

# Constitutive Modeling – Implementation, Calibration, V&V

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Mechanics of Materials

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# Outline

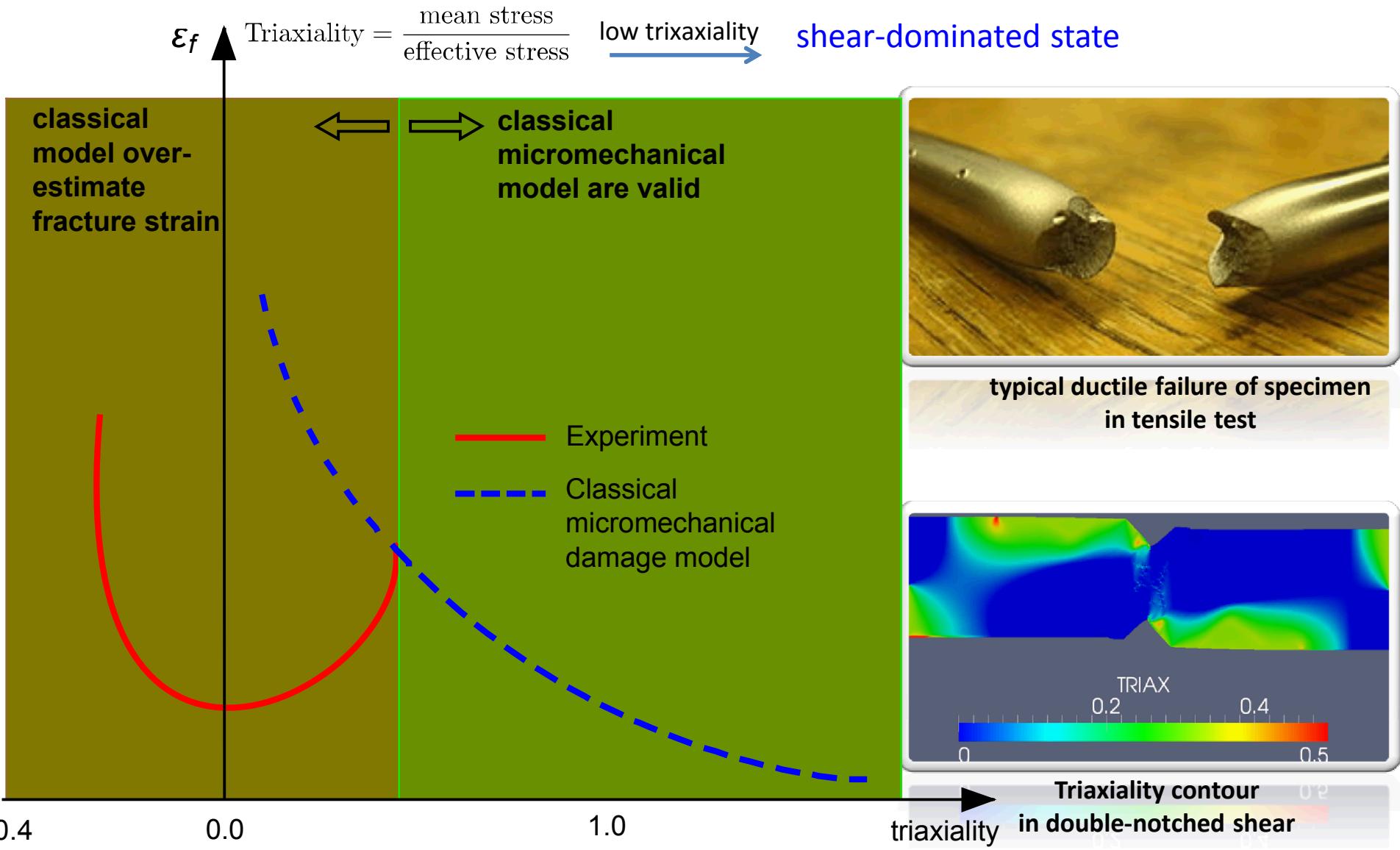
## **Shear-dominated ductile failure**

- Shear-modified Gurson damage model
  - Model formulation
  - Numerical implementation and verification
- Model Calibration and Validation
  - Experiments for 6061-T651 Aluminum
  - Optimization-based parameter calibration (use Dakota, with Kyle Karlson)

## **Cap-plasticity model for porous geomaterials**

- Model formulation
- Numerical implementation and verification
- 3D penetration problem on Salem limestone (couple cap plasticity model with poro-mechanical problem)

# Ductile Failure and Stress Triaxiality



## Schematic representation of the strain to failure of a ductile metal

# Classical Gurson Damage Model

## The macroscopic yield surface

$$\Phi(\boldsymbol{\tau}, Y, f) = \frac{3}{2} \frac{\mathbf{s} : \mathbf{s}}{Y^2} + \boxed{2q_1 f \cosh\left(\frac{3q_2 p}{2Y}\right)} - q_3 f^2 - 1 = 0$$

← pressure dependent

$p = \text{tr}(\boldsymbol{\tau})/3$  mean stress

$\mathbf{s} = \text{dev}(\boldsymbol{\tau})$  deviatoric stress tensor

$Y$  current effective stress of the damage-free matrix material

$f$  void volume fraction ← damage parameter

$q_1, q_2, q_3$  model fitting parameters [Tvergaard 1990]

damage-free  $f = 0$



$$\Phi = \frac{3}{2} \frac{\mathbf{s} : \mathbf{s}}{Y^2} - 1$$

OR  $\Phi = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}Y$

yield surface for J2  
plasticity!

## Hardening law for matrix material

- Saturation-type

$$Y = Y_0 + Y_\infty [1 - \exp(-\delta \varepsilon_q)] + K \varepsilon_q$$

- Power-law

$$Y = Y_0 (1 + E \varepsilon_q / Y_0)^N$$

- Hardening minus recovery model

$$Y = Y_0(\theta) + 2\mu(\theta) \varepsilon_{ss}$$

## Evolution of eqps

$$\dot{\varepsilon}_q Y (1 - f) = \boldsymbol{\tau} : \left( \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \right)$$

where

$$\frac{\partial \Phi}{\partial \boldsymbol{\tau}} = \mathbf{s} + \frac{1}{3} q_1 q_2 Y f \sinh(v) \mathbf{1}$$

# Shear Modification

## Classical damage evolution law

$$\dot{f} = \dot{f}_g + \dot{f}_{nu} \quad \dot{f}_{nu} = A\dot{\varepsilon}_q \quad A(\varepsilon_q) = \begin{cases} \frac{f_N}{s_N \sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\varepsilon_q - \epsilon_N}{s_N}\right)^2\right], & p \geq 0 \\ 0, & p < 0 \end{cases}$$

original void growth law, physically based and derived by [Gurson 1977]

$$\dot{f}_g = (1 - f) \operatorname{tr} \left( \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \right) \quad \text{← predicts no void growth under shear state}$$

Recent experiment evidence suggests classical model over estimate the fracture strain

## Shear-modified damage growth law

Introducing third-stress-invariant dependent [Nahshon-Hutchinson 2008]

$$\omega(\boldsymbol{\tau}) = 1 - \left( \frac{27J_3}{2\tau_e^3} \right)^2 \quad \text{where} \quad \tau_e := \sqrt{3/2} \|\mathbf{s}\| \quad \text{effective stress} \\ J_3 := \det(\mathbf{s}) \quad \text{third stress invariant}$$

$$\dot{f}_g = (1 - f) \operatorname{tr} \left( \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \right) + k_\omega f \frac{\omega(\boldsymbol{\tau})}{\tau_e} \mathbf{s} : \left( \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \right)$$

$k_\omega$  material constant that sets the magnitude of the damage growth rate in pure shear states

# Hyperelastic Constitutive Relation

## Strain energy function

$$\Psi = \Psi^{\text{vol}}[J_e] + \Psi^{\text{iso}}[\hat{\mathbf{b}}_e]$$

The volumetric and isochoric parts

$$\Psi^{\text{vol}}[J_e] = \frac{1}{2}\kappa(\ln J_e)^2, \quad \Psi^{\text{iso}}[\hat{\mathbf{b}}_e] = \frac{1}{4}\mu \ln \hat{\mathbf{b}}_e : \ln \hat{\mathbf{b}}_e$$

where

$$\hat{\mathbf{b}}_e := J_e^{-2/3} \mathbf{b}_e \quad \kappa \text{ bulk modulus}$$

$$J_e := \det \mathbf{F}_e \quad \mu \text{ shear modulus}$$

$$\mathbf{b}_e := \mathbf{F}_e \mathbf{F}_e^T$$

## Elastic constitutive law and the Kirchhoff stress

$$\boldsymbol{\tau} = \kappa \ln J_e \mathbf{g}^{-1} + \mu \ln \hat{\mathbf{b}}_e$$

The Kirchhoff pressure and deviatoric stress tensor

$$p = \frac{1}{3} \text{tr}(\boldsymbol{\tau}) = \frac{1}{2}\kappa \ln \det \mathbf{b}_e$$

$$\mathbf{s} = \text{dev}(\boldsymbol{\tau}) = \mu \text{dev} \ln \mathbf{b}_e$$

## Flow rule

from principle of maximum dissipation

$$-\frac{1}{2} L_v(\mathbf{b}_e) \cdot \mathbf{b}_e^{-1} = \gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}$$

# Numerical implementation

An implicit objective integration algorithm is implemented for integrating stress response over a finite time step. Backward Euler is applied to rate equations.

## Local unknown vector (4x1)

$$\mathbf{X} = \{p, f, \varepsilon_q, \Delta\gamma\}$$

## Local nonlinear system of equations (4x1)

$$R_1(\mathbf{X}) = \frac{1}{2}\mathbf{s} : \mathbf{s} - \frac{1}{2}\psi Y^2$$

$$R_2(\mathbf{X}) = p - p^{\text{tr}} + q_1 q_2 \kappa \Delta\gamma Y f \sinh(v)$$

$$R_3(\mathbf{X}) = f - f_n - q_1 q_2 (1 - f) \Delta\gamma Y f \sinh(v) - \sqrt{\frac{2}{3}} \Delta\gamma k_\omega f \omega(\boldsymbol{\tau}) \|\mathbf{s}\| - A(\varepsilon_q - \varepsilon_{q(n)})$$

$$R_4(\mathbf{X}) = \varepsilon_q - \varepsilon_{q(n)} - \frac{\Delta\gamma}{Y(1 - f)} (\mathbf{s} : \mathbf{s} + q_1 q_2 p Y f \sinh(v))$$

Iterative solution procedure like the Newton's method requires consistent linearisation, therefore the computation of local Jacobian matrix (4x4)  $\mathbf{J} = \partial \mathbf{R} / \partial \mathbf{X}$

difficulty and time-consuming to derive analytical expression!

## Remarks

Forward Automatic Differentiation (FAD) is used to obtain local Jacobian matrix.

LocalNonlinearSolver is used to solve the linearized equation, and upon convergence, compute the system sensitivity information.

## Implicit integration algorithm for shear-modified Gurson damage model

GIVEN:  $\varepsilon_{q(n)}$ ,  $f_n$ ,  $\mathbf{b}_{e(n)}$  and  $\mathbf{F}$

FIND:  $\boldsymbol{\tau}$ ,  $\varepsilon_q$ ,  $f$ ,  $\mathbf{b}_e(\mathbf{F}_p)$

STEP 1. Compute trial elastic left Cauchy-Green tensor  $\mathbf{b}_e^{\text{tr}}$

STEP 2. Compute trial Kirchhoff pressure and deviatoric tensor  $p^{\text{tr}}, \mathbf{s}^{\text{tr}}$

STEP 3. Check yielding:  $\Phi^{\text{tr}}(p^{\text{tr}}, \mathbf{s}^{\text{tr}}, \varepsilon_{q(n)}, f_n) > 0$  ?

No, set  $p = p^{\text{tr}}$ ,  $\mathbf{s} = \mathbf{s}^{\text{tr}}$ ,  $\mathbf{b}_e = \mathbf{b}_e^{\text{tr}}$ ,  $\varepsilon_q = \varepsilon_{q(n)}$ ,  $f = f_n$  and exit

STEP 4. Yes, local Newton loop

4.1 Initialize  $\mathbf{X}^k$  and iteration count  $k = 0$

4.2 Assemble residual  $\mathbf{R}(\mathbf{X}^k)$

4.3 Check convergence:  $\| \mathbf{R} \| < tol$  ?

Yes, converged and go to STEP 5

4.4 No, compute local Jacobian matrix  $\mathbf{J} = \partial \mathbf{R} / \partial \mathbf{X}$  

4.5 Solve system of equations  $\mathbf{J} \cdot \delta \mathbf{X} = \mathbf{R}$  for  $\delta \mathbf{X}$  

4.6 Update  $\mathbf{X}^{k+1} = \mathbf{X}^k - \delta \mathbf{X}$ ,  $k \rightarrow k + 1$  and go to 4.2

STEP 5. Update  $\boldsymbol{\tau} = \mathbf{s} + pg$ , and  $\varepsilon_q, f, \mathbf{F}_p^*$

\*The plastic deformation gradient is updated upon local convergence

$$\mathbf{F}_p = \exp \left( \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \right) \cdot \mathbf{F}_{b(n)}$$

This integration needs to be done for each global iteration within a global loading step.

## example code from GursonFD\_Def.hpp using FAD and NonLinearSolver

```
// initialize local unknown vector
X[0] = dgam;  X[1] = p;  X[2] = fvoid;  X[3] = eq;

{// local Newton-Raphson loop

// initialize DFadType local unknown vector Xfad
// Note that since Xfad is a temporary variable that gets changed within local
iterations
// when we initialize Xfad, we only pass in the values of X, NOT the system
sensitivity information
for (std::size_t i = 0; i < 4; ++i) {
    Xval[i] = Sacado::ScalarValue<ScalarT>::eval(X[i]);
    Xfad[i] = DFadType(4, i, Xval[i]);
}
:
:
// local system of equations
Rfad[0] = Phi;
Rfad[1] = pfad - p
    + dgam * q1 * q2 * kappa * Ybar * fvoidfad * std::sinh(tmp);
Rfad[2] = fvoidfad - fvoid - dfg - dfn;
Rfad[3] = eqfad - eq - deq;

// get ScalarT Residual
for (int i = 0; i < 4; i++)
    R[i] = Rfad[i].val();

// get local Jacobian
for (int i = 0; i < 4; i++)
    for (int j = 0; j < 4; j++)
        dRdX[i + 4 * j] = Rfad[i].dx(j);
:
:
// call LocalNonlinearSolver
solver.solve(dRdX, X, R); ← LocalNonlinearSolver
} // end local Newton loop

// compute sensitivity information w.r.t system parameters, and pack back to X
solver.computeFadInfo(dRdX, X, R); ← compute system sensitivity
```

← “unpack” system sensitivity information

local Jacobian matrix (4x4)  
$$J = \frac{\partial \mathbf{R}}{\partial \mathbf{X}}$$

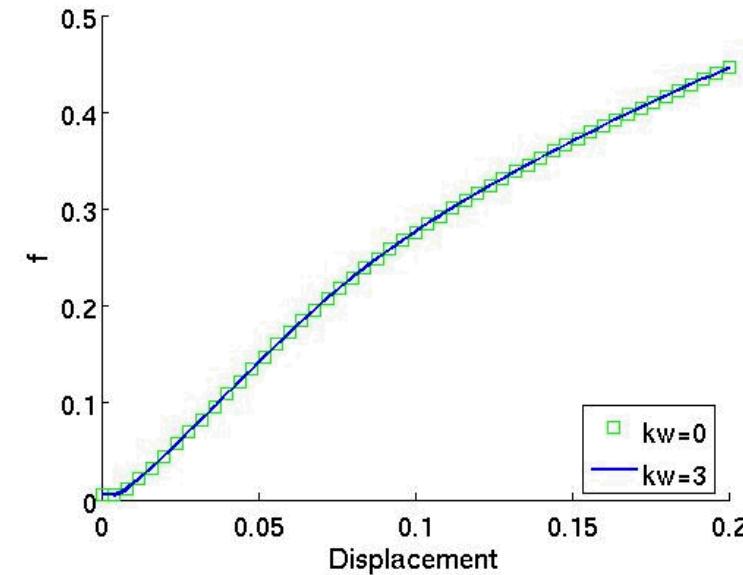
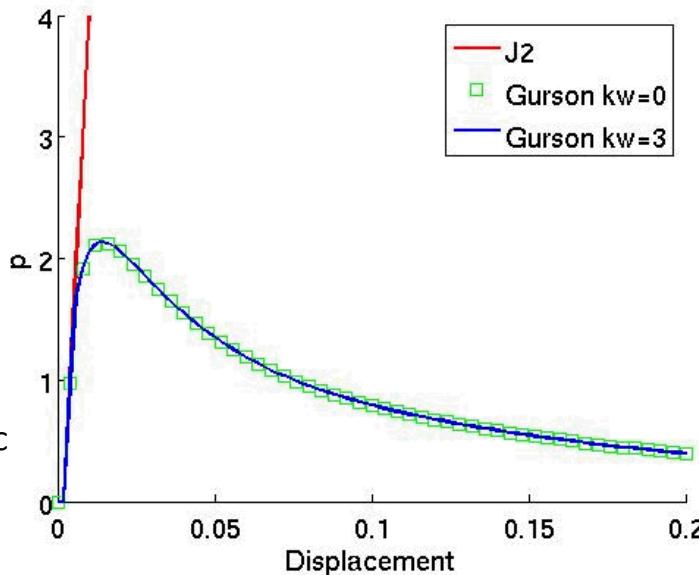
← LocalNonlinearSolver

← compute system sensitivity

# Verification: element tests

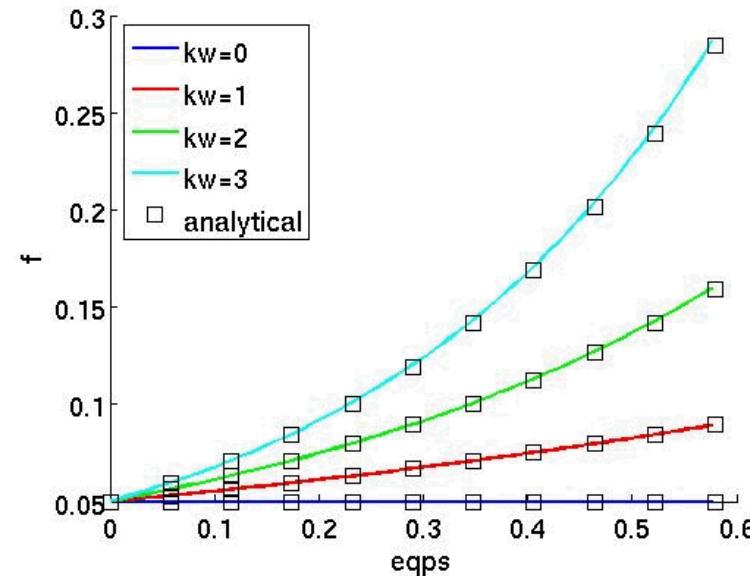
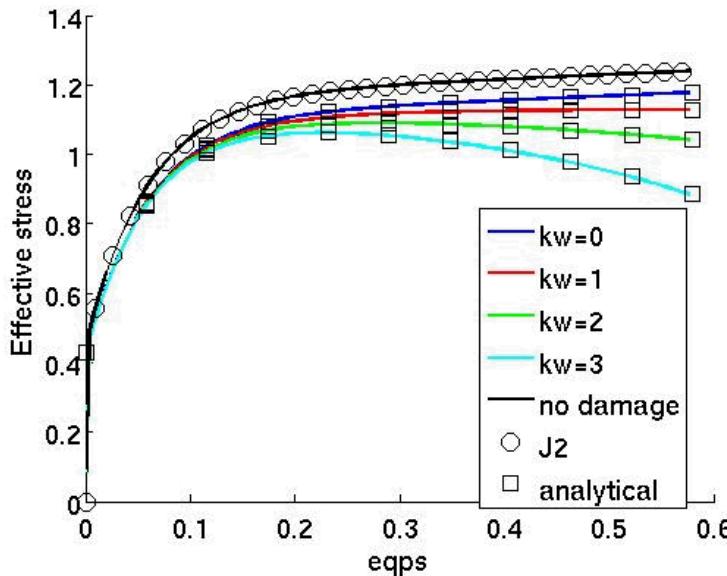
## hydrostatic extension

- J2 predicts no plasticity (pressure-independent).
- Gurson model response independent of shear term, because it's purely hydrostatic stress state.



## simple shear

- Analytical solution can be derived if void nucleation is neglected.
- Damage free Gurson recovers J2 model.
- Without shear term, the classical Gurson model predicts no damage growth.



# Outline

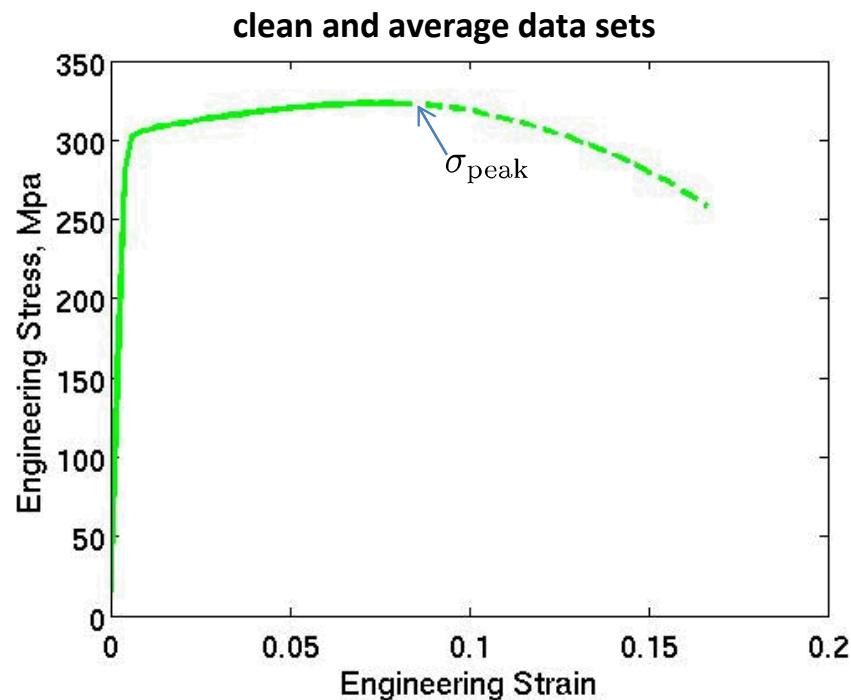
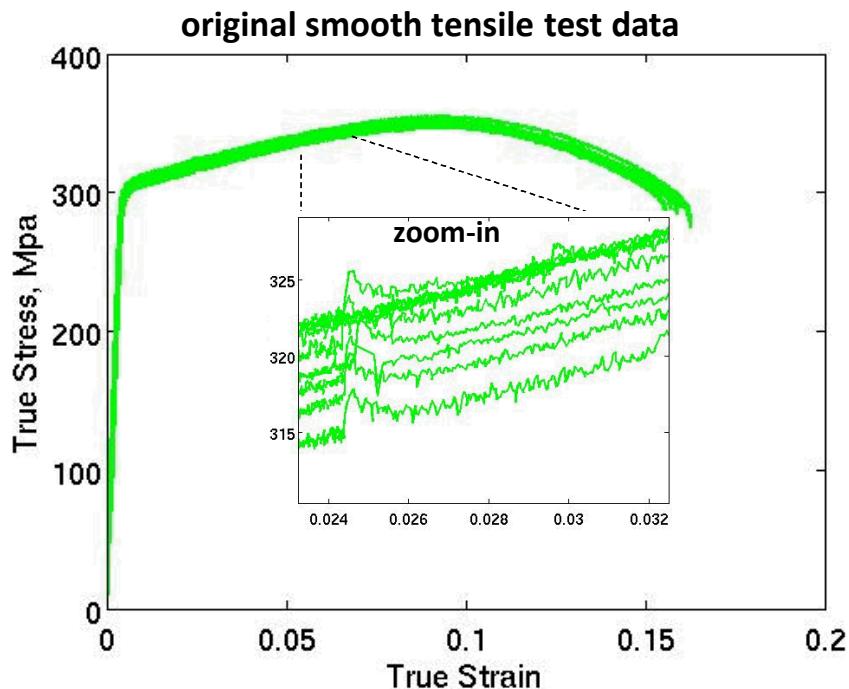
## Shear-dominated ductile failure

- Shear-modified Gurson damage model
  - Hyper-elastic formulation
  - Numerical implementation and verification
- Model Calibration and Validation
  - Experiments for 6061-T651 Aluminum
  - Optimization-based parameter calibration (Use **Dakota**, with Kyle Karlson)

## Cap-plasticity model for geomaterials

- Model formulation
- Numerical implementation and verification
- 3D penetration problem on Salem limestone (couple cap plasticity model with poro-mechanical problem)

# Smooth Tensile Test for 6061-T651 Aluminum



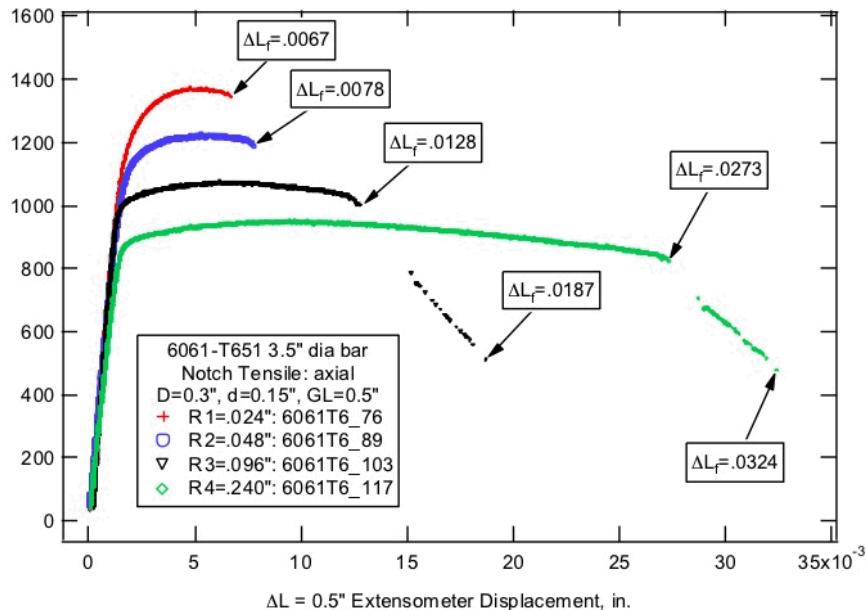
- 8 sets of experimental data
- Non-smooth and non-unique data points
- Calibrate model to fit engineering stress-strain curve up to peak load



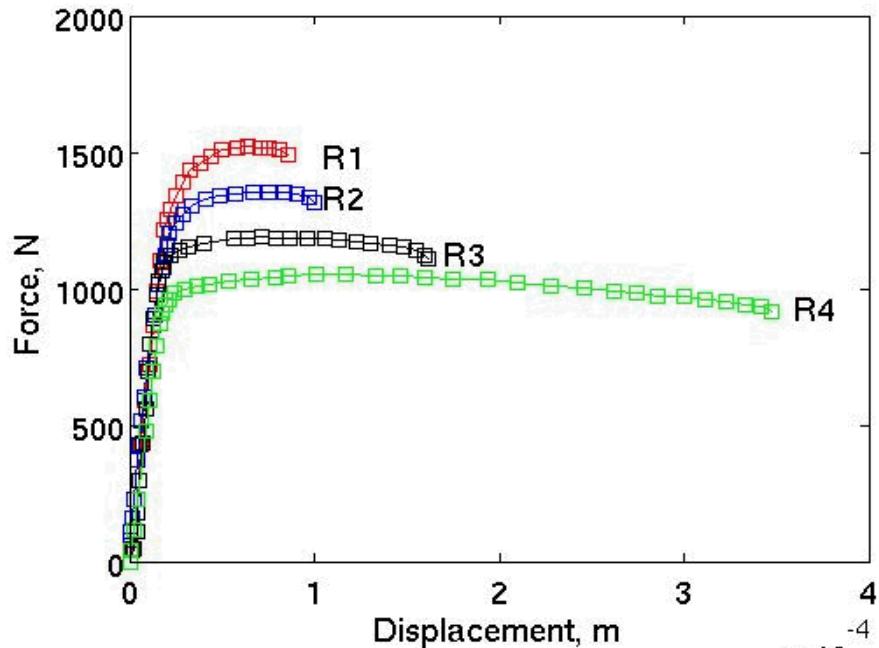
Tensile specimen: Notched and smooth

# Notched Tensile Test for 6061-T651 Aluminum

original notched tensile test data



Digitalized data for notched tensile tests



- 4 different notch radius
- original figure is digitalized
- Notched tensile test used for calibration, also “validation”.



Tensile specimen: Notched and smooth

# Model Calibration

## Parameters to calibrate in the damage model

Besides elastic constants, for shear-modified Gurson model, the following parameters need to be calibrated

- the matrix strain hardening parameters  $Y_0, N$   **Smooth tensile test**
- the macroscopic yield surface coefficients  $q_1, q_2, q_3$   **keep constant**
- initial void volume fraction  $f_0$   **keep constant**
- void nucleation law  $f_N, \epsilon_N, s_N$   **Notched tensile**
- shear damage parameter  $k_\omega$   **Shear test**
- mesh size  $D_0$   **mesh refinement study**

## Optimization-based model calibration

- Define objective function

$$f(p_1, \dots, p_N) = \frac{1}{2} \sum_{i=1}^n [F_i(p_1, \dots, p_N) - \bar{F}_i]^2$$

 response (simulation)       target (experiment)

- Find the parameter set  $(p_1, \dots, p_N)$  that minimizes the objective function (maximize the agreement between simulation response and experiment)

# Model calibration

## Optimization-based model calibration

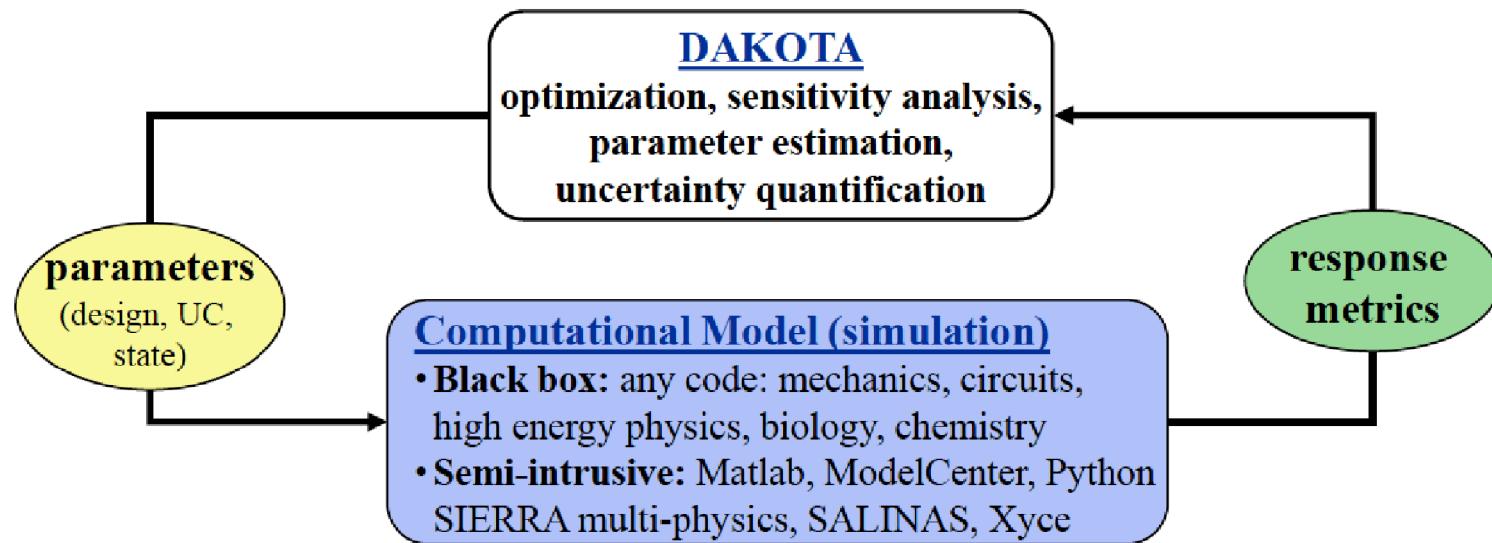
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↑ response (simulation)      ↑ target (experiment)

- Solution of the optimization problem requires iterative process
- Requires computing derivative of objective function w.r.t. parameter sets (Use FAD in Albany?)

# *Dakota* for automating the parameter variation process



# Model calibration

## Optimization-based model calibration

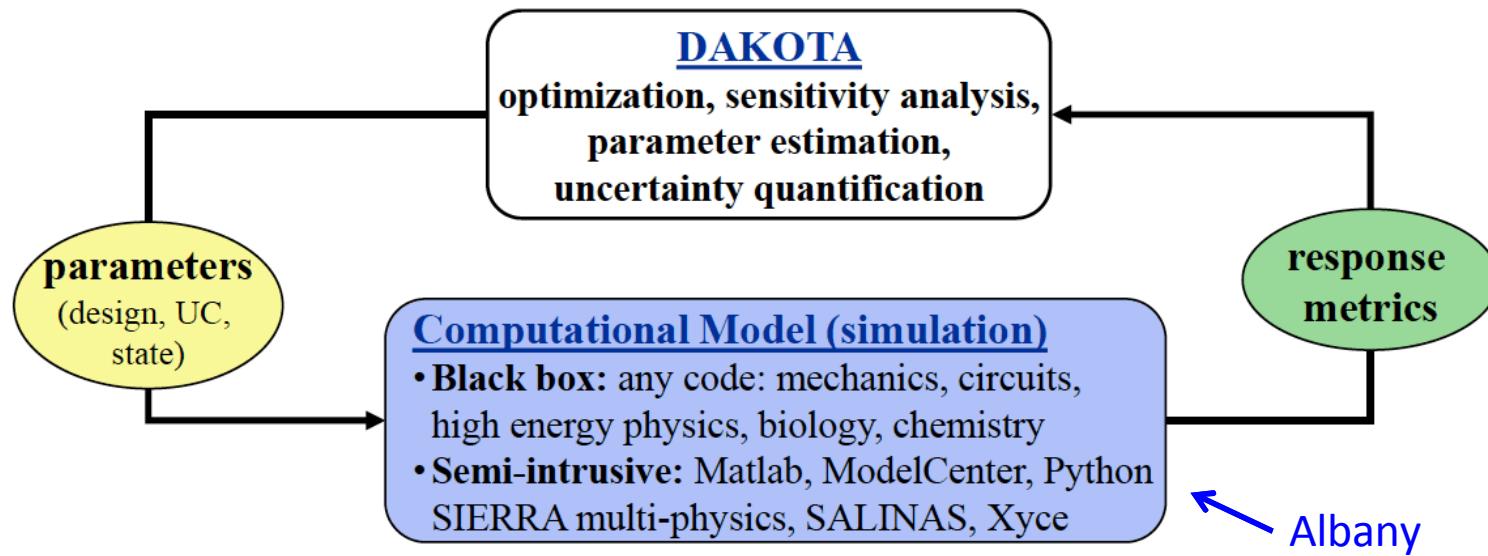
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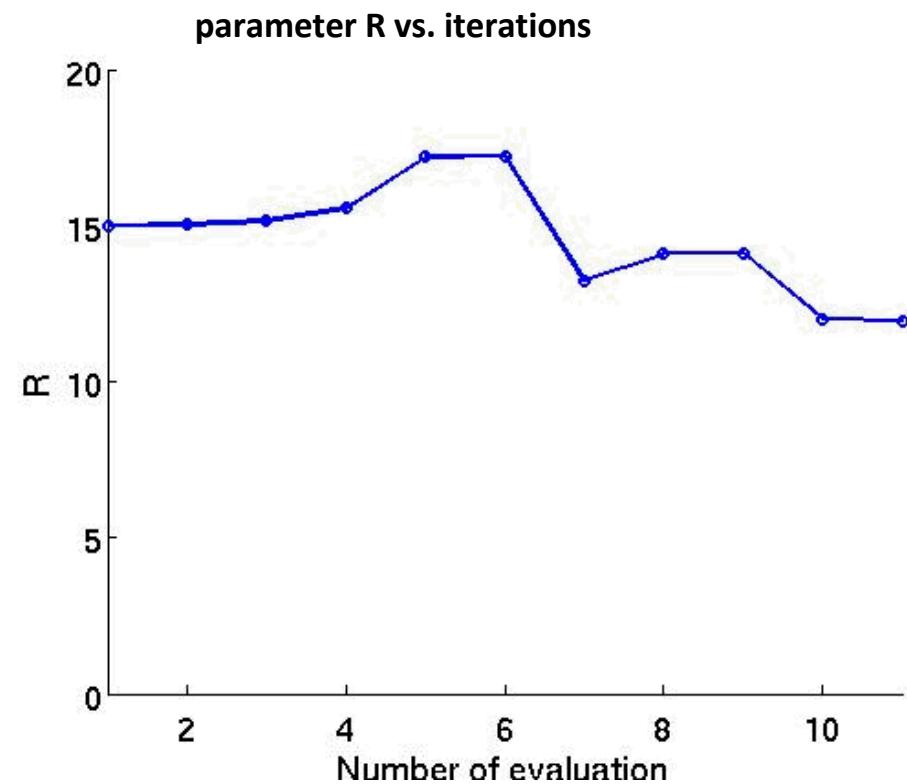
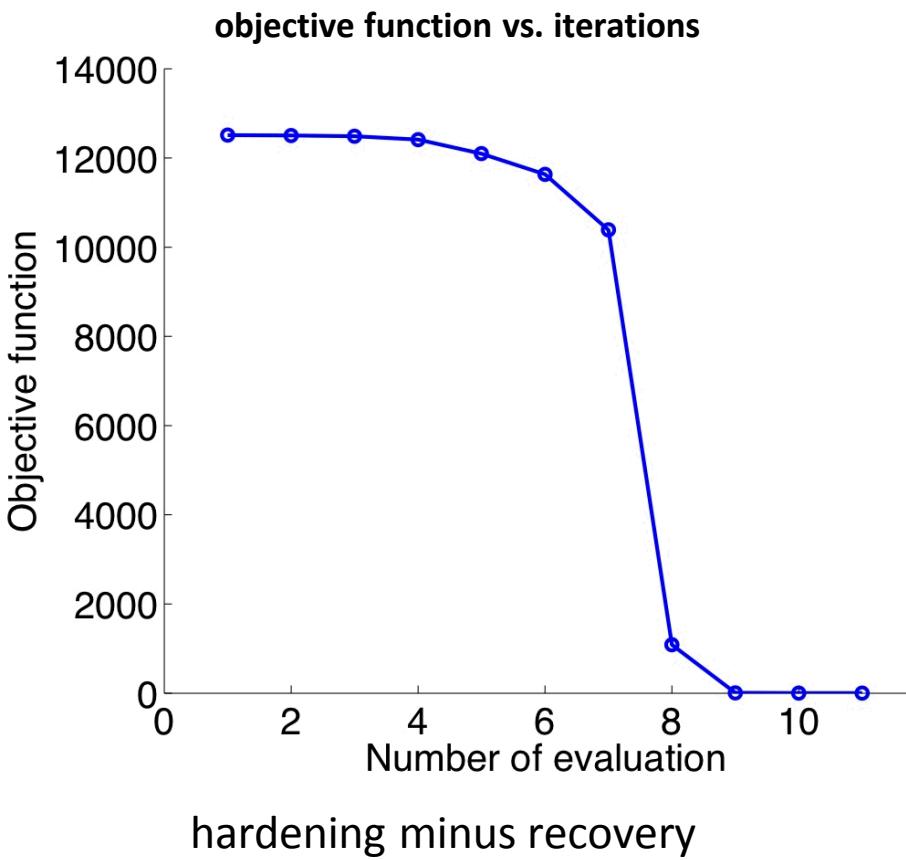
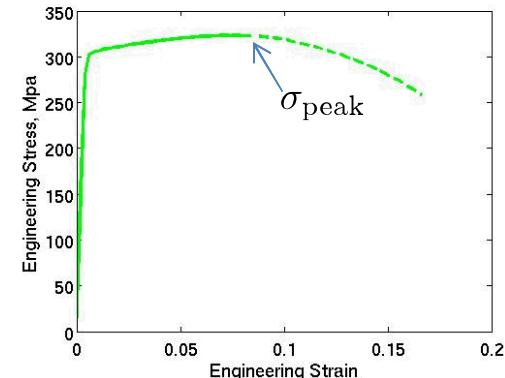
## **Dakota for automating the parameter variation process**



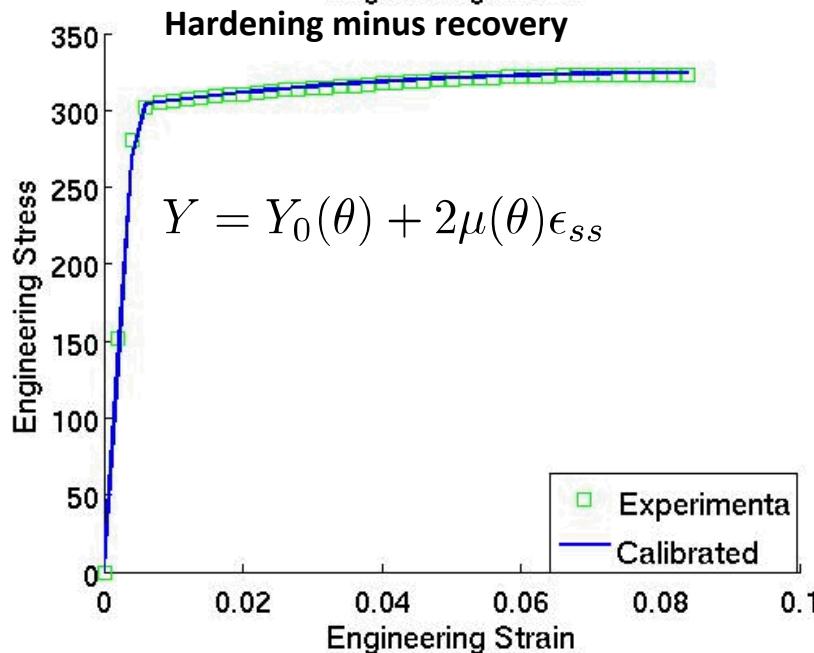
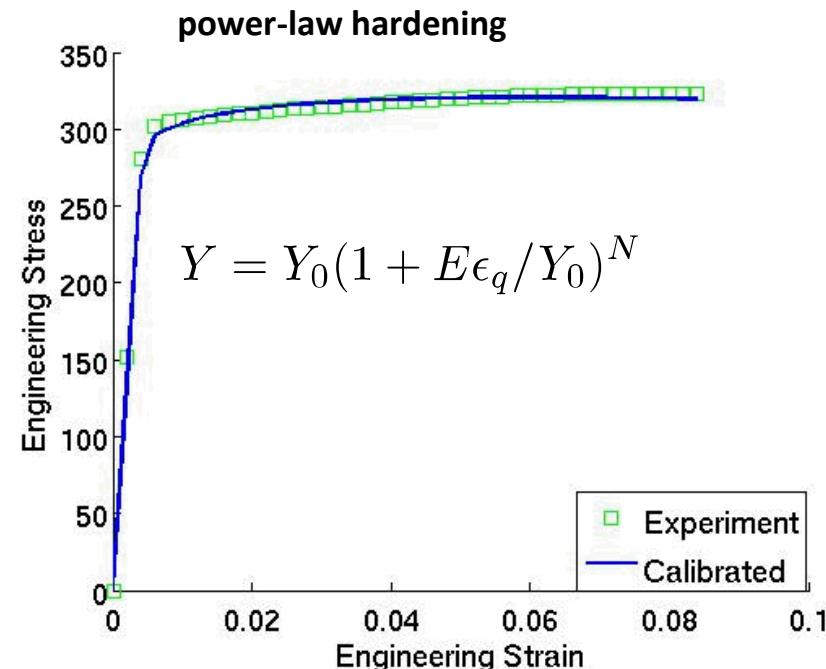
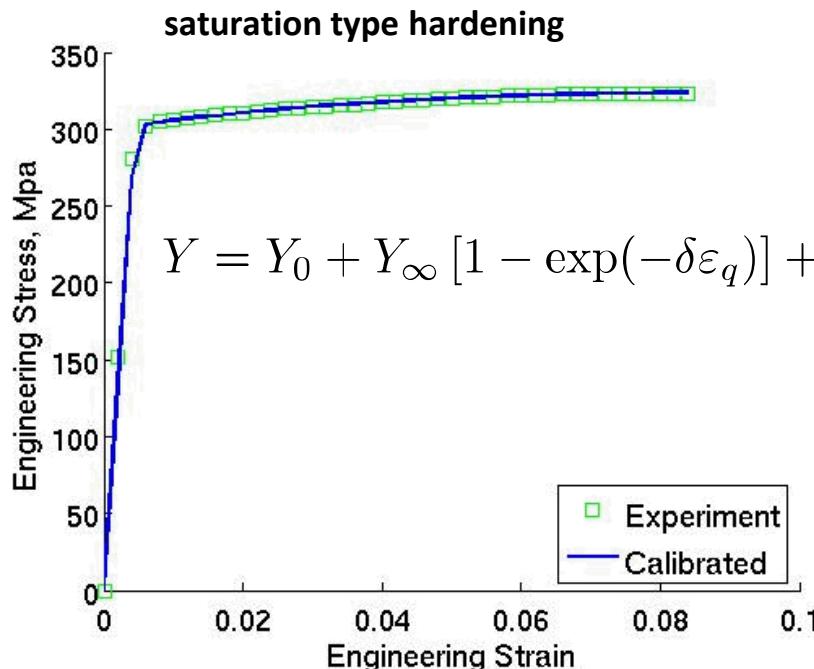
# Calibration of the matrix strain hardening parameters

- Calibration up to peak load
- Dakota Least-square method
- Numerical gradient computed by finite difference

$$f(p_1, \dots, p_N) = \frac{1}{2} \sum_{i=1}^n [F_i(p_1, \dots, p_N) - \bar{F}_i]^2$$



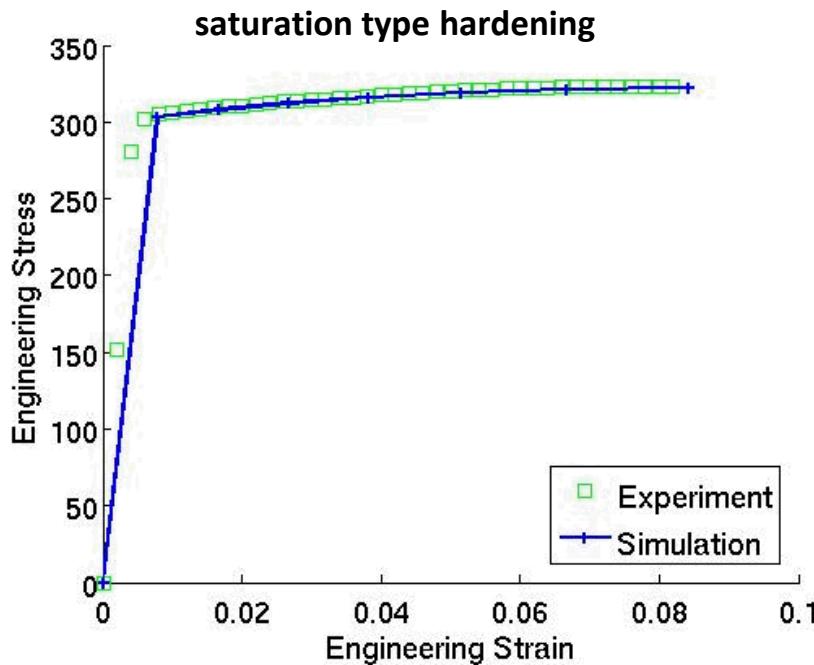
## Calibration the matrix strain hardening parameters



- Single element calibration
- different hardening laws are calibrated

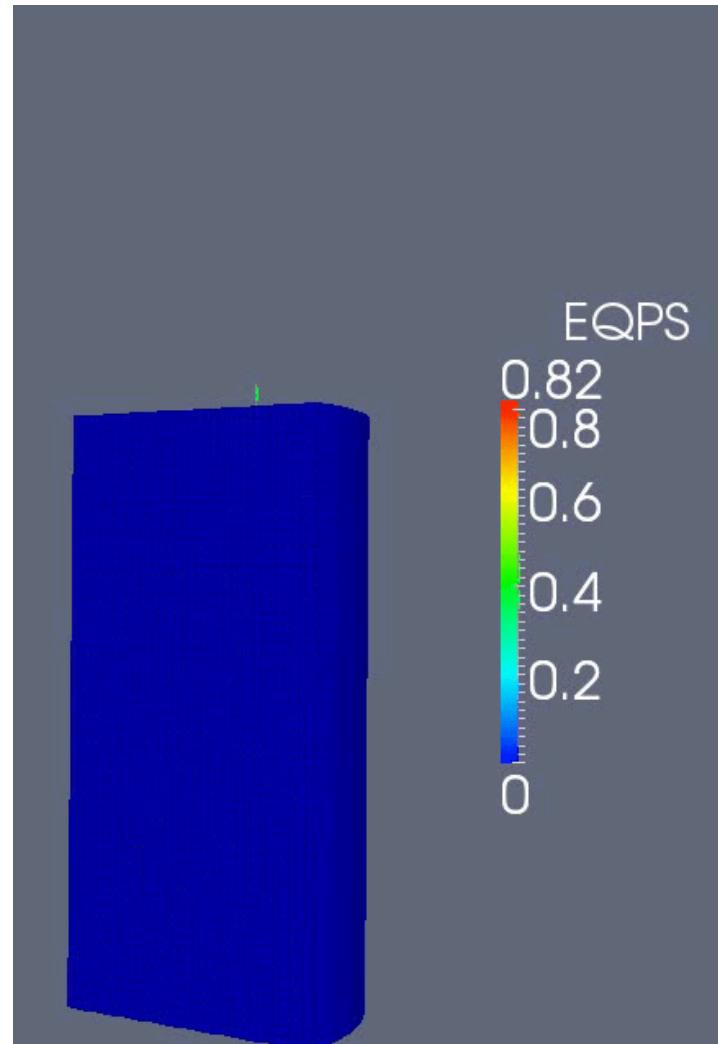
# Smooth tensile tests

- Verify the calibrated parameters from single element calibration
- Due to symmetry, only one-eighth of the sample is simulated
- Damage not included (does not affect pre-peak response)



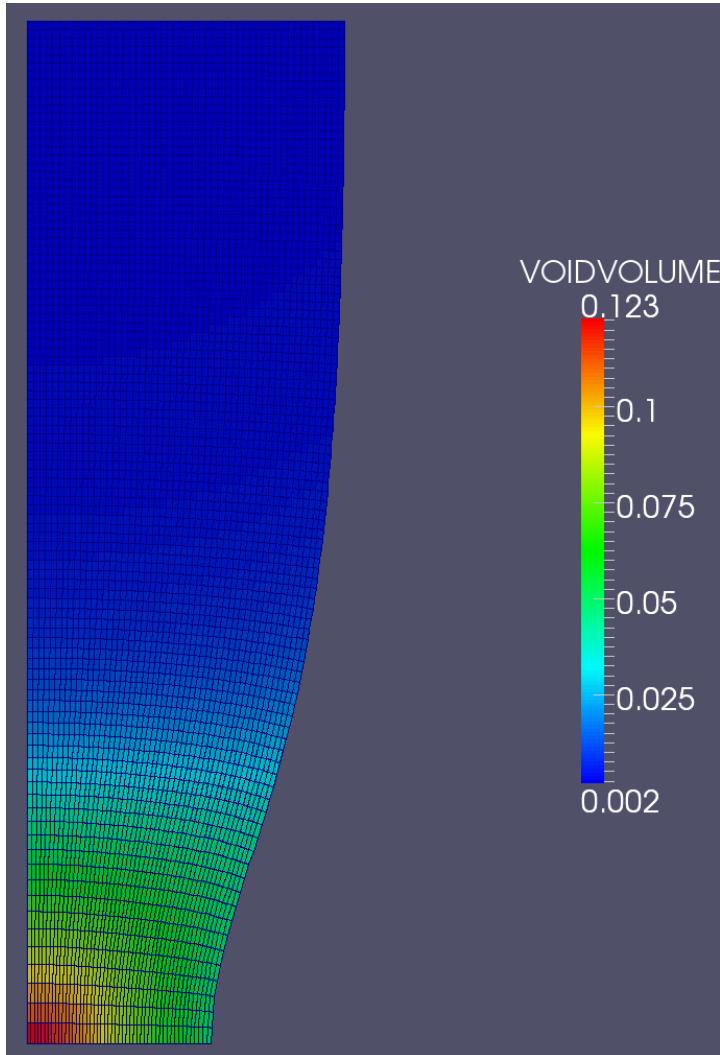
## material parameters

calibrated:	constant:	
$Y_0 = 303.3$ MPa	$f_0 = 0$	$q_1 = 1.5$
$Y_\infty = 376.9$ MPa	$k_\omega = 0$	$q_2 = 1.0$
$K = 30.4$ MPa	$f_N = 0$	$q_3 = 2.25$
		$\delta = 12.4$

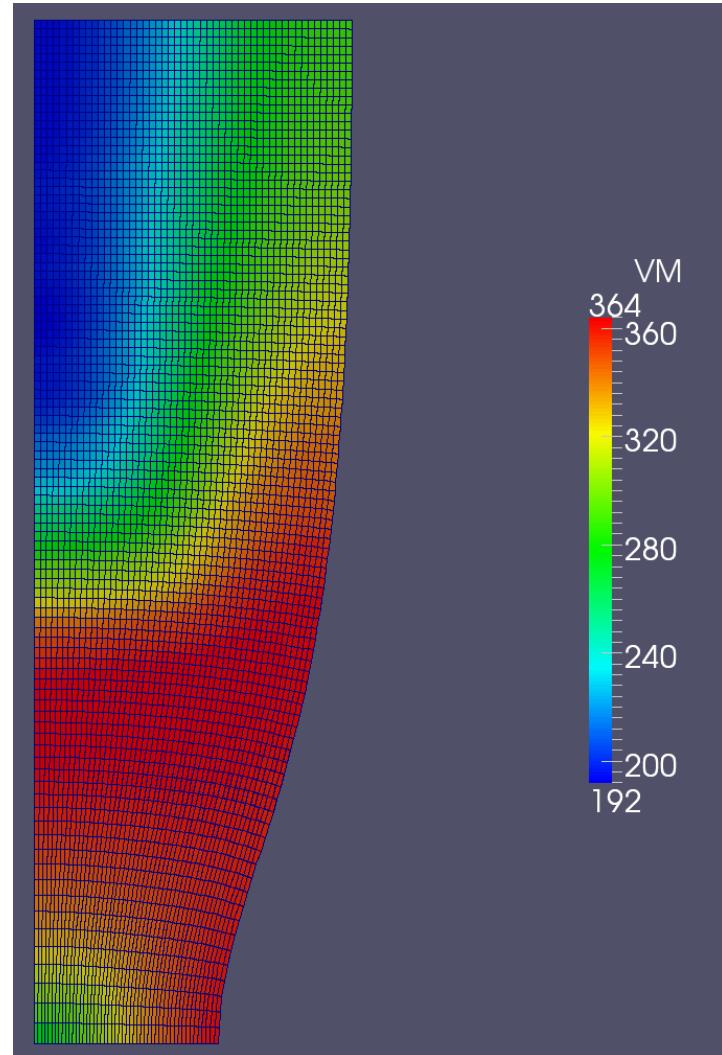


# Smooth tensile tests

damage parameter

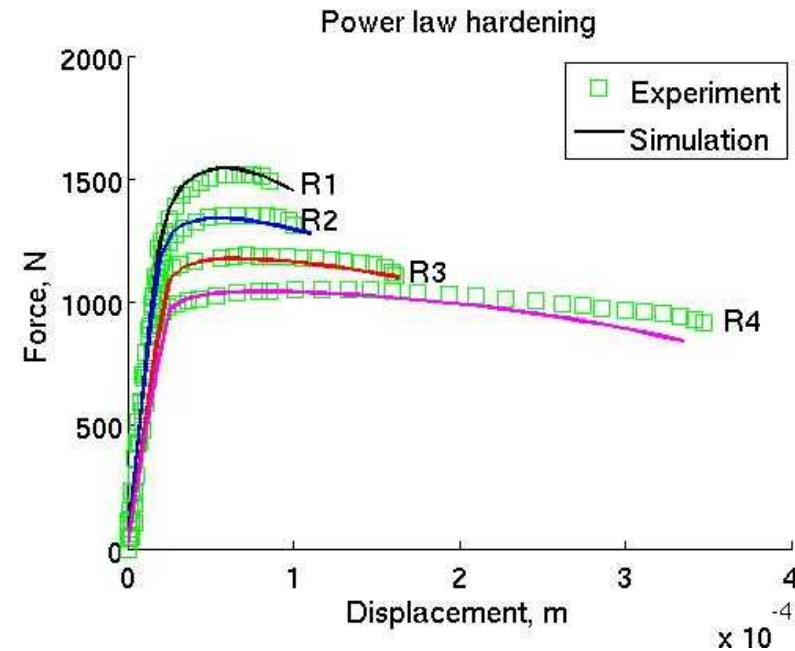
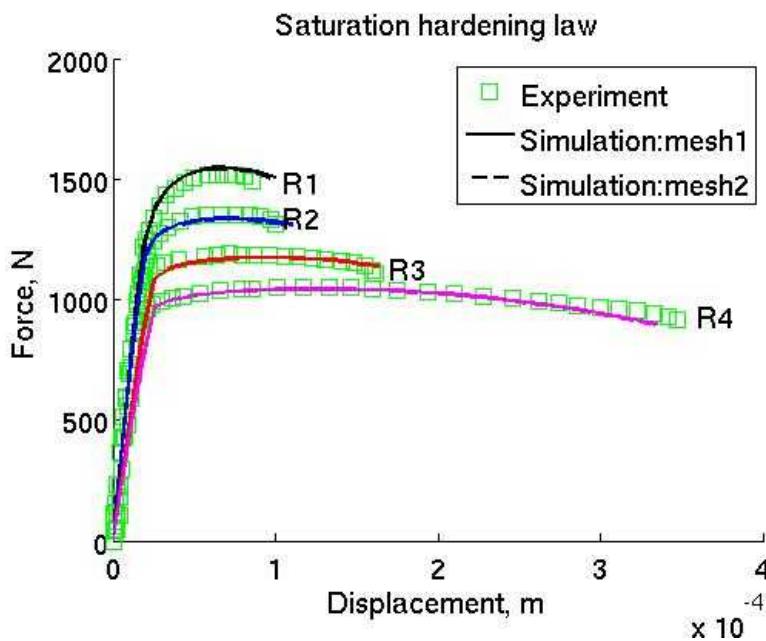


Von Mises stress

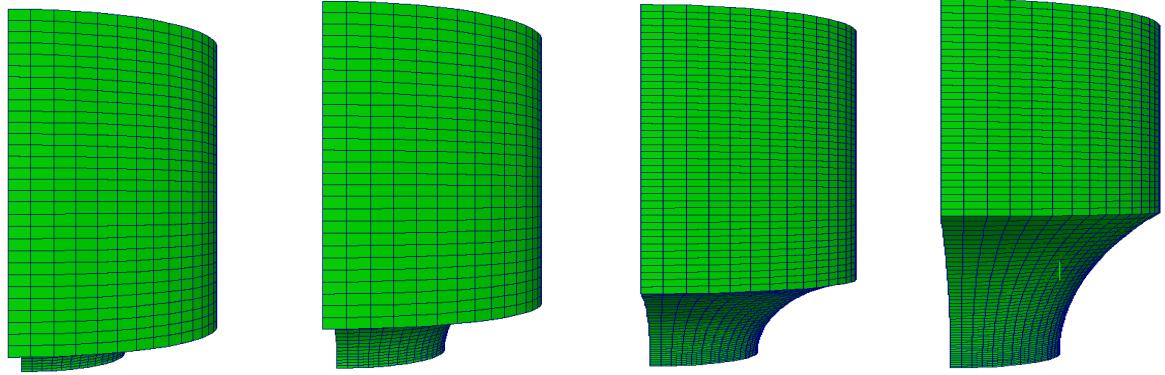


# Notched Tensile Tests

- Introduce damage in the model (use constant from literature)
- Use calibrated hardening law from smooth tensile test (“validate”)
- Four different notch radius, one eighth of the sample modeled



FE mesh for four different radius



damage parameters

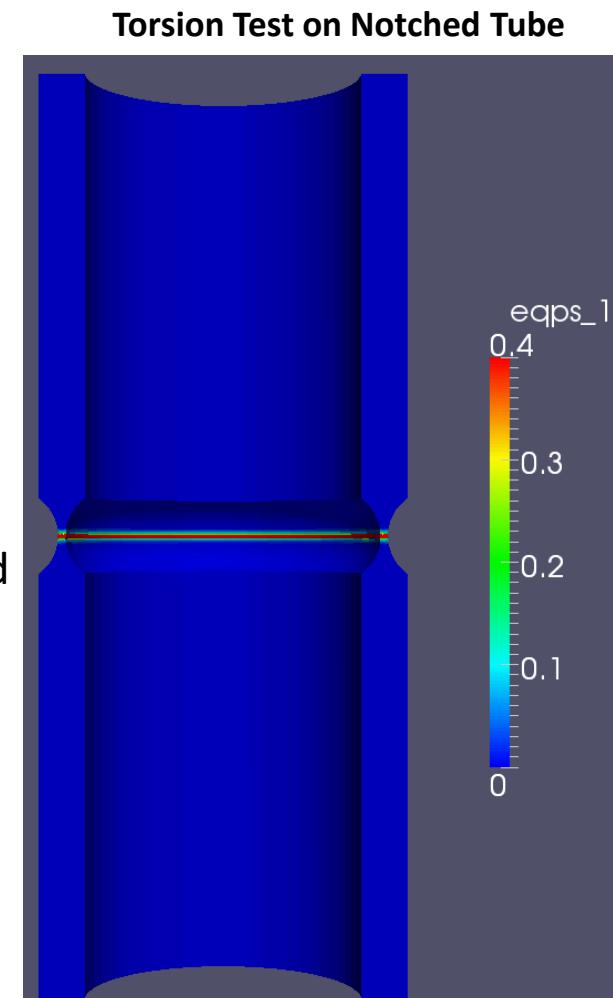
$$f_0 = 0.002$$

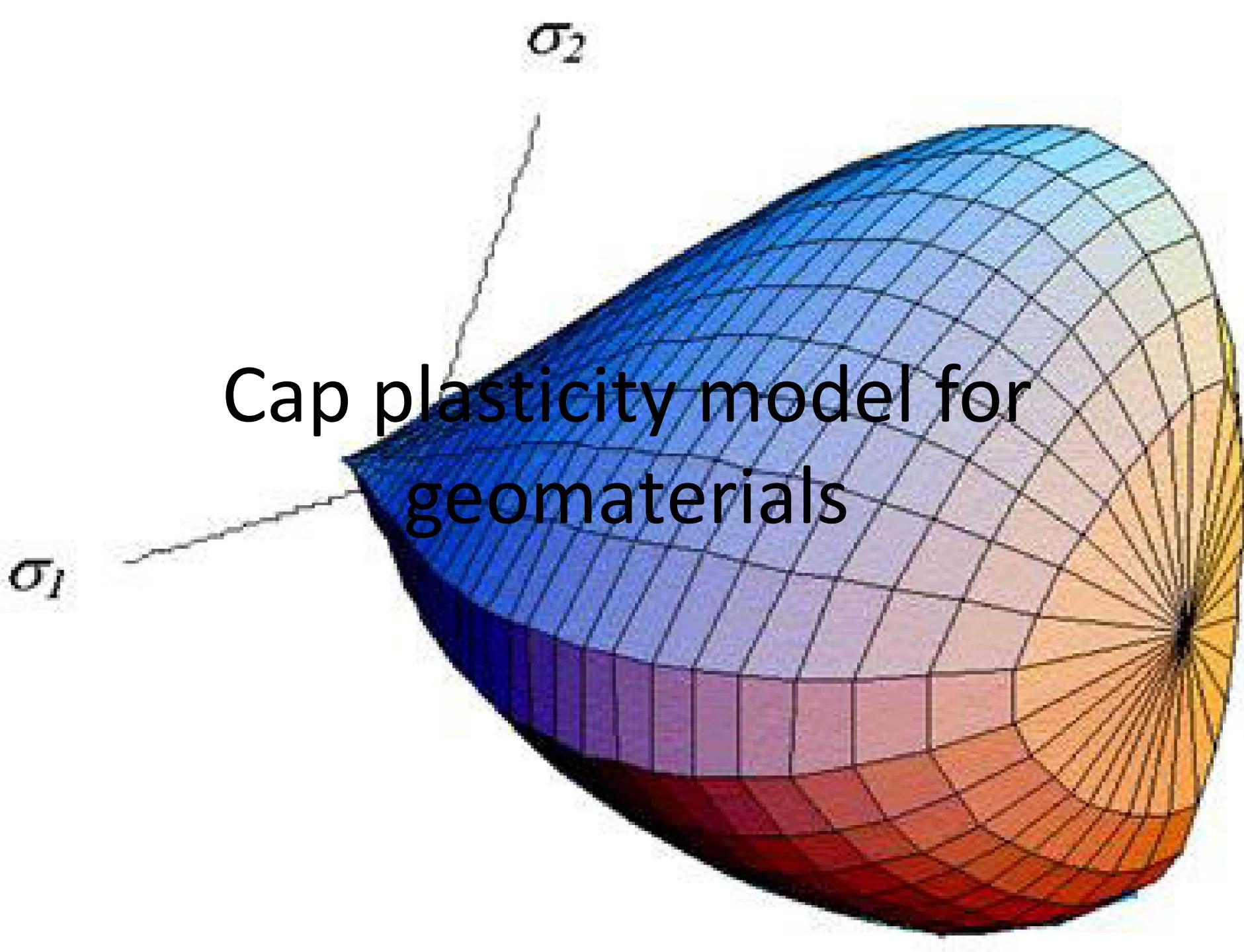
$$k_\omega = 0$$

$$f_N = 0.04$$

# Remarks and ongoing work

- Develop and implement a hyper-elastic formulation of the shear-modified Gurson model
- Use **FAD** and **LocalNonlinearSolver** assisting the implementation of the model
- Use **Dakota** to automate process of optimization-based parameter calibration
- Parameter Calibration:
  - Parameters for matrix hardening law calibrated using single element
  - Void nucleation parameter will require multi-element (specimen-scale computation) calibration using notched tensile test
  - The optimization process may not always converge and may not converge to local minimum
- Shear damage parameter calibration requires high fidelity test: Notched Tube





# Cap plasticity model

- For modeling complicated behavior of porous geomaterials, such as sandstone, limestone
- Capable of capturing shear localization in low porosity geomaterials, as well as compaction band in high porosity geomaterials
- Three invariant, isotropic and kinematic hardening, non-associative plasticity

## Yield surface and plastic potential

$$f(I_1, J_2, J_3, \alpha, \kappa) = (\Gamma(\beta))^2 J_2 - F_c(F_f - N)^2 = 0$$

$$g(I_1, J_2, J_3, \alpha, \kappa) = (\Gamma(\beta))^2 J_2 - F_c^g(F_f^g - N)^2$$

where the exponential shear failure surface

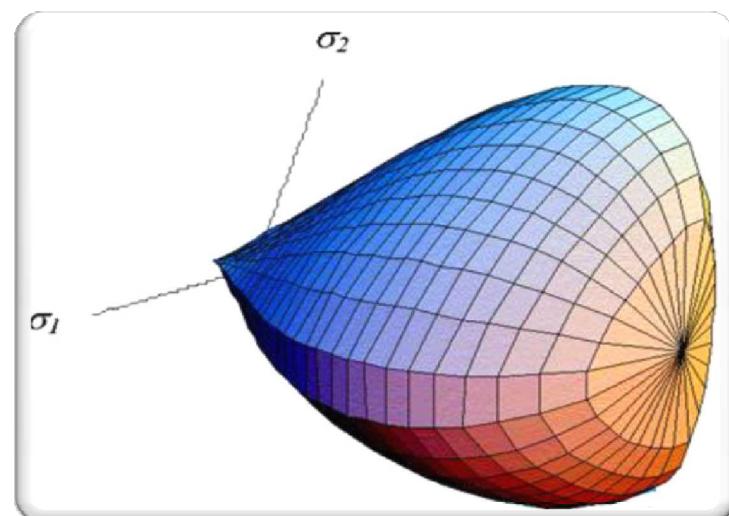
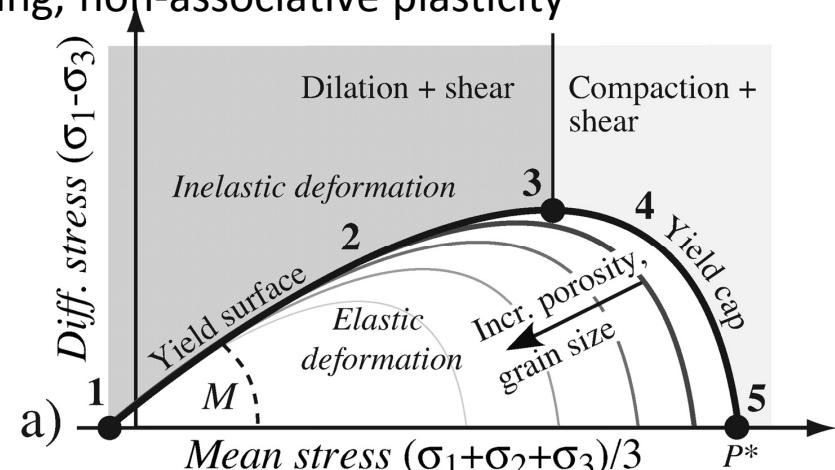
$$F_f(I_1) = A - C \exp(BI_1) - \theta I_1$$

$$F_f^g(I_1) = A - C \exp(LI_1) - \phi I_1$$

$\Gamma(\beta)$  is a function of the Lode angle, and takes into account differences in compression and extension

$$\beta = -\frac{1}{3} \sin^{-1} \left( \frac{3\sqrt{3}J_3}{2(J_2)^{3/2}} \right)$$

$$\Gamma(\beta) = \frac{1}{2} \left( 1 + \sin 3\beta + \frac{1}{\psi} (1 - \sin 3\beta) \right)$$



# Cap plasticity model

$F_c$  provides an smooth elliptical cap to the yield function

$$F_c(I_1, \kappa) = 1 - H(\kappa - I_1) \left( \frac{I_1 - \kappa}{X(\kappa) - \kappa} \right)^2$$

where function X (the intersection of the cap surface with the mean stress axis in median plane)

$$X(\kappa) = \kappa - RF_f(\kappa)$$

## Evolution laws for kinematic hardening

$$\dot{\alpha} = \dot{\gamma} h^\alpha(\alpha)$$

$$h^\alpha = c^\alpha G^\alpha(\alpha) \operatorname{dev}\left(\frac{\partial g}{\partial \sigma}\right)$$

where G is a function limits the growth of the back stress as it approaches the failure surface

$$G^\alpha(\alpha) = 1 - \frac{\sqrt{J_2^\alpha}}{N}, \quad J_2^\alpha = \frac{1}{2} \alpha : \alpha$$

## Evolution laws for isotropic hardening

$$\dot{\kappa} = \dot{\gamma} h^\kappa(\kappa)$$

$$h^\kappa = \frac{\operatorname{tr}(\partial g / \partial \sigma)}{\partial \epsilon_v^p / \partial \kappa}$$

where the following form of volumetric strain is used

$$\epsilon_v^p = W(\exp[D_1(X(\kappa) - X_0) - D_2(X(\kappa) - X_0)^2] - 1)$$

# Numerical implementation

- Both implicit and explicit scheme has been used to integrate the cap plasticity model
- Explicit scheme:
  - an normal stress correction algorithm has been implemented to prevent stress drifting from yield surface.
  - no local system of equation needs to be solved.
  - smaller time steps are generally required
- Implicit scheme:
  - require iterative solution of local system of equation
  - larger time steps can be used

**Local unknown vector (13x1)**

$$\mathbf{X} = \{\sigma, \alpha, \kappa, \Delta\gamma\}$$

**Local nonlinear system of equations (13x1)**

**Remarks**

**Forward Automatic Differentiation (FAD)** is used to obtain local Jacobian matrix.

**LocalNonlinearSolver** is used to solve the linearized equation, and upon convergence, compute the system sensitivity information.

## example code from CapImplicit\_Def.hpp using FAD and NonLinearSolver

```
// initialize local unknown vector
X[0] = sigmaVal(0, 0); X[1] = sigmaVal(1, 1); X[2] = sigmaVal(2, 2);
X[3] = sigmaVal(1, 2); X[4] = sigmaVal(0, 2); X[5] = sigmaVal(0, 1);
X[6] = alphaVal(0, 0); X[7] = alphaVal(1, 1); X[8] = alphaVal(1, 2);
X[9] = alphaVal(0, 2); X[10] = alphaVal(0, 1);
X[11] = kappaVal; X[12] = dgammaVal;

{// local Newton-Raphson loop

for (int i = 0; i < 13; ++i) {
    XVal[i] = Sacado::ScalarValue<ScalarT>::eval(X [i]);
    Xfad[i] = DFadType(13, i, XVal[i]);
}

:
:

// local system of equations (13 x 1)
:
:

// get ScalarT Residual
for (int i = 0; i < 13; i++)
    R[i] = Rfad[i].val();

// get local Jacobian
for (int i = 0; i < 13; i++)
    for (int j = 0; j < 13; j++)
        dRdX[i + 13 * j] = Rfad[i].dx(j); } } local Jacobian matrix (13x13)

$$J = \partial \mathbf{R} / \partial \mathbf{X}$$


if (kappa_flag == true) {
    for (int j = 0; j < 13; j++)
        dRdX[11 + 13 * j] = 0.0;
    dRdX[11 + 13 * 11] = 1.0;
}
:

:

// call LocalNonlinearSolver
solver.solve(dRdX, X, R); } LocalNonlinearSolver

}// end local Newton loop

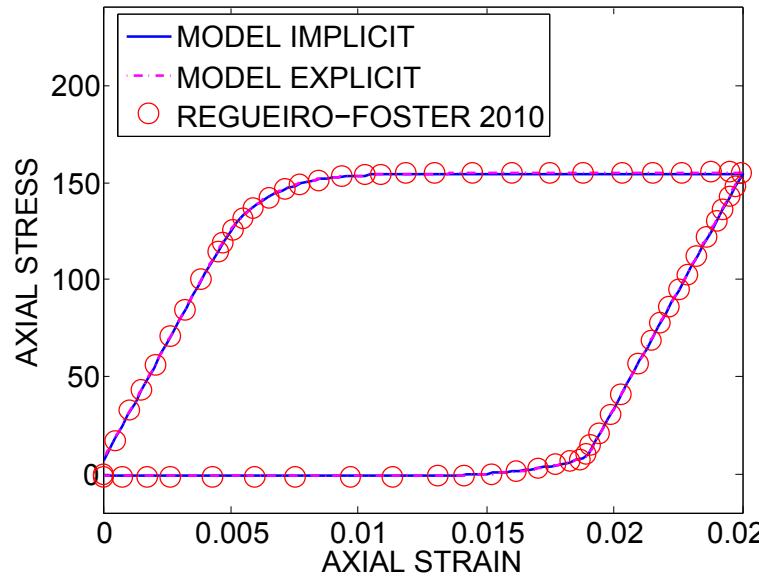
// compute sensitivity information w.r.t system parameters, and pack back to X
solver.computeFadInfo(dRdX, X, R); } compute system sensitivity
```

# Material Parameters for Salem Sandstone

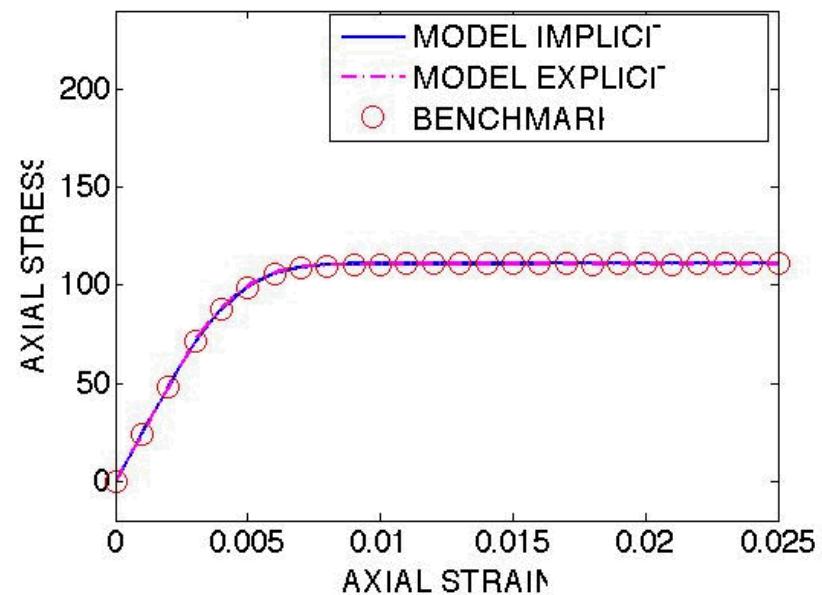
Parameter	Value	Unit
$E$	22,547	MPa
$\nu$	0.2524	dimensionless
$A$	689.2	MPa
$B, L$	$2.94e - 4, 1.0e - 4$	1/MPa
$C$	675.2	MPa
$\theta, \phi$	0.0	rad
$R, Q$	28.0	dimensionless
$\kappa_0$	-8.05	MPa
$W$	0.08	dimensionless
$D_1$	$1.47e - 3$	1/MPa
$D_2$	0.0	$1/\text{MPa}^2$
$c^\alpha$	1e5	MPa
$\psi$	1.0	dimensionless
$N$	6.0	MPa

# Verification: element tests

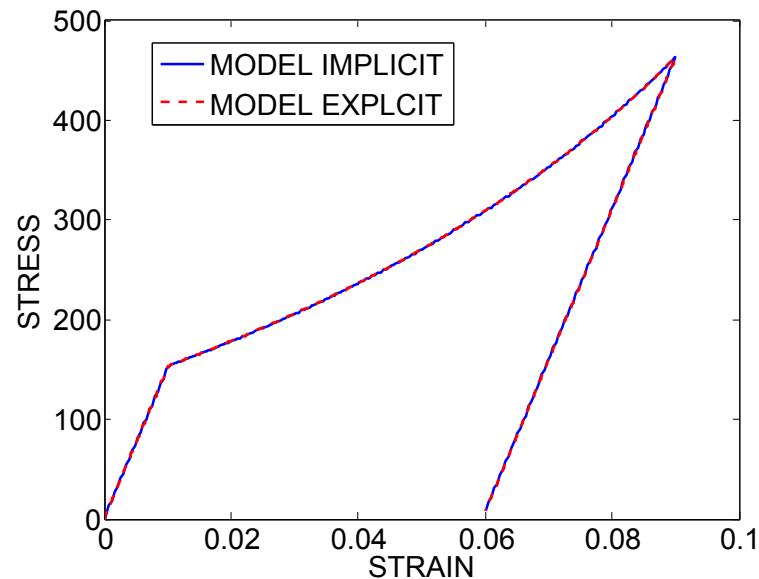
## plane strain compression



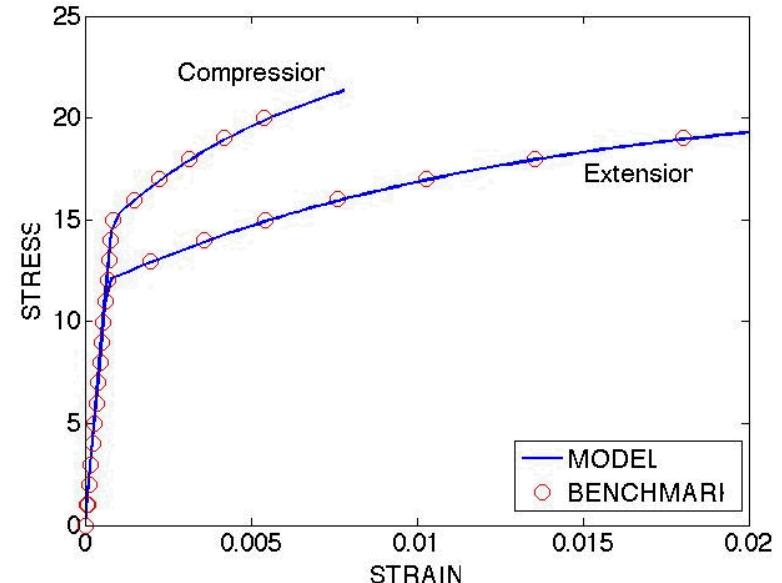
## plane stress



## volumetric extension



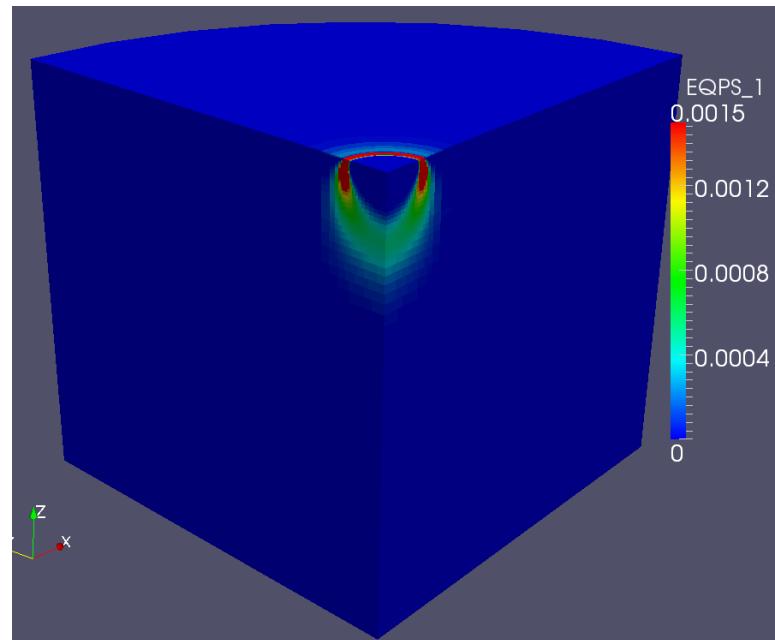
## Triaxial compression and extension



# 3D Penetration Problem on Salem Limestone

Couple cap plasticity model with poro-mechanical problem in LCM

eqps contour



pore-pressure evolution

