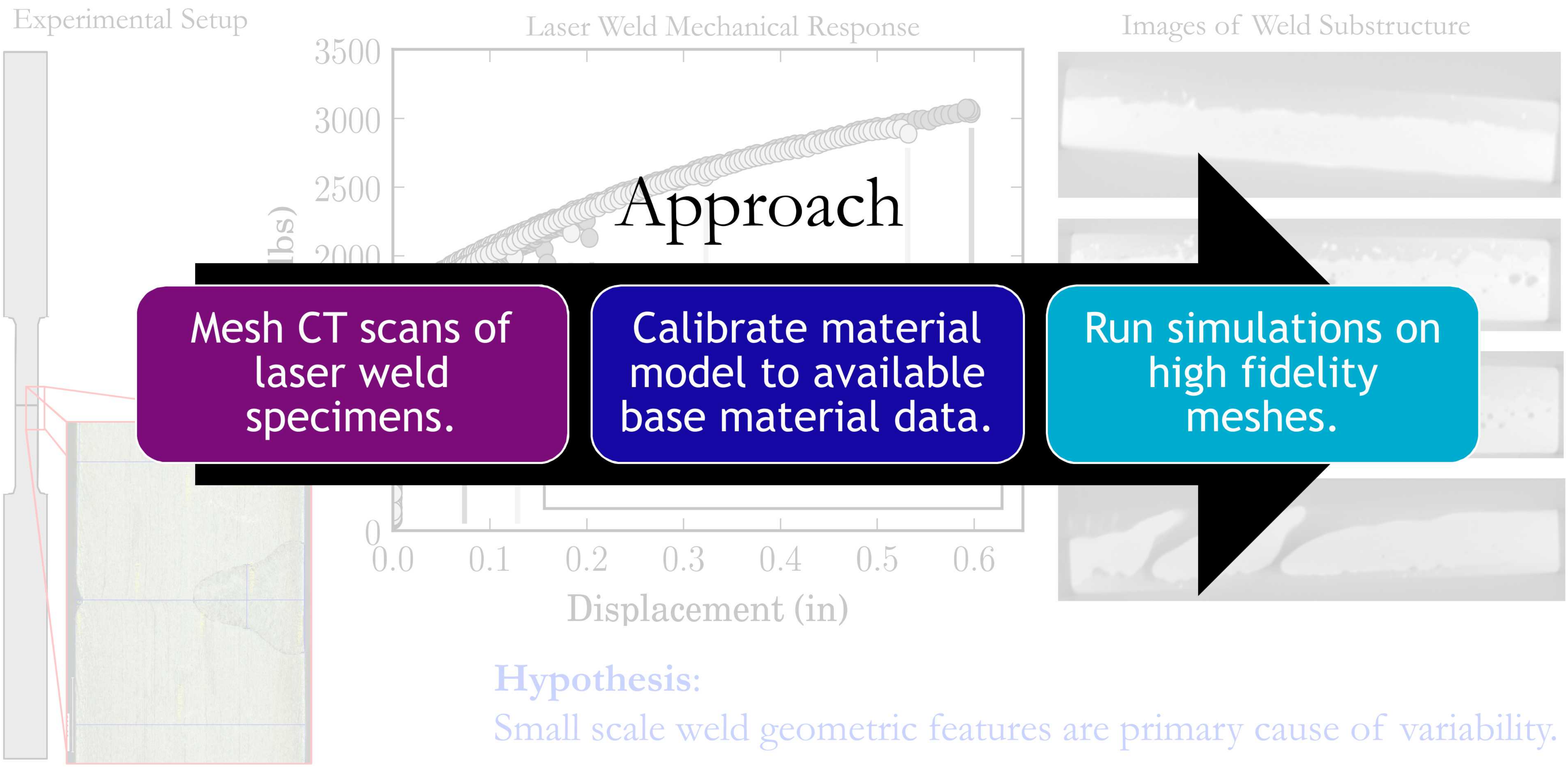


Hypothesis:

Small scale weld geometric features are primary cause of variability.

Experimental data provided by John Madison, Helena Jin

Determining Cause of Laser Weld Mechanical Variability



Approach

Mesh CT scans of laser weld specimens.

Calibrate material model to available base material data.

Run simulations on high fidelity meshes.

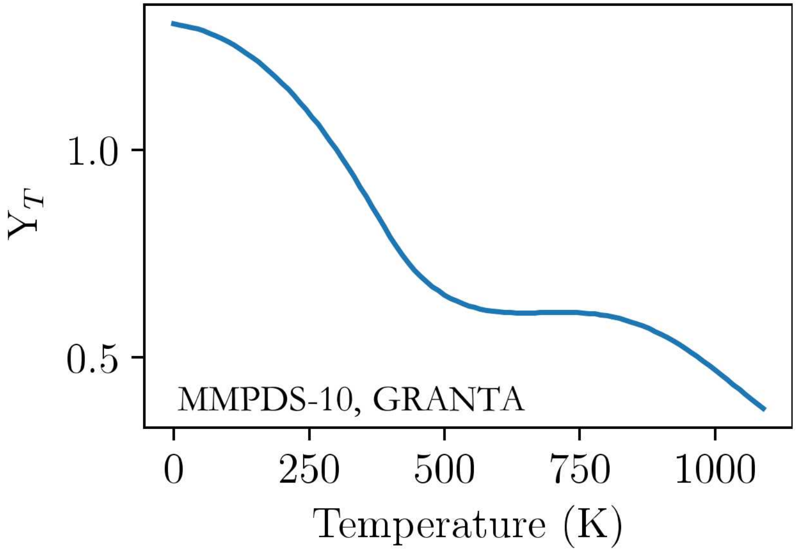
Hypothesis:

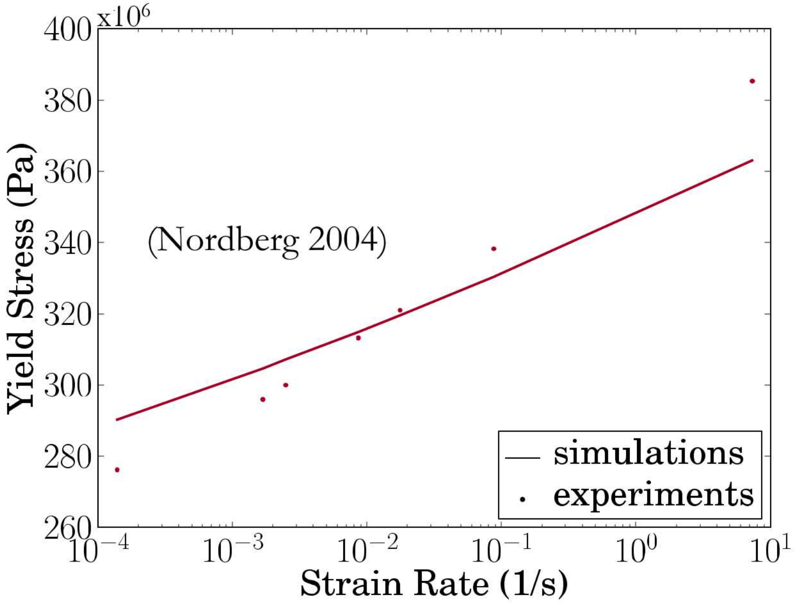
Small scale weld geometric features are primary cause of variability.

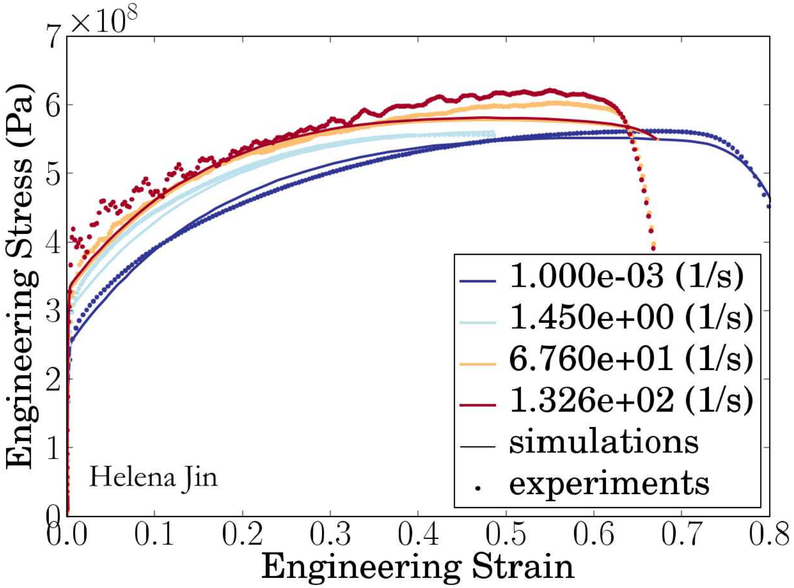
Experimental data provided by John Madison, Helena Jin

Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen







Material Parameter Calibration: Plasticity Calibration

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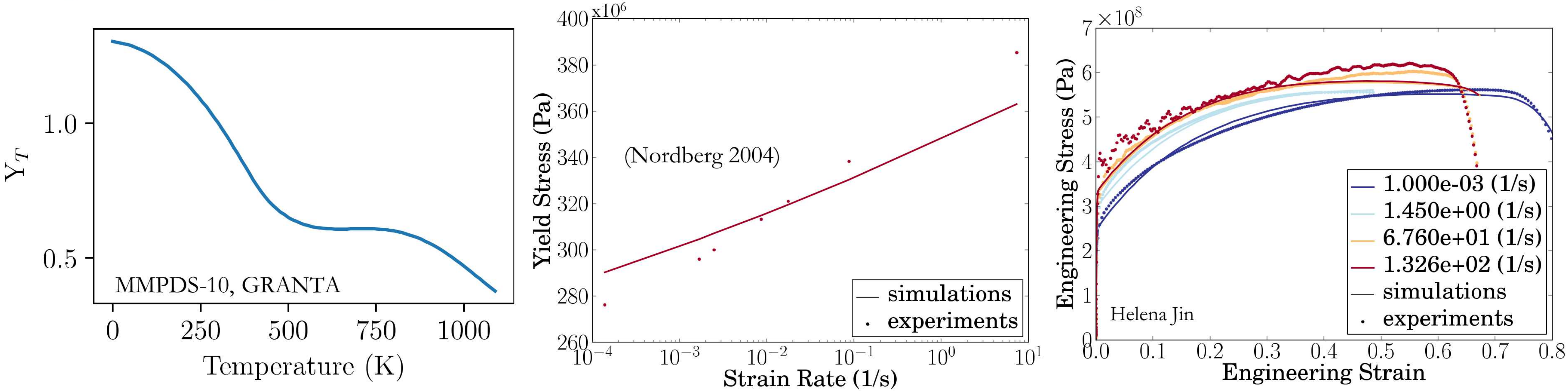
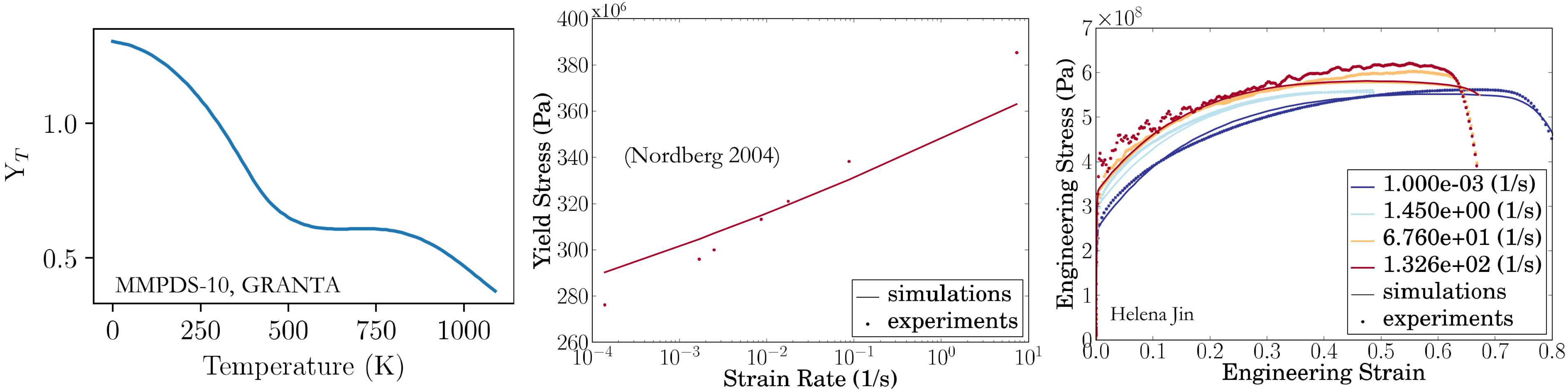


Temperature/rate dependent plasticity calibration

Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen



Temperature/rate dependent plasticity calibration

Yield condition:

$$Y_0 Y_T(\theta)\left[1+\sinh^{-1}\left\{\left(\frac{\dot{\epsilon}_{eq}}{f}\right)^{1/n}\right\}\right]+\kappa=\sigma_{eq}(\hat{\sigma}_{ij})$$

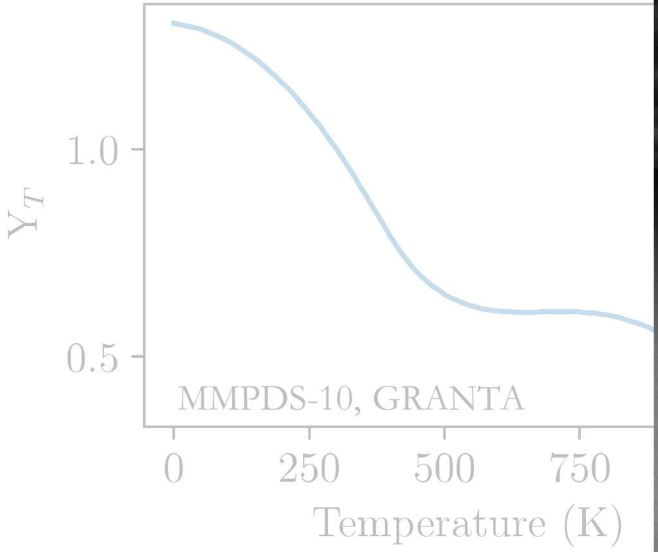
Hardening behavior:

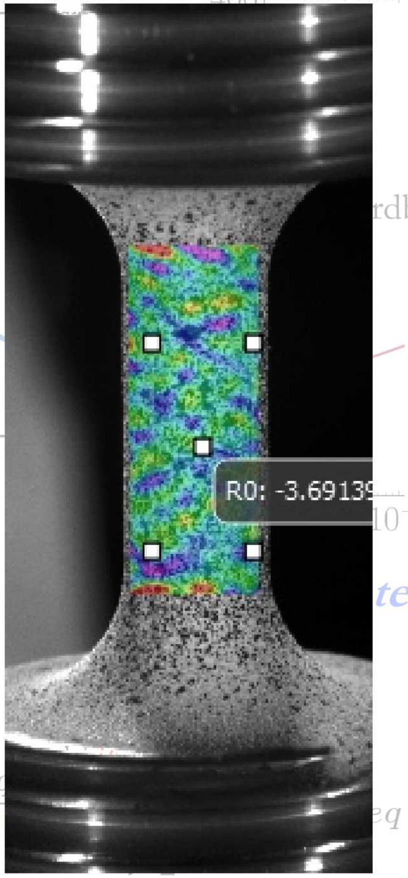
$$\dot{\kappa}=\left[H\left(1+\frac{\zeta}{\kappa}\right)-R_d\kappa\right]\dot{\epsilon}_{eq}$$

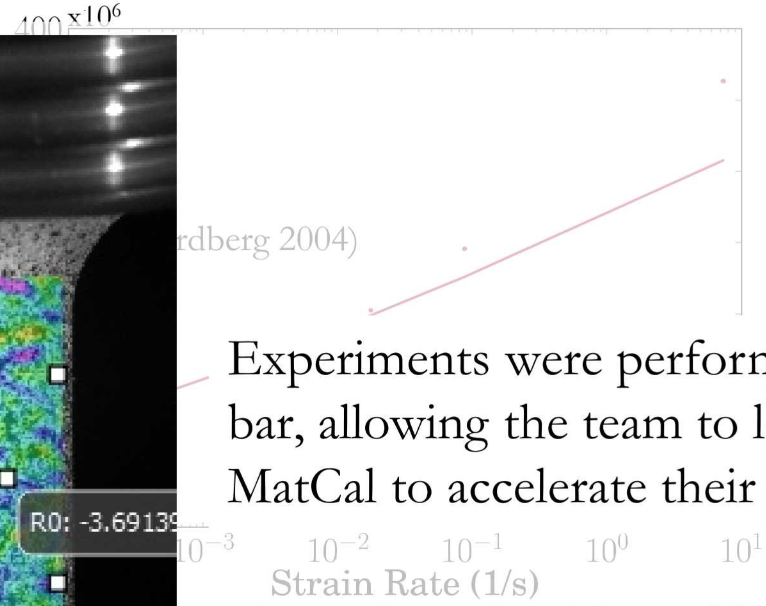
$$\frac{d}{dt}\left(\frac{\zeta}{\mu}\right)=h_{\zeta}\left(\frac{\zeta}{\mu}\right)\dot{\epsilon}_{eq}$$

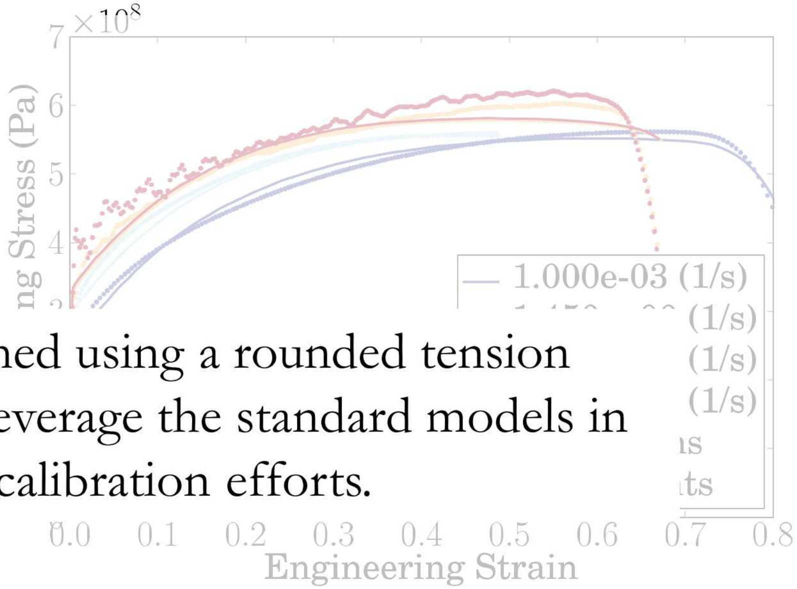
Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen









Experiments were performed using a rounded tension bar, allowing the team to leverage the standard models in MatCal to accelerate their calibration efforts.

te dependent plasticity calibration

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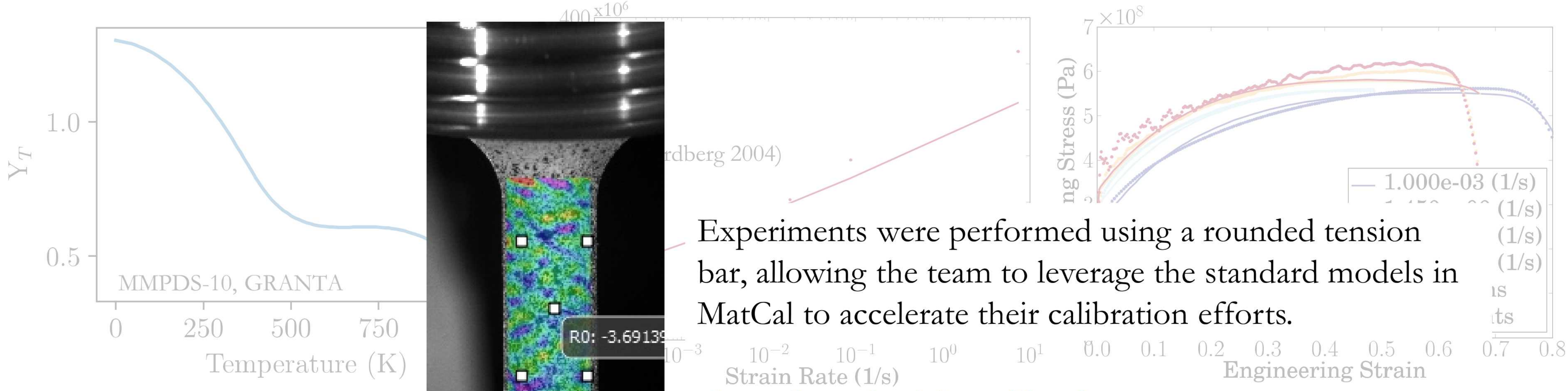
Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen → **MatCal Pointed to Material Block**



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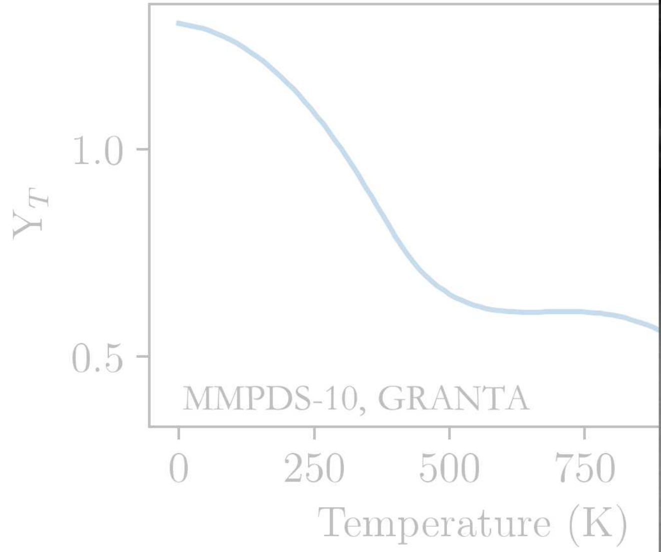
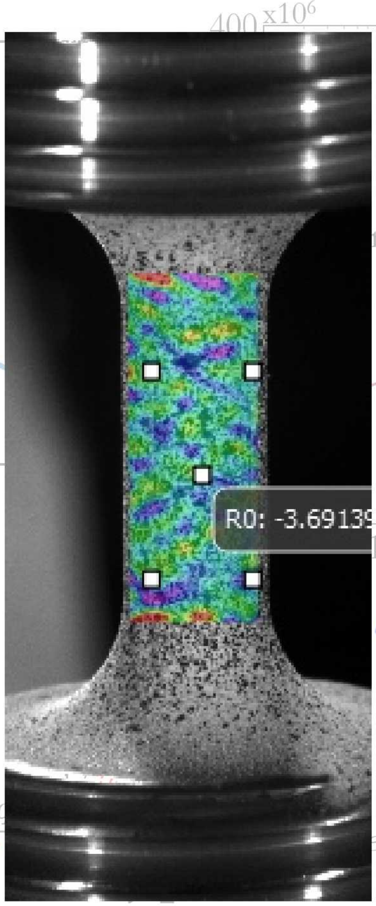
Material Parameter Calibration: Plasticity Calibration

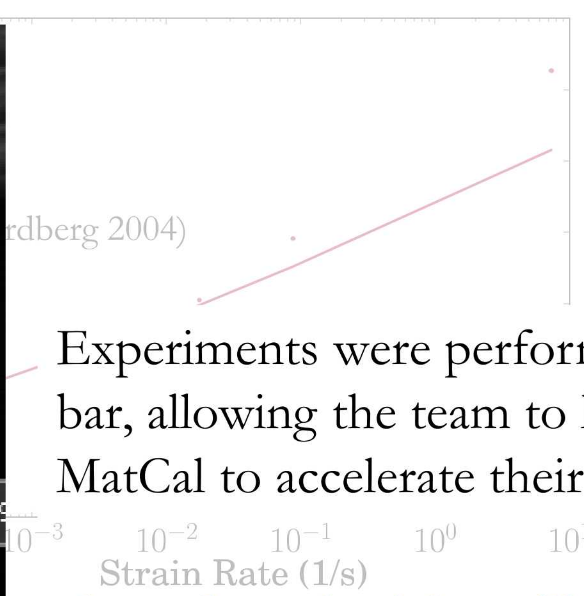
Plasticity Model Chosen

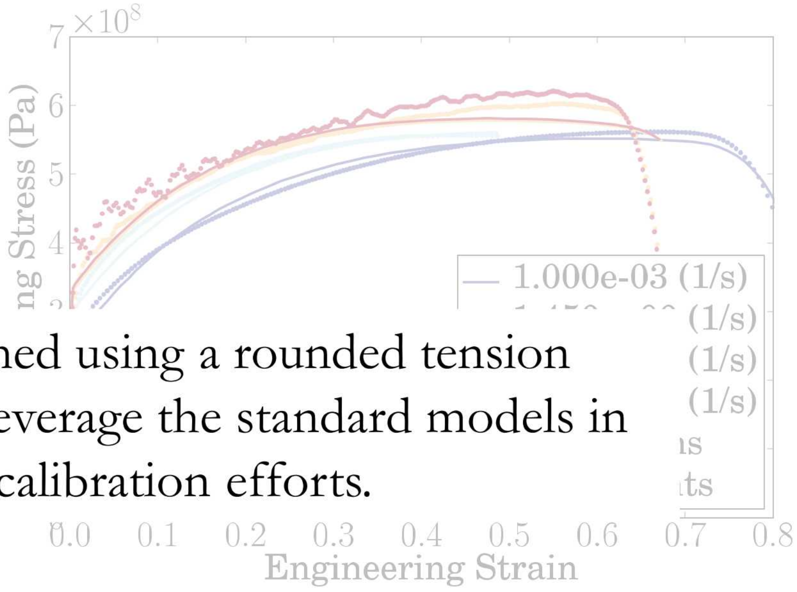
MatCal Pointed to Material Block

MatCal Pointed to Experimental Data









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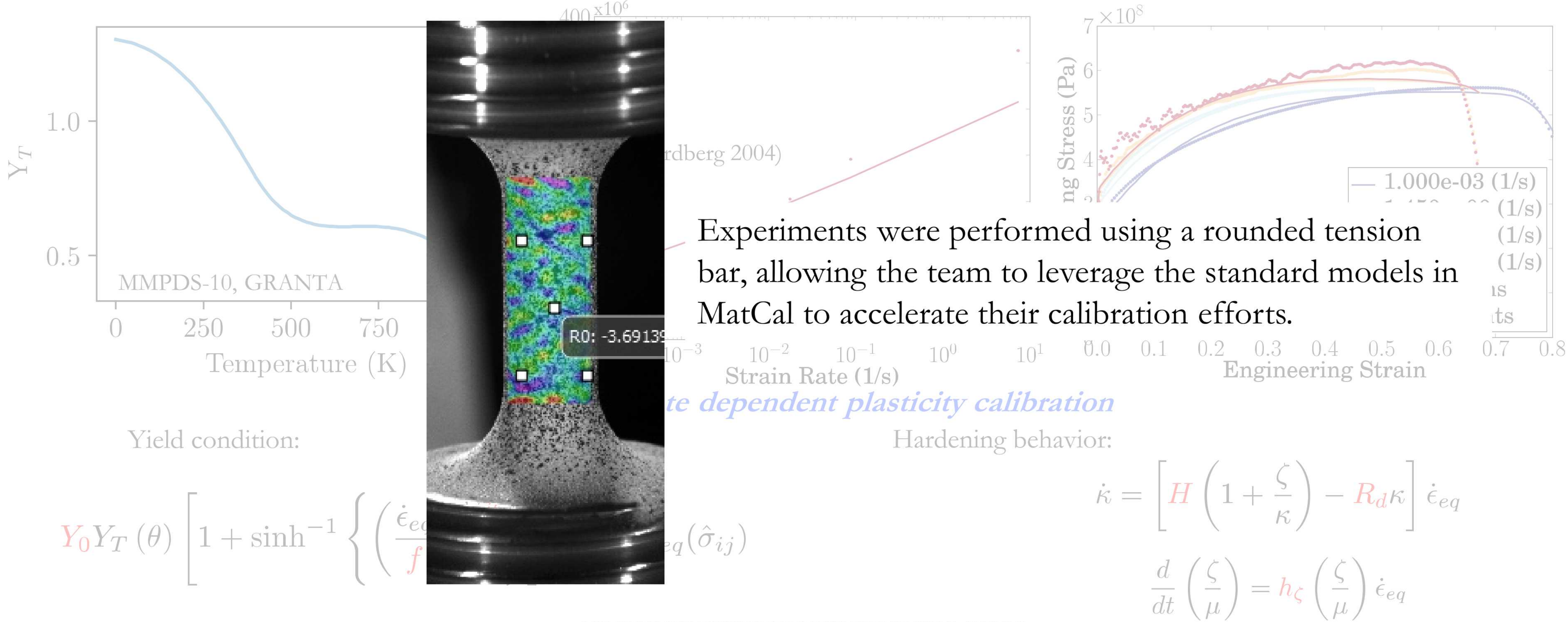
Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen → MatCal Pointed to Material Block → MatCal Pointed to Experimental Data → Push Go



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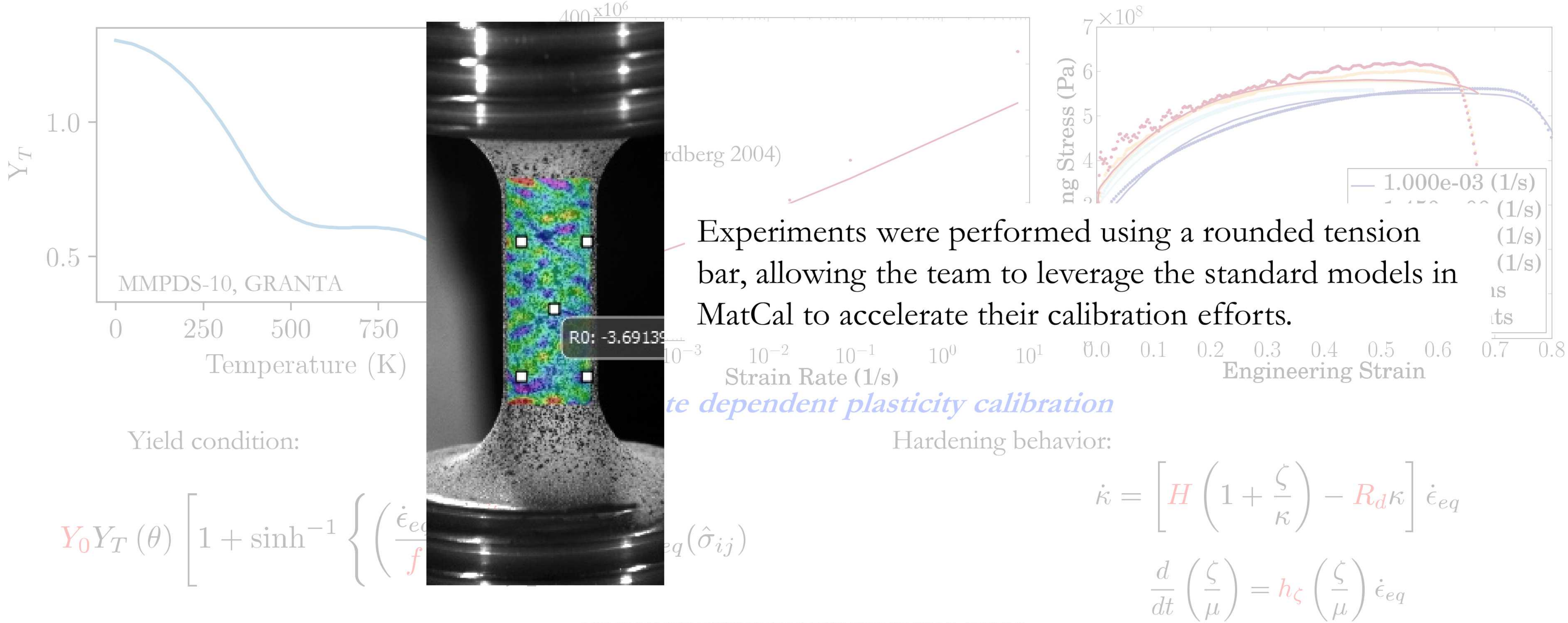
Material Parameter Calibration: Plasticity Calibration

Plasticity Model Chosen → MatCal Pointed to Material Block → MatCal Pointed to Experimental Data → Push Go → Next day have calibrated Material Parameters



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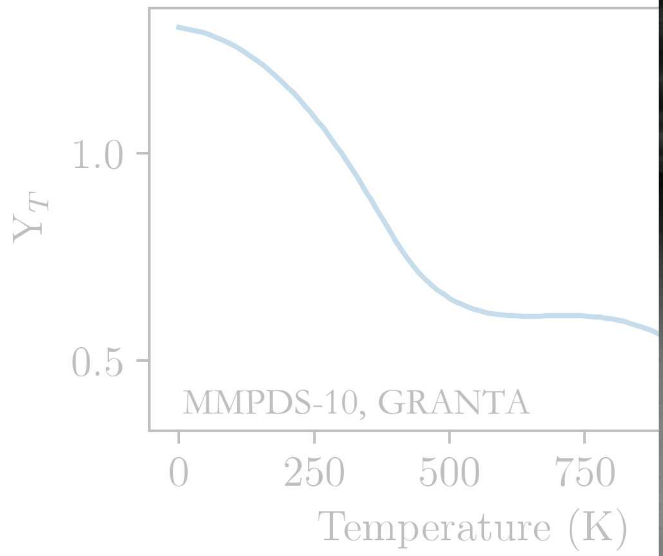
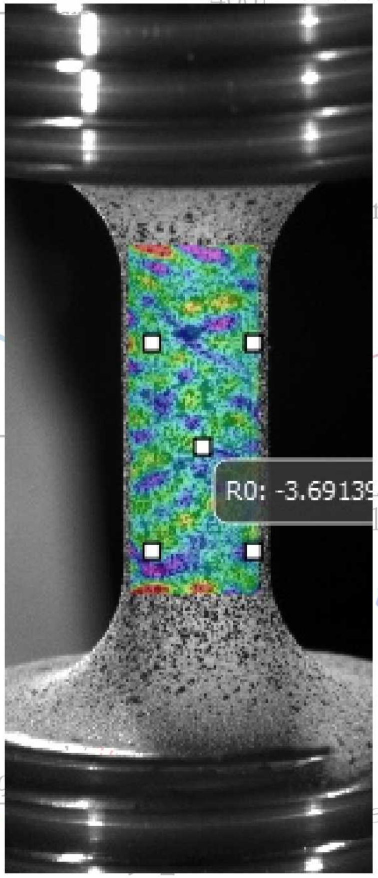
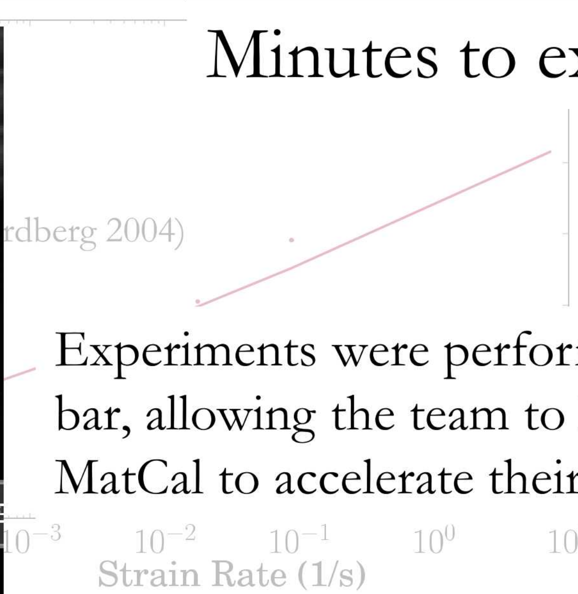
Material Parameter Calibration: Plasticity Calibration

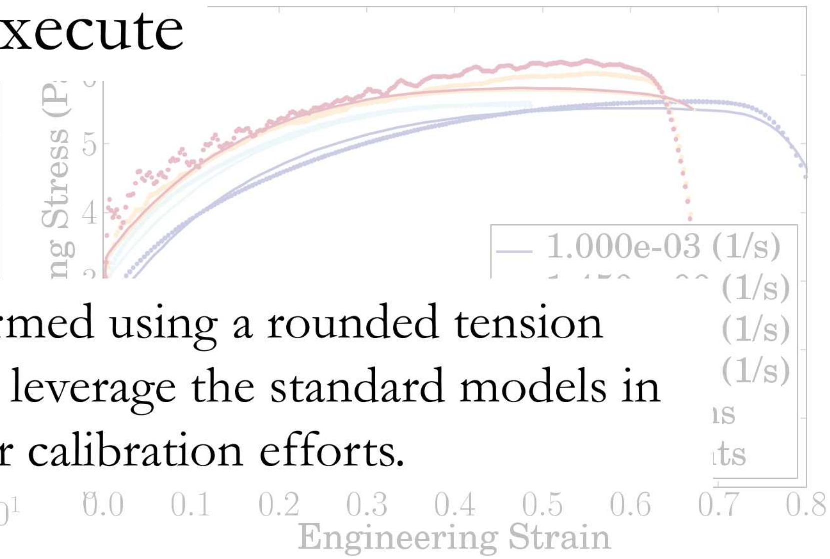
- Plasticity Model Chosen
- MatCal Pointed to Material Block
- MatCal Pointed to Experimental Data
- Push Go
- Next day have calibrated Material Parameters

Minutes to execute









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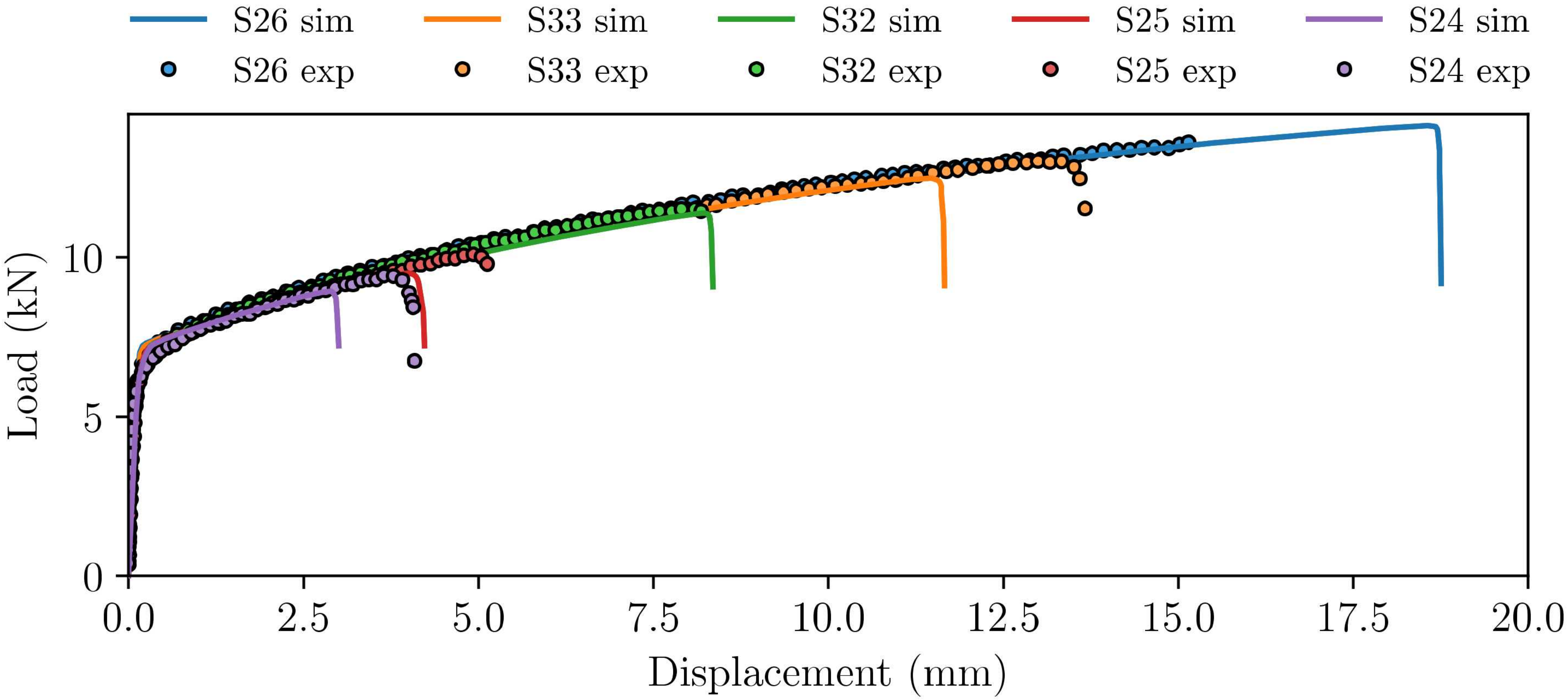
Predict Variability Attributable to only Geometry



Von Mises Stress:

Specimen S24 (high porosity, shallow weld)

Specimen S25 (abnormal geometry)

Specimen S32 (low porosity)

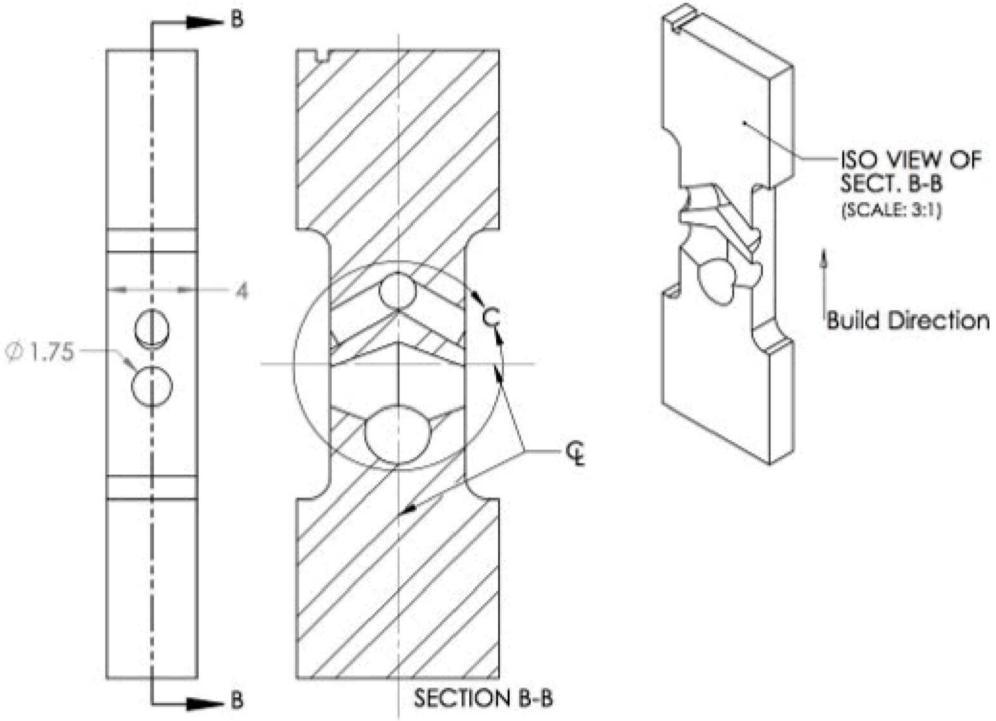
Specimen S33 (low porosity, deep weld)

Specimen S26 (medium porosity, deep weld)

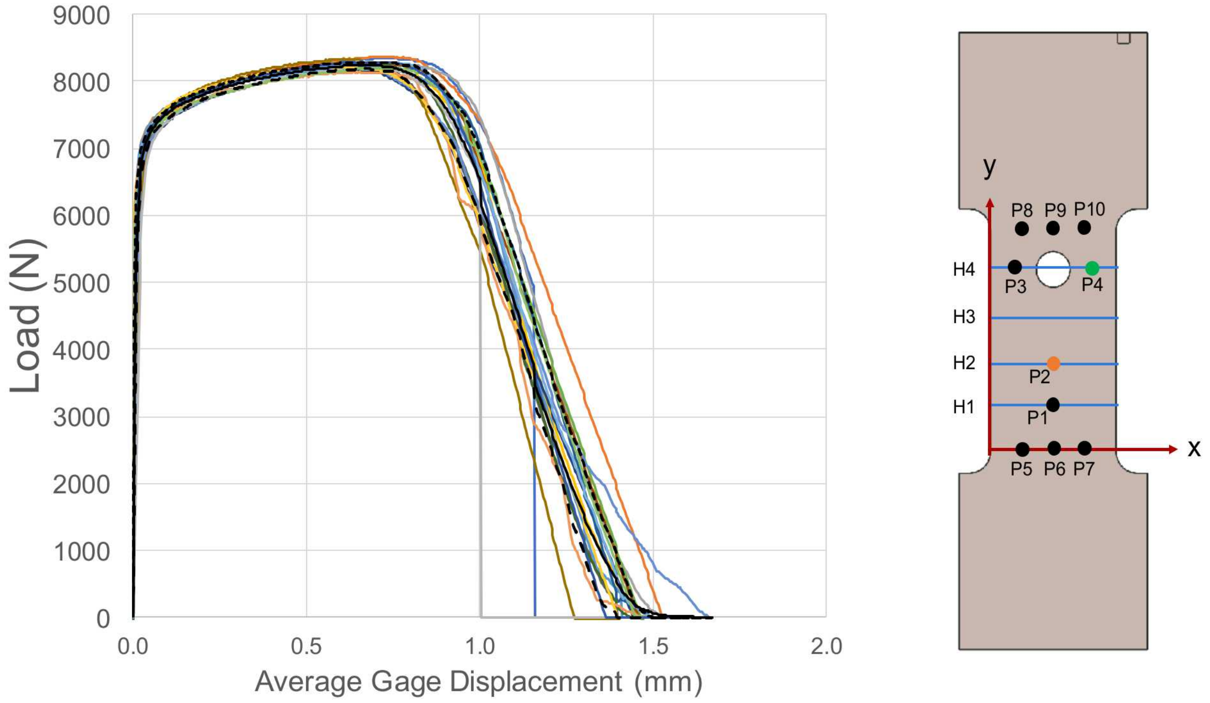
A MatCal Success: Sandia Fracture Challenge 3 (SFC3)

Challenge:

Given a novel AM 316 stainless steel specimen geometry, make a blind prediction of the loading and failure behavior, and provide uncertainty measurements.



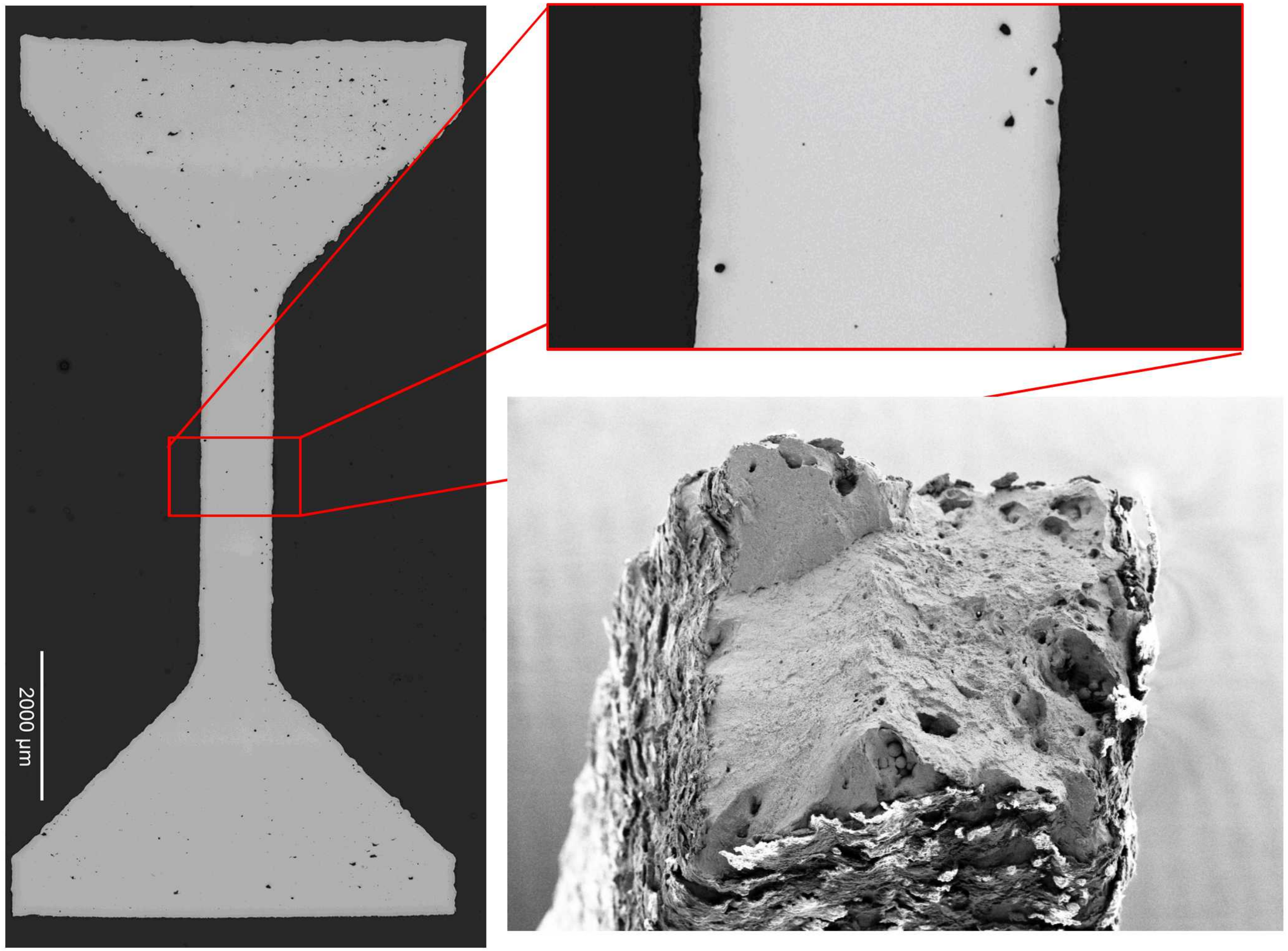
Specimen Geometry



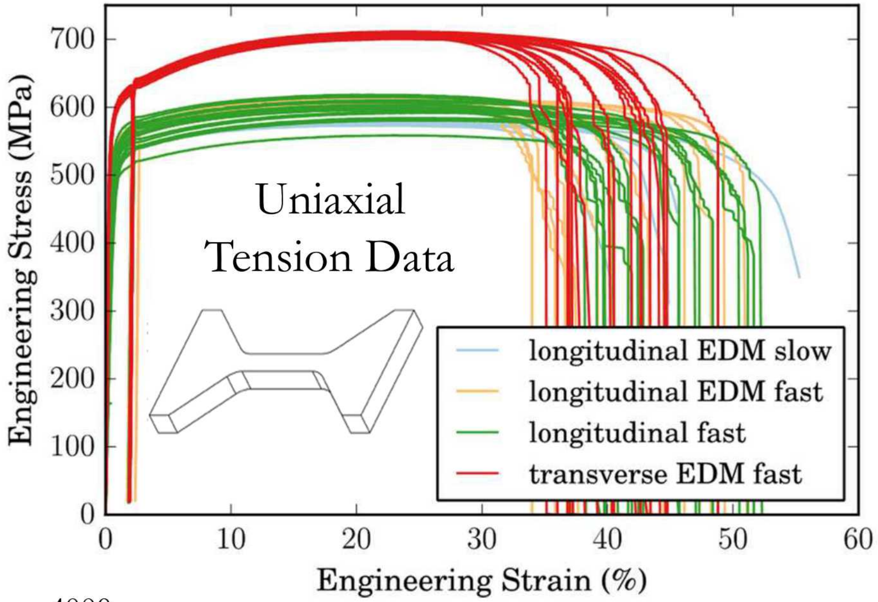
Needed to predict both local and global responses for the specimen.

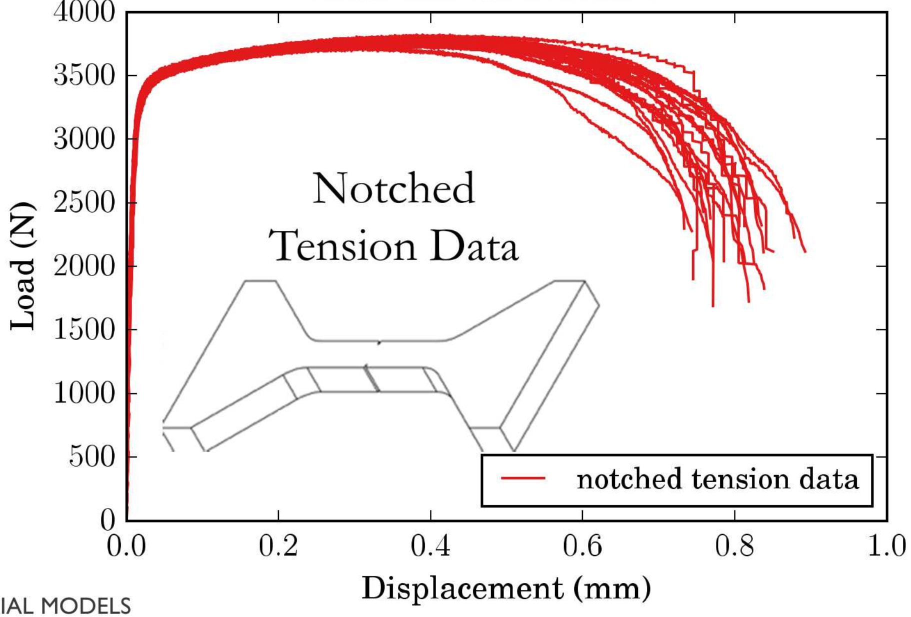
SFC3: Information Provided

Test Sample Geometry Information

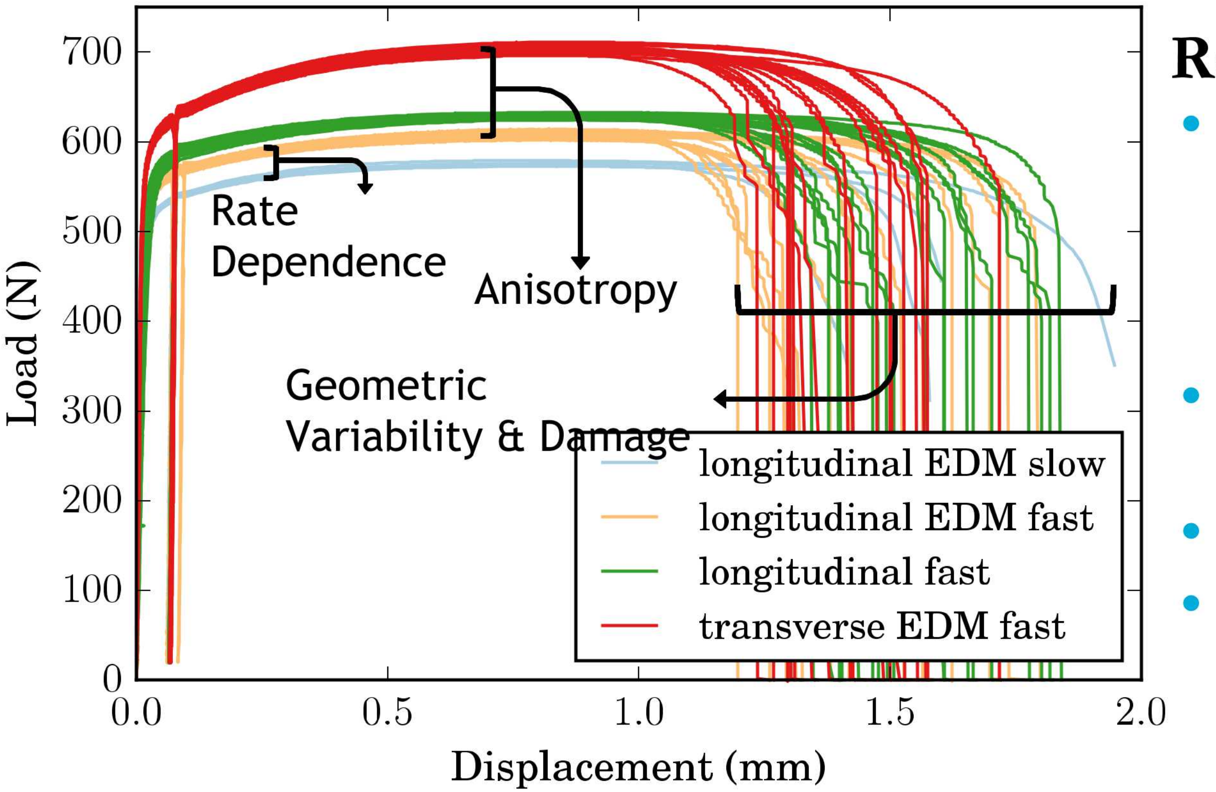


Tension Test Data





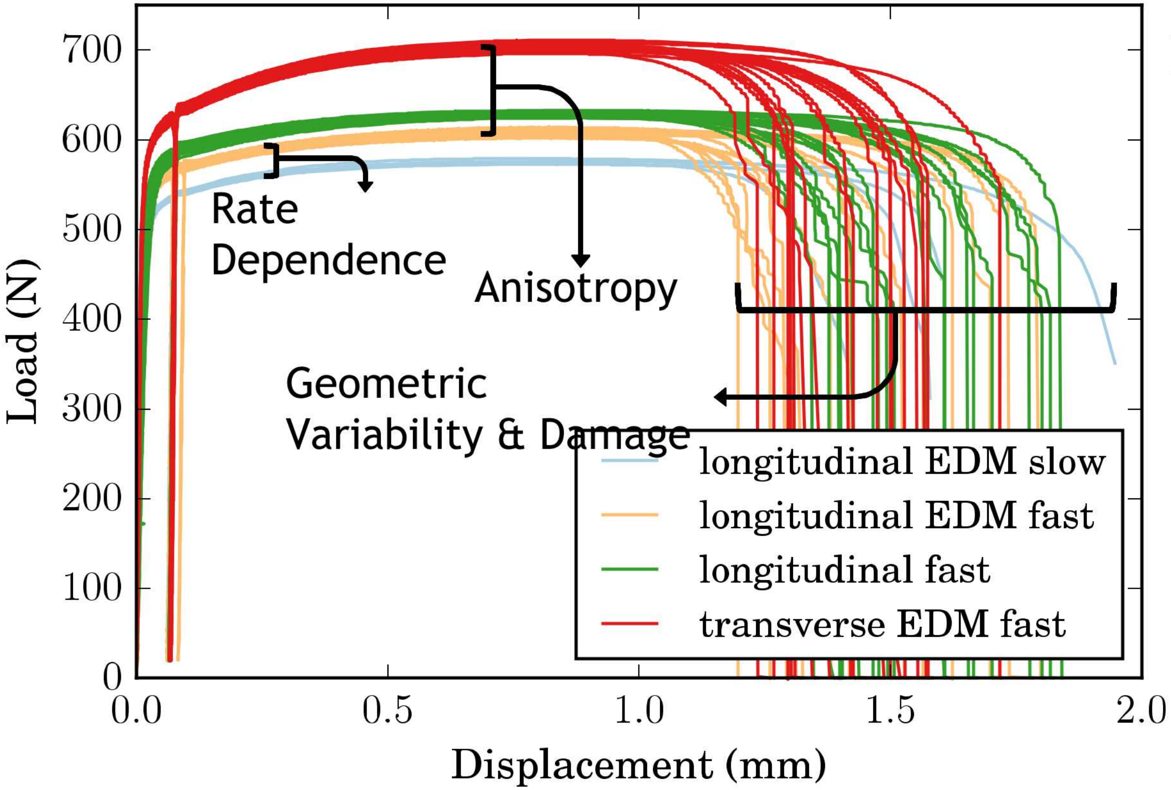
SFC3: MatCal's Role-Model Selection



Relevant material phenomena:

- Nonlinear hardening
  - Investigated: Voce, Power-law, and Voce + pre-strain due to residual stress
- Temperature and rate dependence
- Plastic anisotropy
- Failure: Void nucleation/growth

SFC3: MatCal's Role-Model Selection



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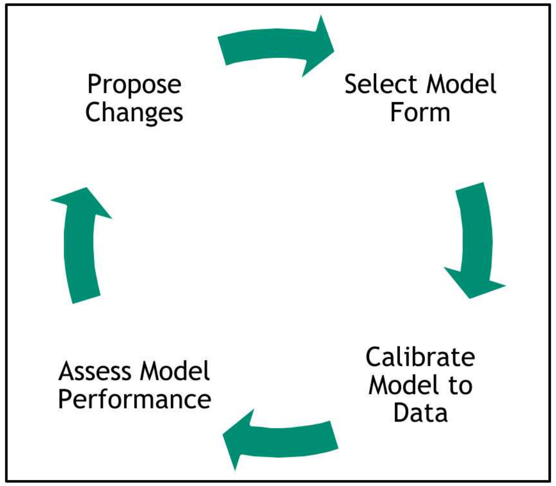
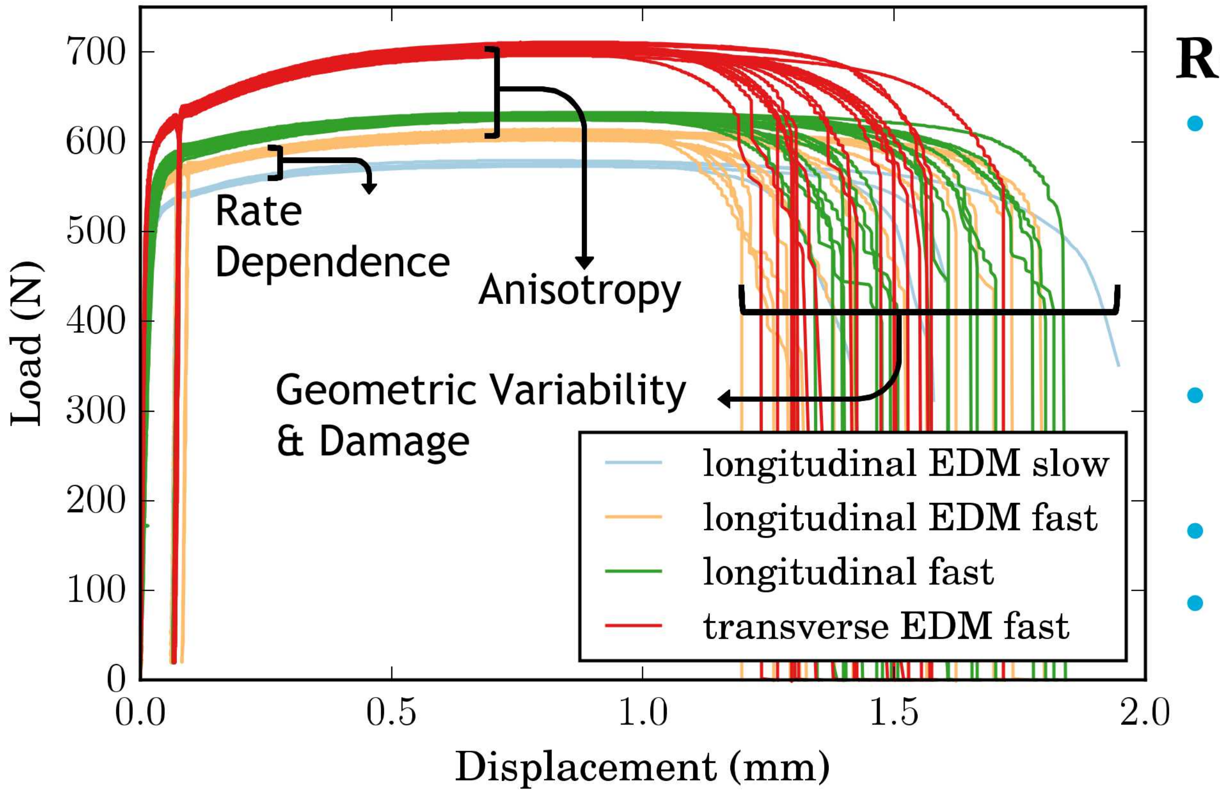


SFC3: MatCal's Role-Model Selection



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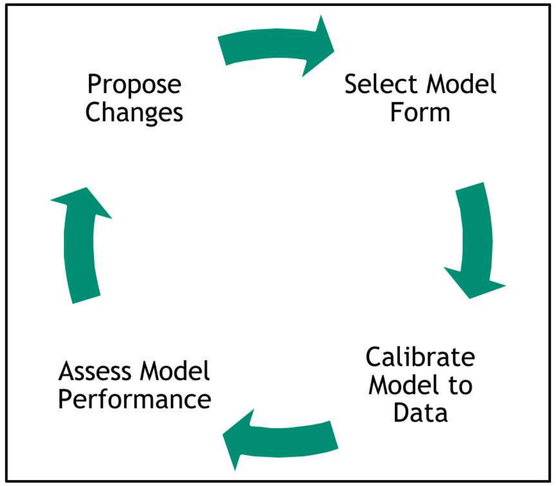

Propose Changes

Select Model Form

Calibrate Model to Data

Assess Model Performance

Final material model form chosen: **16 unknown parameters**

$$\sigma_f = Y_0\left\{1+\sinh^{-1}\left[\left(\frac{\dot{\epsilon}_p}{f}\right)^{1/n}\right]\right\} + A(\epsilon_p)^b$$

Power-law hardening with rate dependent yield

$$\theta^2(\hat{\sigma}_{ij}) = F(\hat{\sigma}_{22}-\hat{\sigma}_{33})^2 + G(\hat{\sigma}_{33}-\hat{\sigma}_{11})^2 + H(\hat{\sigma}_{11}-\hat{\sigma}_{22})^2 + 2L\hat{\sigma}_{23}^2 + 2M\hat{\sigma}_{31}^2 + 2N\hat{\sigma}_{12}^2$$

Hill yield surface

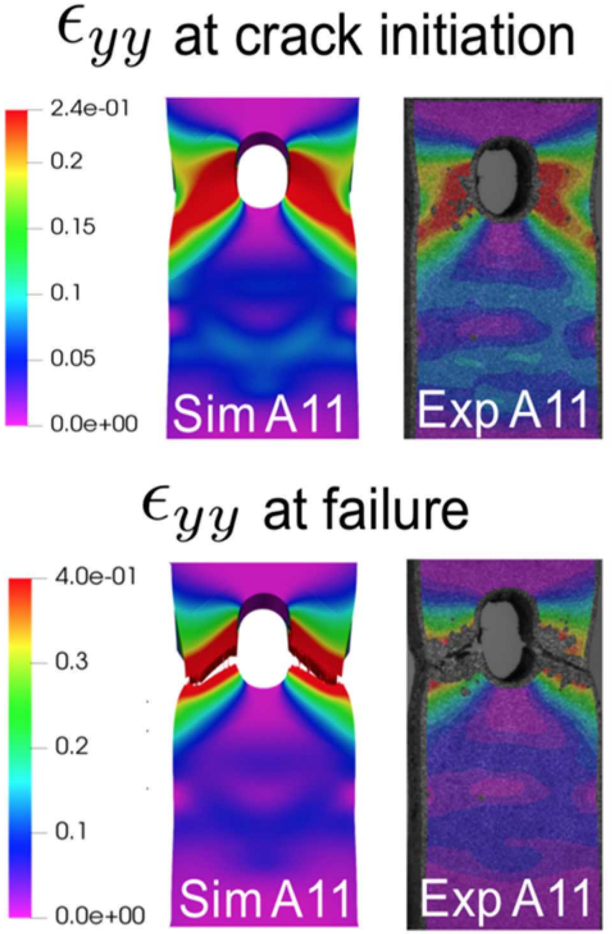
$$\dot{v_v} = \sqrt{\frac{2}{3}}\dot{\epsilon}_p\frac{1}{\eta}(1+\eta v_v)\left[(1+\eta v_v)^{m+1}-1\right] \cdot\sinh\left[\frac{2(2m-1)}{2m+1}\frac{\langle p\rangle}{\sigma_f}\right] - (v_v - v_0)\frac{\dot{\eta}}{\eta}$$

$$\dot{\eta} = \eta\dot{\epsilon}_p\left(N_1\left[\frac{4}{27}-\frac{J_3^2}{J_2^3}\right] + N_3\left[\frac{|p|}{\sigma_f}\right]\right)$$

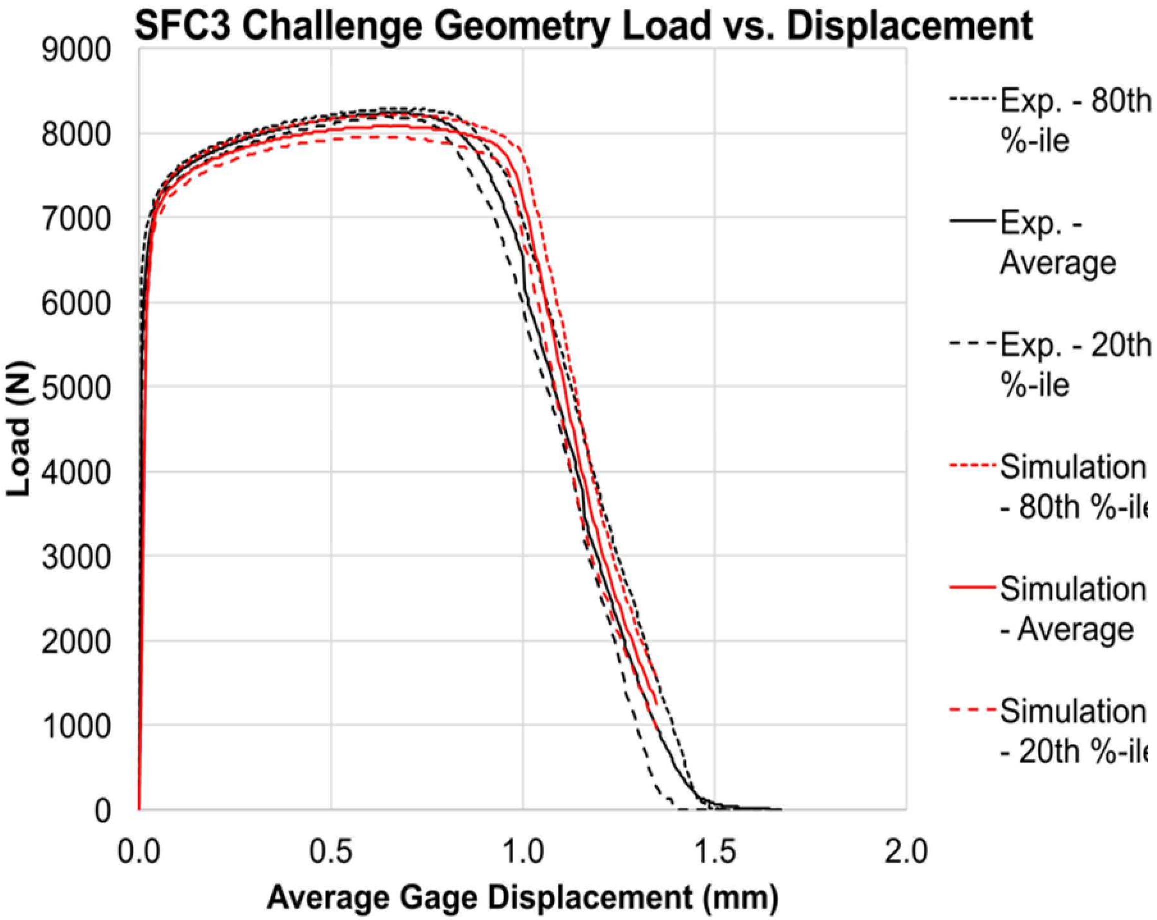
Void nucleation & growth

MatCal Enabled Prediction Deemed Most Accurate

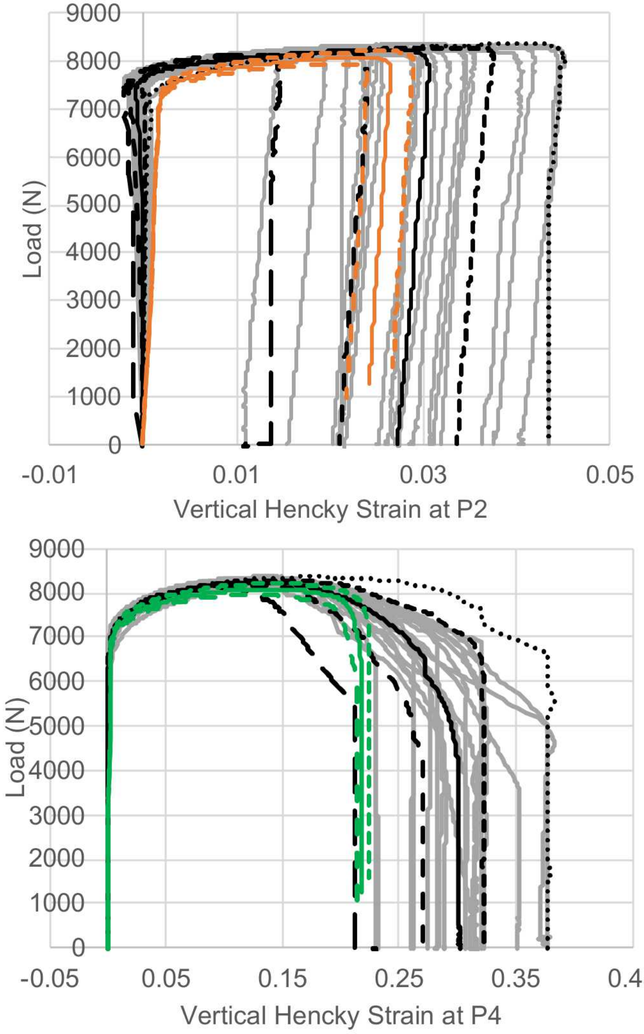
Qualitative



Global



Local



International Journal of Fracture:
Sandia Fracture Challenge 3: detailing the Sandia Team Q failure prediction strategy

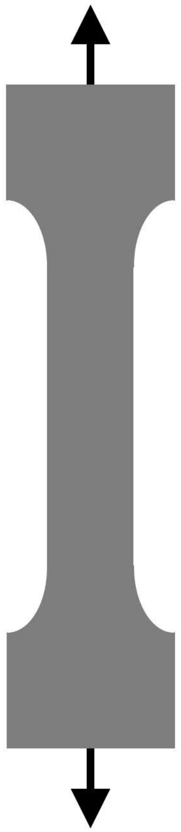
Advanced Calibration with Full-Field Data

Elizabeth Jones, Sandia National Laboratories

NSE CROSS-SITE MEETING ON CALIBRATED
MATERIAL MODELS

There are two main classes of calibration techniques.

Traditional



Advanced

There are two main classes of calibration techniques.

Traditional

- Simple geometries
- Global data (i.e. engineering stress and extensometer strain)
- Uniaxial (i.e. tension only; shear only)

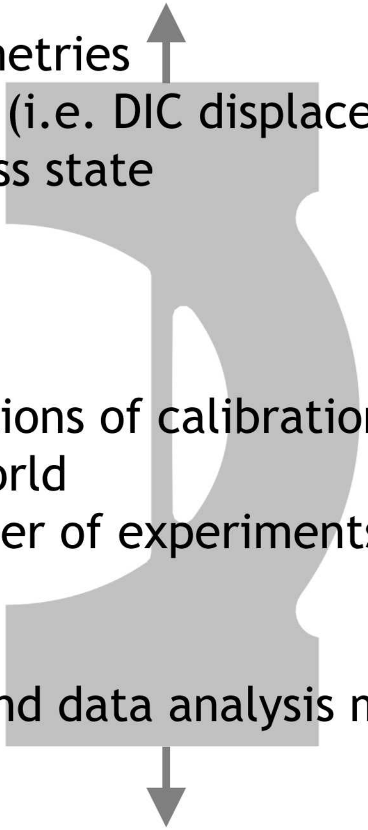
Advantages

- Simple experiments
- Data easy to interpret

Disadvantages

- Uniaxial stress state does not reflect real-world loading conditions
- Multiple experiments required to fit a complex material model

Advanced



- Arbitrary geometries
- Full-field data (i.e. DIC displacements)
- Multiaxial stress state

Advantages

- Loading conditions of calibration specimen reflect real-world
- Reduced number of experiments

Disadvantages

- Experiments and data analysis more complicated

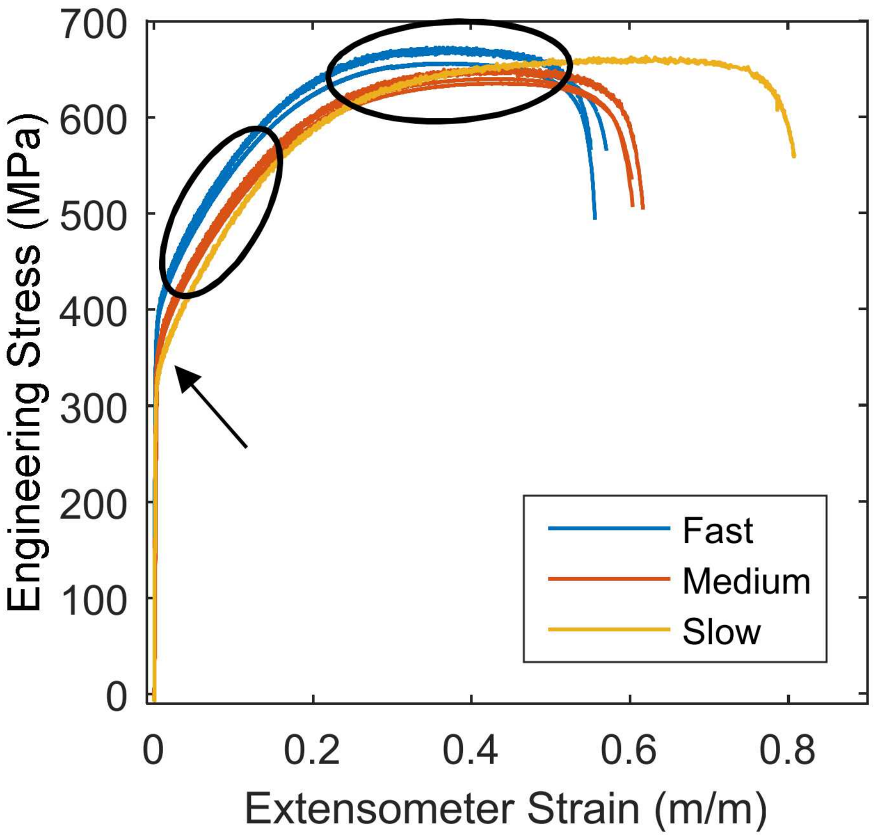
Method 1: The BCJ model was calibrated using traditional techniques and global, uniaxial tensile data.

$$\sigma_f(p,\dot{p},\boldsymbol{\xi}) = \underbrace{\sigma_Y\left\{1+\operatorname{asinh}\left[\left(\frac{\dot{p}}{b}\right)^{1/m}\right]\right\}}_{\text{Strain rate dependence of initial yield}} + \underbrace{\frac{H}{R_d}\left[1-\exp(-R_d p)\right]}_{\text{Isotropic hardening}}$$

$$\text{Temperature dependence}\begin{cases}\sigma_y(\theta) = \sigma_1 - \sigma_2\theta \qquad H(\theta) = H_1 - H_2\theta \\ R_d(\theta) = R_{d1}\exp\left(\frac{-R_{d2}}{\theta}\right) + R_{d3}\end{cases}$$

Experiment

- Material: 304L stainless steel rolled sheet, 1.5 mm thick
- Dog bone gauge section: 50.8 mm x 12.7 mm
- Three nominal strain rates (s^{-1}):
    - $1.0 \cdot 10^{-4}$
    - $3.2 \cdot 10^{-3}$
    - $1.0 \cdot 10^{-1}$
- Virtual extensometer from DIC (22 mm)



Material Identification

- Finite-element model updating (FEMU) with MatCal
- Cost function built from simulated and experimental stress/strain curves

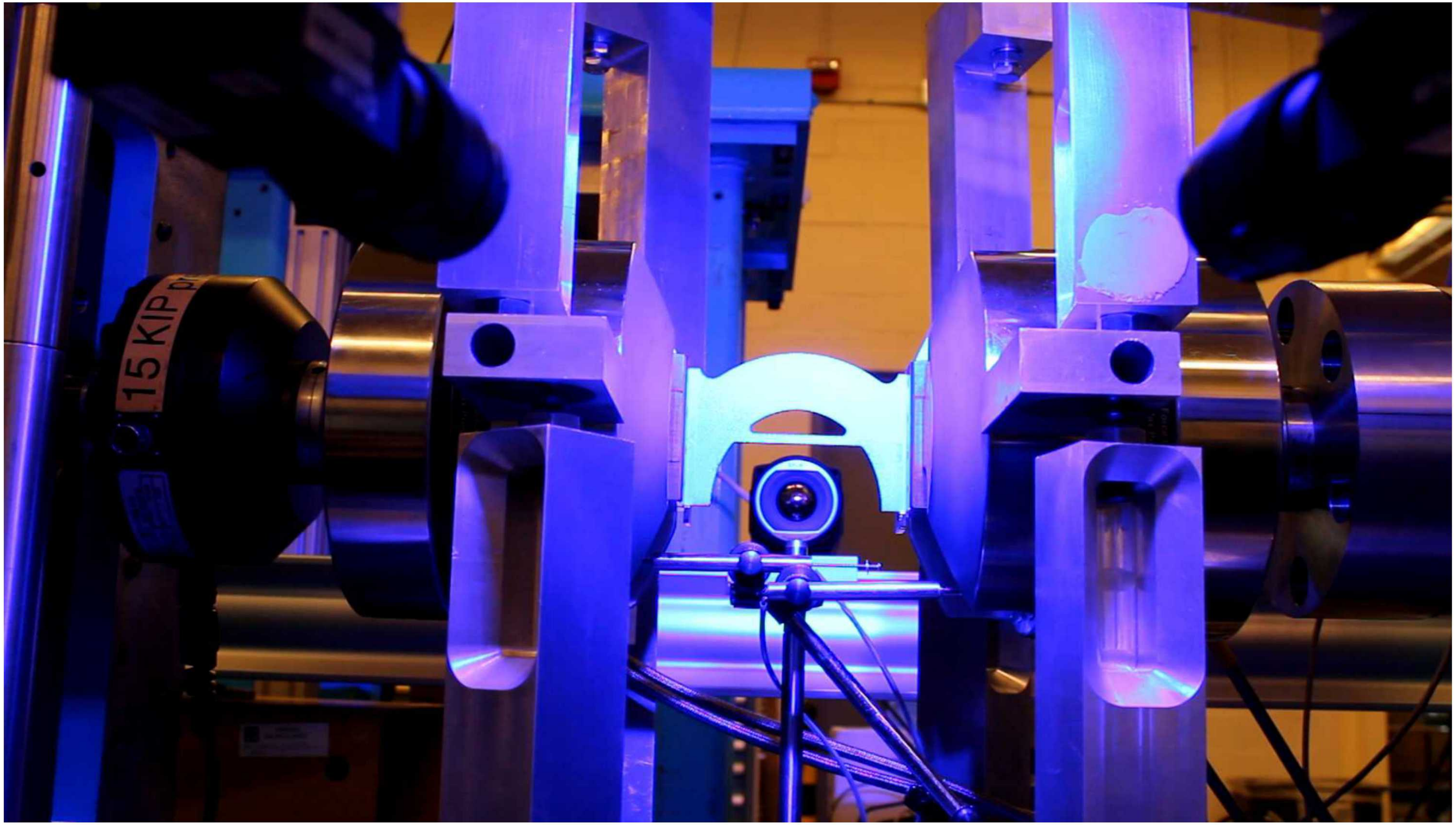
Method 1: The BCJ model was calibrated using traditional techniques and global, uniaxial tensile data.

Traditional Calibration

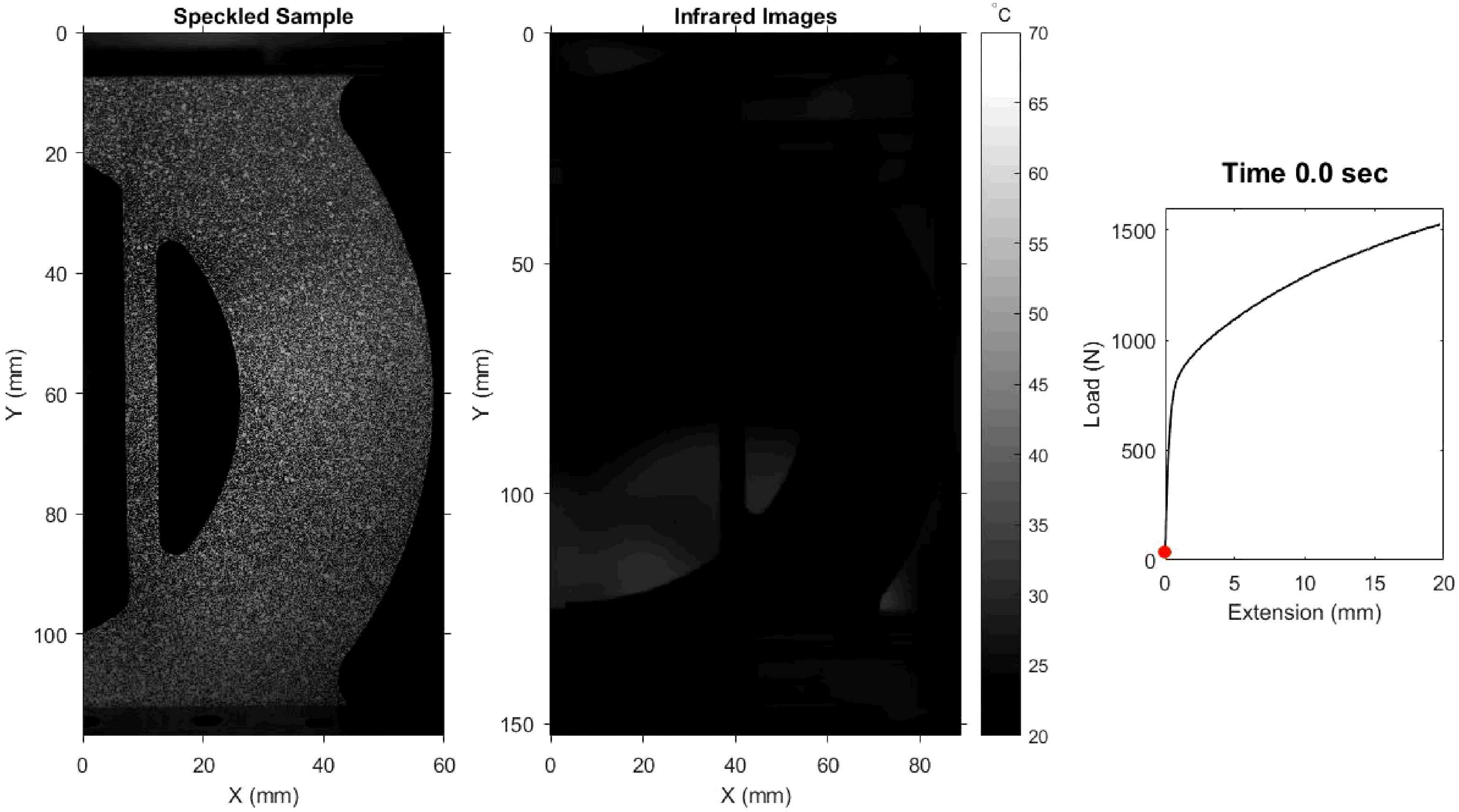
1. Only global load/extensometer data is used.

2. Many tests are required to capture strain-rate dependence.

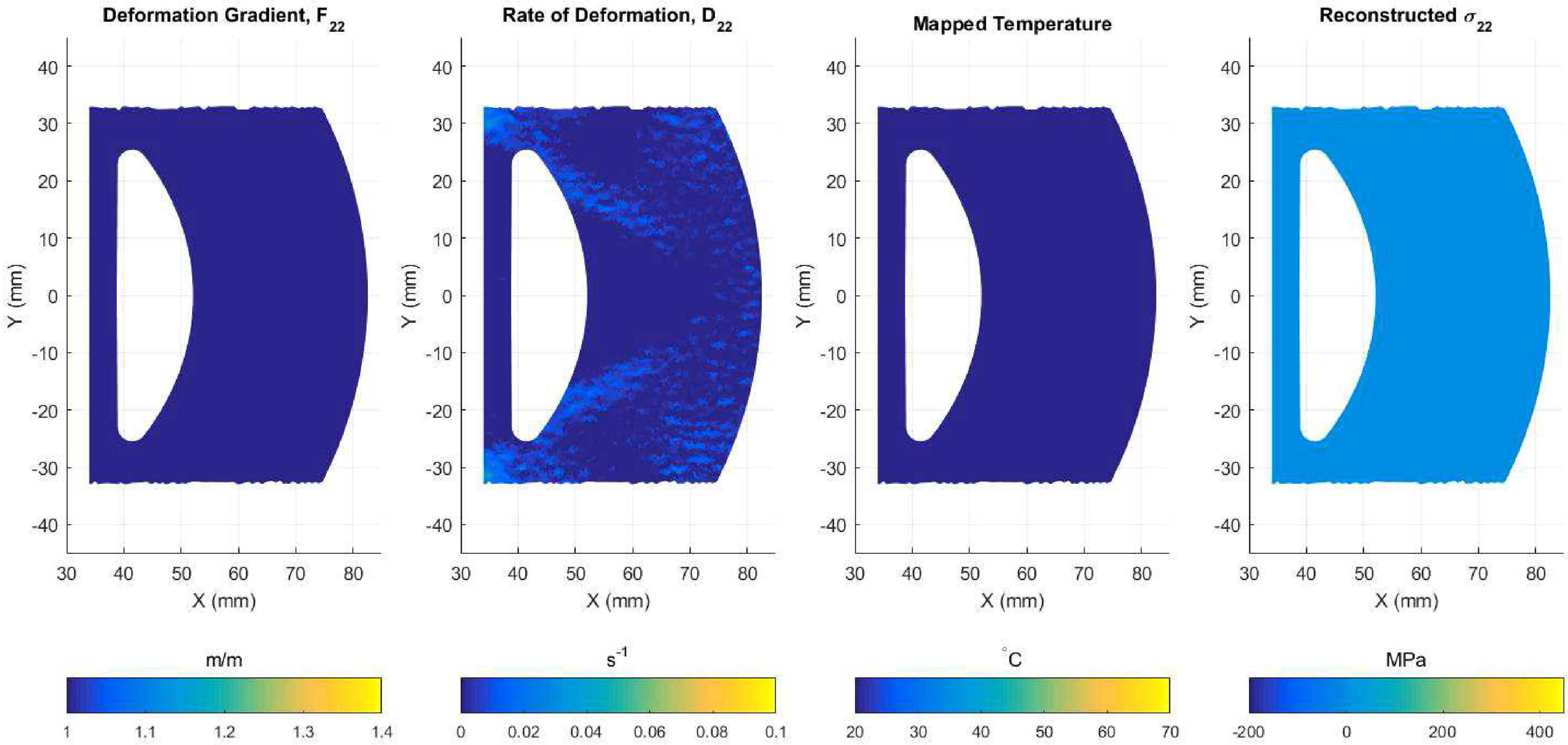
Method 2: The BCJ model was calibrated using the Virtual Fields Method and full-field DIC data.



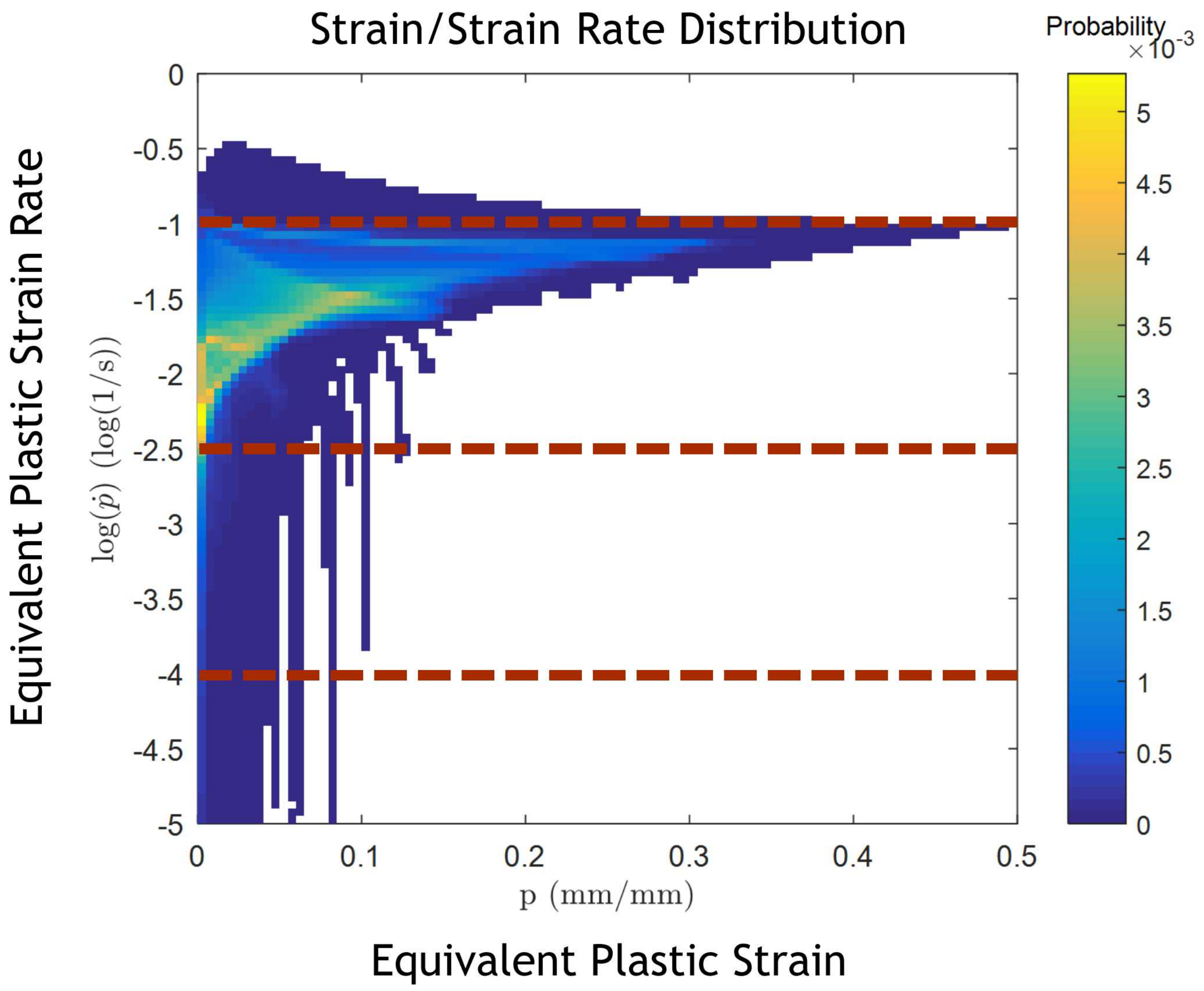
Raw data includes images of a patterned specimen for DIC, IR for temperature measurements, and resultant force.



Derived data includes strain, strain rate, temperature, and reconstructed stress



Complex specimen geometry induces strain rate heterogeneity in the sample.



Virtual Fields Method is a **powerful inverse technique** that capitalizes on full-field data.

- Principle of virtual power
  - $$\underbrace{\int_{V_o} \Pi : \dot{F}^* \, dV}_{\textit{Internal Power, } P_{int}} = \underbrace{f \cdot \overline{v^*}}_{\textit{External Power, } P_{ext}}$$
- Cost function
  - $$\Psi = \sum\nolimits_{\text{time}} [P_{int} - P_{ext}]^2$$

Π	First Piola-Kirchoff Stress
f	Resultant Load
V	Sample Volume
v^*	Virtual Velocity
$\dot{F}^*$	Virtual Velocity Gradient

Stress is a function of:

- Strain, strain rate, temperature
- Material model

Measured experimentally

Kinematically admissible
Selected judiciously

Pierron and Grédiac (2012) *The Virtual Fields Method*. Springer.

Method 2: The BCJ model was calibrated using the Virtual Fields Method and full-field DIC data.

Advanced Calibration

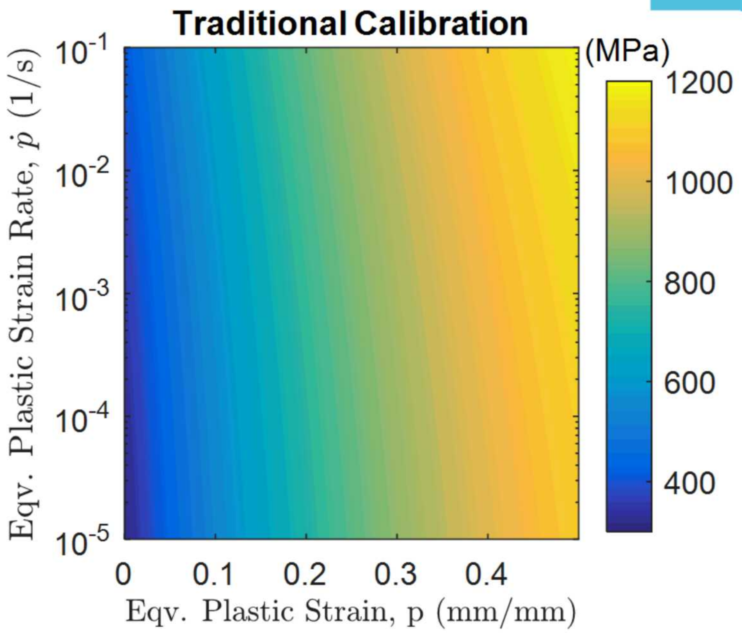
1. Full-field data is used.

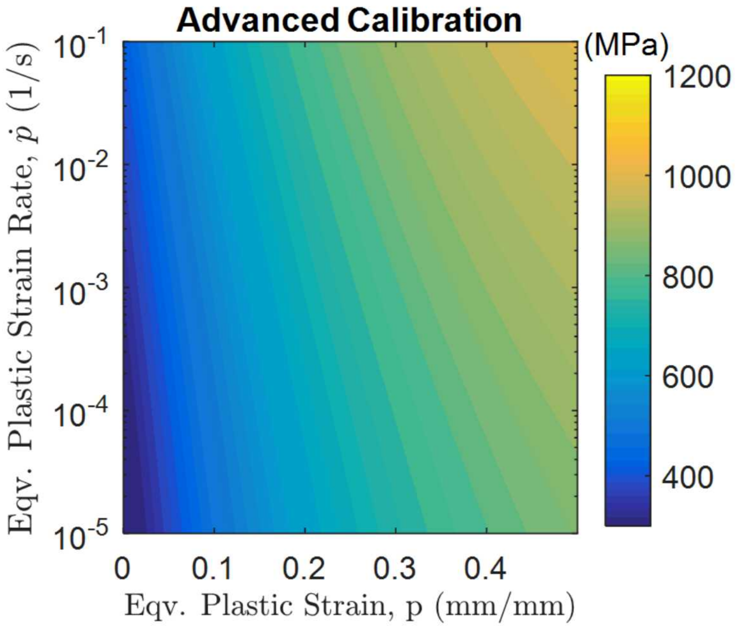
2. A single test is used to capture strain-rate dependence.

The two calibration methods identify similar, but different, model parameters.

$$\sigma_f(p,\dot{p},\boldsymbol{\xi}) = \sigma_Y\left\{1+\operatorname{asinh}\left[\left(\frac{\dot{p}}{b}\right)^{1/m}\right]\right\}+\frac{H}{R_d}[1-\exp(-R_d p)]$$

Parameter	Symbol	Units	Traditional Calibration	Advanced Calibration
Quasi-static yield stress	σ_y	MPa	253.8	163.9
Hardening	H	MPa	2538	2682
Dynamic recovery	R_d	--	2.110	3.845
Rate-dependent coefficient	b	s^{-1}	4.728	$2.372\cdot10^{-4}$
Rate-dependent exponent	m	--	9.229	7.306





Summary

- Model calibration is a difficult but critical component of engineering analysis
- Complex material behavior requires complex models.
- MatCal provides a **verified and validated** tool for model calibration
  - MatCal wraps existing Sandia and external tools, with the aim to reduce the time analysts spend performing material calibration by providing a standardized and verified tool specifically tailored to this purpose.
  - MatCal aims to improve the visibility and traceability of calibration work through a GRANTA interface.
  - MatCal aims to be a future catalyst for more advanced calibration methods.

- Advanced methods of calibration are required to increase data richness, reduce cases of "under-resolved" data or "non-unique" solutions, and improve experimental efficiency.