

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)

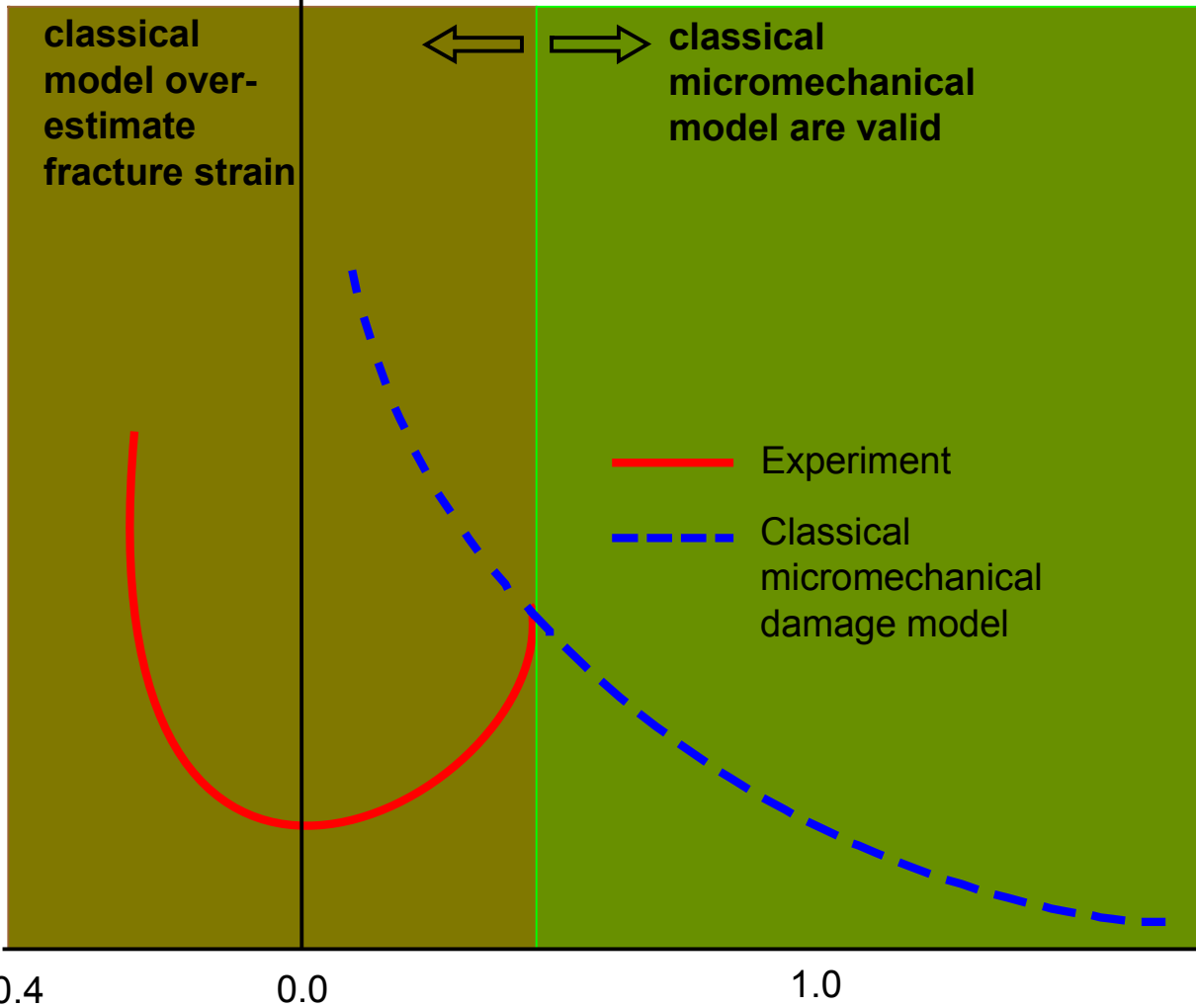
Cap-plasticity model for porous geomaterials

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

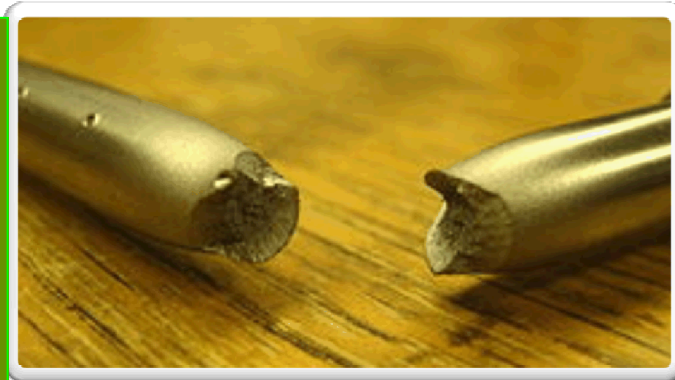
Ductile Failure and Stress Triaxiality

$$\text{Triaxiality} = \frac{\text{mean stress}}{\text{effective stress}}$$

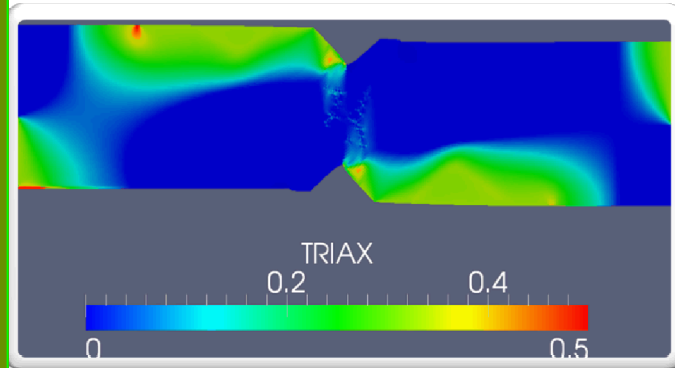
low triaxiality \rightarrow shear-dominated state



Schematic representation of the strain to failure of a ductile metal



typical ductile failure of specimen in tensile test



Triaxiality contour in double-notched shear

Classical Gurson Damage Model

The macroscopic yield surface

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

← pressure dependent

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

$\boldsymbol{s} = \text{dev}(\boldsymbol{\tau})$ 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 $f = 0$



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

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

yield surface for J2
plasticity!

Hardening law for matrix material

- Saturation-type

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

- Power-law

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

- Hardening minus recovery model

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

Evolution of eqps

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

where

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

Shear Modification

Classical damage evolution law

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

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

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

Recent experiment evidence suggests classical model over estimate the fracture strain

Shear-modified damage growth law

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

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

$$J_3 := \det(\mathbf{s}) \quad \text{third stress invariant}$$

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

k_ω 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

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

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

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

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 principal 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^{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

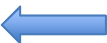
STEP 4. Yes, local Newton loop

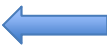
4.1 Initialize \mathbf{X}^k and iteration count $k = 0$

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

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

Yes, converged and go to STEP 5

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

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

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 $\boldsymbol{\tau} = \mathbf{s} + p\mathbf{g}$, 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);
} // end local Newton loop

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

← “unpack” system sensitivity information

} local Jacobian matrix (4x4)
 $J = \partial R / \partial X$

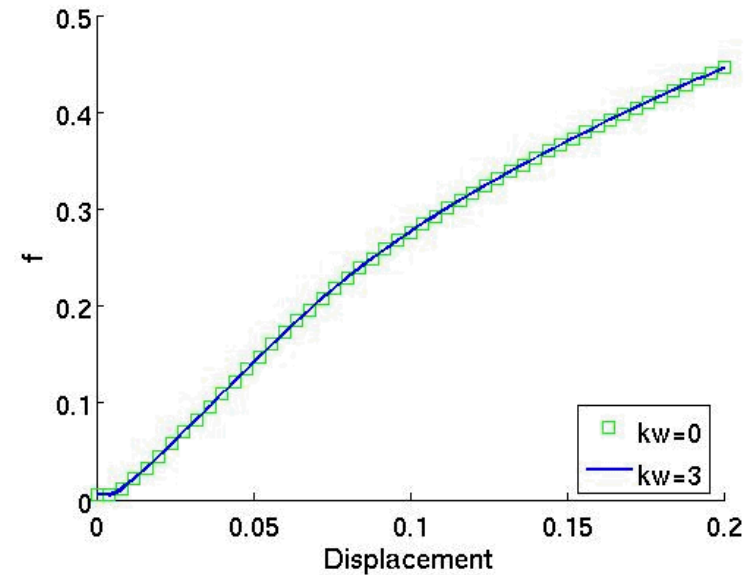
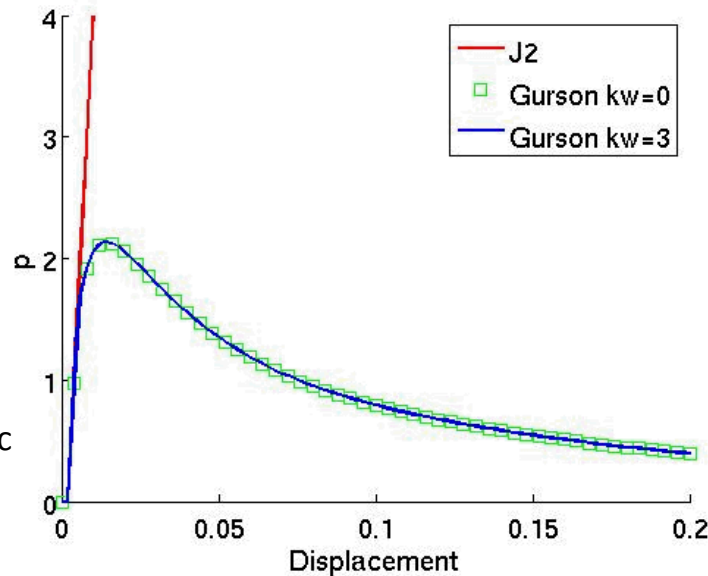
← LocalNonlinearSolver

← compute system sensitivity

Verification: element tests

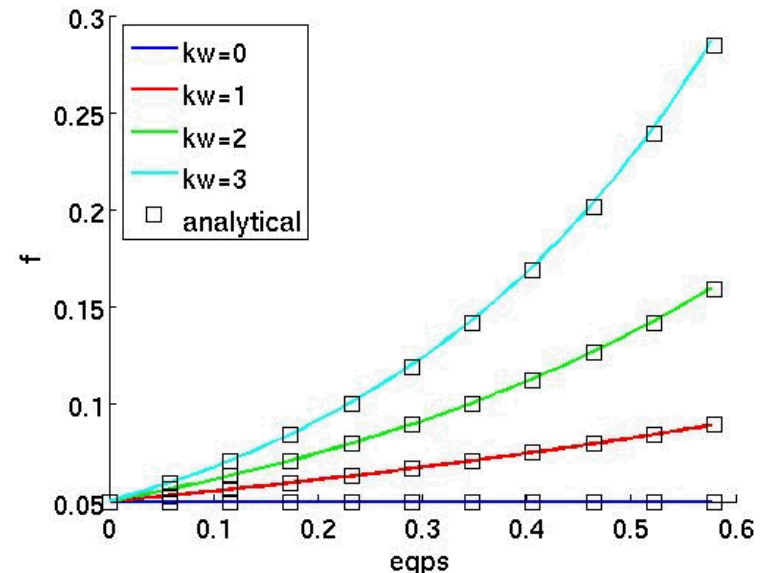
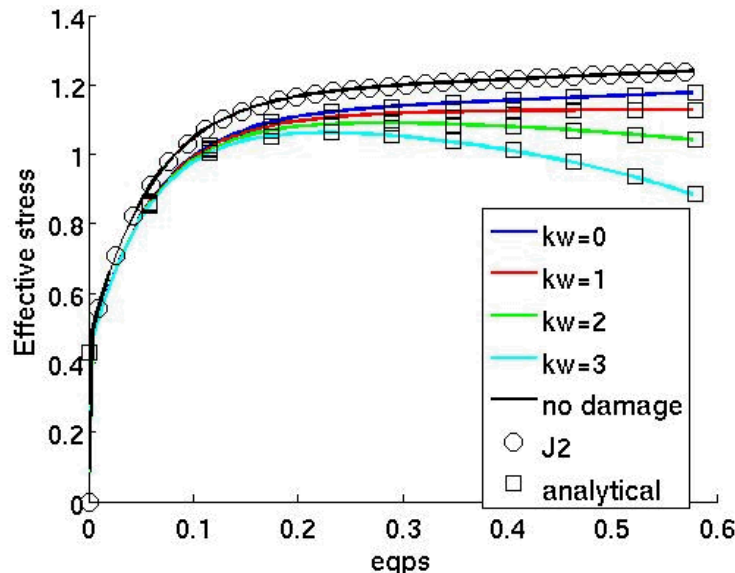
hydrostatic extensioin

- 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

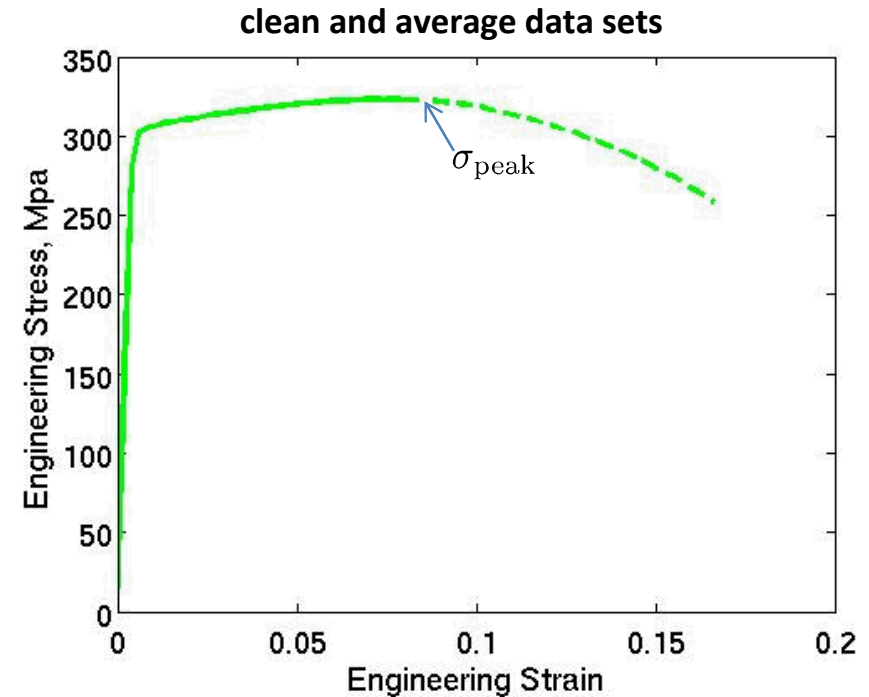
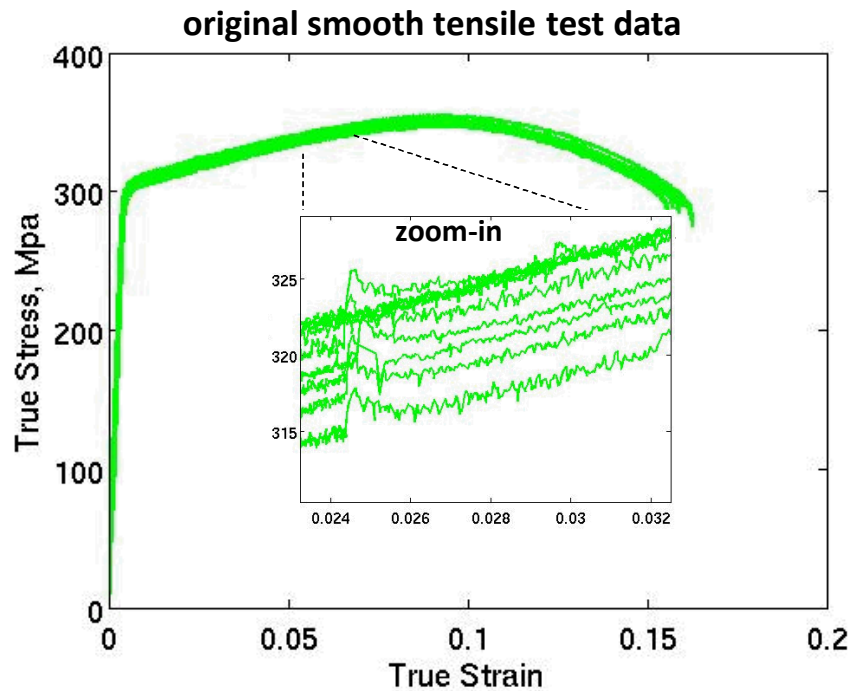
Shear-dominated ductile failure

- 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)

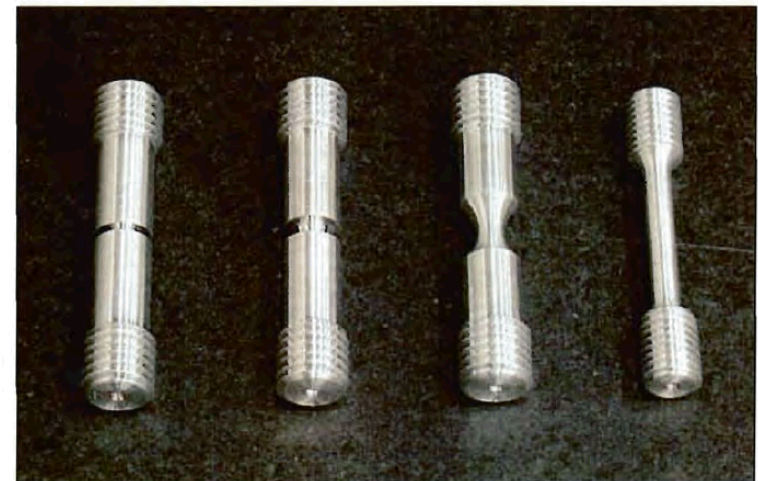
Cap-plasticity model for geomaterials

- Model formulation
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Smooth Tensile Test for 6061-T651 Aluminum



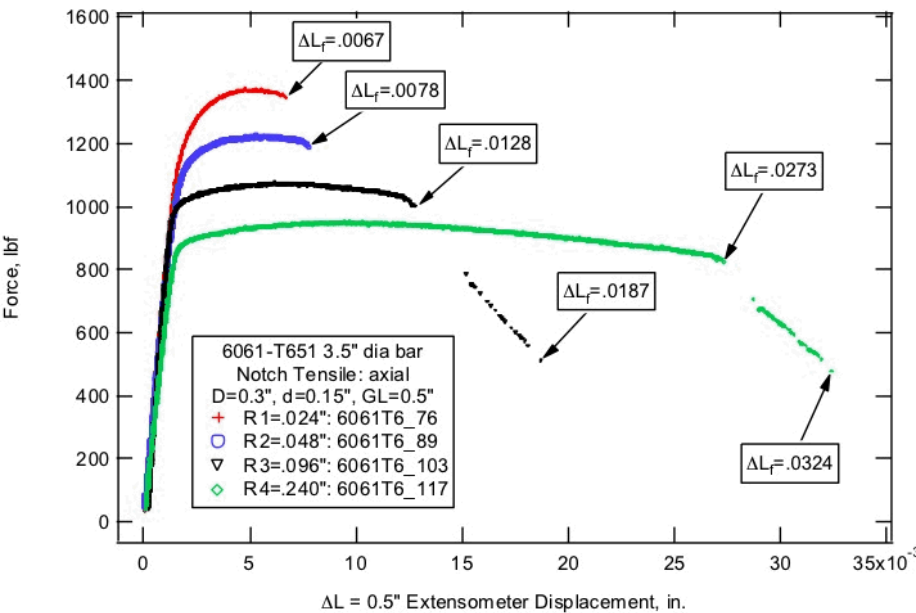
- 8 sets of experimental data
- Non-smooth and non-unique data points
- Calibrate model to fit engineering stress-strain curve up to peak load



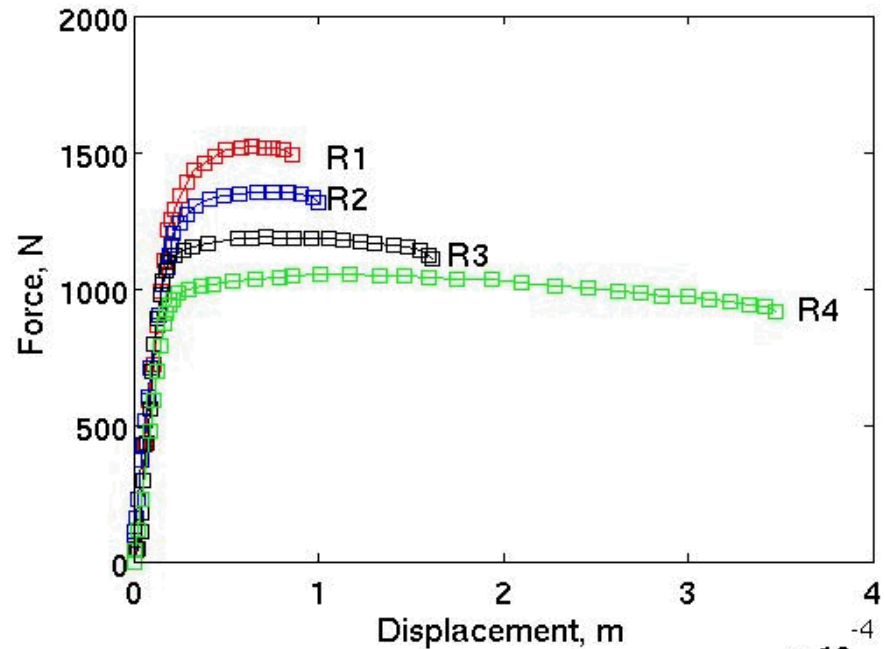
Tensile specimen: Notched and smooth

Notched Tensile Test for 6061-T651 Aluminum

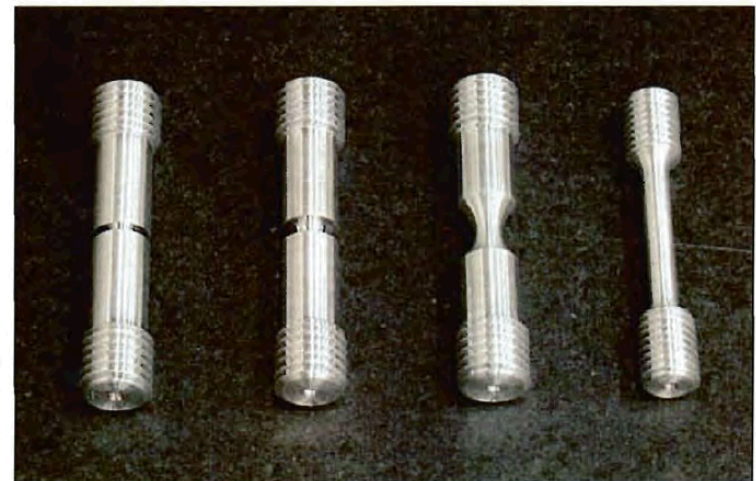
original notched tensile test data



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, ϵ_N, s_N  Notched tensile
- shear damage parameter k_ω  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

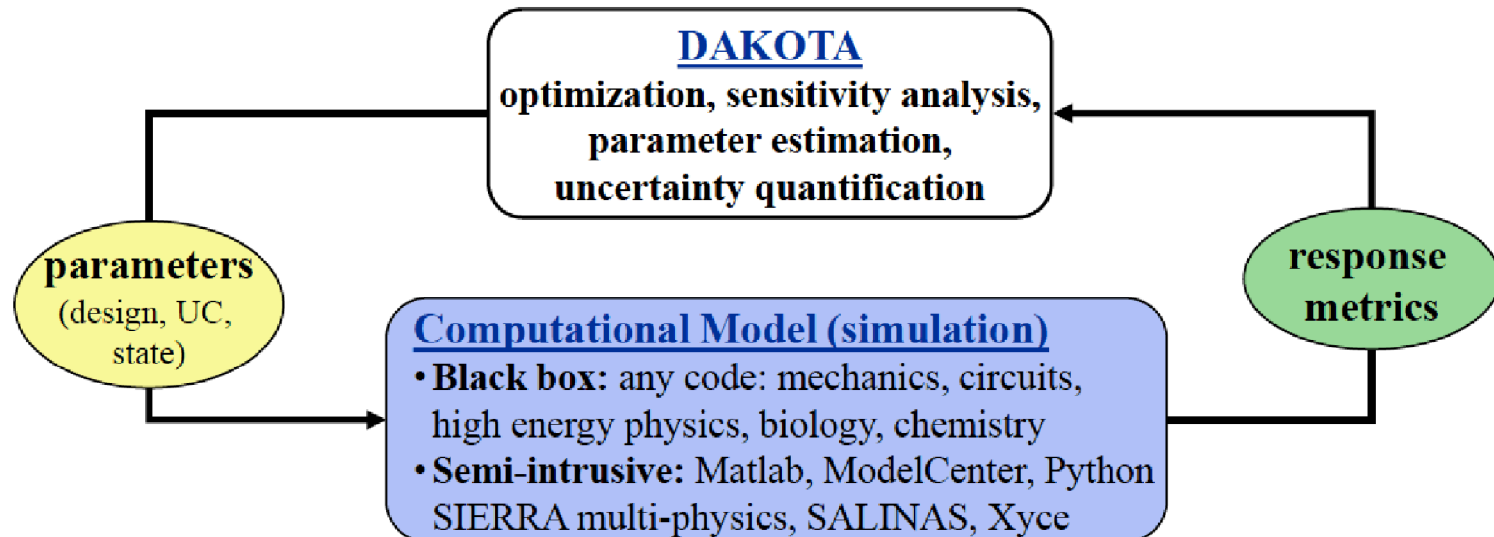
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response (simulation) target (experiment)

- 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

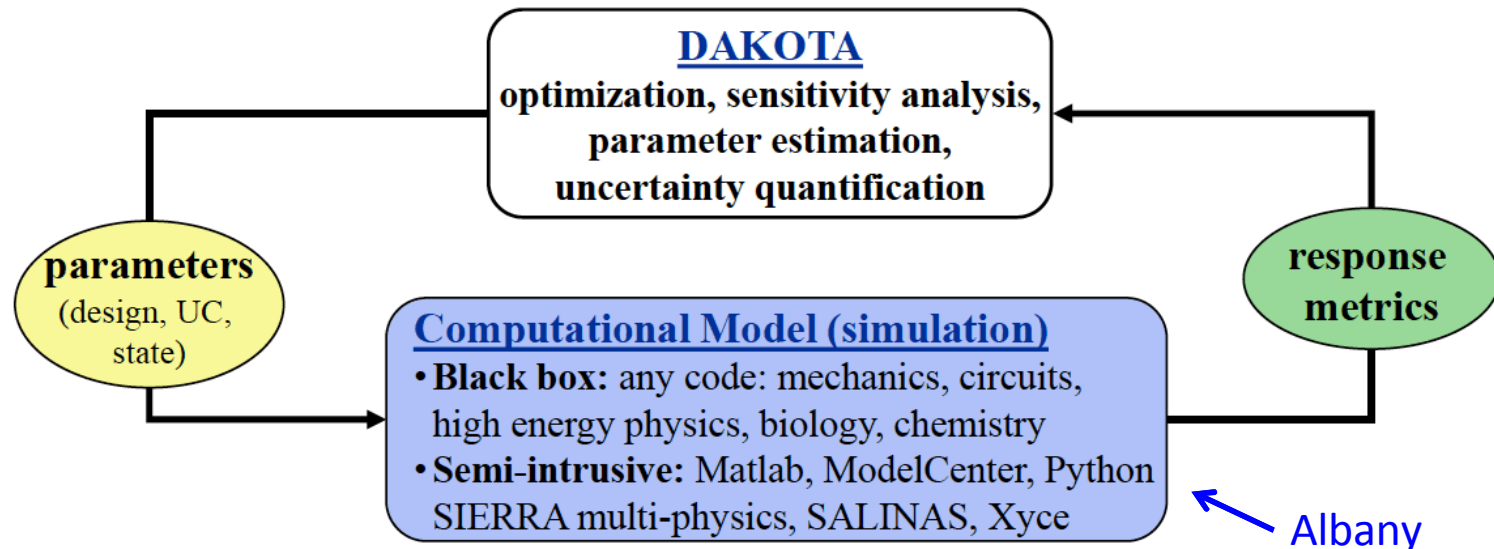
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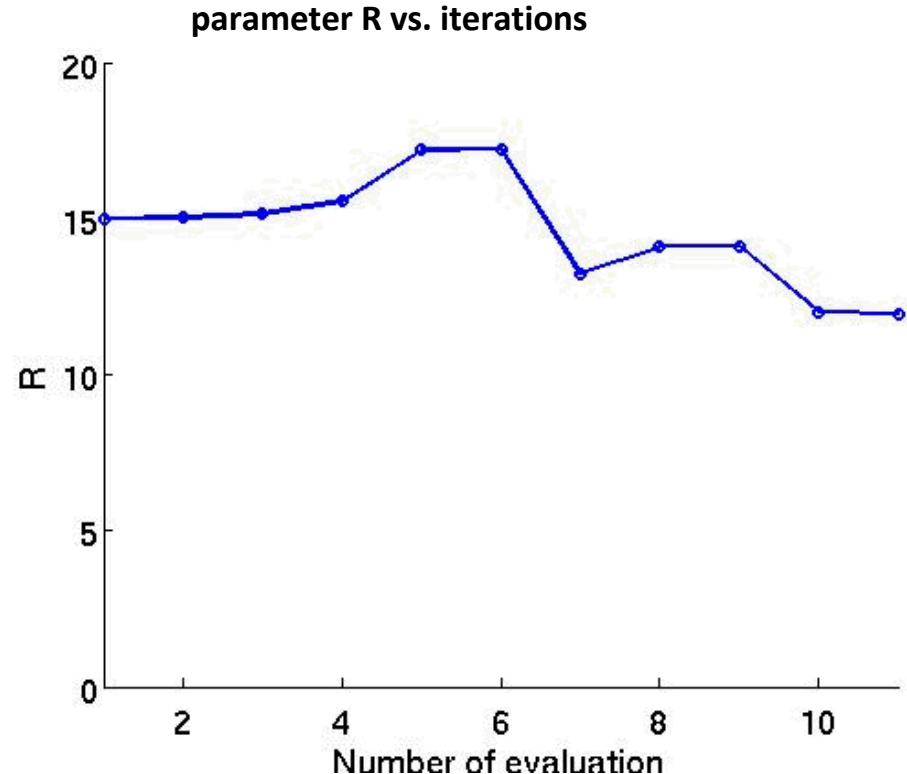
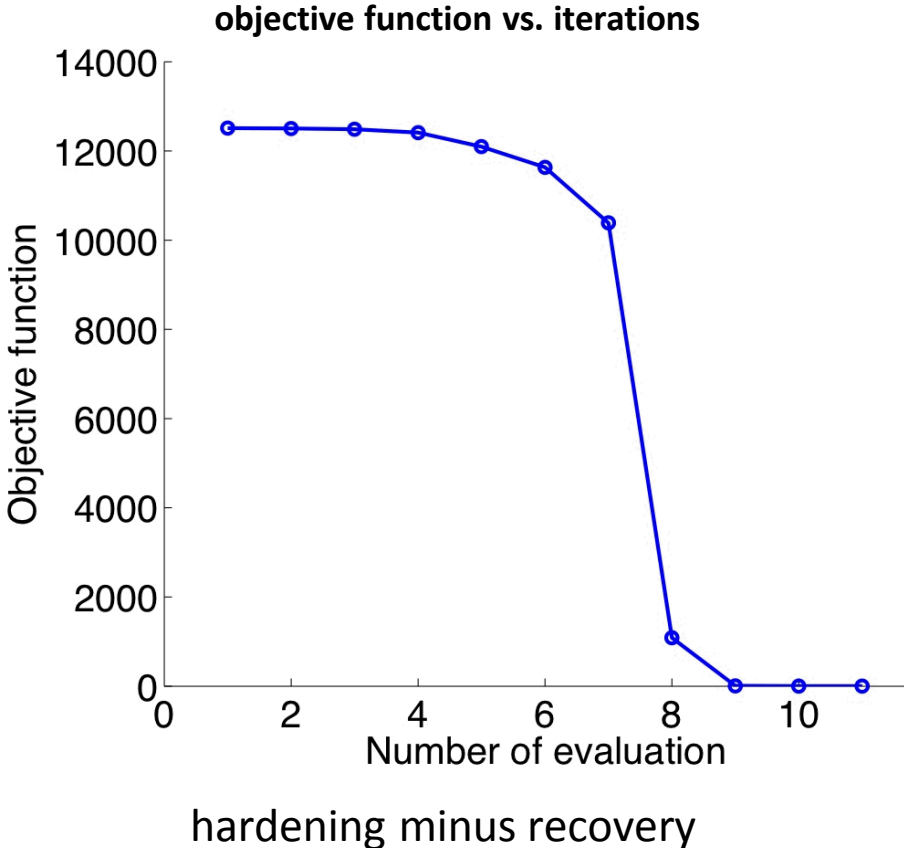
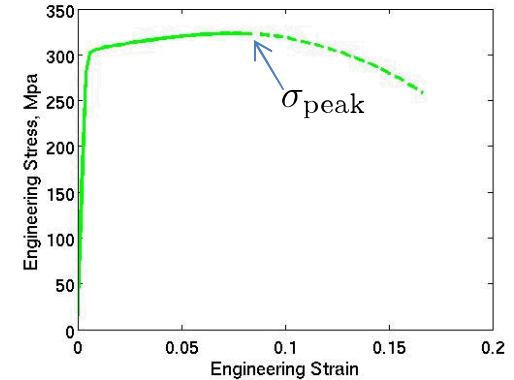
Dakota for automating the parameter variation process



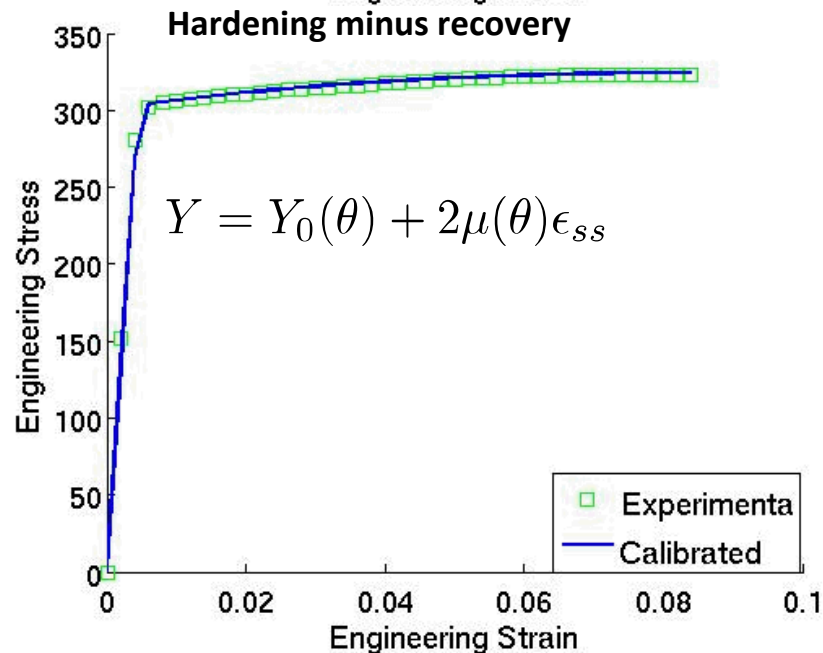
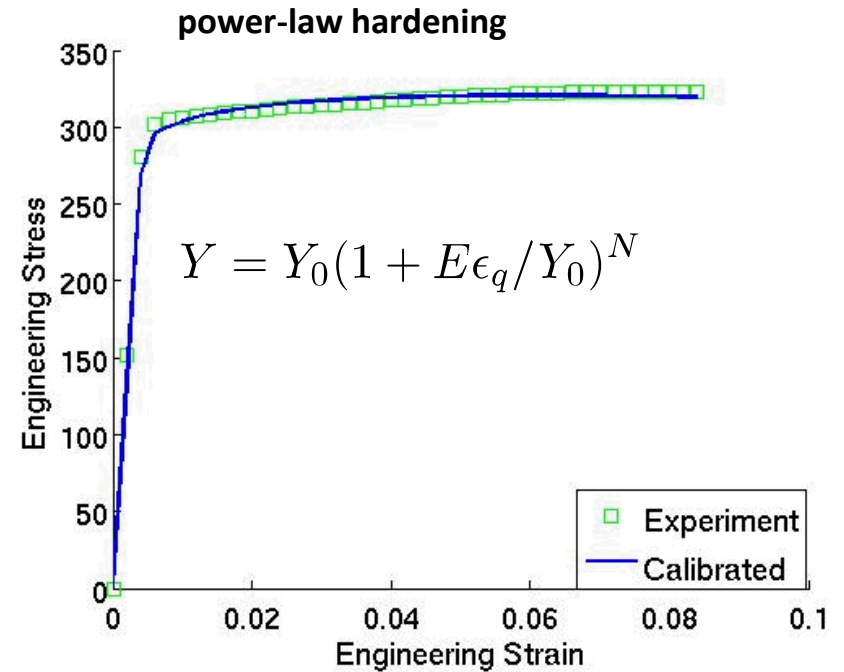
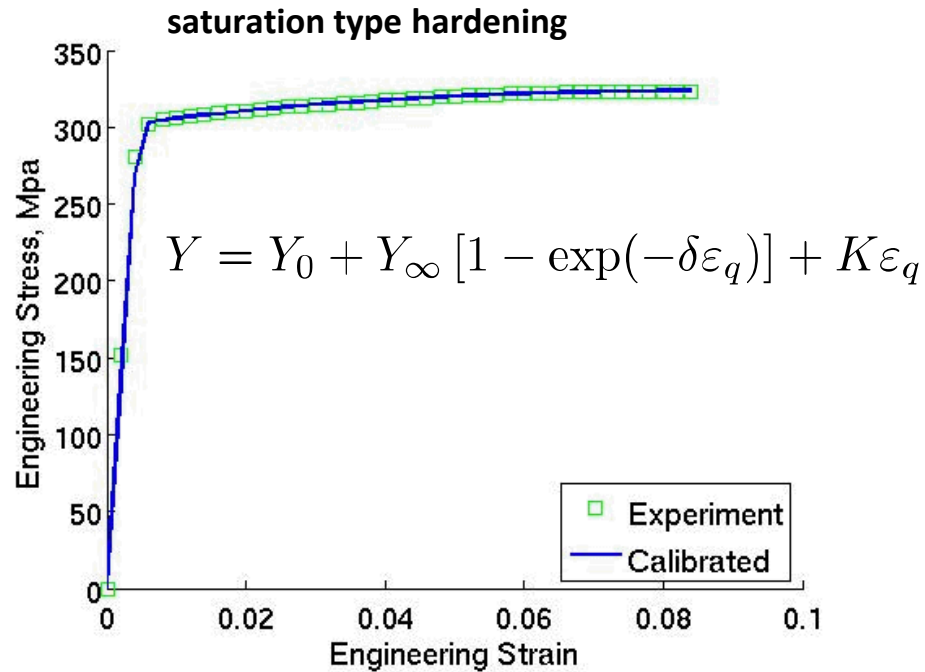
Calibration of the matrix strain hardening parameters

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

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



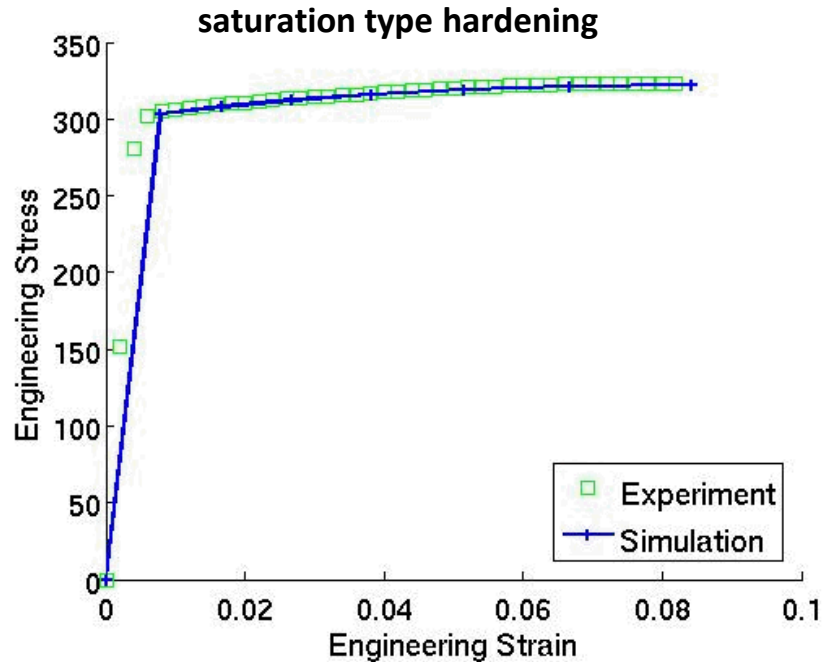
Calibration the matrix strain hardening parameters



- 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:

$$Y_0 = 303.3 \text{ MPa}$$

$$Y_\infty = 376.9 \text{ MPa}$$

$$K = 30.4 \text{ MPa}$$

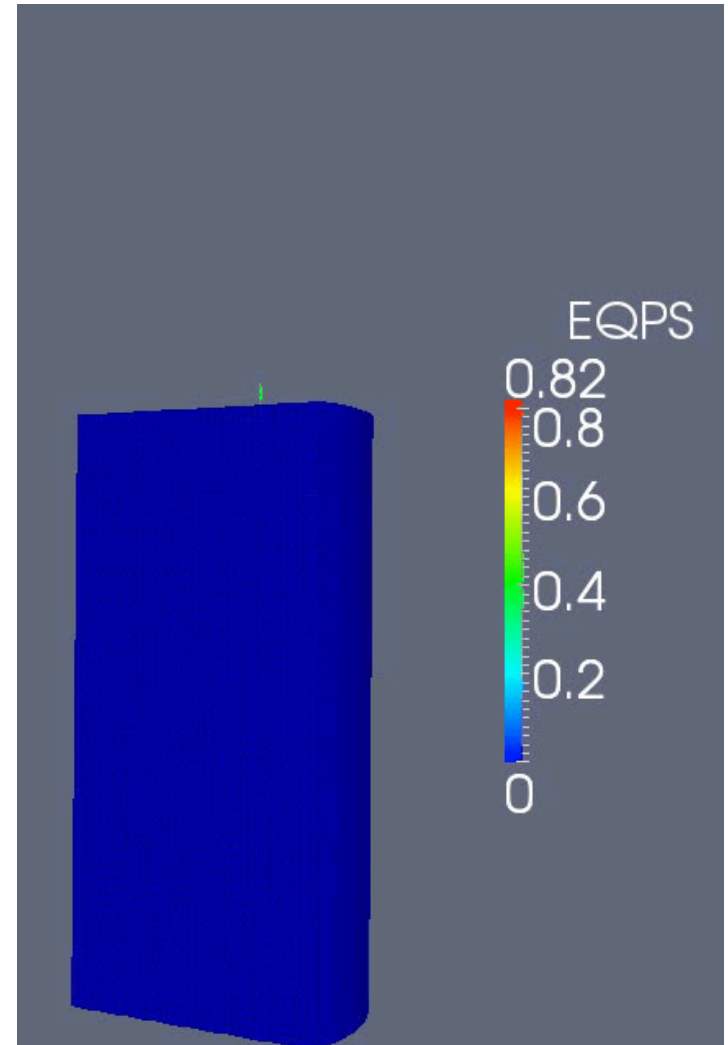
$$\delta = 12.4$$

constant:

$$f_0 = 0 \quad q_1 = 1.5$$

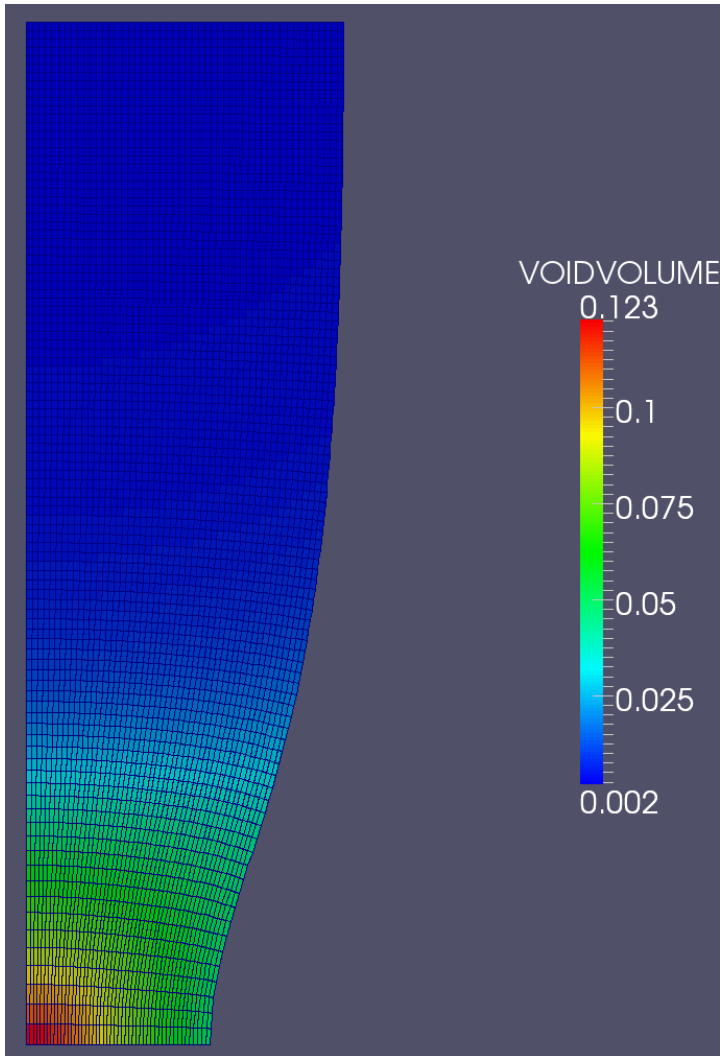
$$k_\omega = 0 \quad q_2 = 1.0$$

$$f_N = 0 \quad q_3 = 2.25$$

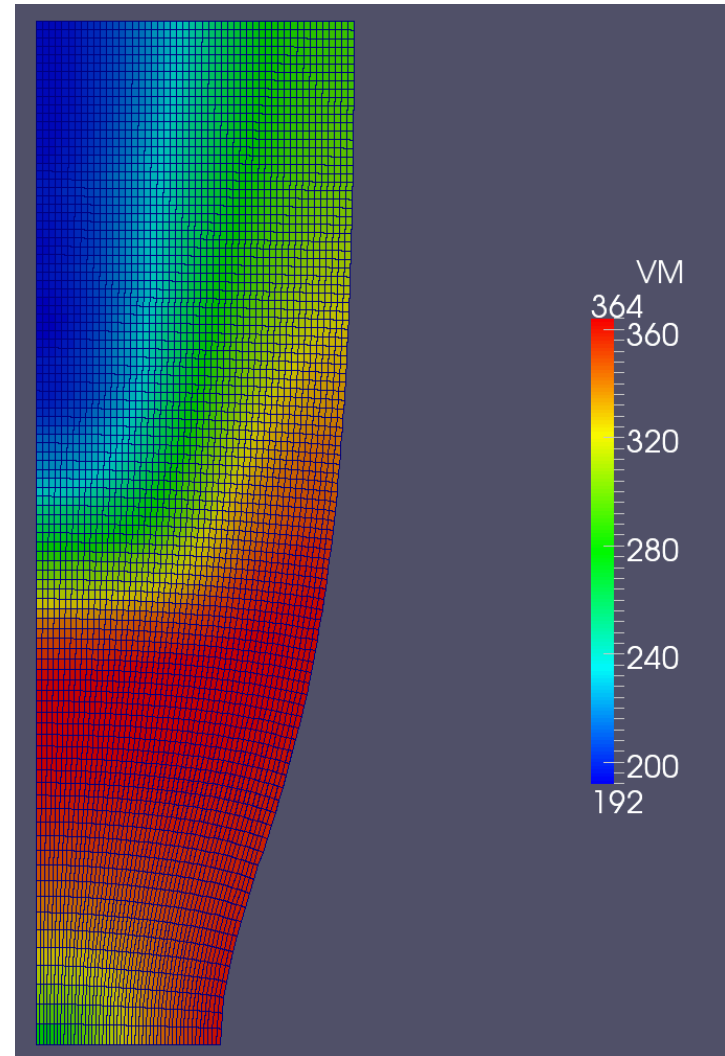


Smooth tensile tests

damage parameter

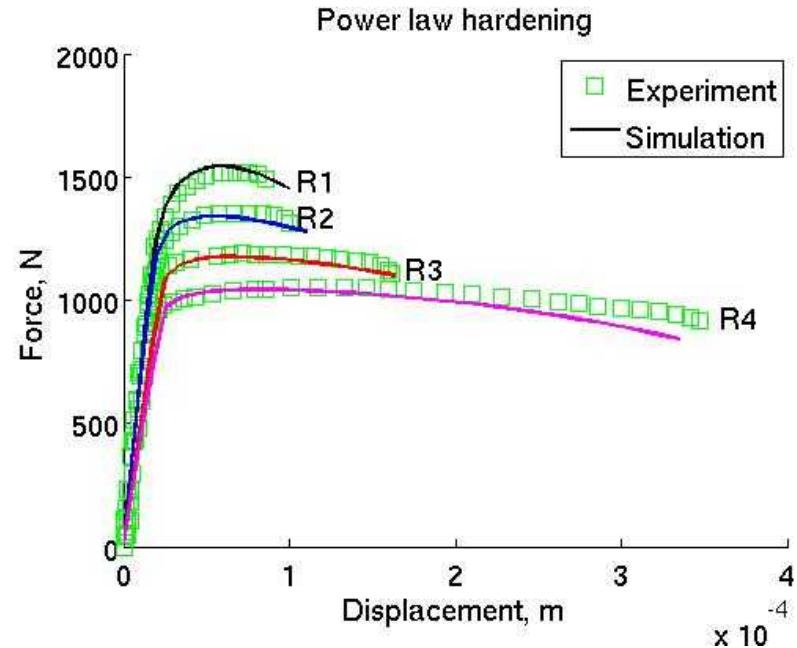
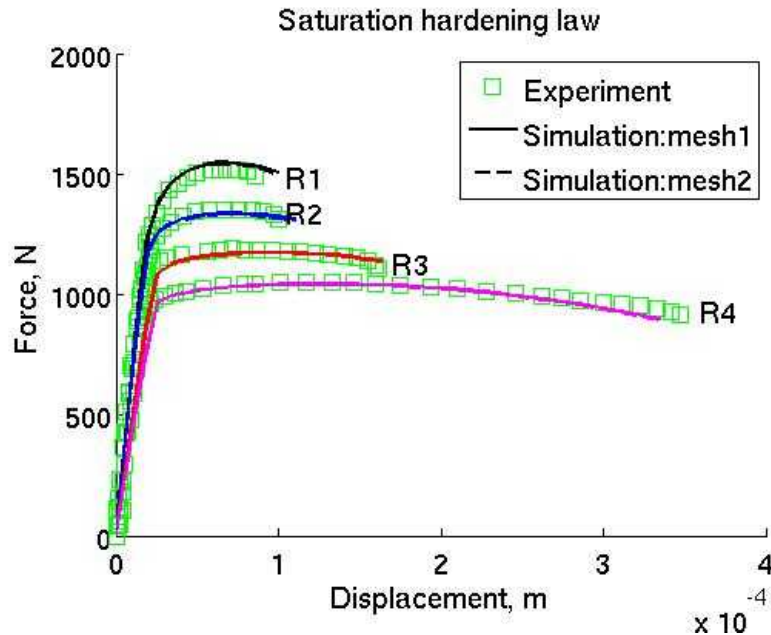


Von Mises stress

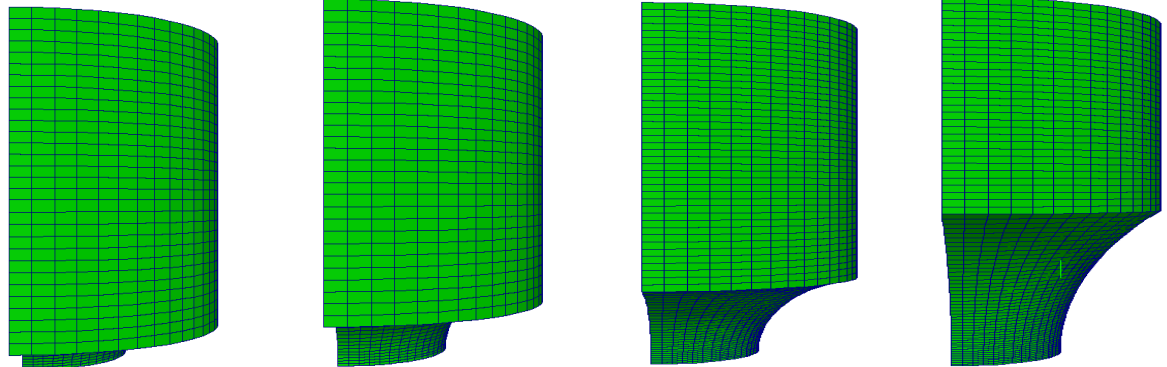


Notched Tensile Tests

- 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

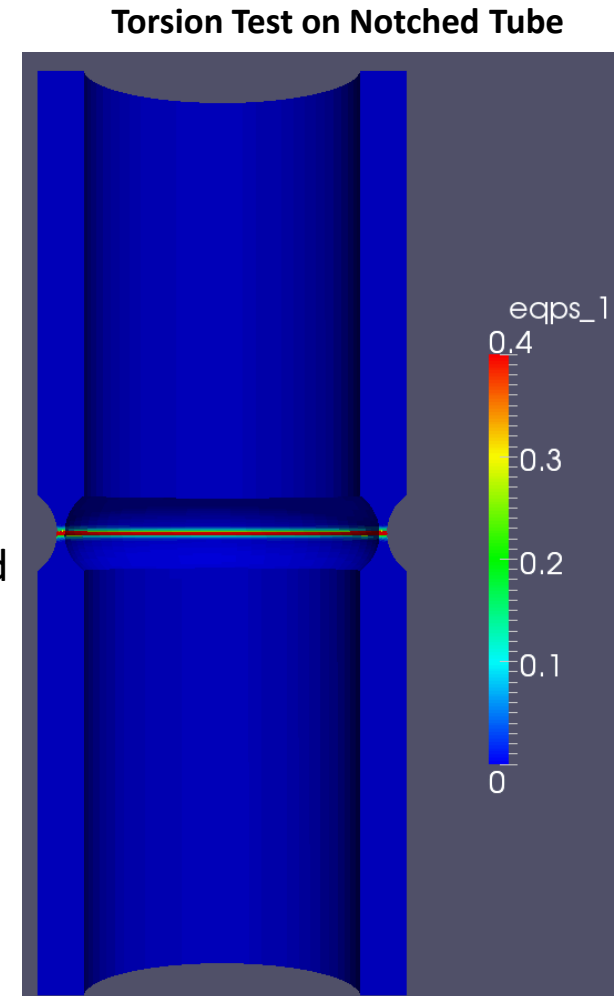
$$f_0 = 0.002$$

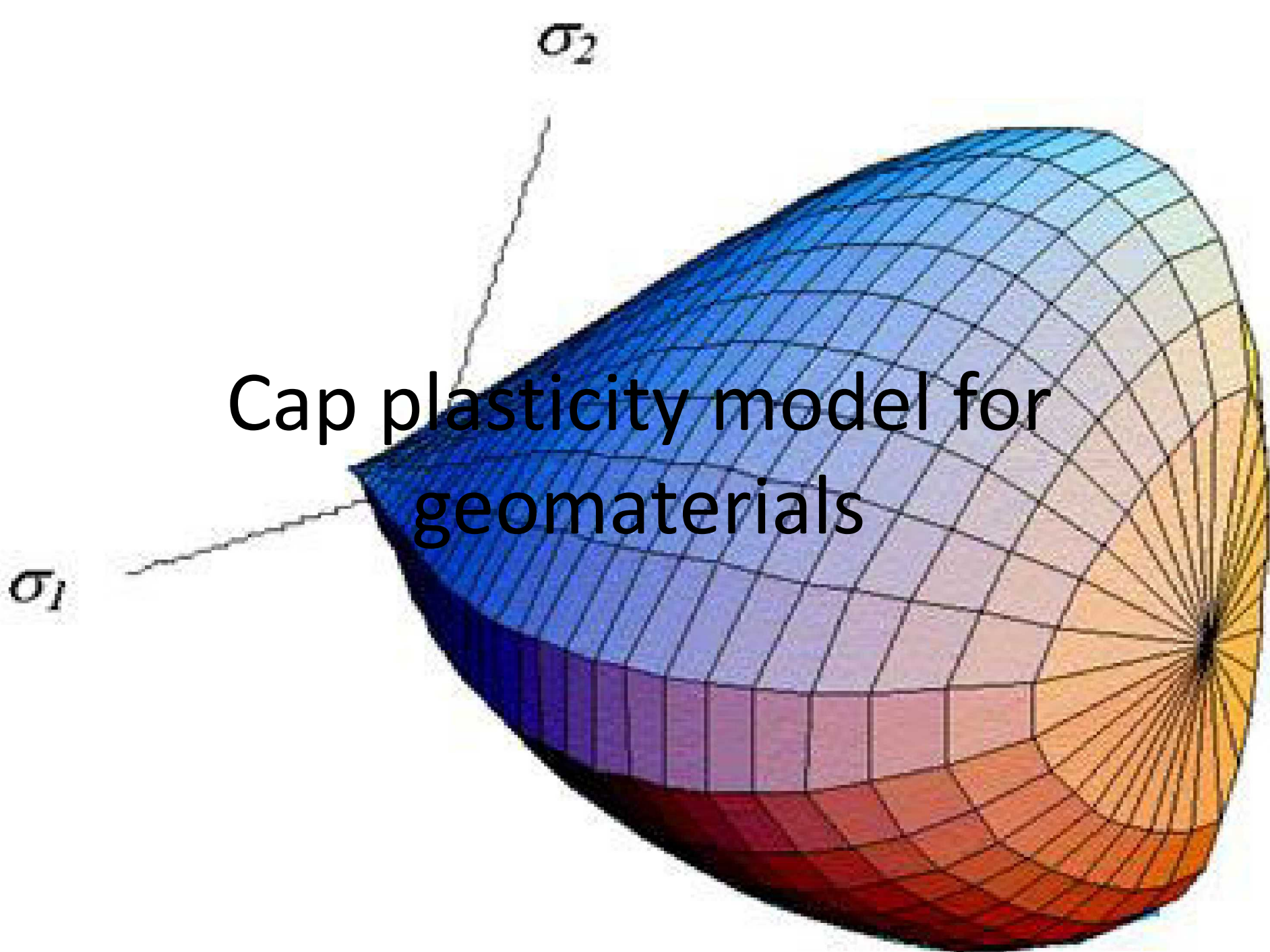
$$k_\omega = 0$$

$$f_N = 0.04$$

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

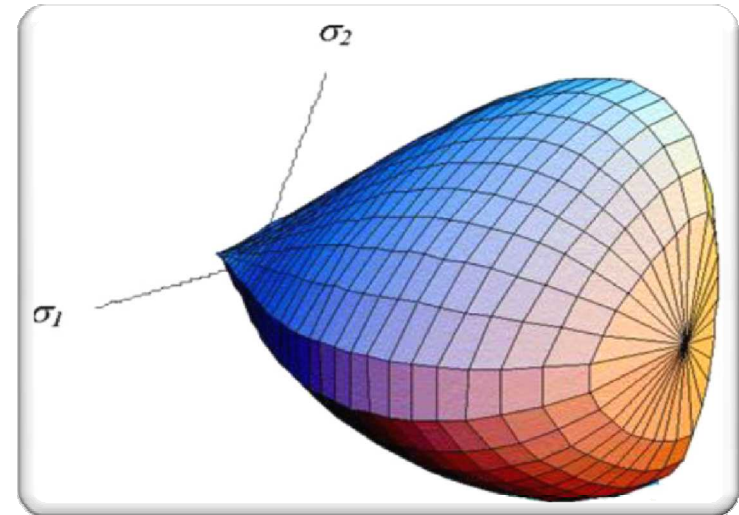
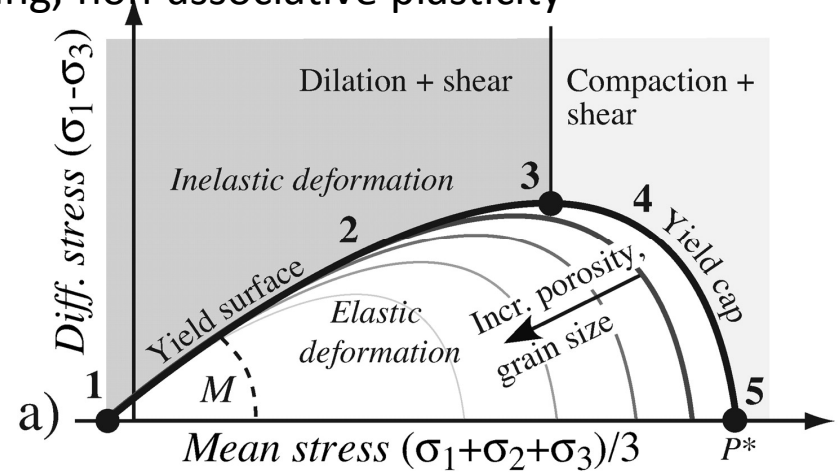
$$F_f(I_1) = A - C \exp(BI_1) - \theta I_1$$

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

$\Gamma(\beta)$ 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 a 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 that 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)

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

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);

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);
} // end local Newton loop

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

← “unpack” system sensitivity information

} local Jacobian matrix (13x13)
 $J = \partial R / \partial X$

← LocalNonlinearSolver

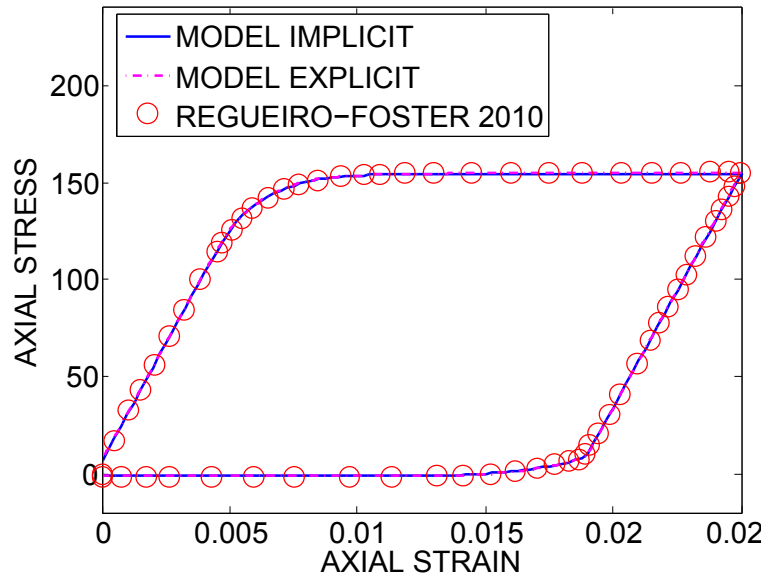
← compute system sensitivity

Material Parameters for Salem Sandstone

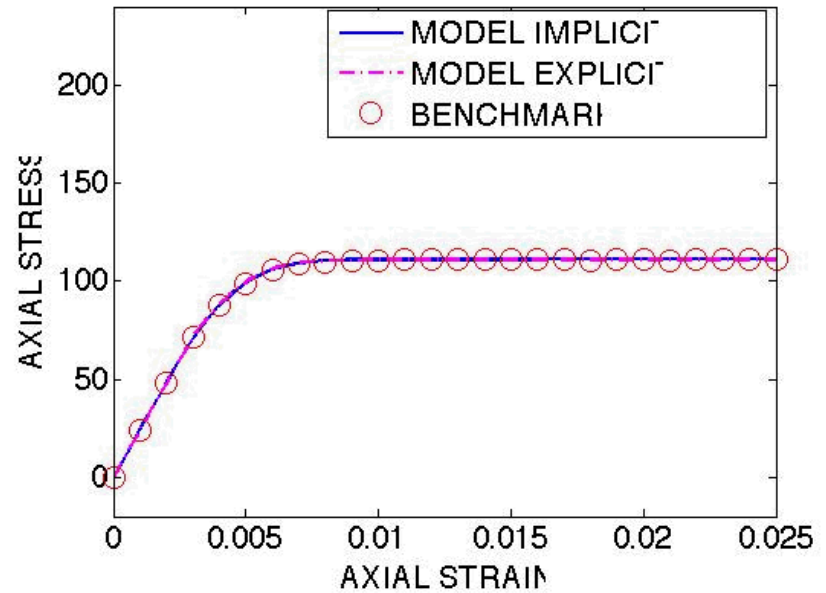
Parameter	Value	Unit
E	22,547	MPa
ν	0.2524	dimensionless
A	689.2	MPa
B, L	$2.94e - 4, 1.0e - 4$	1/MPa
C	675.2	MPa
θ, ϕ	0.0	rad
R, Q	28.0	dimensionless
κ_0	-8.05	MPa
W	0.08	dimensionless
D_1	$1.47e - 3$	1/MPa
D_2	0.0	1/MPa ²
c^α	1e5	MPa
ψ	1.0	dimensionless
N	6.0	MPa

Verification: element tests

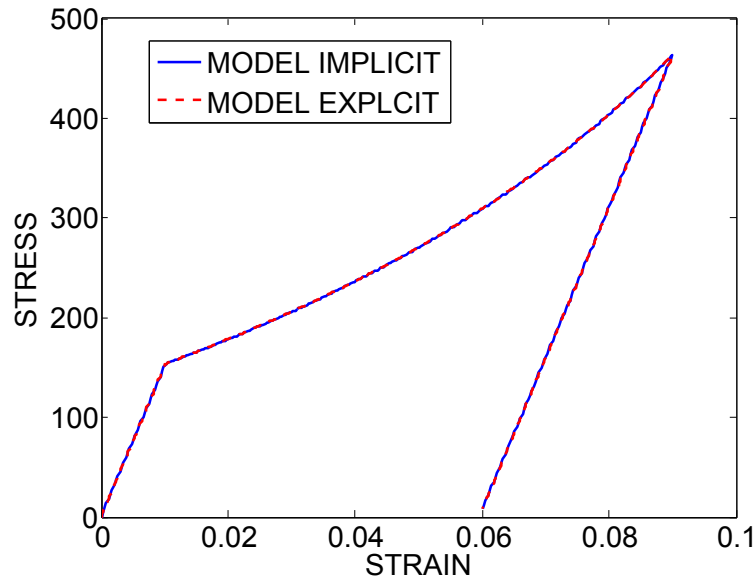
plane strain compression



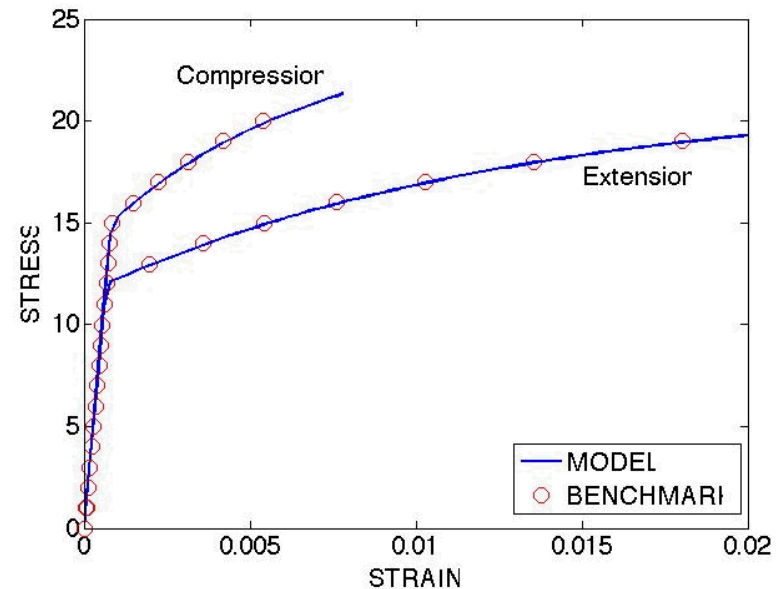
plane stress



volumetric extension



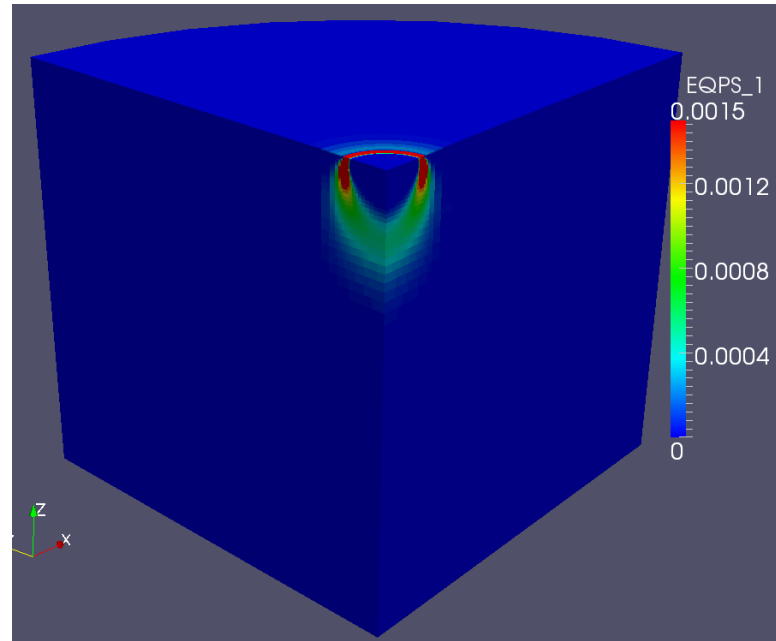
Triaxial compression and extension



3D Penetration Problem on Salem Limestone

Couple cap plasticity model with poro-mechanical problem in LCM

eqps contour



pore-pressure evolution

