SANDIA REPORT

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Printed June 2015

A Modified Gurson Model: Formulation and Implementation

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A Modified Gurson Model: Formulation and Implementation

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Abstract

In this report a modified Gurson modeled is presented. It can be used to model ductile behavior up to and including material failure. The formulation incorporates the Gurson failure surface, including void nucleation, growth, and coalescence, with a J_2 yield surface with user-defined hardening behavior. Aspects of the formulation and implementation will be discussed.

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Chapter 1

Introduction

The purpose of this work is to present a modified Gurson constitutive model for use in capturing the behavior of ductile materials in the failure regime. The Gurson model has been used extensively in metal plasticity, starting with [4], and the modified Gurson model described here was recently proposed by [7], and extended to include void nucleation in [8]. In this treatment we incorporate a hyperelastic strain energy potential to define the underlying model of elasticity, and investigate a fully implicit Newton algorithm for integration of the evolution equations associated with the state variables used to define the constitutive response.

Chapter 2

Model Formulation

This section should begin with a short description about the origins of the model, including the desire to capture porous solid behavior related to void growth with an inelastic body. Then some comments about the thermodynamic motivation to place it within a hyperelastic framework. It should include sections on the flow rule and each piece of the void volume fraction evolution equation.

2.1 Background

The original Gurson model was developed by [4] based on rigorous micromechanical analysis of a characteristic volume element with spherical or cylindrical-shaped voids surrounded by rigid plastic matrix materials. This model was motivated by experimental observations of dilational plastic deformation during ductile fracture in porous metals, which generates considerable porosity due to the growth and nucleation of voids. Tvergaard and Needleman [14] later improved the original Gurson model by introducing additional parameters into the yield function and by introducing an effective void volume fraction term to account for coalescence of voids that better capture the damage growth rates. This model is known as the 'Gurson-Tvergaard-Needleman' or the GTN model.

One important limitation of the original Gurson or the GTN model is that the void growth (i.e., the damage) depends only on the mean stress. In a shear-dominated state, such as in a projectile penetration problem, the model is unable to predict damage growth if continuous void nucleation is not invoked. This limitation motivates a modification of the original void growth law to include a shear term proposed in [7]. This modification, though phenomenological in nature, has been shown to improve the prediction of the Gurson model in situations where shear stress dominates [7, 8].

The original Gurson model and the recent shear modification were both formulated either with a small deformation assumption or within a hypoelastic framework. The large deformation typically encountered in a ductile failure simulation would render the small deformation formulation inappropriate. As for the hypoelastic formulation, there are well known drawbacks such as the non-zero work done in a closed cycle of elastic deformation, which violates the most important axiom of an elastic response ([1]).

To avoid the above problems, in this section, the shear-modified Gurson model in [7, 8] will be reformulated within a large deformation hyperelastic constitutive framework. Since the elastic response is derived from a hyperelastic potential, the work done in a closed elastic deformation loop vanishes exactly. Furthermore, the hyperelastic formulation eliminates the need for incrementally objective stress update algorithms and can be easily integrated with frame-invariant formulations of anisotropic elasticity and anisotropic plastic yielding ([1]).

2.2 Preliminaries for large deformation hyperelastic formulation

2.2.1 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. [11] 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 $\bar{\boldsymbol{b}}^e$

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

2.2.2 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

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

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

$$\Psi^{\text{vol}}[J^e] = \frac{1}{2}\kappa(\ln J^e)^2 \tag{2.11}$$

$$\Psi^{\text{iso}}[\bar{\boldsymbol{b}}^e] = \mu(\frac{1}{2}\ln \bar{\boldsymbol{b}}^e) : (\frac{1}{2}\ln \bar{\boldsymbol{b}}^e) \tag{2.12}$$

where κ and μ are the bulk and shear modulus, and the elastic logarithmic Hencky strains $\frac{1}{2}\ln \boldsymbol{b}^e$ is used as the strain measure ([13]). The elastic constitutive law and the Kirchhoff stresses are given as

$$\boldsymbol{\tau} = \kappa \ln J^e \boldsymbol{g}^{-1} + \mu \ln \bar{\boldsymbol{b}}^e = \kappa(\ln \boldsymbol{b}^e : \boldsymbol{g})\boldsymbol{g}^{-1} + \mu \operatorname{dev} \ln \boldsymbol{b}^e \tag{2.13}$$

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

$$p = \frac{1}{3}\operatorname{tr}(\boldsymbol{\tau}) = \frac{1}{2}\kappa \operatorname{tr} \ln \boldsymbol{b}^e = \frac{1}{2}\kappa \ln \det \boldsymbol{b}^e \tag{2.14}$$

$$\boldsymbol{s} = \operatorname{dev}(\boldsymbol{\tau}) = \mu \operatorname{dev} \ln \boldsymbol{b}^e \tag{2.15}$$

2.3 Constitutive relations of the 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.

2.3.1 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

$$\Phi = \|\boldsymbol{s}\| - \sqrt{\frac{2}{3}}\operatorname{sign}(\psi)\sqrt{|\psi|}Y \tag{2.16}$$

where ψ contains contributions from the damage in the material and Y is the Kirchhoff yield stress. This yield function (2.16) is a linear form, in terms of $\|\boldsymbol{s}\|$, of the Gurson yield criteria. This particular form is implemented to facilitate comparisons with existing J_2-like models in the Albany analysis code [9], where the yield functions are mostly written as linear functions of $\|\boldsymbol{s}\|$.

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

$$\psi = 1 + f^2 - 2f\cosh(v), \quad v = \frac{3p}{2Y} \tag{2.17}$$

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.

2.3.2 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 [11] for metal is written as

$$Y = Y_0 + Y_\infty \left[1 - \exp(-\delta\varepsilon_q)\right] + K\varepsilon_q \tag{2.18}$$

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

$$\dot{\varepsilon}_q Y(1-f) = \boldsymbol{\tau} : \left(\gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}}\right) \tag{2.19}$$

Substituting yield function Φ into (2.19) to obtain the expression to compute $\dot{\varepsilon}_q$

$$\dot{\varepsilon}_q = \frac{1}{1-f}\left(\gamma\sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{pt}{Y}\right) \tag{2.20}$$

2.3.3 Flow rule

Following the standard procedure of the principle of maximum dissipation, Simo and Miehe [10] proposed a general form of associate flow rule, which is adopted in the current formulation and is given as

$$-\frac{1}{2}L_v(\boldsymbol{b}^e)\cdot\boldsymbol{b}^{-e} = \gamma\frac{\partial\Phi}{\partial\boldsymbol{\tau}} = \gamma\boldsymbol{n} + \frac{1}{3}t\mathbf{1} \tag{2.21}$$

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 (2.16) leads to the following

$$\boldsymbol{n} = \frac{\boldsymbol{s}}{\|\boldsymbol{s}\|} \tag{2.22}$$

$$t = \operatorname{tr}\left(\gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) = \sqrt{\frac{3}{2}} \gamma f \sinh(\frac{3p}{2Y}) \frac{1}{\sqrt{|\psi|}} \operatorname{sign}(\psi) \tag{2.23}$$

2.3.4 Evolution of void volume fraction

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, $\dot{f}_n$.

$$\dot{f} = \dot{f}_g + \dot{f}_n \tag{2.24}$$

In the original Gurson model [4], the void growth part $\dot{f}_g$ was related to the plastic volume change as

$$\dot{f}_g = (1 - f) \operatorname{tr}\left(\gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) \tag{2.25}$$

To account for the void growth under shear-dominated stress state, the void growth law (2.25) was extended in [7] by adding a term that depends on the third stress invariant. This shear-modified void growth equation is written as

$$\dot{f}_g = (1 - f) \operatorname{tr}\left(\gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) + k_\omega f \frac{\omega(\boldsymbol{\tau})}{\tau_e} \boldsymbol{s} : \left(\gamma \frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) \tag{2.26}$$

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 [7]. The function $\omega(\boldsymbol{\tau})$ includes the effect of the third stress invariant on void growth and is given as

$$\omega(\boldsymbol{\tau}) = 1 - \left(\frac{27 J_3}{2\tau_e^3}\right)^2 \tag{2.27}$$

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

Substituting the yield function (2.16) and the expression for $\omega(\boldsymbol{\tau})$ (2.27) into the void growth law (2.26) yields

$$\dot{f}_g = (1-f)t + \sqrt{\frac{2}{3}}\gamma k_\omega f \omega(\boldsymbol{\tau}) \tag{2.28}$$

The effective increase in damage due to plastic strain controlled nucleation is given by [3] as

$$\dot{f}_{nu} = A\dot{\varepsilon}_q \tag{2.29}$$

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

$$A = \begin{cases} \frac{f_N}{s_N\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\varepsilon_q - \epsilon_N}{s_N}\right)^2\right], & p \geq 0 \\ 0, & p < 0 \end{cases} \tag{2.30}$$

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.

Chapter 3

Implementation

This section should discuss implementation aspects of the large deformation hyperelastic model and the implicit integration scheme. I based the Sierra implementation off of the Albany version, so that would be a good place to start. In both places we are using Sacado to compute derivative for the local consistent tangent, so we should talk about what that buys us.

Details of the numerical implementation of the large deformation hyperelastic Gurson model are discussed in this section. A fully implicit integration scheme ([11, 13]) is implemented to integrate the flow rule, the evolution equation for the internal variable (e.g., ε_q), and the evolution equation for the void volume fraction f over a finite time step $\Delta t = t_{n+1} - t_n$. The integration scheme consists of an elastic trial state followed by a plastic correction. Stresses and the internal variables are updated at time t_{n+1} given their known values at time t_n and the deformation gradient $\boldsymbol{F}_{n+1}$.

The implicit integration scheme results a set of nonlinear discrete equations for integrating the stress and internal variables, which requires an iterative solution method such as the Newton's method. In the Newton's method, precise derivatives are necessary to assemble the local Jacobian matrix that is essential to achieve an optimal asymptotic convergence rate. In this work, a technique called the forward automatic differentiation (FAD) will be used to compute necessary derivatives. The implementation will leverage the existing FAD capability of the Sacado package in Sandia National Laboratories' Trilinos framework [5].

3.1 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 (2.21) such that

$$-\frac{1}{2}\dot{\boldsymbol{C}}^{-p} \cdot \boldsymbol{C}^{p} = \gamma \boldsymbol{F}^{-1} \cdot \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \cdot \boldsymbol{F} \tag{3.1}$$

where γ is the plastic multiplier. Then, the application of the exponential mapping to (3.1) yields an incremental objective integration algorithm

$$\boldsymbol{C}^{-p}_{n+1} = \boldsymbol{F}^{-1}_{n+1} \cdot \exp\left(-2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{F}_{n+1} \cdot \boldsymbol{C}^{-p}_{n} \tag{3.2}$$

Applying the push-forward operation to (3.2) yields an update algorithm for the elastic left Cauchy-Green tensor $\boldsymbol{b}^e_{n+1}$ as

$$\boldsymbol{b}^e_{n+1} = \exp\left(-2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{b}^{e\,\mathrm{tr}} \tag{3.3}$$

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

$$\boldsymbol{b}^{e\,\mathrm{tr}} = \boldsymbol{F}_{n+1} \cdot \boldsymbol{C}^{-p}_{n} \cdot \boldsymbol{F}^{T}_{n+1} \tag{3.4}$$

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

$$\ln \boldsymbol{b}^e_{n+1} = \ln \boldsymbol{b}^{e\,\mathrm{tr}} - 2\Delta\gamma \frac{\partial \Phi_{n+1}}{\partial \boldsymbol{\tau}} \tag{3.5}$$

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

$$p_{n+1} = p^{\mathrm{tr}} - \kappa t \tag{3.6}$$

$$\boldsymbol{s}_{n+1} = \boldsymbol{s}^{\mathrm{tr}} - 2\mu\Delta\gamma\boldsymbol{n} \tag{3.7}$$

where $\boldsymbol{n}$ and t are given by (2.22), (2.23) and are evaluated at time t_{n+1}, and p^{tr} and $\boldsymbol{s}^{\mathrm{tr}}$ are the trial states given by

$$p^{\mathrm{tr}} = \kappa \ln J^{e\,\mathrm{tr}}, \quad J^{e\,\mathrm{tr}} = \det(\boldsymbol{b}^{e\,\mathrm{tr}})^{1/2} \tag{3.8}$$

$$\boldsymbol{s}^{\mathrm{tr}} = \mu \,\mathrm{dev} \ln \boldsymbol{b}^{e\,\mathrm{tr}} \tag{3.9}$$

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 (2.24) and (2.20). The resulting discrete equations are

$$f_{n+1} = f_n + (1 - f_{n+1})t + \sqrt{\frac{2}{3}}\Delta\gamma k_\omega f_{n+1}\omega(\boldsymbol{\tau}) + A_{n+1}(\varepsilon_{q(n+1)} - \varepsilon_{q(n)}) \tag{3.10}$$

$$\varepsilon_{q(n+1)} = \varepsilon_{q(n)} + \frac{1}{1 - f_{n+1}}\left(\Delta\gamma\sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{p_{n+1}t}{Y}\right) \tag{3.11}$$

3.2 Local nonlinear system of equations

The discrete form of the rate equations (3.3), (3.6), (3.7), (3.10) and (3.11) 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

$$R_1(\boldsymbol{X}) = \|\boldsymbol{s}^{\mathrm{tr}}\| - 2\mu\Delta\gamma - \sqrt{\frac{2}{3}}\mathrm{sign}(\psi)\sqrt{|\psi|}Y \tag{3.12}$$

$$R_2(\boldsymbol{X}) = p - p^{\mathrm{tr}} + \kappa t \tag{3.13}$$

$$R_3(\boldsymbol{X}) = f - f_n - (1-f)t - \sqrt{\frac{2}{3}}\Delta\gamma k_\omega f\omega(\boldsymbol{\tau}) - A(\varepsilon_q - \varepsilon_{q(n)}) \tag{3.14}$$

$$R_4(\boldsymbol{X}) = \varepsilon_q - \varepsilon_{q(n)} - \frac{1}{1-f}\left(\Delta\gamma\sqrt{\frac{2|\psi|}{3}}\mathrm{sign}(\psi) + \frac{pt}{Y}\right) \tag{3.15}$$

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

$$\boldsymbol{X} = \{p, f, \varepsilon_q, \Delta\gamma\} \tag{3.16}$$

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 $\boldsymbol{b}_e^{\mathrm{tr}}$ (3.4)
STEP 2. Compute trial stresses $p^{\mathrm{tr}}, \boldsymbol{s}^{\mathrm{tr}}$ (3.8), (3.9)
STEP 3. Check yielding (2.16): $\Phi^{\mathrm{tr}}(p^{\mathrm{tr}}, \boldsymbol{s}^{\mathrm{tr}}, \varepsilon_{q(n)}, f_n) > 0$?
No, set $p = p^{\mathrm{tr}}, \boldsymbol{s} = \boldsymbol{s}^{\mathrm{tr}}, \boldsymbol{b}^e = \boldsymbol{b}^{e\,\mathrm{tr}}, \varepsilon_q = \varepsilon_{q(n)}, f = f_n$ and exit
STEP 4. Yes, local Newton loop
4.1 Initialize $\boldsymbol{X}^k$ (3.16) and the iteration count $k = 0$
4.2 Assemble the residual equations $\boldsymbol{R}(\boldsymbol{X}^k)$ (3.12) - (3.15)
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 $\boldsymbol{X}^{k+1} = \boldsymbol{X}^k - \delta \boldsymbol{X}$, $k \rightarrow k+1$ 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 (3.1) and (3.4) to compute trial state, is updated using

$$\boldsymbol{F}^p = \exp\left(\frac{\partial \Phi}{\partial \boldsymbol{\tau}}\right) \cdot \boldsymbol{F}_n^p \tag{3.17}$$

In the Newton's iterative solution method, it requires consistent linearization of the system of equation (3.12) - (3.15), 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 [6, 12]. 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 [2] for applications of FAD to constitutive modeling in small- and large-deformation computational inelasticity.

3.3 FAD: a numerical exact way of computing consistent tangent

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 (3.12)- (3.15), with respect to the unknown vector (3.16). The implementation is presented in Sandia National Laboratories' Albany analysis code[9], 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.

Chapter 4

Numerical Examples

This section could be renamed to Numerical Examples, and should include any and all verification/validation work. To be clear, for the purpose of the SAND report, we don't require any validation. I will have to include a description of the Sierra input parameters for use in their user's manual, but obviously I'll worry about that.

To demonstrate the model, the plasticity parameters were fit to data obtained from the tensile testing of an A286 alloy. Subsequently, some of the parameters governing the failure behavior of the model were varied to study their effects. The data collection and parameter fitting details are outside of the scope of this report, and the results of this process can be seen in Figure 4.1 and Table 4.1, where the ranges of the relevant parameters are listed as appropriate for the study. Note that in Figure 4.1, as for other multi-linear hardening models in Sierra, the `YIELD_STRESS` parameter aligns with the first non-zero true strain point in the curve.

4.1 Uniaxial Tension

In this section we investigate the behavior of the model in a state of uniaxial tension. In particular, we will observe the stress and void volume fraction response for a variety of failure parameter combinations to develop an understanding of the behavior of the model. Figure 4.2 shows the model behavior for various values of the shear parameter k_ω, and evidently it has little to no effect on the response for this stress state.

In Figure 4.3 a set of nucleation parameters are specified and also evaluated in the uniaxial tension scenario. In this case the volume fraction of nucleated voids f_N, is varied, while the mean value and standard deviation of failure strain, ϵ_N and s_N respectively, are specified and held constant. Observe that the von Mises stress component is somewhat reduced, to a greater extent as the volume fraction of nucleated voids is increased. Also observe that the void volume fraction grows by approximately the specified volume fraction of nucleated voids, accelerated the apparent void growth until the total void volume fraction of nucleated void has been exhausted. Afterwards, the trajectory returns to that of the void growth

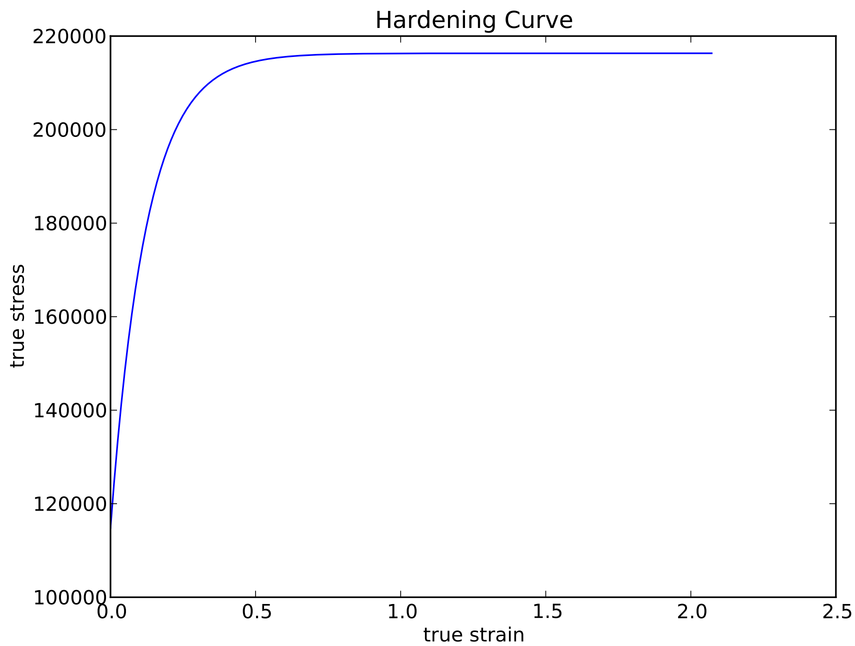
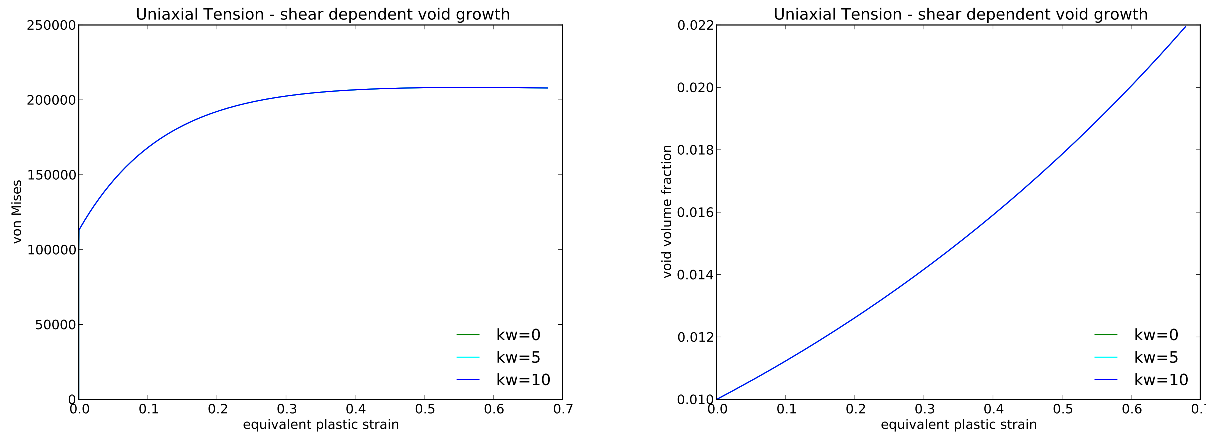


Figure 4.1. True stress versus true strain, obtained from a fitting the tensile behavior of an A286 steel alloy.

Parameters	
YOUNGS_MODULUS	29.0e6 *psi*
POISSONS_RATIO	0.3
YIELD_STRESS	1.14794e5 *psi*
Q1	1.5
Q2	1.0
Q3	2.25
KW	{0,5,10}
INITIAL_VOID	{0.0001,0.001,0.01}
EN	{0.0,0.1,0.2}
SN	0.1
FN	{0.0,0.1,0.2}
CRITICAL_VOID	0.5
FAILURE_VOID	0.6667
HARDENING_FUNCTION	see Figure 4.1

Table 4.1. Input parameters for the Gurson model in Sierra and the ranges over which parameters were varied in the present study.



(a) stress

(b) void volume fraction

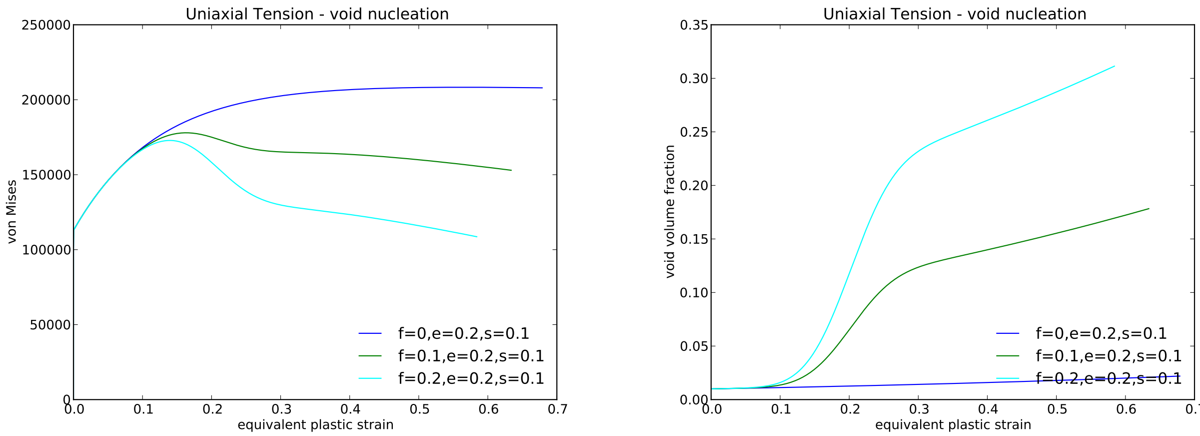
Figure 4.2. Von Mises stress component and void volume fraction plotted against equivalent plastic strain. The shear void growth parameter has an insignificant effect on the response of the material point in tension.

without augmentation.

4.2 Simple Shear

In this section we investigate the behavior of the two components of the failure model, specifically the shear dependent void growth and the void nucleation terms, in the context of simple shear. To test this problem we use the plasticity parameters developed in the previous section and study the response of the model to with various failure parameters. In Figure 4.4 we vary the shear parameter, k_ω, which governs the rate of void growth in shear dominated states of stress as per (2.26). Observe that in the extreme case for simple shear k_ω can accelerate void growth to the point of complete material failure corresponding to the shear stress component reaching a value of zero.

In Figure 4.5 a set of nucleation parameters are specified and also evaluated in the simple shear scenario. In this case the volume fraction of nucleated voids f_N, is varied, while the mean value and standard deviation of failure strain, ϵ_N and s_N respectively, are specified and held constant. Observe that the shear stress component is somewhat reduced, to a greater extent as the volume fraction of nucleated voids is increased. Also observe that the void

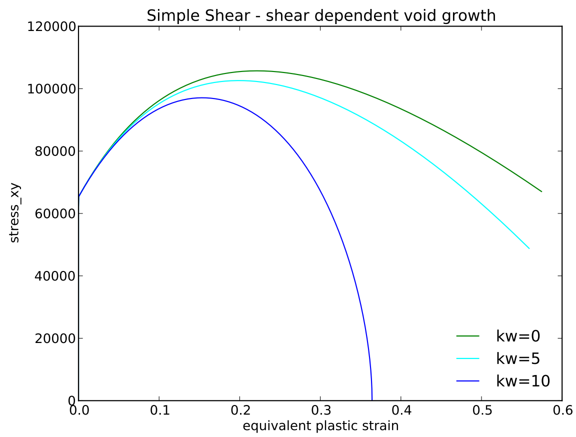


(a) stress

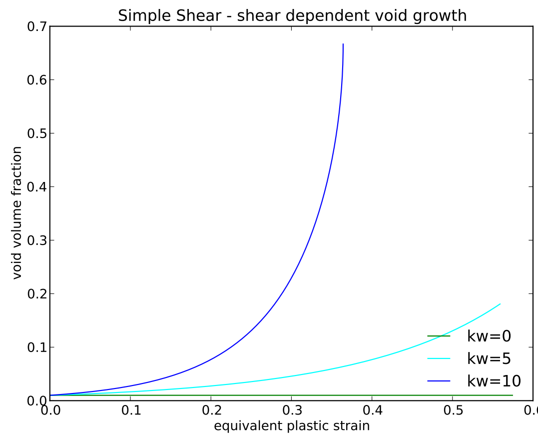
(b) void volume fraction

Figure 4.3. Von Mises component and void volume fraction plotted against equivalent plastic strain. The void nucleation parameters have some effect on the response of the material point in uniaxial tension.

volume fraction grows by approximately the specified volume fraction of nucleated voids, in particular, where f_N is zero, the void volume fraction does not deviate from zero.

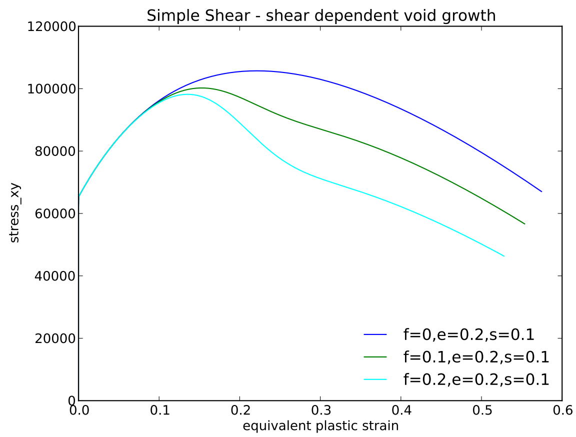


(a) stress

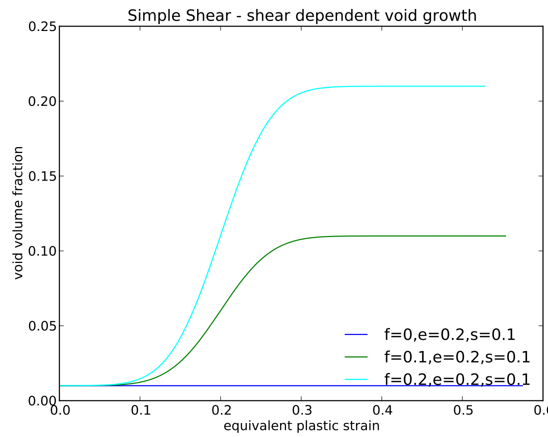


(b) void volume fraction

Figure 4.4. Shear stress component and void volume fraction plotted against equivalent plastic strain. The shear void growth parameter has a pronounced effect on the response of the material point in simple shear.



(a) stress



(b) void volume fraction

Figure 4.5. Shear stress component and void volume fraction plotted against equivalent plastic strain. The void nucleation parameters have some effect on the response of the material point in simple shear.

Chapter 5

Conclusions

This should be a summary and short discussion about the strengths and weaknesses of the model. Nothing too fancy, just practice for the journal article.

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