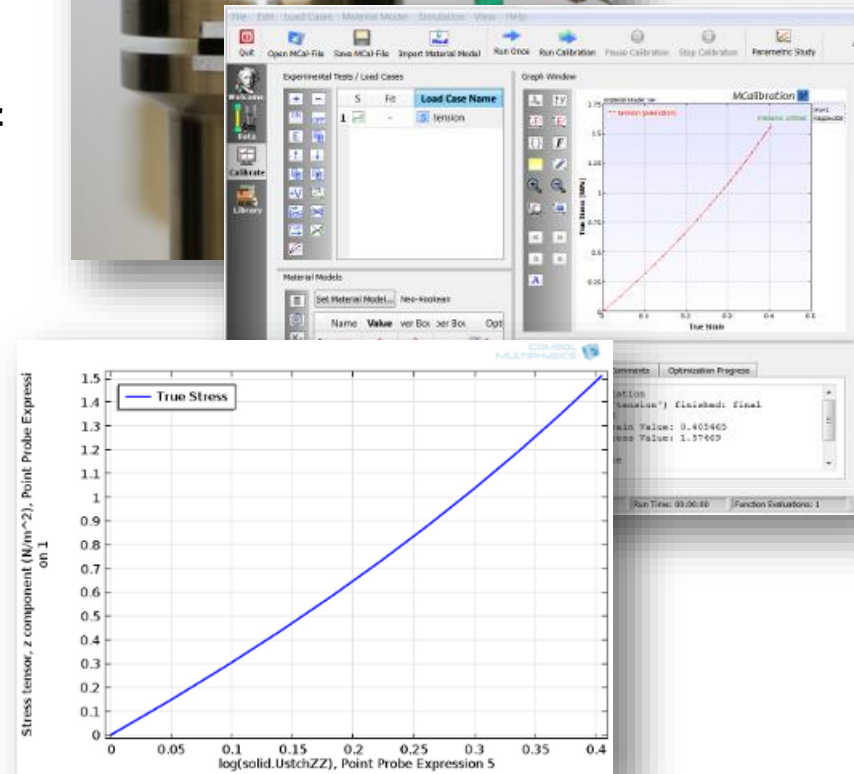
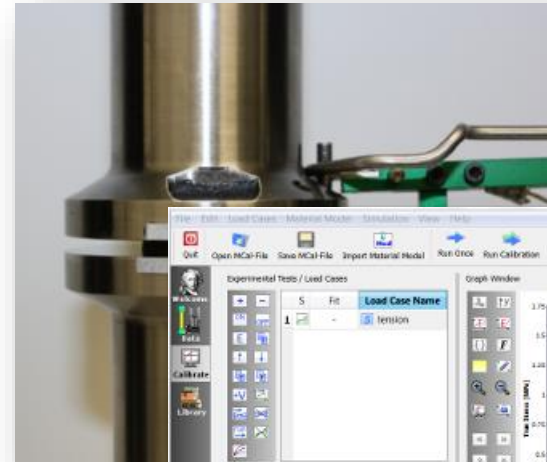


# Non-Linear Mechanical Modeling of Thermoplastics using COMSOL Multiphysics

Jorgen Bergstrom, Ph.D.  
Nagi Elabbasi, Ph.D.

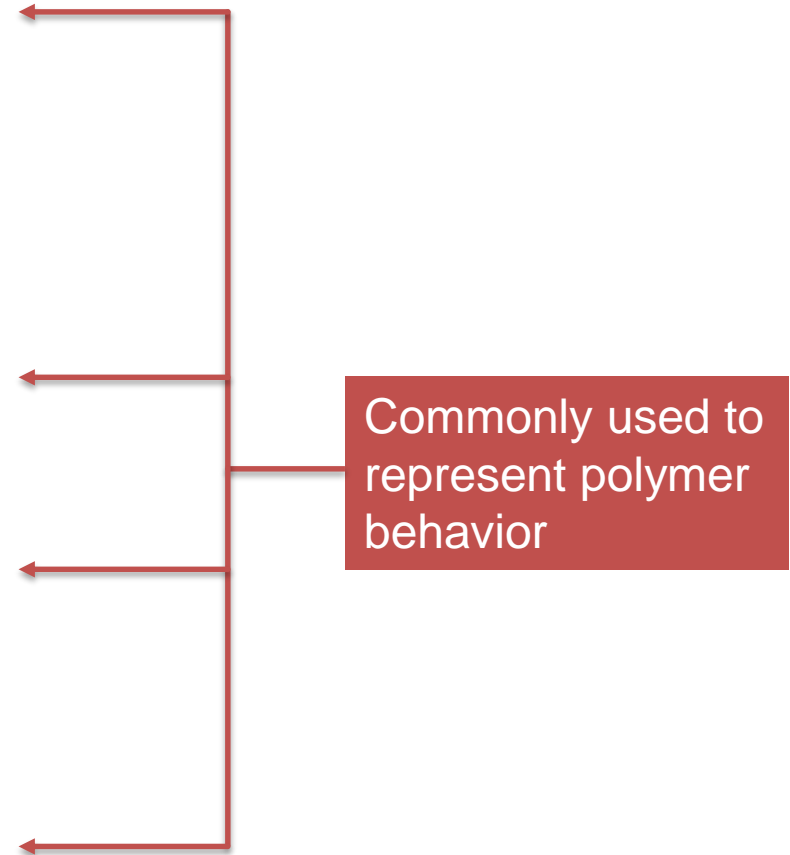
# Outline

- Introduction to material models for structural FEA
- COMSOL External Material Functionality
- Example Problem: modeling of PEEK
  - Experimental data
  - Material model calibration
  - Material model validation using COMSOL
- Summary



# COMSOL Solid Mechanics Materials

- **Elastoplastic Material**
- Fatigue
- General Stress-Strain Relation
- Geomechanics Material
- **Hyperelastic Material**
- Linear Elastic Material
- **Linear Viscoelastic Material**
- Nonlinear Elastic Material
- Poroelastic Material
- **External Material Functionality**

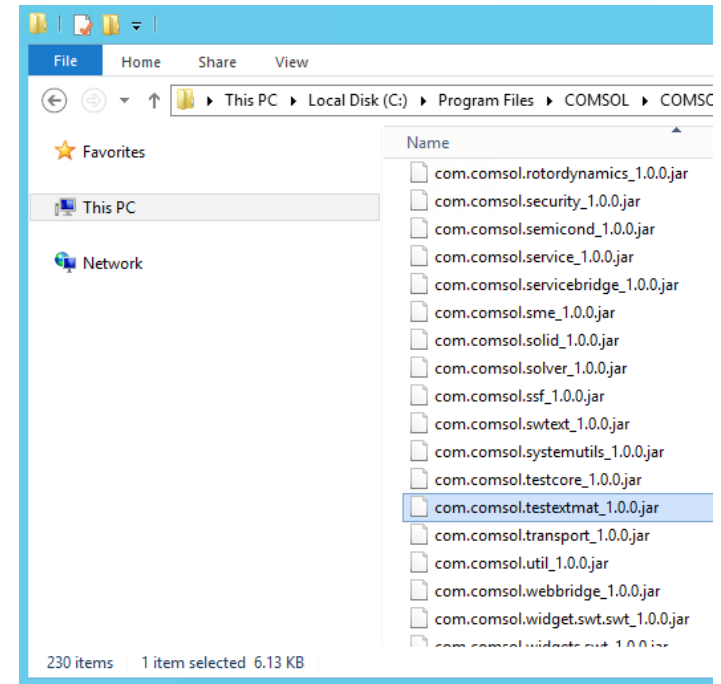


# External Material Model with COMSOL

```

EXPORT int
eval(double *time0,           // Time at previous step, scalar
     double *time1,           // Time at current step, scalar
     double *temp0,           // Temperature at previous step
     double *temp1,           // Temperature at current step
     double *F0,               // Deformation gradient at previous step
     double *F1,               // Deformation gradient at current step
     double *PK2_stress,       // Second Piola-Kirchhoff stress tensor
     double *Jac,              // Jacobian d(PK2_stress[i],F1)
     double *elastEner,        // Elastic energy, scalar, state
     double *plastEner,        // Plastic energy, scalar, state
     int *nProps,              // Number of material model properties
     double *props,            // Material model properties
     int *nStates,             // number of states, scalar, state
     double *states)           // States, nStates vector
{
    int res = 0;
    COMSOL_POLYUMOD(time0, time1, temp0, temp1, F0, F1,
                    PK2_stress, Jac, elastEner, plastEner, nProps,
                    props, nStates, states, &res);
    return res;
}

```



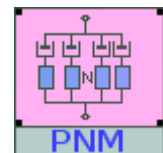
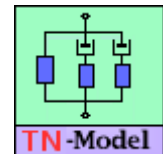
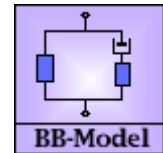
1. Write code for user-material model
2. Compile code to shared-library format
3. Copy jar-file to COMSOL plugins directory
4. Define the material parameters in COMSOL



The PolyUMod library is available for COMSOL

# PolyUMod Library

- Commercially available library available from Veryst Engineering
- More than 15 different highly accurate non-linear viscoplastic material models, e.g.:
  - Bergstrom-Boyce (BB) Model
    - *Suitable for rubbers and elastomer-like materials*
    - *Captures: strain rate effects, hysteresis*
  - Three Network (TN) Model
    - *Suitable for isotropic thermoplastics*
    - *Captures: strain rate effects, viscoplastic flow and recovery*
  - Parallel Network (TN) Model
    - *Suitable for highly non-linear and/or anisotropic materials*
    - *Captures: strain rate effects, viscoplastic flow and recovery*

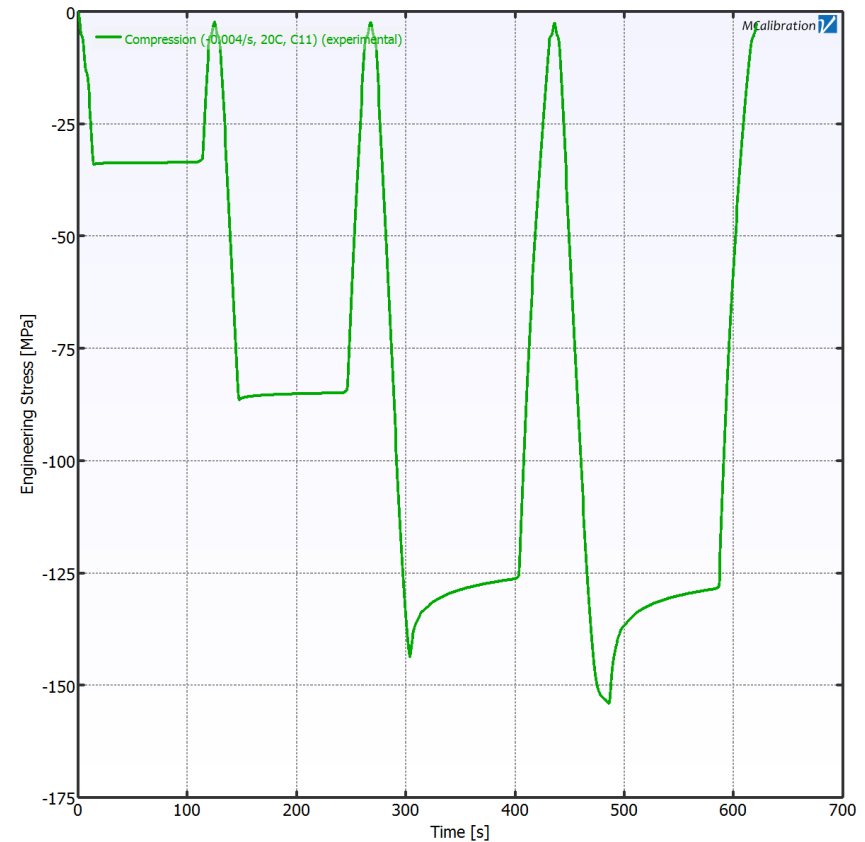
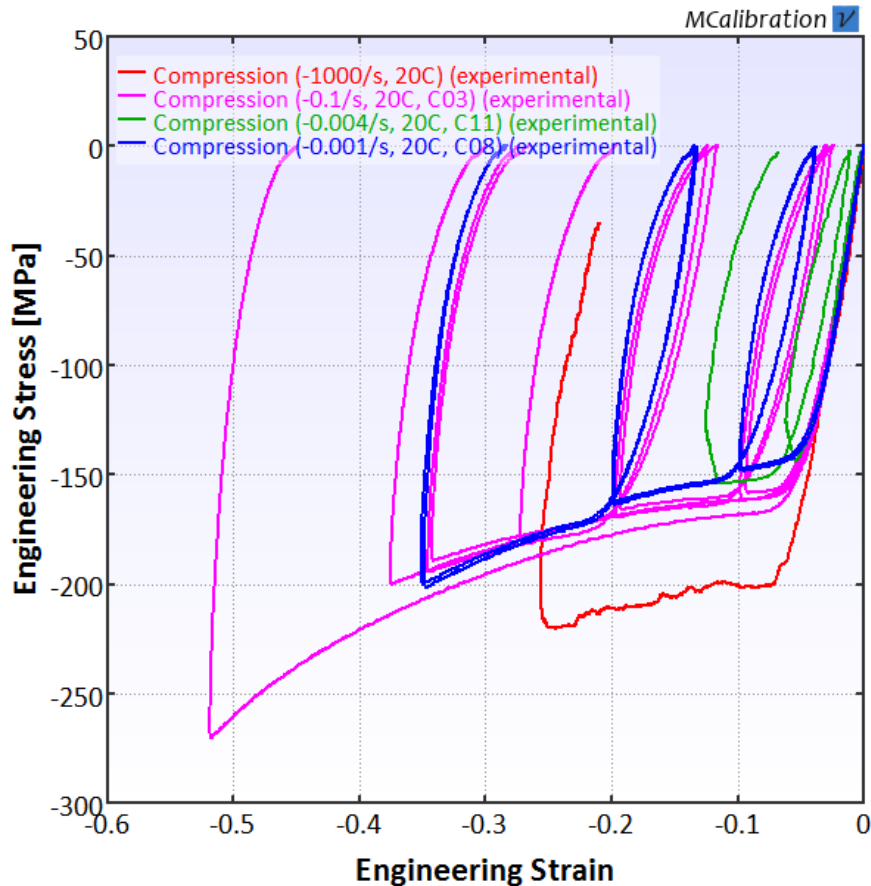


# Polyether Ether Ketone (PEEK)

- Good mechanical properties ( $E \approx 4 \text{ GPa}$ ,  $\sigma_{ut} \approx 100 \text{ MPa}$ )
- Good wear resistance
- Inert, generally biocompatible
- Orthopedic applications:
  - Spinal implants/spacers
  - Fixation (screws, plates, etc.)
  - Biomedical textiles (wovens, braids)
- Sealing applications (HPHT)

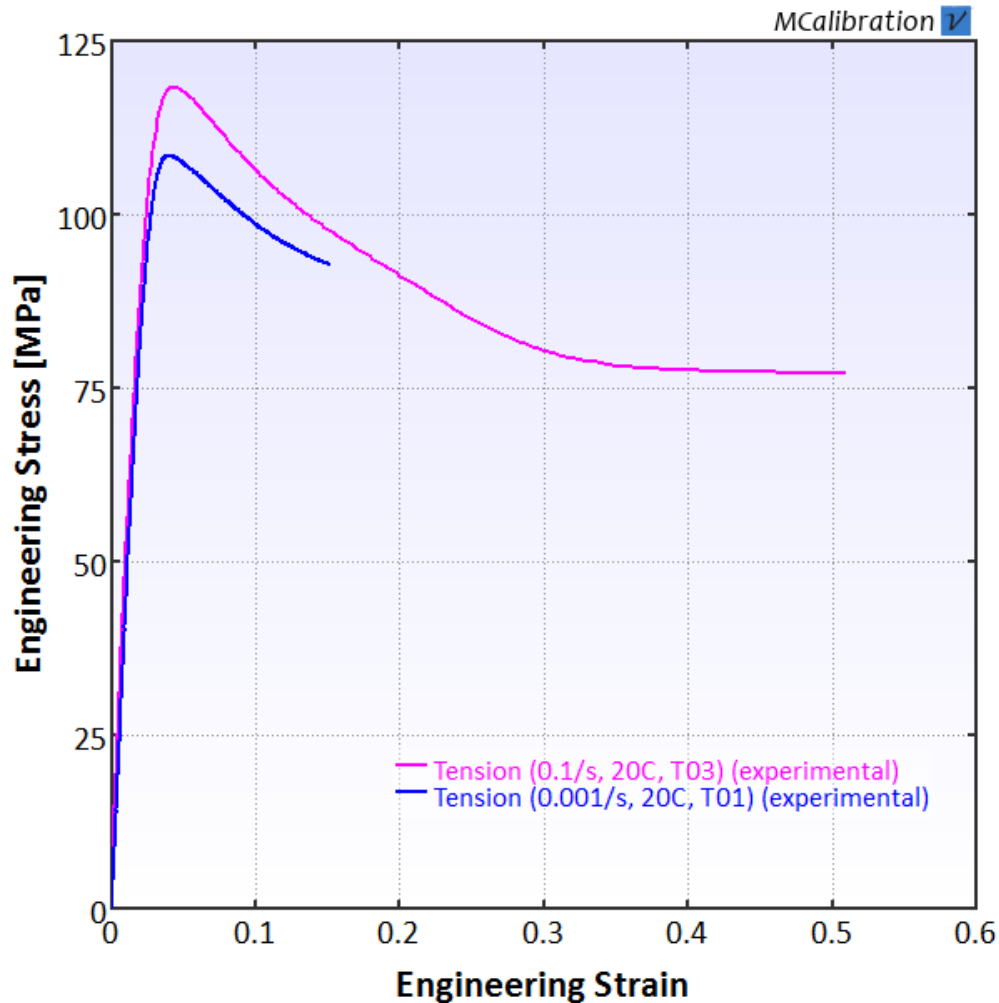


# Experimental Test: Uniaxial Compression



Uniaxial Compression

# Experimental Test: Uniaxial Tension

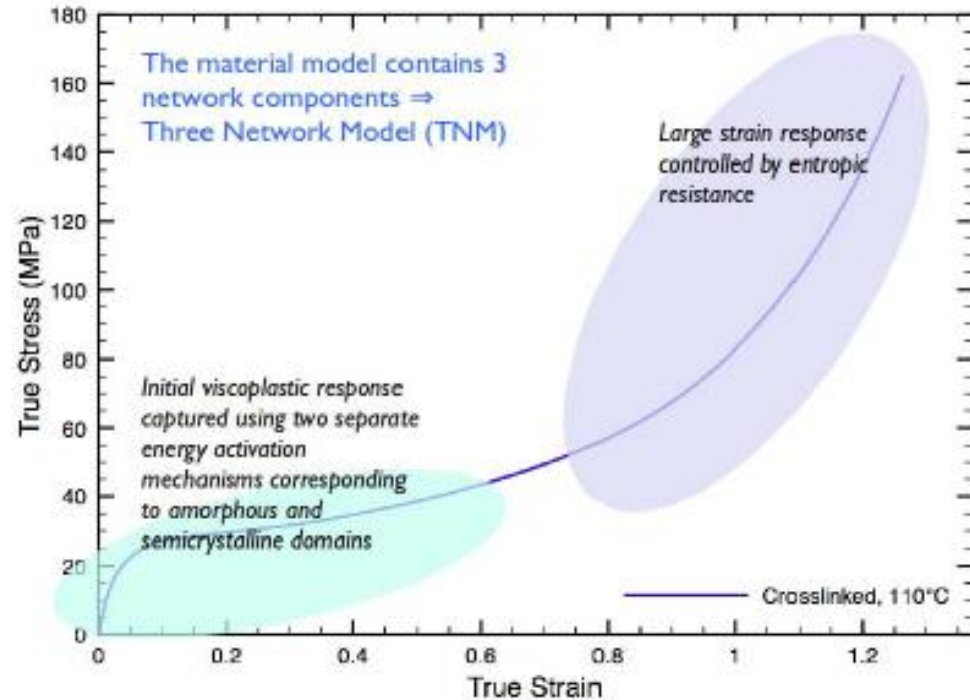
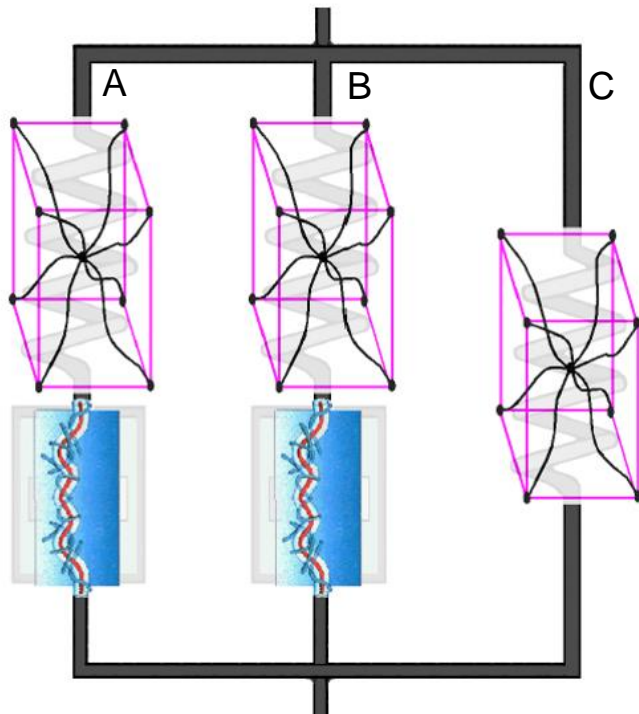


Viscoplastic response with slight softening after yield

Uniaxial Tension



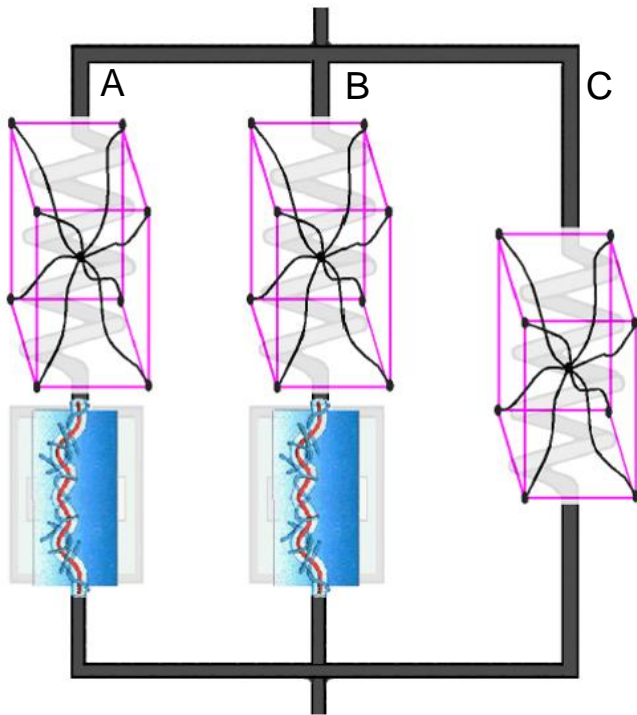
# Three Network (TN) Model



The **Three Network (TN) model** is a micromechanism inspired modeling framework suitable for thermoplastics. The TN model is available in the PolyUMod library.

Bergstrom, Bischoff, "An Advanced Thermomechanical Constitutive Model for UHMWPE," Int. J. Structural Changes in Solids, Vol 2, No 1, pp. 31-39, 2010

# TN Model Theory



- The stress in each network is defined by the Arruda-Boyce Eight Chain model:

$$\sigma = \frac{\mu_A}{J^e \bar{\lambda}^e} \frac{\mathcal{L}^{-1}(\bar{\lambda}^e / \lambda_L)}{\mathcal{L}^{-1}(1 / \lambda_L)} \text{dev}[b^e] + \kappa (J^e - 1) \mathbf{1}$$

- The shear modulus in Network 2 evolves with the plastic strain:

$$\dot{\mu} = -\beta [\mu_i - \mu_f] \dot{\gamma}$$

- The flow in each network is defined by a reptation inspired equation:

$$\dot{\gamma} = \dot{\gamma}_0 \left( \frac{\tau}{\hat{t} + aR(p)} \right)^m$$

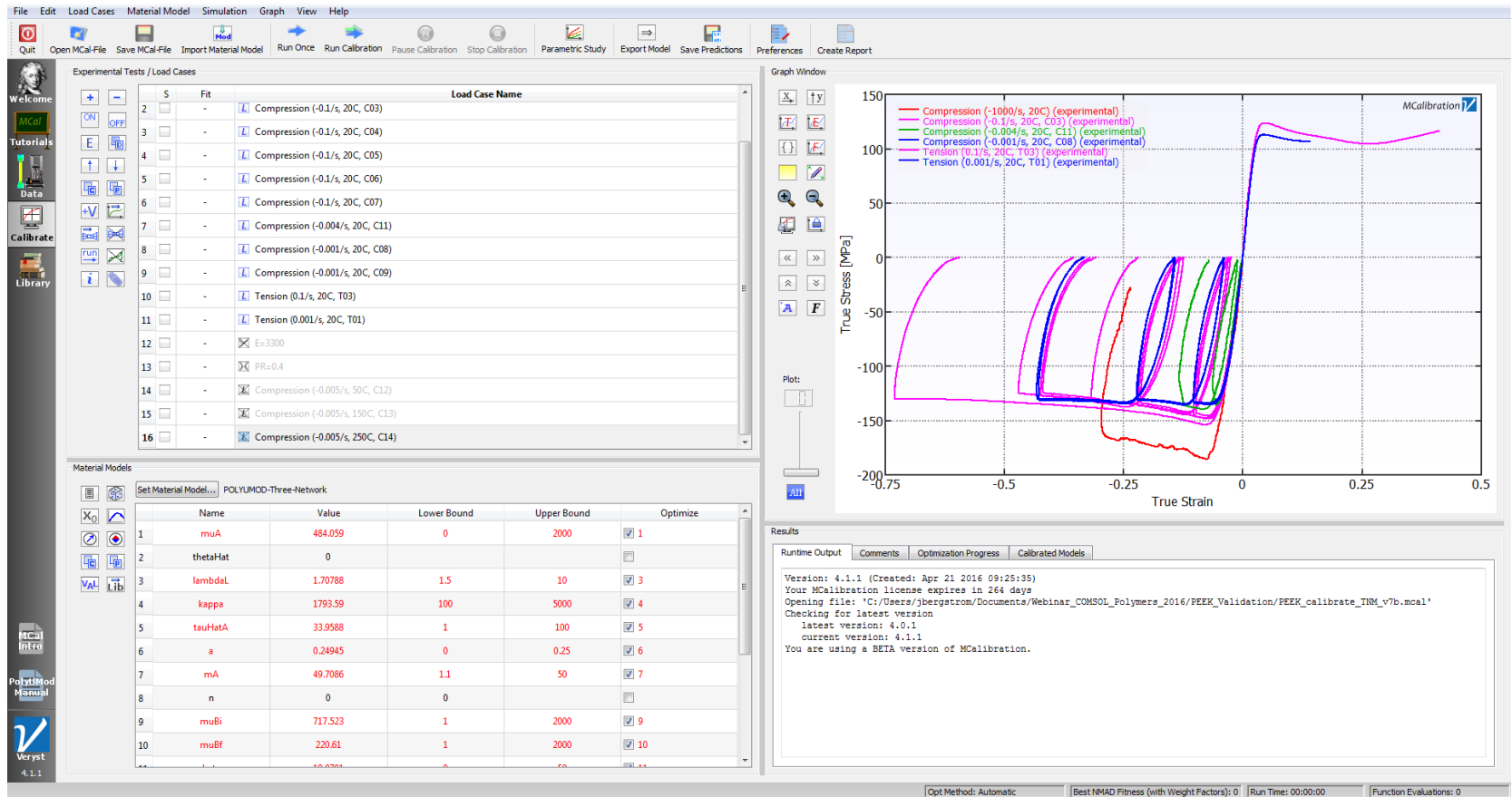
# TN Model Parameters

Index	Symbol	Parameter Name	Unit*	Description
1	$\mu_A$	muA	S	Shear modulus of network A
2	$\hat{\theta}$	thetaHat	T	Temperature factor
3	$\lambda_L$	lambdaL	-	Locking stretch
4	$\kappa$	kappa	S	Bulk modulus
5	$\hat{\tau}_A$	tauHatA	S	Flow resistance of network A
6	$a$	a	-	Pressure dependence of flow
7	$m_A$	mA	-	Stress exponential of network A
8	$n$	n	-	Temperature exponential
9	$\mu_{Bi}$	muBi	S	Initial shear modulus of network B
10	$\mu_{Bf}$	muBf	S	Final shear modulus of network B
11	$\beta$	beta	-	Evolution rate of $\mu_B$
12	$\hat{\tau}_B$	tauHatB	S	Flow resistance of network B
13	$m_B$	mB	-	Stress exponential of network B
14	$\mu_C$	muC	S	Shear modulus of network C
15	$q$	q	-	Relative contribution of $I_2$ of network C
16	$\alpha$	alpha	T <sup>-1</sup>	Thermal expansion coefficient
17	$\theta_0$	theta0	T	Thermal expansion reference temperature

\*where: - = dimensionless, S = stress, T = temperature, f = frequency

- The TN model needs up to 17 parameters that need to be determined from experimental data

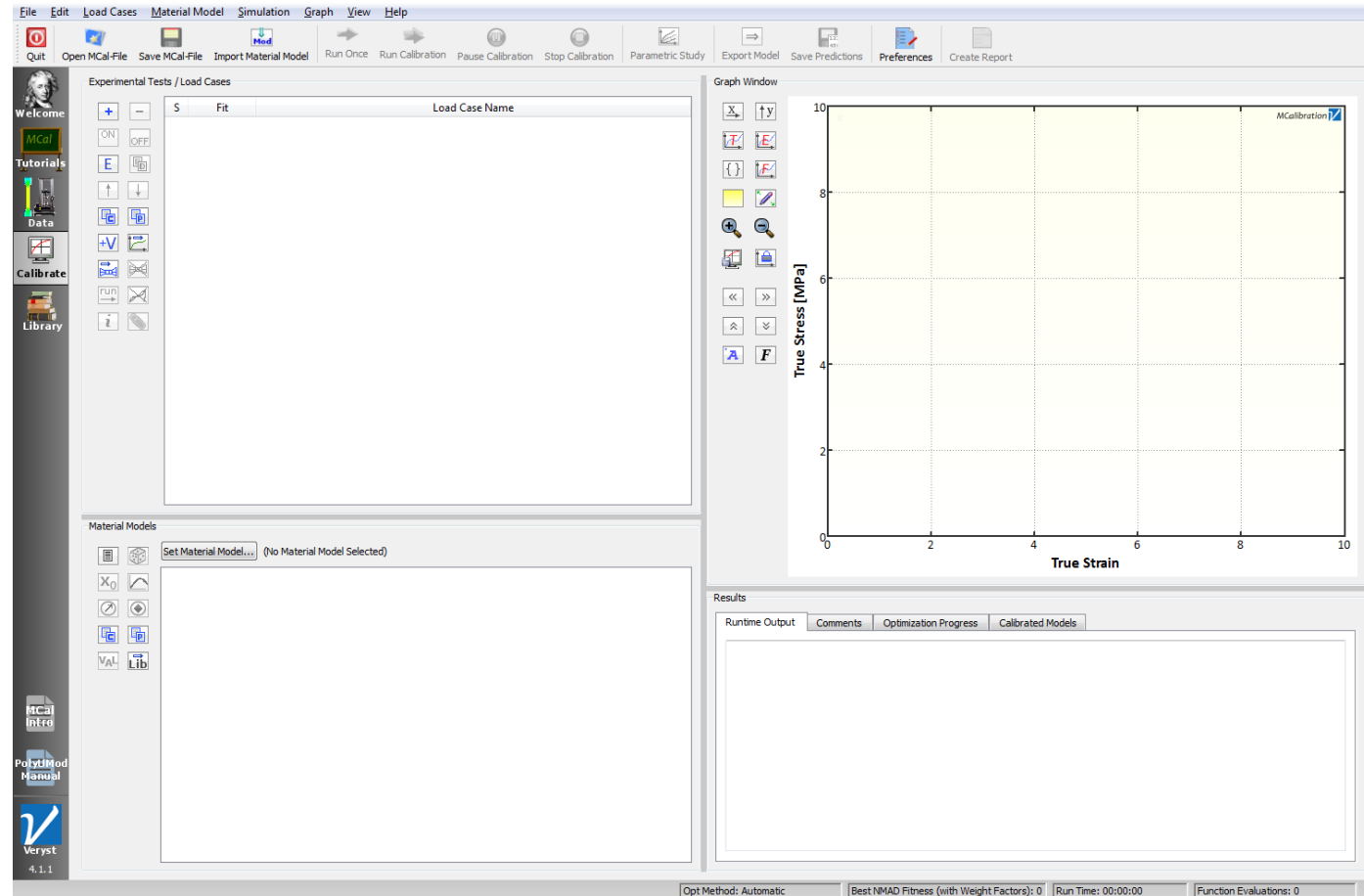
# Material Model Calibrations



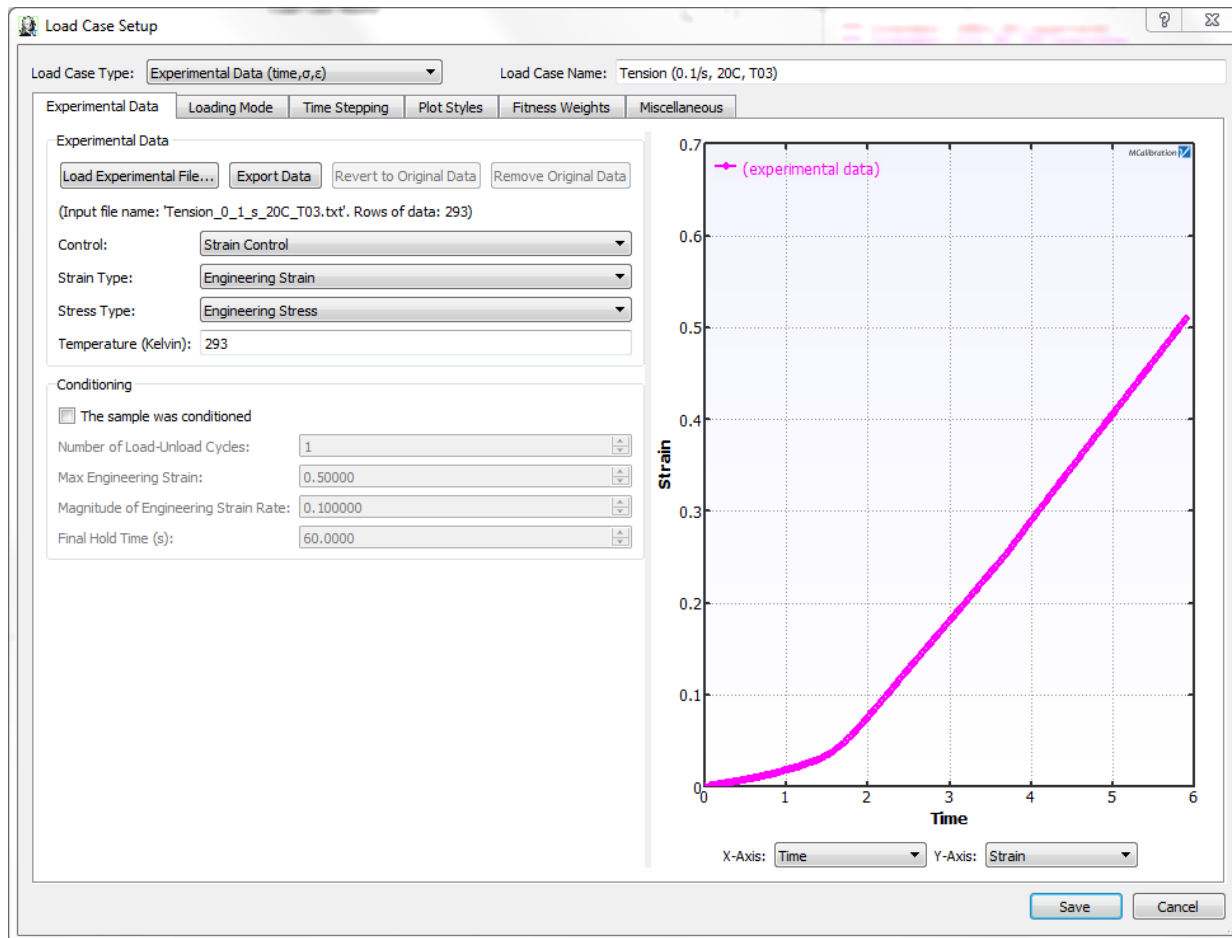
The TN model was calibrated using the MCalibration<sup>®</sup> software from Veryst Engineering.

# MCalibration Example - 1

- Start the software and read in the experimental data

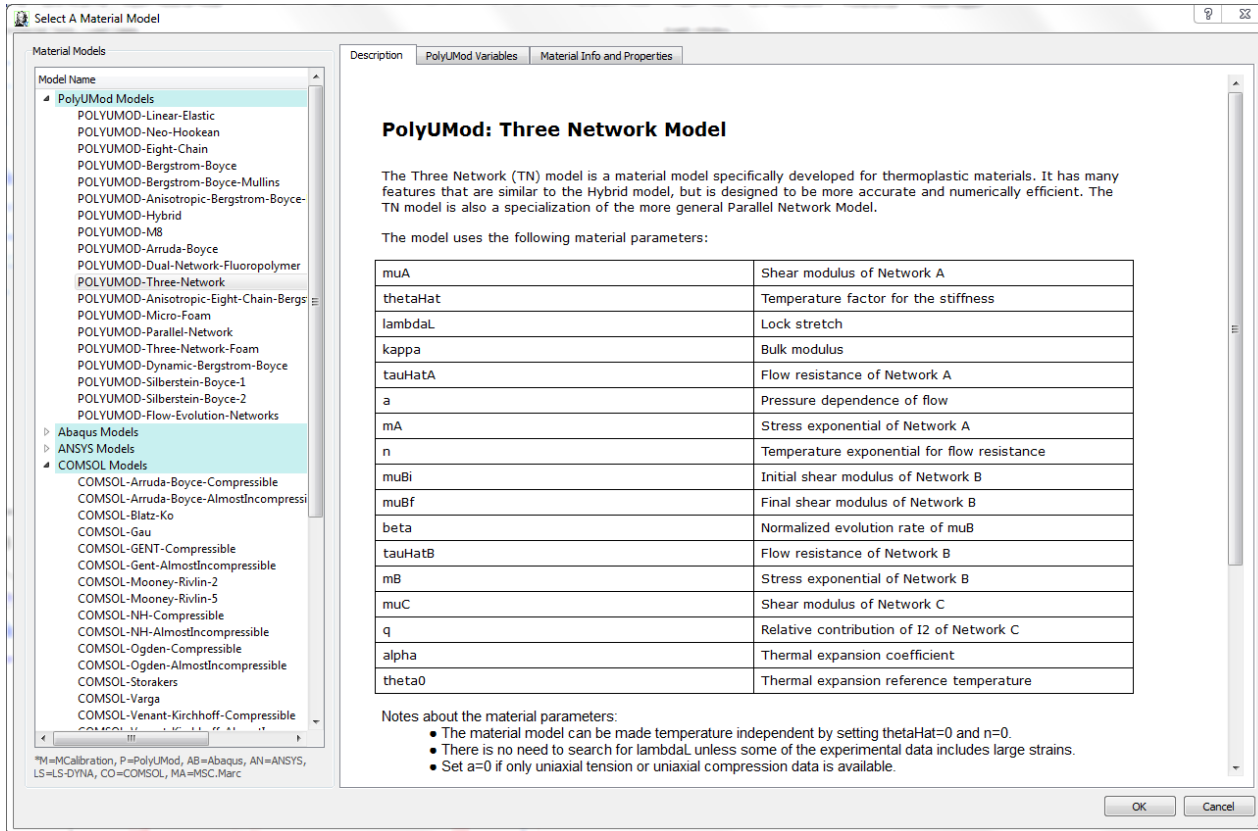


# MCalibration Example – 2



- The experimental data is loaded using a Load Case dialog
- This figure shows a tension load case
- Repeat this step for all experiments

# MCalibration Example – 3



**Select A Material Model**

Material Models

Model Name

- PolyUMod Models
    - POLYUMOD-Linear-Elastic
    - POLYUMOD-Neo-Hookean
    - POLYUMOD-Eight-Chain
    - POLYUMOD-Bergstrom-Boyce
    - POLYUMOD-Bergstrom-Boyce-Mullins
    - POLYUMOD-Anisotropic-Bergstrom-Boyce
    - POLYUMOD-Hybrid
    - POLYUMOD-M8
    - POLYUMOD-Arruda-Boyce
    - POLYUMOD-Dual-Network-Fluoropolymer
    - POLYUMOD-Three-Network
    - POLYUMOD-Anisotropic-Eight-Chain-Bergs
    - POLYUMOD-Micro-Foam
    - POLYUMOD-Parallel-Network
    - POLYUMOD-Three-Network-Foam
    - POLYUMOD-Dynamic-Bergstrom-Boyce
    - POLYUMOD-Silberstein-Boyce-1
    - POLYUMOD-Silberstein-Boyce-2
    - POLYUMOD-Flow-Evolution-Networks
  - Abaqus Models
  - ANSYS Models
  - COMSOL Models
    - COMSOL-Arruda-Boyce-Compressible
    - COMSOL-Arruda-Boyce-AlmostIncompressi
    - COMSOL-Blatz-Ko
    - COMSOL-Gau
    - COMSOL-GENT-Compressible
    - COMSOL-Gent-AlmostIncompressible
    - COMSOL-Mooney-Rivlin-2
    - COMSOL-Mooney-Rivlin-5
    - COMSOL-NH-Compressible
    - COMSOL-NH-AlmostIncompressible
    - COMSOL-Ogden-Compressible
    - COMSOL-Ogden-AlmostIncompressible
    - COMSOL-Storakers
    - COMSOL-Varga
    - COMSOL-Venant-Kirchhoff-Compressible

Description

PolyUMod Variables

Material Info and Properties

**PolyUMod: Three Network Model**

The Three Network (TN) model is a material model specifically developed for thermoplastic materials. It has many features that are similar to the Hybrid model, but is designed to be more accurate and numerically efficient. The TN model is also a specialization of the more general Parallel Network Model.

The model uses the following material parameters:

muA	Shear modulus of Network A
thetaHat	Temperature factor for the stiffness
lambdaL	Lock stretch
kappa	Bulk modulus
tauHata	Flow resistance of Network A
a	Pressure dependence of flow
mA	Stress exponential of Network A
n	Temperature exponential for flow resistance
muBi	Initial shear modulus of Network B
muBf	Final shear modulus of Network B
beta	Normalized evolution rate of muB
tauHatB	Flow resistance of Network B
mB	Stress exponential of Network B
muC	Shear modulus of Network C
q	Relative contribution of I2 of Network C
alpha	Thermal expansion coefficient
theta0	Thermal expansion reference temperature

Notes about the material parameters:

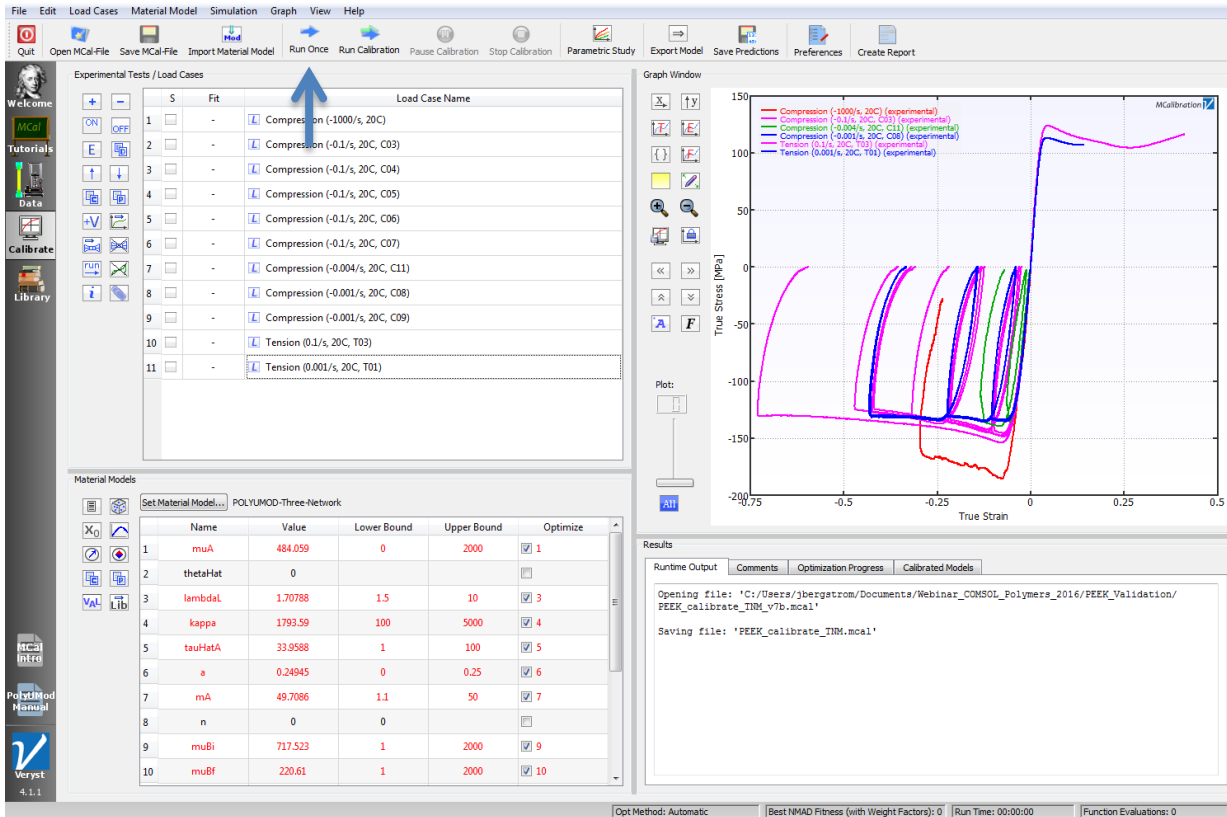
- The material model can be made temperature independent by setting thetaHat=0 and n=0.
- There is no need to search for lambdaL unless some of the experimental data includes large strains.
- Set a=0 if only uniaxial tension or uniaxial compression data is available.

OK Cancel

\*M=MCalibration, P=PolyUMod, AB=Abaqus, AN=ANSYS, LS=LS-DYNA, CO=COMSOL, MA=MSC.Marc

- Then select a material model to calibrate
- In this example we will select the TN model

# MCalibration Example – 4



Experimental Tests / Load Cases

S	Fit	Load Case Name
1	-	Compression (-1000/s, 20C)
2	-	Compression (-0.1/s, 20C, C03)
3	-	Compression (-0.1/s, 20C, C04)
4	-	Compression (-0.1/s, 20C, C05)
5	-	Compression (-0.1/s, 20C, C06)
6	-	Compression (-0.1/s, 20C, C07)
7	-	Compression (-0.004/s, 20C, C11)
8	-	Compression (-0.001/s, 20C, C08)
9	-	Compression (-0.001/s, 20C, C09)
10	-	Tension (0.1/s, 20C, T03)
11	-	Tension (0.001/s, 20C, T01)

Material Models

Name	Value	Lower Bound	Upper Bound	Optimize	
1	muA	484.059	0	2000	<input checked="" type="checkbox"/>
2	thetaHat	0			<input type="checkbox"/>
3	lambdaL	1.70788	1.5	10	<input checked="" type="checkbox"/>
4	kappa	1793.59	100	5000	<input checked="" type="checkbox"/>
5	tauHatA	33.9588	1	100	<input checked="" type="checkbox"/>
6	a	0.24945	0	0.25	<input checked="" type="checkbox"/>
7	mA	49.7086	1.1	50	<input checked="" type="checkbox"/>
8	n	0	0		<input type="checkbox"/>
9	muBi	717.523	1	2000	<input checked="" type="checkbox"/>
10	muBf	220.61	1	2000	<input checked="" type="checkbox"/>

Graph Window

True Stress [MPa]

True Strain

Results

```

Runtime Output
Comments
Optimization Progress
Calibrated Models

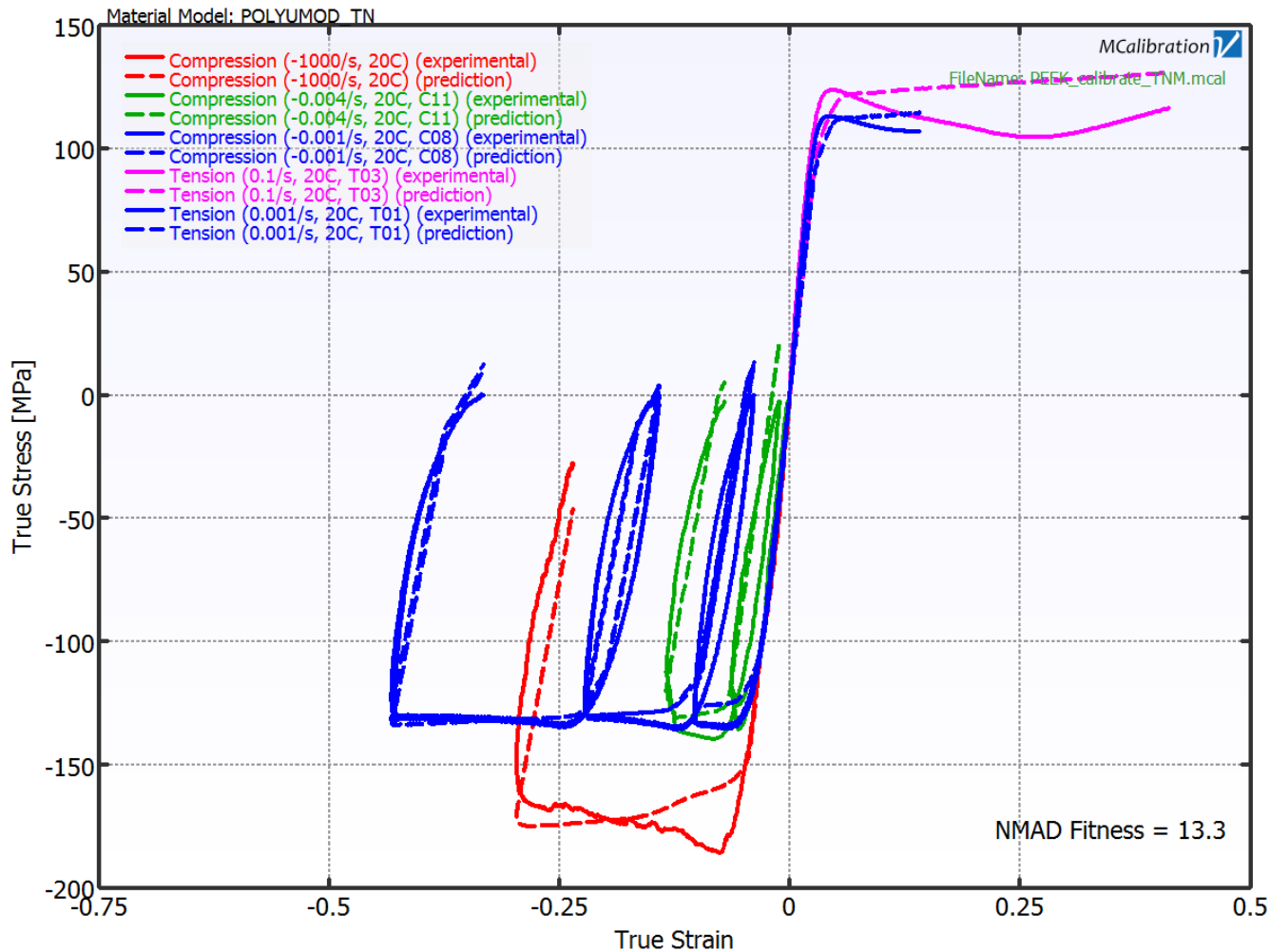
Opening file: 'C:/Users/jbergstrom/Documents/Webinar_CONSOL_Polymers_2016/PEEK_Validation/PEEK_calibrate_T01_v7b.mcal'
Saving file: 'PEEK_calibrate_T01.mcal'
  
```

Opt Method: Automatic | Best NMAD Fitness (with Weight Factors): 0 | Run Time: 00:00:00 | Function Evaluations: 0

- Then simply click “Run Calibration” to automatically adjust the material parameters to best match the experimental data
- The stress calculations are performed within MCalibration



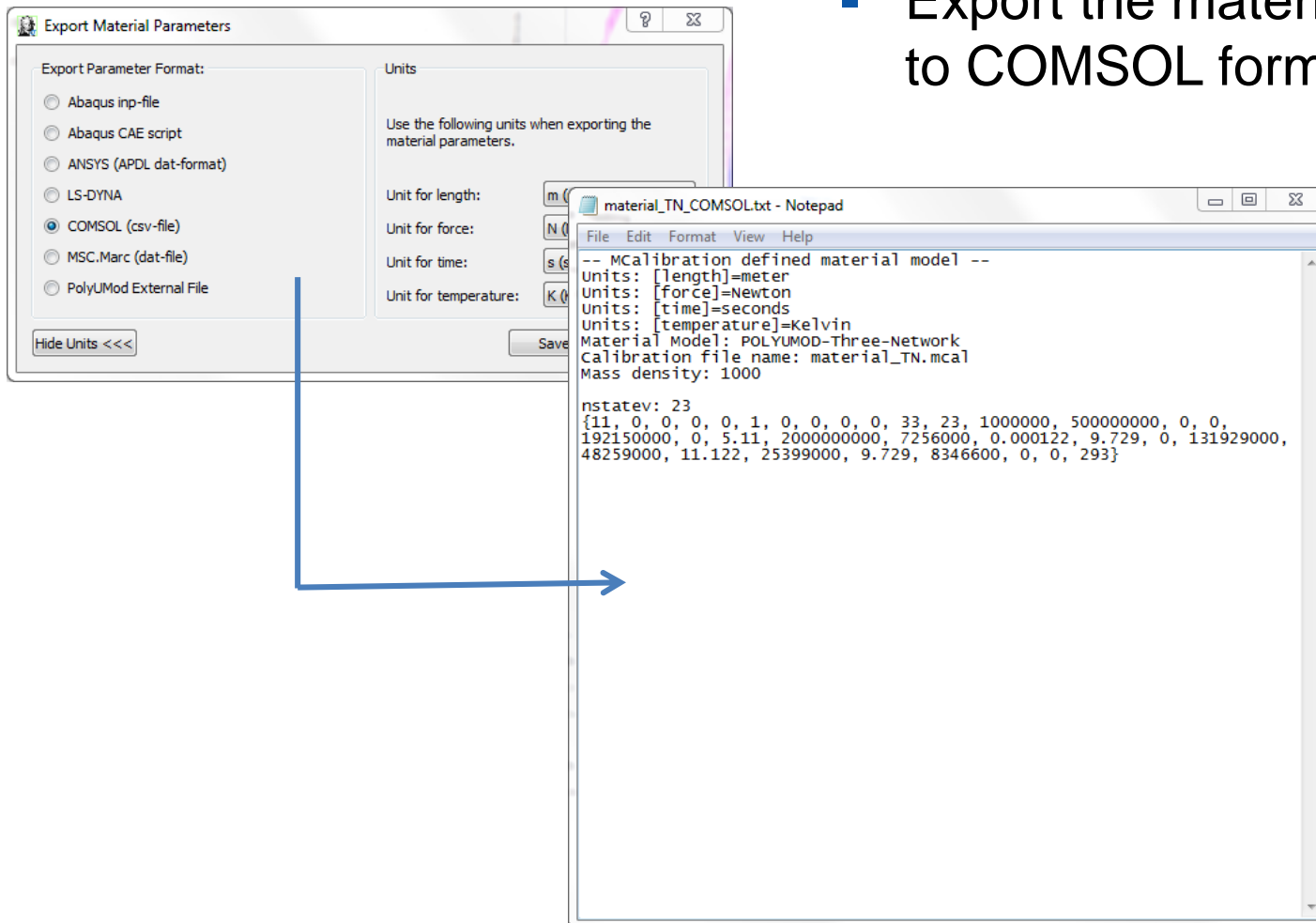
# MCalibration Example – 5



- Comparison between experimental data and material model predictions
- The TN model accurately captures the uniaxial tension and compression response

# MCalibration Example - 6

- Export the material model to COMSOL format



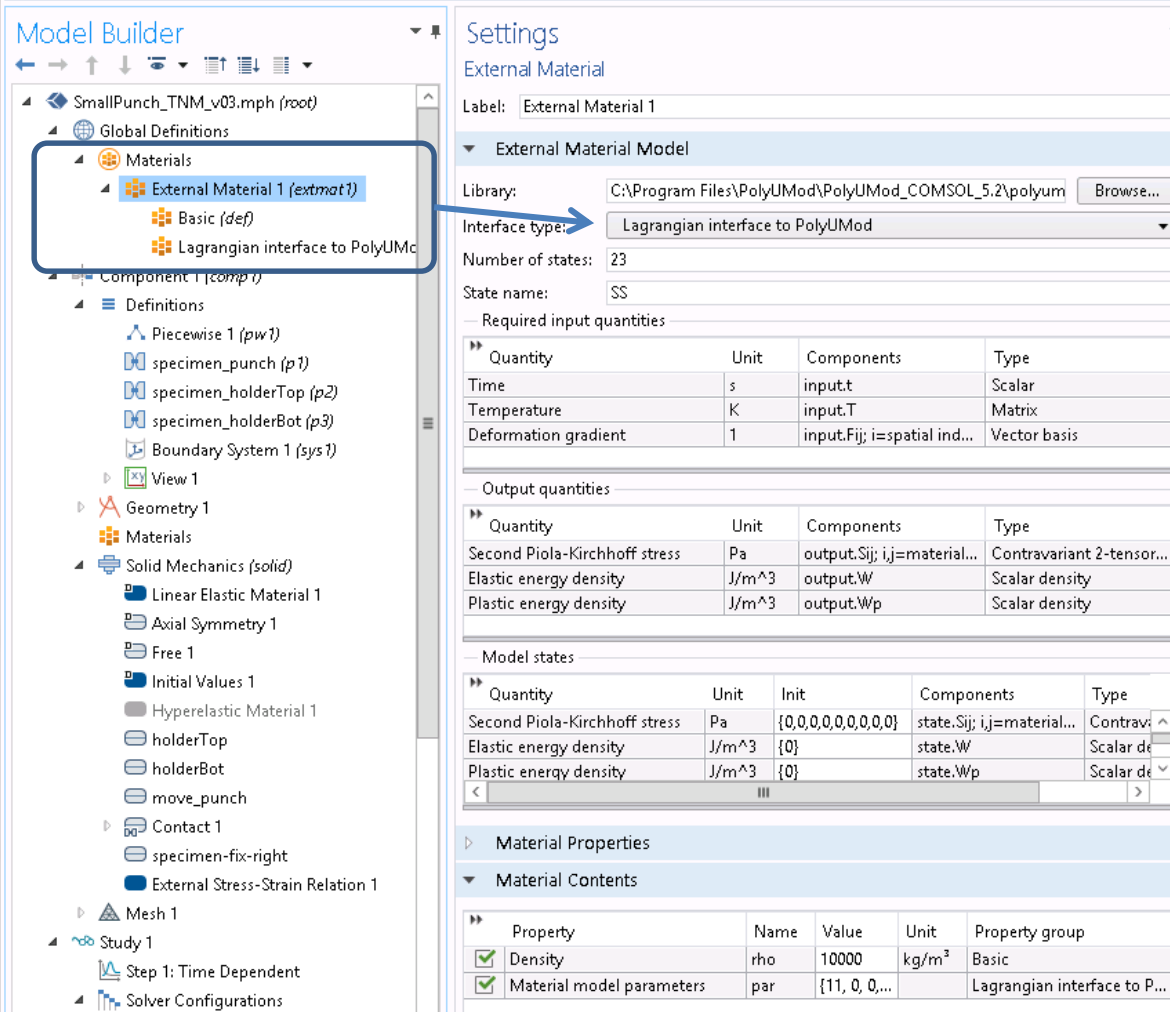
The screenshot shows the 'Export Material Parameters' dialog box with the 'COMSOL (csv-file)' option selected. A blue arrow points from this option to a Notepad window titled 'material\_TN\_COMSOL.txt'. The Notepad window contains the following text:

```

-- MCalibration defined material model --
Units: [length]=meter
Units: [force]=Newton
Units: [time]=seconds
Units: [temperature]=Kelvin
Material Model: POLYUMOD-Three-Network
Calibration file name: material_TN.mcal
Mass density: 1000

nstatev: 23
{11, 0, 0, 0, 0, 1, 0, 0, 0, 0, 33, 23, 1000000, 500000000, 0, 0,
192150000, 0, 5.11, 2000000000, 7256000, 0.000122, 9.729, 0, 131929000,
48259000, 11.122, 25399000, 9.729, 8346600, 0, 0, 293}
  
```

# MCalibration Example - 7



**Settings**  
External Material

Label: External Material 1

External Material Model

Library: C:\Program Files\PolyUMod\PolyUMod\_COMSOL\_5.2\polyum Browse...

Interface type: Lagrangian interface to PolyUMod

Number of states: 23

State name: SS

Required input quantities

Quantity	Unit	Components	Type
Time	s	input.t	Scalar
Temperature	K	input.T	Matrix
Deformation gradient	1	input.Fij; i=spatial ind...	Vector basis

Output quantities

Quantity	Unit	Components	Type
Second Piola-Kirchhoff stress	Pa	output.Sij; i,j=material...	Contravariant 2-tensor...
Elastic energy density	J/m <sup>3</sup>	output.W	Scalar density
Plastic energy density	J/m <sup>3</sup>	output.Wp	Scalar density

Model states

Quantity	Unit	Init	Components	Type
Second Piola-Kirchhoff stress	Pa	{0,0,0,0,0,0,0,0}	state.Sij; i,j=material...	Contravi...
Elastic energy density	J/m <sup>3</sup>	{0}	state.W	Scalar de...
Plastic energy density	J/m <sup>3</sup>	{0}	state.Wp	Scalar de...

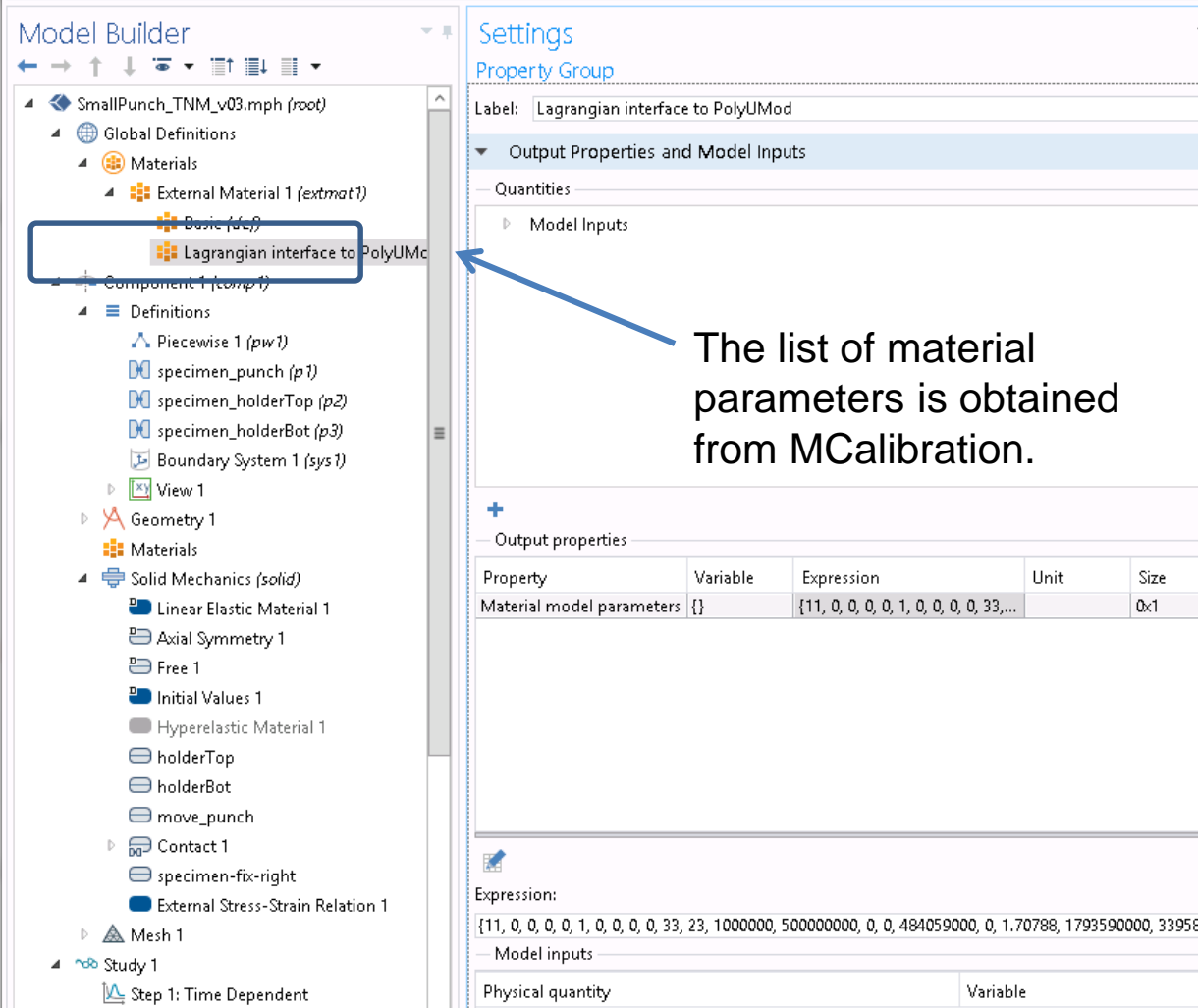
Material Properties

Material Contents

Property	Name	Value	Unit	Property group
<input checked="" type="checkbox"/> Density	rho	10000	kg/m <sup>3</sup>	Basic
<input checked="" type="checkbox"/> Material model parameters	par	{11, 0, 0, ...}		Lagrangian interface to P...

- The calibrated material model can then be entered into COMSOL Version 5.2 (and later) using the interface for external material models
- This interface can be used to model advanced nonlinear viscoplastic material models using the PolyUMod® library from Veryst Engineering

# COMSOL External Material Functionality



The screenshot shows the COMSOL Model Builder interface. In the left-hand 'Model Builder' tree, the 'Materials' section is expanded to show 'External Material 1 (extmat1)', which contains a sub-entry 'Lagrangian interface to PolyUMod'. This entry is highlighted with a blue box. An arrow points from this box to the 'Settings' pane on the right.

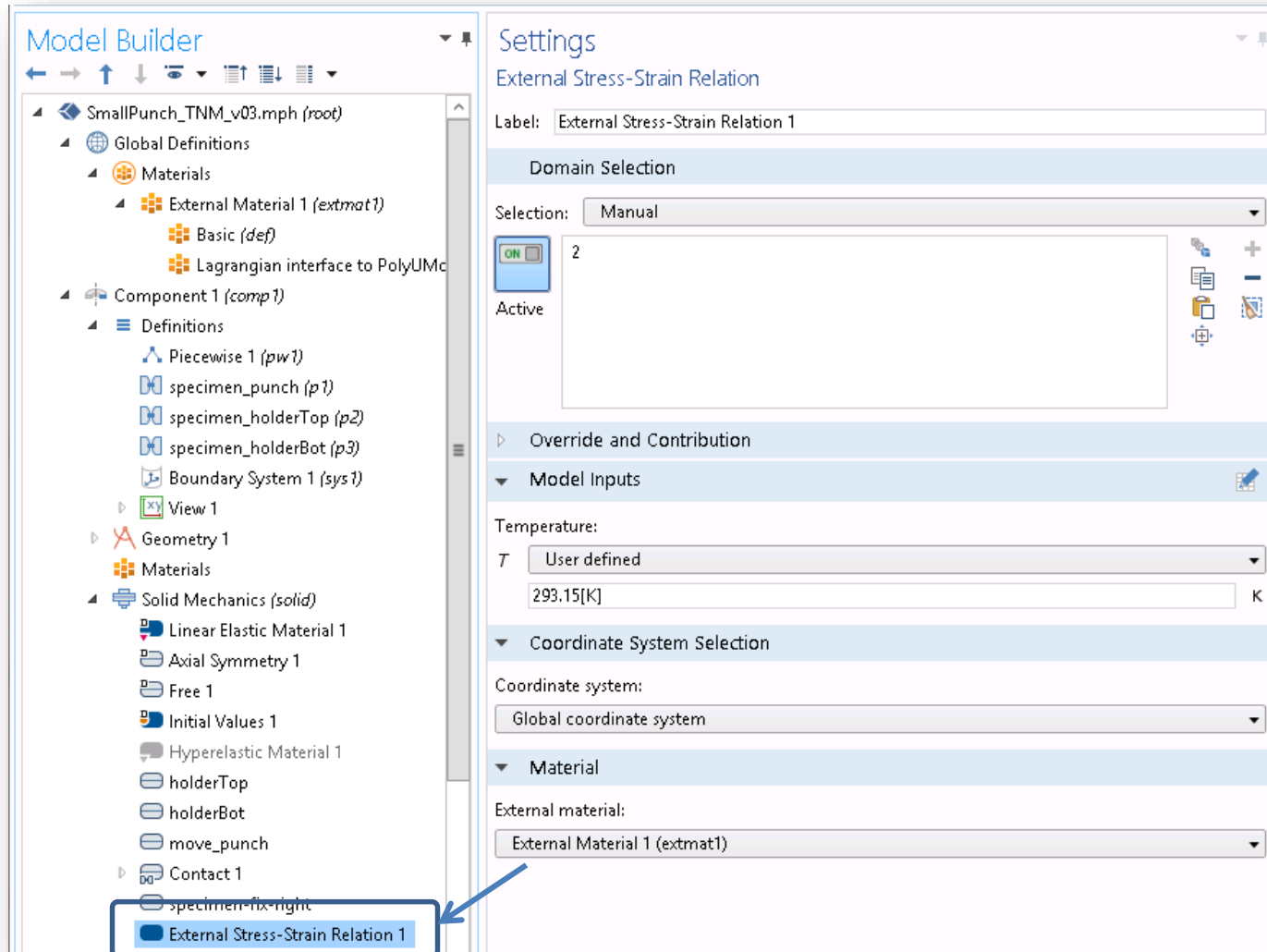
The 'Settings' pane shows the 'Property Group' for 'Lagrangian interface to PolyUMod'. Under 'Output Properties and Model Inputs', the 'Model Inputs' section is expanded. A text box with an arrow pointing to this section contains the text: 'The list of material parameters is obtained from MCalibration.'

Below the 'Model Inputs' section, the 'Output properties' section contains a table with the following data:

Property	Variable	Expression	Unit	Size
Material model parameters	{}	{11, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 33, ...		0x1

At the bottom of the 'Settings' pane, the 'Expression' field is visible, containing a long list of numerical values: {11, 0, 0, 0, 1, 0, 0, 0, 0, 33, 23, 1000000, 500000000, 0, 0, 484059000, 0, 1.70788, 1793590000, 33958}.

# COMSOL External Material Functionality

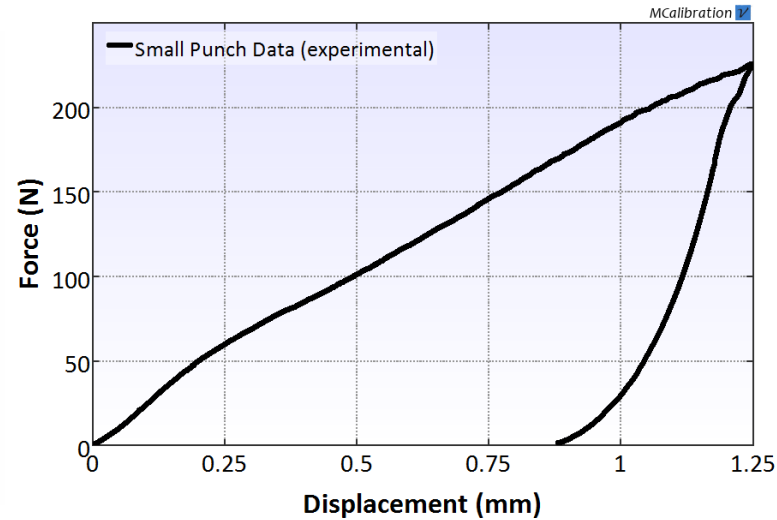
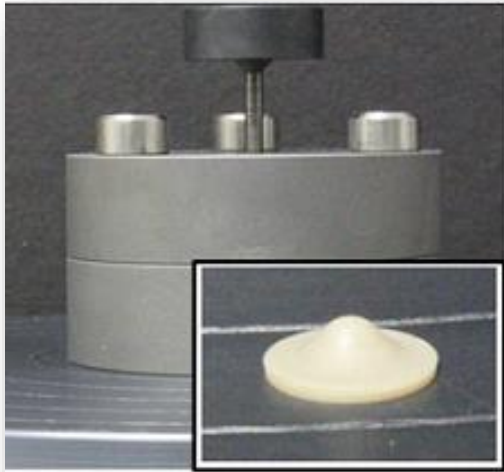


The screenshot displays the COMSOL Model Builder interface. On the left, the **Model Builder** tree shows the hierarchy: **SmallPunch\_TNM\_v03.mph (root)** > **Global Definitions** > **Materials** > **External Material 1 (extmat1)**. A blue box highlights **External Stress-Strain Relation 1** in the **Definitions** list, with a blue arrow pointing to the **Settings** panel on the right.

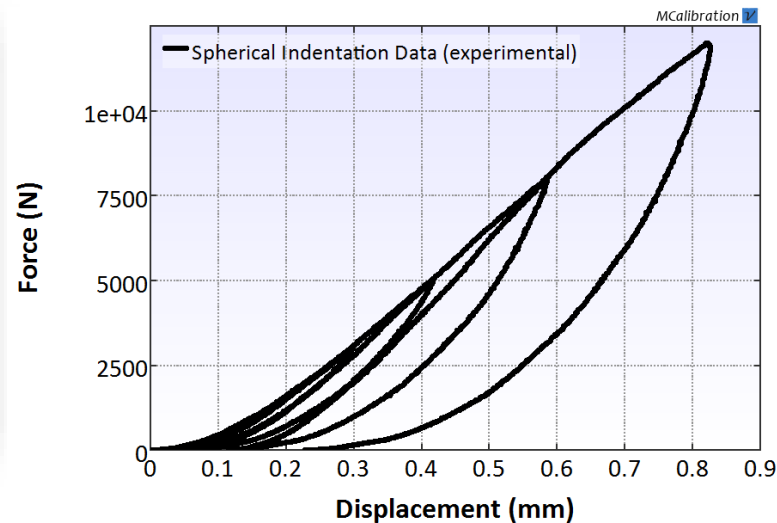
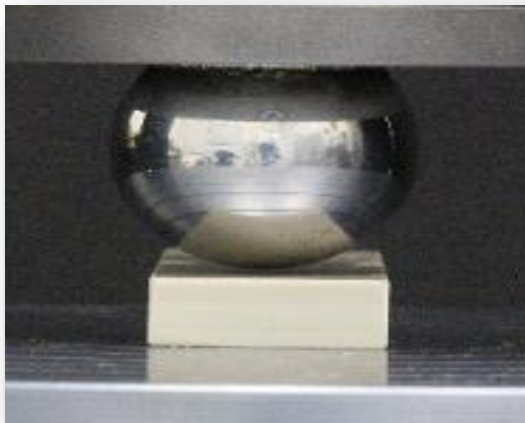
The **Settings** panel for **External Stress-Strain Relation** includes the following configuration:

- Label:** External Stress-Strain Relation 1
- Domain Selection:** Selection: Manual
- Active:** ON (checked), 2
- Override and Contribution:** (Expanded)
- Model Inputs:** (Expanded)
- Temperature:** T: User defined, 293.15[K]
- Coordinate System Selection:** Coordinate system: Global coordinate system
- Material:** External material: External Material 1 (extmat1)

# Multiaxial Validation Testing

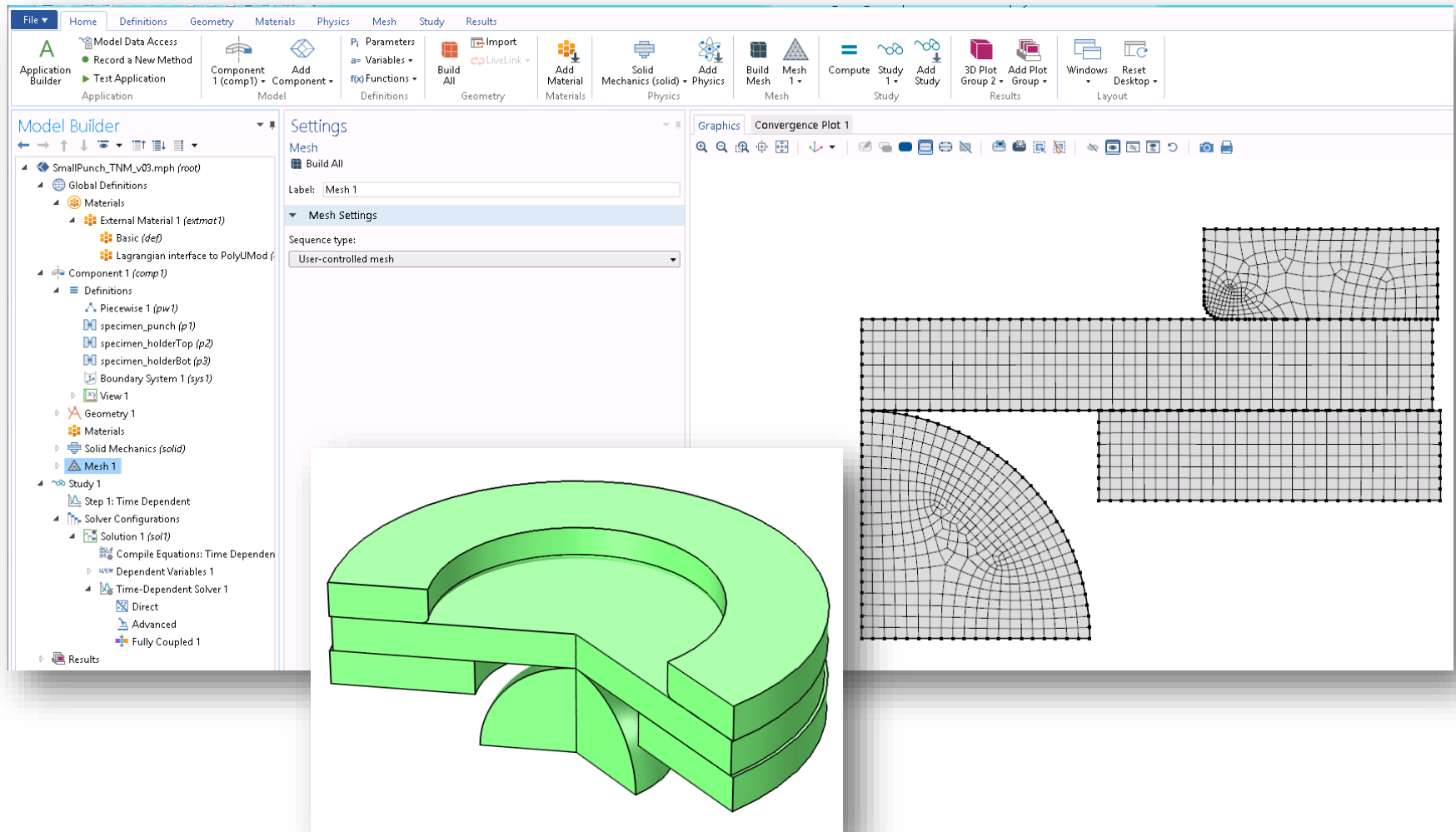


Small punch testing (ASTM F2183)



Spherical Indentation Testing

# COMSOL: Small Punch Simulation

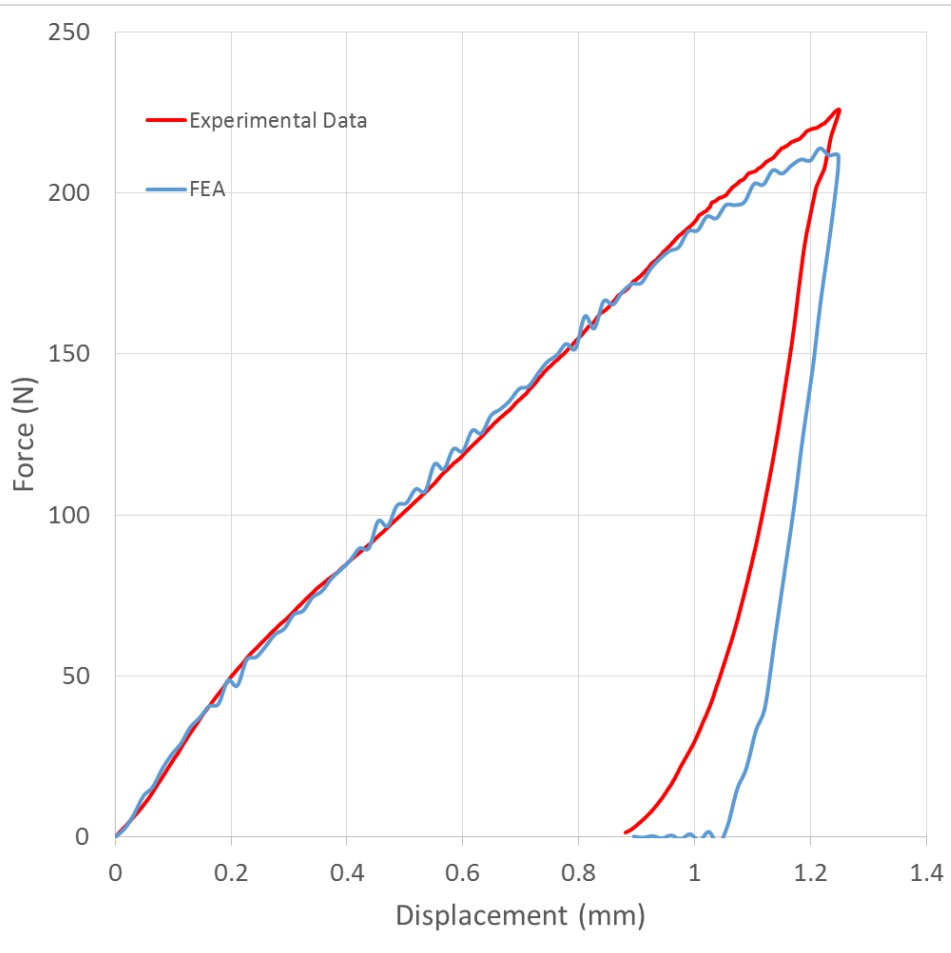


The screenshot displays the COMSOL Multiphysics software interface for a small punch simulation. The main window is divided into several panes:

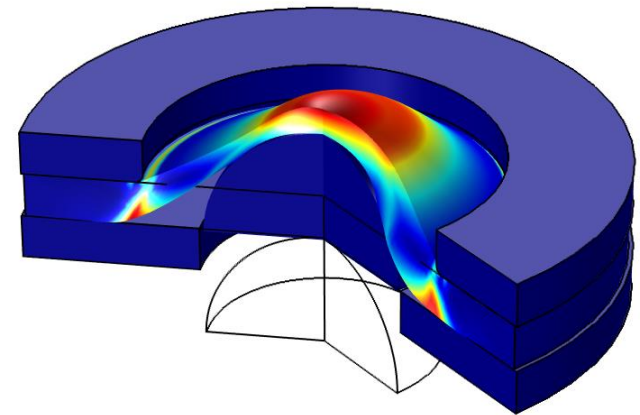
- Model Builder:** Shows the hierarchical structure of the model. The tree includes:
  - SmallPunch\_TNM\_v03.mph (root)
    - Global Definitions
    - Materials
      - External Material 1 (extmat1)
        - Basic (def)
        - Lagrangian interface to PolyUMod (f)
    - Component 1 (comp1)
      - Definitions
        - Piecewise 1 (pw1)
        - specimen\_punch (p1)
        - specimen\_holderTop (p2)
        - specimen\_holderBot (p3)
        - Boundary System 1 (sys1)
      - View 1
      - Geometry 1
      - Materials
      - Solid Mechanics (solid)
      - Mesh 1
    - Study 1
      - Step 1: Time Dependent
      - Solver Configurations
        - Solution 1 (sol1)
          - Compile Equations: Time Dependent
          - Dependent Variables 1
            - Time-Dependent Solver 1
              - Direct
              - Advanced
              - Fully Coupled 1

- Settings:** Shows the configuration for the selected 'Mesh 1' object. The 'Mesh Settings' section is expanded, showing 'Sequence type' set to 'User-controlled mesh'.
- Graphics:** Displays a 2D mesh plot of the specimen and holder components. The mesh is refined at the sharp corners and the contact area of the punch.
- 3D View:** A 3D perspective view of the model, showing a green specimen being punched by a holder. The specimen is a semi-circular ring with a central hole, and the holder consists of two semi-circular blocks.

# COMSOL: Small Punch Test



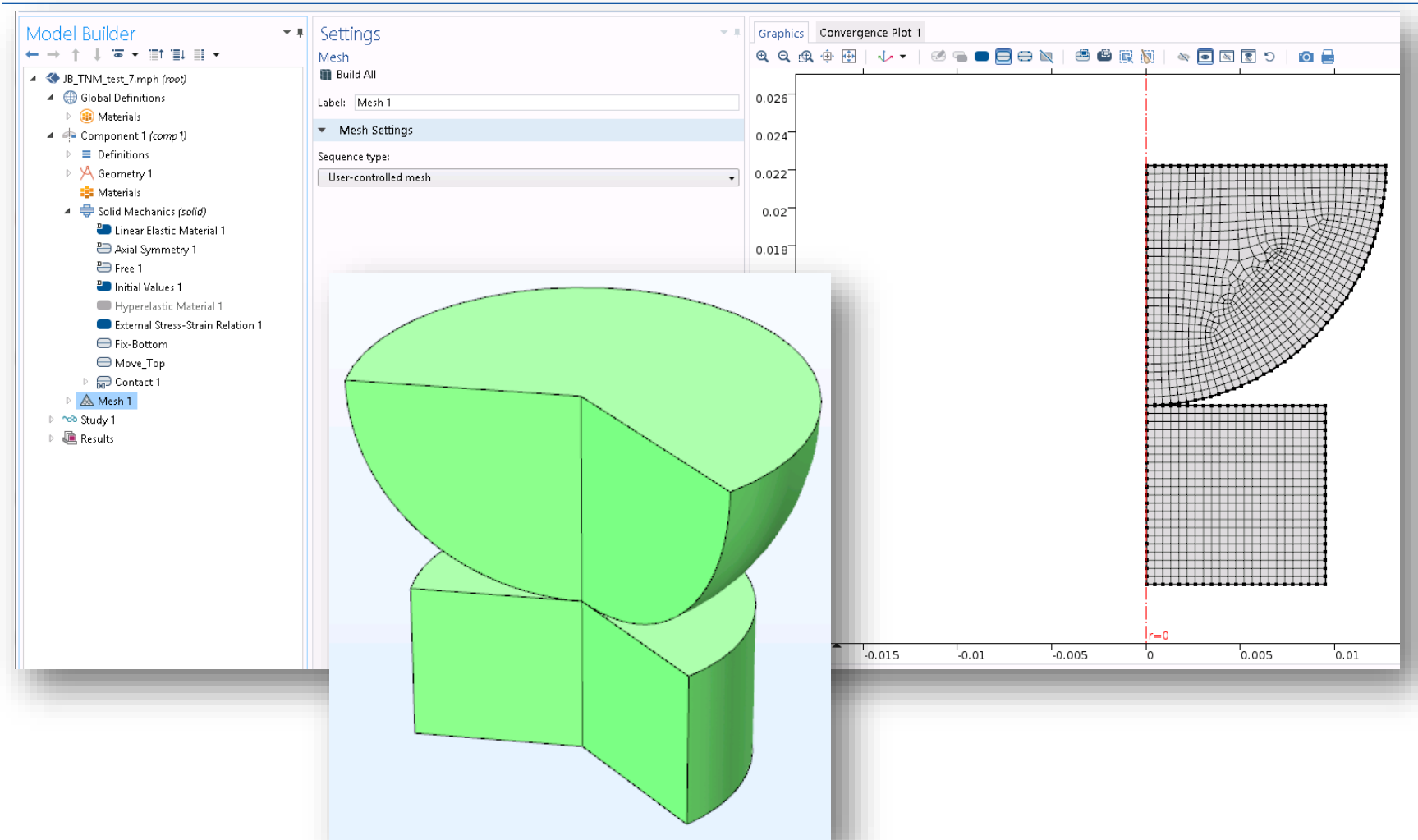
- The COMSOL model is in excellent agreement with the experimental data



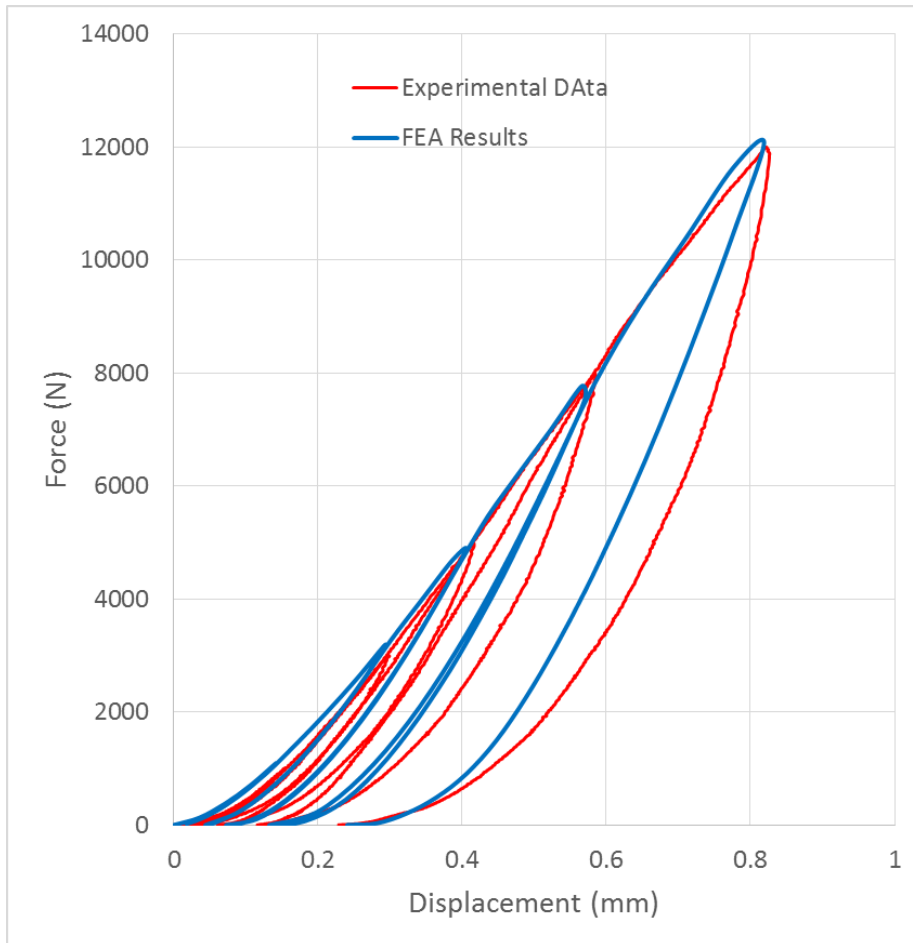
Axisymmetric model



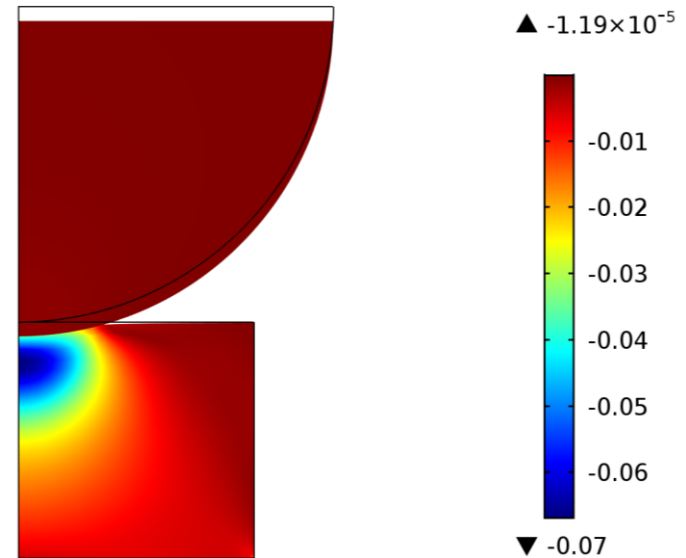
# COMSOL: Indentation



# COMSOL: Indentation



Time=50.919 s Surface: Third principal strain (1)



- The TN model is in excellent agreement with the experimental validation data

# Summary

---

Accurate COMSOL non-linear structural FE analysis requires:

- Careful experimental testing
- Selection of an appropriate material model
  - The External Material Functionality in COMSOL can be used to introduce very accurate viscoplastic material models
- Material model calibration
  - The MCalibration software is very useful for model calibration
- Material model validation (optional)
- FE model setup and simulation