On the formulation and numerical integration of a shear-modified Gurson model for ductile failure simulation at finite strain

Author Information

June 10, 2015

1 Introduction

TODO: add literature review

2 Preliminaries for finite deformation hyperelastic formulation

2.1 Kinematic preliminaries

To set the stage for the hyperelastic formulation, the kinematic preliminaries for large deformation elastoplasticity are summarized in this section, along with the quantities and relations that will be used in subsequent model development.

An essential feature of this elastoplasticity framework is the multiplicative decomposition of the deformation gradient $\boldsymbol{F}$ into an elastic part $\boldsymbol{F}^e$ and a plastic part $\boldsymbol{F}^p$

$$\boldsymbol{F} = \boldsymbol{F}^e \cdot \boldsymbol{F}^p. \tag{2.1}$$

This decomposition introduces the notion of an intermediate local configuration (cf. [8] and the references therein for the motivation and micromechanical basis for such a decomposition).

Next, we introduce a set of strain measures associated with the multiplicative decomposition that will be used extensively in the model development. First is the right Cauchy-Green tensor $\boldsymbol{C}$, and its plastic counterpart $\boldsymbol{C}^p$, which are defined in the reference configuration

$$\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F} \tag{2.2}$$

$$\boldsymbol{C}^p = \boldsymbol{F}^{pT} \cdot \boldsymbol{F}^p \tag{2.3}$$

where $\boldsymbol{F}^T$ is the transpose of $\boldsymbol{F}$.

In the current configuration we consider the left Cauchy-Green tensor $\boldsymbol{b}$, and its elastic counterpart $\boldsymbol{b}^e$

$$\boldsymbol{b} = \boldsymbol{F} \cdot \boldsymbol{F}^T \tag{2.4}$$

$$\boldsymbol{b}^e = \boldsymbol{F}^e \cdot \boldsymbol{F}^{eT} \tag{2.5}$$

The above fundamental strain measures are related via pull-back and push-forward operations

$$\boldsymbol{C}^{-p} = \boldsymbol{F}^{-1} \cdot \boldsymbol{b}^{e} \cdot \boldsymbol{F}^{-T} \tag{2.6}$$

$$\boldsymbol{b}^{e} = \boldsymbol{F} \cdot \boldsymbol{C}^{-p} \cdot \boldsymbol{F}^{T} \tag{2.7}$$

In metal plasticity, a standard assumption is that plastic flow is isochoric (volume-preserving), i.e. $\det(\boldsymbol{F}^{p}) = 1$, which implies

$$J = \det(\boldsymbol{F}) = \det(\boldsymbol{F}^{e}) \tag{2.8}$$

Defining $J^{e} = \det(\boldsymbol{F}^{e})$, we have the volume preserving part of the elastic left Cauchy-Green tensor $\bar{\boldsymbol{b}}^{e}$

$$\bar{\boldsymbol{b}}^{e} = J^{e^{-2/3}} \boldsymbol{b}^{e} = J^{-2/3} \boldsymbol{b}^{e}. \tag{2.9}$$

2.2 Hyperelastic constitutive relation

The starting point of the hyperelastic constitutive formulation is the assumption of the existence of a strain-energy function, which is proposed to have the following form

$$\Psi = \Psi^{\mathrm{vol}}[J^{e}] + \Psi^{\mathrm{iso}}[\bar{\boldsymbol{b}}^{e}] \tag{2.10}$$

Here the strain-energy function Ψ is a decoupled function of the volumetric part (i.e., $J^{e} = \det \boldsymbol{F}^{e}$) and the isochoric part (i.e., $\bar{\boldsymbol{b}}^{e}$) of the elastic deformation. The volumetric and the isochoric parts of the strain-energy function are given as

$$\Psi^{\mathrm{vol}}[J^{e}] = \frac{\kappa}{4} \left(J^{e2} - 1 - \ln \mathrm{J}^{\mathrm{e2}} \right) \tag{2.11}$$

$$\Psi^{\mathrm{iso}}[\bar{\boldsymbol{b}}^{e}] = \frac{\mu}{2} \left(\mathrm{tr}(\bar{\boldsymbol{b}}^{\mathrm{e}}) - 3 \right) \tag{2.12}$$

where κ and μ are the bulk and shear modulus. Here we are following the developments of ([10]), however we employ a different choice of strain energy-functions. The elastic constitutive law and the Kirchhoff stresses are given as

$$\boldsymbol{\tau} = J^{e} p \mathbf{1} + \boldsymbol{s} \tag{2.13}$$

The Kirchhoff pressure p and the deviatoric stress tensor $\boldsymbol{s}$ are related to the elastic strain measure as

$$p = \frac{1}{3} \mathrm{tr}(\boldsymbol{\tau}) = \frac{\kappa}{2} \left(J^{e2} - 1 \right) / J^{e} \tag{2.14}$$

$$\boldsymbol{s} = \mathrm{dev}(\boldsymbol{\tau}) = \mu \, \mathrm{dev}(\bar{\boldsymbol{b}}^{e}) \tag{2.15}$$

3 Formulation of the finite deformation Gurson model

Within the previously described large deformation hyperelastic framework, key components of the constitutive relations of the shear-modified Gurson model are presented in this section, including the yield function, the hardening law, the flow rule and the evolution law for the shear-modified void growth.

3.1 Yield function

The yield function Φ of the Gurson model can be written in terms of the previously defined Kirchhoff mean stress p and deviatoric stress tensor $\boldsymbol{s}$ as

$$\Phi = \frac{1}{2}\boldsymbol{s} : \boldsymbol{s} - \frac{1}{3}\psi Y^2 \tag{3.1}$$

where ψ contains contributions from the damage in the material and Y is the Kirchhoff yield stress. This yield function (3.1) is a quadratic version form. This particular variant of the yield function was chosen as it proved to exhibit superior properties of robustness in convergence in the nonlinear solution algorithm outline below.

The function ψ directly relates to the void volume fraction of the porous solid and is given as

$$\psi = 1 + q_3 f^2 - 2q_1 f \cosh(v), \quad v = \frac{3q_2 p}{2Y} \tag{3.2}$$

where p is the Kirchhoff pressure defined in (2.14), and f is the void volume fraction of the porous solid. The Kirchhoff yield stress Y describes the hardening of the undamaged matrix material. Also, the constants $q_1, q_2 2, q_3$ are the accepted additional yield parameters often present in GTN type models.

3.2 Hardening law

The hardening law relates the yield strength Y to some measure of plastic deformation. One example of a nonlinear hardening law proposed by [8] for metal is written as

$$Y = Y_0 + Y_\infty \left[1 - \exp(-\delta \varepsilon_q)\right] + K\varepsilon_q \tag{3.3}$$

where ε_q is the equivalent plastic strain, Y_0 is the initial yield strength, Y_∞ is the residual flow stress, K is the hardening coefficient, and δ is the saturation exponent. Other forms of hardening law can also be used depending on the observed material behavior.

The plastic work increment in the matrix material is equal to the macroscopic plastic work increment, which can be used to derive the evolution equation for the equivalent plastic strain ε_q as

$$\dot{\varepsilon}_q Y(1-f) = \boldsymbol{\tau} : \left(\gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) \tag{3.4}$$

Substituting yield function Φ into (3.4) to obtain the expression to compute $\dot{\varepsilon}_q$

$$\dot{\varepsilon}_q = \frac{1}{1-f}\left(\gamma \sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{pt}{Y}\right) \tag{3.5}$$

3.3 Flow rule

Following the standard procedure of the principle of maximum dissipation, Simo and Miehe [7] proposed a general form of associate flow rule, which is adopted in the current formulation and is given as

$$-\frac{1}{2}L_v(\boldsymbol{b}^e)\cdot\boldsymbol{b}^{-e}=\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}=\gamma\boldsymbol{n}+\frac{1}{3}t\mathbf{1} \tag{3.6}$$

where $L_v(\boldsymbol{b}^e)=\boldsymbol{F}\cdot\dot{\boldsymbol{C}}^{-p}\cdot\boldsymbol{F}^T$ is the Lie derivative, and $\boldsymbol{n}$ and t are the deviatoric and volumetric component of the gradient term, respectively. Substituting the yield function (3.1) leads to the following

$$\boldsymbol{n}=\frac{\boldsymbol{s}}{\|\boldsymbol{s}\|} \tag{3.7}$$

$$t=\operatorname{tr}\left(\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}\right)=\sqrt{\frac{3}{2}}\gamma f\sinh(\frac{3p}{2Y})\frac{1}{\sqrt{|\psi|}}\operatorname{sign}(\psi) \tag{3.8}$$

3.4 Evolution of void volume fraction and shear modification

The void volume fraction f is the internal variable that characterizes the material damage. The rate of change in total void volume fraction, $\dot{f}$, is typically given by the sum of contributions due to the void growth, $\dot{f}_g$, and the nucleation of new voids, $\dot{f}_n$.

$$\dot{f}=\dot{f}_g+\dot{f}_n \tag{3.9}$$

In the original Gurson model [3], the void growth part $\dot{f}_g$ was related to the plastic volume change as

$$\dot{f}_g=(1-f)\operatorname{tr}\left(\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}\right) \tag{3.10}$$

To account for the void growth under shear-dominated stress state, the void growth law (3.10) was extended in [5] by adding a term that depends on the third stress invariant. This shear-modified void growth equation is written as

$$\dot{f}_g=(1-f)\operatorname{tr}\left(\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}\right)+k_\omega f\frac{\omega(\boldsymbol{\tau})}{\tau_e}\boldsymbol{s}:\left(\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}\right) \tag{3.11}$$

where $\tau_e=\sqrt{3/2}\|\boldsymbol{s}\|$ is the effective deviatoric Kirchhoff stress, k_ω is a material constant that sets the magnitude of the damage growth rate in pure shear states [5]. The function $\omega(\boldsymbol{\tau})$ includes the effect of the third stress invariant on void growth and is given as

$$\omega(\boldsymbol{\tau})=1-\left(\frac{27J_3}{2\tau_e^3}\right)^2 \tag{3.12}$$

where $J_3=\det(\boldsymbol{s})$ is the third invariant of deviatoric Kirchhoff stress tensor.

Substituting the yield function (3.1) and the expression for $\omega(\boldsymbol{\tau})$ (3.12) into the void growth law (3.11) yields

$$\dot{f}_g = (1-f)t + \sqrt{\frac{2}{3}}\gamma k_\omega f \omega(\boldsymbol{\tau}) \tag{3.13}$$

The effective increase in damage due to plastic strain controlled nucleation is given by [2] as

$$\dot{f}_{nu} = A\dot{\varepsilon}_q \tag{3.14}$$

where the parameter A is defined as a function of the matrix equivalent plastic strain ε_q

$$A = \begin{cases} \frac{f_N}{s_N\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\varepsilon_q - \epsilon_N}{s_N}\right)^2\right], & p \geq 0 \\ 0, & p < 0 \end{cases} \tag{3.15}$$

where the nucleation strain follows a normal distribution with a mean value ϵ_N and a standard deviation s_N with the volume fraction of the nucleated voids given by f_N.

4 Integration of constitutive equations

4.1 Discrete form of the rate equations

To derive the discrete form of the rate equations, the starting point is to write the evolution equations in the material (reference) configuration. For the flow rule, a pull-back operation is applied to (3.6) such that

$$-\frac{1}{2}\dot{\boldsymbol{C}}^{-p} \cdot \boldsymbol{C}^p = \gamma \boldsymbol{F}^{-1} \cdot \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \cdot \boldsymbol{F} \tag{4.1}$$

where γ is the plastic multiplier. Then, the application of the exponential mapping to (4.1) yields an incremental objective integration algorithm

$$\boldsymbol{C}^{-p}_{n+1} = \boldsymbol{F}^{-1}_{n+1} \cdot \exp\left(-2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{F}_{n+1} \cdot \boldsymbol{C}^{-p}_n \tag{4.2}$$

Applying the push-forward operation to (4.2) yields an update algorithm for the elastic left Cauchy-Green tensor $\boldsymbol{b}^e_{n+1}$ as

$$\boldsymbol{b}^e_{n+1} = \exp\left(-2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{b}^{e\,\mathrm{tr}} \tag{4.3}$$

where the trial elastic left Cauchy-Green tensor $\boldsymbol{b}^{e\,\mathrm{tr}}$ is given by

$$\boldsymbol{b}^{e\,\mathrm{tr}} = \boldsymbol{F}_{n+1} \cdot \boldsymbol{C}^{-p}_n \cdot \boldsymbol{F}^T_{n+1} \tag{4.4}$$

From elastic and plastic isotropy, $\boldsymbol{b}^e_{n+1}, \boldsymbol{b}^{e\,\mathrm{tr}}$ and $\boldsymbol{\tau}$ have identical principal axes. Then, the logarithmic Hencky strains follow as

$$\ln \boldsymbol{b}^e_{n+1} = \ln \boldsymbol{b}^{e\,\mathrm{tr}} - 2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}} \tag{4.5}$$

Using the elastic constitutive relations (2.14) and (2.15), the Kirchhoff pressure and deviatoric stress tensor at time t_{n+1} can be obtained as

$$p_{n+1} = p^{\mathrm{tr}} - \kappa t \tag{4.6}$$

$$\boldsymbol{s}_{n+1} = \boldsymbol{s}^{\mathrm{tr}} - 2\mu\Delta\gamma\boldsymbol{n} \tag{4.7}$$

where $\boldsymbol{n}$ and t are given by (3.7), (3.8) and are evaluated at time t_{n+1}, and p^{tr} and $\boldsymbol{s}^{\mathrm{tr}}$ are the trial states given by

$$p^{\mathrm{tr}} = \kappa \ln J^{e\,\mathrm{tr}}, \quad J^{e\,\mathrm{tr}} = \det(\boldsymbol{b}^{e\,\mathrm{tr}})^{1/2} \tag{4.8}$$

$$\boldsymbol{s}^{\mathrm{tr}} = \mu\,\mathrm{dev}\ln\boldsymbol{b}^{e\,\mathrm{tr}} \tag{4.9}$$

The discrete form of evolution equations for internal variable ε_q and the void volume fraction f are obtained by apply backward Euler scheme to their evolution equations (3.9) and (3.5). The resulting discrete equations are

$$f_{n+1} = f_n + (1 - f_{n+1})t + \sqrt{\frac{2}{3}}\Delta\gamma k_\omega f_{n+1}\omega(\boldsymbol{\tau}) + A_{n+1}(\varepsilon_{q(n+1)} - \varepsilon_{q(n)}) \tag{4.10}$$

$$\varepsilon_{q(n+1)} = \varepsilon_{q(n)} + \frac{1}{1 - f_{n+1}}\left(\Delta\gamma\sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{p_{n+1}t}{Y}\right) \tag{4.11}$$

4.2 Local nonlinear system of equations

The discrete form of the rate equations (4.3), (4.6), (4.7), (4.10) and (4.11) include four unknowns quantities relate to the stresses and internal state variables at time t_{n+1}, which are the pressure p, the equivalent plastic strain ε_q, the void volume fraction f, and the plastic multiplier $\Delta\gamma$.

The unknowns will be obtained from solving the following nonlinear system of equations. For simplicity, in the following, we will omit the index $n+1$ referring to the current time t_{n+1}. The resulting nonlinear system of equations are

$$R_1(\boldsymbol{X}) = \|\boldsymbol{s}^{\mathrm{tr}}\| - 2\mu\Delta\gamma - \sqrt{\frac{2}{3}}\mathrm{sign}(\psi)\sqrt{|\psi|}Y \tag{4.12}$$

$$R_2(\boldsymbol{X}) = p - p^{\mathrm{tr}} + \kappa t \tag{4.13}$$

$$R_3(\boldsymbol{X}) = f - f_n - (1 - f)t - \sqrt{\frac{2}{3}}\Delta\gamma k_\omega f\omega(\boldsymbol{\tau}) - A(\varepsilon_q - \varepsilon_{q(n)}) \tag{4.14}$$

$$R_4(\boldsymbol{X}) = \varepsilon_q - \varepsilon_{q(n)} - \frac{1}{1 - f}\left(\Delta\gamma\sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{pt}{Y}\right) \tag{4.15}$$

where, the vector of unknowns $\boldsymbol{X}$ is

$$\boldsymbol{X} = \{p, f, \varepsilon_q, \Delta\gamma\} \tag{4.16}$$

The above nonlinear system of equations can be solved through iterative solution method such as the Newton's method. The implicit algorithm for integrating the shear-modified large deformation Gurson model is summarized in the following box.

Box 1. Implicit algorithm for integrating shear-modified large deformation Gurson model

GIVEN: $\varepsilon_{q(n)}, f_n, \boldsymbol{b}_n^e$ and $\boldsymbol{F}$
FIND: $\boldsymbol{\tau}, \varepsilon_q, f, \boldsymbol{b}^e$(or $\boldsymbol{F}^p$) at time t_{n+1}
STEP 1. Compute trial elastic left Cauchy-Green tensor $\boldsymbol{b}_e^{\text{tr}}$ (4.4)
STEP 2. Compute trial stresses $p^{\text{tr}}, \boldsymbol{s}^{\text{tr}}$ (4.8), (4.9)
STEP 3. Check yielding (3.1): $\Phi^{\text{tr}}(p^{\text{tr}}, \boldsymbol{s}^{\text{tr}}, \varepsilon_{q(n)}, f_n) > 0$?
No, set $p = p^{\text{tr}}, \boldsymbol{s} = \boldsymbol{s}^{\text{tr}}, \boldsymbol{b}^e = \boldsymbol{b}^{e\,\text{tr}}, \varepsilon_q = \varepsilon_{q(n)}, f = f_n$ and exit
STEP 4. Yes, local Newton loop
4.1 Initialize $\boldsymbol{X}^k$ (4.16) and the iteration count $k = 0$
4.2 Assemble the residual equations $\boldsymbol{R}(\boldsymbol{X}^k)$ (4.12) - (4.15)
4.3 Check convergence: $\| \boldsymbol{R} \| < tolerance$?
Yes, converged and go to STEP 5
4.4 No, compute local Jacobian matrix $\boldsymbol{J} = \partial \boldsymbol{R}/\partial \boldsymbol{X}$
4.5 Solve system of equations $\boldsymbol{J} \cdot \delta \boldsymbol{X} = \boldsymbol{R}$ for $\delta \boldsymbol{X}$
4.6 Update $\boldsymbol{X}^{k+1} = \boldsymbol{X}^k - \delta \boldsymbol{X}$, $k \to k+1$ and go to 4.2
STEP 5. Update $\boldsymbol{\tau} = \boldsymbol{s} + p\boldsymbol{g}$, ε_q, f, and $\boldsymbol{F}^p$

The plastic deformation gradient $\boldsymbol{F}^p$, which is used in (4.1) and (4.4) to compute trial state, is updated using

$$\boldsymbol{F}^p = \exp\left(\frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{F}_n^p \tag{4.17}$$

In the Newton's iterative solution method, it requires consistent linearization of the system of equation (4.12) - (4.15), which necessities a derivative of the objective functions with respect to the independent fields (i.e., the unknowns). The Jacobian derivative of the objective function ($\boldsymbol{J} = \partial \boldsymbol{R}/\partial \boldsymbol{X}$) is commonly referred to as the algorithmic consistent tangent operator in the constitutive model literature [4, 9]. In this work, a technique in computational science called the forward automatic differentiation (FAD) will be used to compute necessary derivatives. FAD provides an efficient and convenient way to evaluate derivatives. It will be detailed in the next section. Interested readers can also refer to [1] for applications of FAD to constitutive modeling in small- and large-deformation computational inelasticity.

5 Numerical implementation and solution procedure

5.1 Albany analysis code and solution procedure

TODO: ref to our Journal of Nuclear Material paper. Include a description of the Albany analysis code and the solution procedure.

5.2 FAD: a numerical exact way of computing consistent tangent

Need to modify to include more details of FAD

The FAD technique is applied towards computing the tangent operator ($\boldsymbol{J} = \partial \boldsymbol{R}/\partial \boldsymbol{X}$) which involves first- and second- derivatives of the local system of residual equations (4.12)- (4.15), with respect to the unknown vector (4.16). The implementation is presented in Sandia National Laboratories' Albany analysis code[6], which utilizes the Sacado package contained in Sandia's Trilinos framework to supply the automatic differentiation capabilities employed. To utilize the FAD technique for computing the local tangent operator, one must template both the system of residual

equations and unknown vectors in terms of a Sacado FAD type data instead of the typical double precision data type. The unknown *state vector* will be the independent variable, while the residual equations will be generic functions dependent on the state vectors. The FAD data type contains not only the value of the data but also the derivative of the data with respect to the independent variables. The derivative information is initialized appropriately and propagated forward through the algorithm. In this way, once the sensitivities are initialized, the Jacobian or tangent operator will be calculated automatically. AD is also employed in the Albany analysis code to form the global system Jacobian, or stiffness matrix, for solving boundary value problems.

6 Verification - benchmark element tests

TODO: add benchmark element test example

7 Ductile failure simulation

7.1 Experimental program and results

TODO: a brief description of the experiment program.

7.2 Numerical simulations

8 Conclusions

References

[1] Qiushi Chen, Jakob T Ostien, Glen Hansen, et al. Automatic differentiation for numerically exact computation of tangent operators in small-and large-deformation computational inelasticity. In *TMS 2014 143rd Annual Meeting & Exhibition, Annual Meeting Supplemental Proceedings*, page 289. John Wiley & Sons, 2014.

[2] CC Chu and A Needleman. Void nucleation effects in biaxially stretched sheets. *Journal of Engineering Materials and Technology(Transactions of the ASME)*, 102(3):249–256, 1980.

[3] Arthur L Gurson. Continuum theory of ductile rupture by void nucleation and growth: Part iâĂŤyield criteria and flow rules for porous ductile media. *Journal of engineering materials and technology*, 99(1):2–15, 1977.

[4] Christian Miehe. Numerical computation of algorithmic (consistent) tangent moduli in large-strain computational inelasticity. *Computer Methods in Applied Mechanics and Engineering*, 134(3):223–240, 1996.

[5] K Nahshon and JW Hutchinson. Modification of the gurson model for shear failure. *European Journal of Mechanics-A/Solids*, 27(1):1–17, 2008.

[6] Andrew G Salinger, Roscoe A Bartett, Quishi Chen, Xujiao Gao, Glen Hansen, Irina Kalashnikova, Alejandro Mota, Richard P Muller, Erik Nielsen, Jakob Ostien, et al. Albany: A component-based partial differential equation code built on trilinos. Technical report, Sandia

National Laboratories Livermore, CA; Sandia National Laboratories (SNL-NM), Albuquerque, NM (United States), 2013.

[7] J Simo and C Miehe. Associative coupled thermoplasticity at finite strains: Formulation, numerical analysis and implementation. *Computer Methods in Applied Mechanics and Engineering*, 98(1):41–104, July 1992. ISSN 00457825. doi: 10.1016/0045-7825(92)90170-O.

[8] J. C. Simo and T. J. R. Hughes. *Computational Inelasticity*. Springer Verlag, 1998.

[9] Juan C Simo and Robert Leroy Taylor. Consistent tangent operators for rate-independent elastoplasticity. *Computer Methods in Applied Mechanics and Engineering*, 48(1):101–118, 1985.

[10] P Steinmann, Ch Miehe, and E Stein. Comparison of different finite deformation inelastic damage models within multiplicative elastoplasticity for ductile materials. *Computational Mechanics*, 13(6):458–474, 1994.