Coupling the Hydrostatic/Deviatoric Material Responses in Shock-Hydro Code Simulations

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Abstract

The state of the art in failure modeling enables assessment of crack nucleation, propagation, and progression to fragmentation due to high velocity impact. Vulnerability assessments suggest a need to track material behavior through failure, to the point of fragmentation and beyond. This field of research is particularly challenging for structures made of porous quasi-brittle materials, such as ceramics used in modern armor systems, due to the complex material response when loading exceeds the quasi-brittle material's elastic limit. Further complications arise when incorporating the quasi-brittle material response in multi-material Eulerian hydrocode simulations.

We describe recent efforts in coupling a ceramic materials response in the post-failure regime with an Eulerian hydro code. Material behavior is modeled by the Kayenta material model [1] and Alegra as the host finite element code [3]. Kayenta, a three invariant phenomenological inelasticity model originally developed for modeling the stress response of geologic materials, has in recent years been used with some success in the modeling of ceramic and other quasi-brittle materials to high velocity impact. Due to the granular nature of ceramic materials, Kayenta allows for significant pressures to develop due to dilatant inelastic flow, even in shear dominated loading where traditional equations of state predict little or no pressure response. When a material's ability to carry further load is compromised, Kayenta allows the material's strength and stiffness to progressively degrade through the evolution of damage to the point of material failure. As material dilatation and damage progress, accommodations are made within Alegra to treat in a consistent manner the evolving state.

I Introduction

When simulating events involving extremes in pressure as a consequence of blast, penetration, and shock loadings, among others, it is necessary to describe the hydrostatic material response by an equation of state. When material strength cannot be neglected, an additional constitutive model must be incorporated to describe the material's deviatoric response as part of the stress update algorithm. For elastic-perfectly-inelastic materials, the deviatoric response is separable from the hydrostatic response and its incorporation with an arbitrary equation of state in a total stress update is straightforward. However, for materials in which the hydrostatic and deviatoric responses are not separable, combining an equation of state and strengh models becomes problematic. The hydrostatic response is not solely a function of the pressure computed by the equation of state. Neglecting the hydrostatic/deviatoric coupling leads to inconsistent material states and can, ultimately, lead to unstable finite element simulations.

In this paper, we described recent efforts coupling the hydrostatic equation of state response with the deviatoric material response in Alegra finite element code. The hydrostatic response considered is given by a Mie-Grüneisen equation of state and the strength response by the Kayenta material model. However, the concepts are general enough for adoption by other shock hydro-codes. An outline of the manuscript is as follows: 1) review of the basic equations of inelasticity and an overview of the Kayenta material model, 2) numerical techniques for coupling the dilatant material response with a high pressure equation of state, and 3) control of excessive tensile states.

II Stress/Strain Relationship for Inelastic Materials

If a material is capable of elastic behavior, a necessary condition of thermodynamic admissibility is that the stress $\underset{\approx}{\boldsymbol{\sigma}}$ be derivable from a strain energy potential

$$\underset{\approx}{\boldsymbol{\sigma}} = \frac{\partial u}{\partial \underset{\approx}{\boldsymbol{\varepsilon}}^{\mathrm{e}}}, \tag{1}$$

where u is the internal energy per unit reference volume and $\underset{\approx}{\boldsymbol{\varepsilon}}^{\mathrm{e}}$[1] is the elastic strain work conjugate to $\underset{\approx}{\boldsymbol{\sigma}}$. The rate of stress is given by the time rate of change of the expression in Equation (1)

$$\dot{\underset{\approx}{\boldsymbol{\sigma}}} = \underset{\approxeq}{\mathbb{C}} : \dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{e}}, \tag{2}$$

where the superposed dot indicates a derivative with respect to time and $\underset{\approxeq}{\mathbb{C}}$ is the elastic stiffness given by

$$\underset{\approxeq}{\mathbb{C}} = \frac{\partial^2 u}{\partial \underset{\approx}{\boldsymbol{\varepsilon}}^{\mathrm{e}} \partial \underset{\approx}{\boldsymbol{\varepsilon}}^{\mathrm{e}}}. \tag{3}$$

For isotropic materials, the internal energy is a function of the elastic strain through its invariants. In this case, Equation (2) reduces to

$$\boxed{\dot{\underset{\approx}{\boldsymbol{\sigma}}} = \kappa \dot{\varepsilon}^{\mathrm{e}}_{v} \underset{\approx}{\boldsymbol{\delta}} + 2\mu \dot{\underset{\approx}{\boldsymbol{\gamma}}}^{\mathrm{e}}, \qquad \text{isotropic material response}} \tag{4}$$

where $\varepsilon^{\mathrm{e}}_{v}$ and $\underset{\approx}{\boldsymbol{\gamma}}^{\mathrm{e}}$ are the volumetric and deviatoric elastic strains, κ and μ are the elastic bulk and shear moduli, and $\underset{\approx}{\boldsymbol{\delta}}$ is the second order identity tensor. In the following, we adopt Equation (4), considering only the isotropic material response.

II.A Inelastic Flow

If the rate of strain $\dot{\underset{\approx}{\boldsymbol{\varepsilon}}}$ is presumed to be the sum of the elastic and inelastic components[2], $\dot{\underset{\approx}{\boldsymbol{\varepsilon}}} = \dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{e}} + \dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{i}}$, the stress/strain relationship in Equation (4) can instead be expressed

$$\dot{\underset{\approx}{\boldsymbol{\sigma}}} = \kappa \left(\dot{\varepsilon}_{\mathrm{v}} - \dot{\varepsilon}^{\mathrm{i}}_{\mathrm{v}}\right) \underset{\approx}{\boldsymbol{\delta}} + 2\mu \left(\dot{\underset{\approx}{\boldsymbol{\gamma}}} - \dot{\underset{\approx}{\boldsymbol{\gamma}}}^{\mathrm{i}}\right), \tag{5}$$

[1] Tensor notations, terminology, and nomenclature are outlined in Appendix A

[2] Here, and throughout this manuscript, we use the term "inelastic" to refer to any inelastic deformation.

where $\dot{\varepsilon}_{\rm v}$, $\dot{\varepsilon}^{\rm i}_{\rm v}$, $\dot{\boldsymbol{\gamma}}$, $\dot{\boldsymbol{\gamma}}^{\rm i}$ are the volumetric and deviatoric parts of the total and inelastic strain rates, respectively.

In classical inelasticity, the boundary between elastically obtainable stress states and stress states unobtainable through inviscid processes is termed the *yield surface*. Mathematically, the yield surface is expressed in terms of a stress dependent *yield function* $f(\boldsymbol{\sigma})$. The *yield criterion* is the statement that $f(\boldsymbol{\sigma}) \le 0 \; \forall \; \boldsymbol{\sigma}$. We say that a material has yielded if for a *trial elastic stress* $\boldsymbol{\sigma}^{\rm trial}$, the yield criterion is violated, or $f(\boldsymbol{\sigma}^{\rm trial}) > 0$. In this case, the material is said to "flow" inelastically. The goal of the inelasticity problem then becomes finding the portion of the strain rate attributible to inelastic deformation such that the yield criterion is satisfied and the solution advanced.

Representing the rate of inelastic strain as the product of its magnitude $\dot{\lambda}$ and (unit) direction $\boldsymbol{m}$, the rate of stress in Equation (5) becomes

$$\dot{\boldsymbol{\sigma}} = \left(\kappa\dot{\varepsilon}_{\rm v} - \frac{1}{3}\dot{\lambda}\,{\rm tr}\,\boldsymbol{p}\right)\boldsymbol{\delta} + 2\mu\dot{\boldsymbol{\gamma}} - \dot{\lambda}\boldsymbol{p}', \qquad \text{general stress/strain relationship} \tag{6}$$

where $\boldsymbol{p} = \mathbb{C}\!:\!\boldsymbol{m}$ is the inelastic return direction and $\boldsymbol{p}' = \dot{\lambda}\left(\boldsymbol{p} - 1/3\,{\rm tr}\,\boldsymbol{p}\boldsymbol{\delta}\right)$ is its deviatoric part. In the literature, one encounters several definitions of the inelastic flow direction $\boldsymbol{m}$. However, only the associated direction of inelastic flow, given by

$$\boldsymbol{m} = \frac{\partial f(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} \bigg/ \left\|\frac{\partial f(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}\right\| \qquad \text{associative flow rule} \tag{7}$$

is known to *not* violate thermodynamics. In this paper, we will adopt the associative flow rule.

II.A.1 Isochoric Inelastic Flow

Isochoric inelastic flow occurs in materials that exhibit inelastic incompressibility during inelastic loading. In these materials, the strength is independent of the confining pressure and the inelastic flow and return direction are purely deviatoric, as shown in Figure 1. In this case ${\rm tr}\,\boldsymbol{p} = 0$ and the stress/strain relationship in Equation (6) reduces to

$$\dot{\boldsymbol{\sigma}} = \kappa\dot{\varepsilon}_{\rm v}\boldsymbol{\delta} + 2\mu\left(\dot{\boldsymbol{\gamma}} - \dot{\lambda}\boldsymbol{m}'\right). \qquad \text{isochoric inelastic flow} \tag{8}$$

where the $'$ indicates the deviatoric part of the argument. In other words, the deviatoric response is fully decoupled from the hydrostatic response. The Von Mises yield criterion is an example of a yield criterion that emits isochoric inelastic flow and is appropriate for materials such as most metals in which the assumption of inelastic incompressibility is acceptable.

II.B Dilatant Inelastic Flow

Dilatant inelastic flow occurs in materials that exhibit inelastic compressibility during inelastic loading. In these materials, the strength is dependent on the confining pressure and the inelastic flow has a hydrostatic component, in addition to the deviatoric component described above and as shown in Figure (2). In this case, the stress/strain relationship in Equation (6) cannot be decoupled in to independent hydrostatic and deviatoric components.

The linear/nonlinear Drucker-Prager yield criterion are examples of yield criteria that emit dilatant inelastic flow and are appropriate for materials in which strength increases with confining pressure, such as geologic and engineered geologic-type materials. For materials that also exhibit an upper limit in the amount of supportable hydrostatic pressure, the yield function is enhanced with the addition of a "cap" on the upper limit of hydrostatic pressure.

III The Kayenta Material Model

Kayenta, an outgrowth of the Sandia GeoModel [1], is a general three invariant phenomenological inelasticity model developed for use with geological and rock-like engineering materials. The Kayenta yield surface,

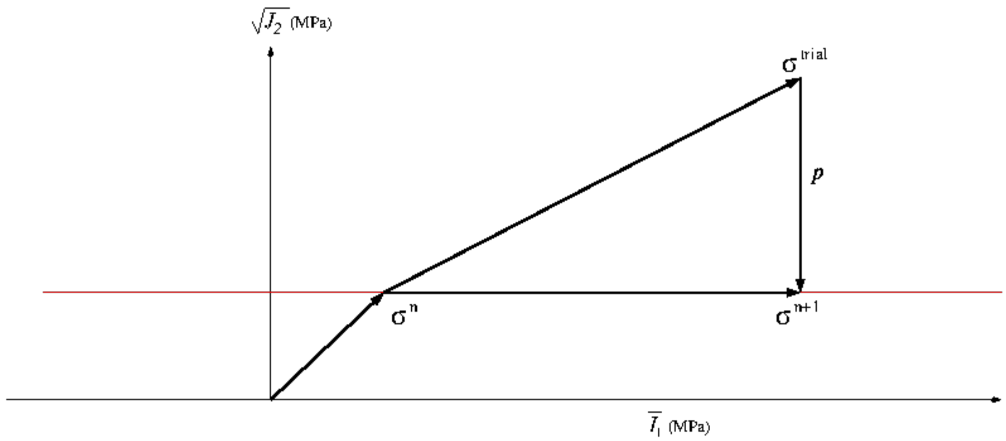


Figure 1: Deviatoric return direction results in isochoric inelastic flow for the Von Mises yield criterion. The x-axes variable $\bar{I}_1$ is the *negative* of the first invariant of the stress tensor ($I_1 = \operatorname{tr} \underset{\approx}{\boldsymbol{\sigma}}$) and the y-axes variable $\sqrt{J_2}$ is the square root of the second "mechanics" invariant of stress ($J_2 = \underset{\approx}{\boldsymbol{\sigma}}' \colon \underset{\approx}{\boldsymbol{\sigma}}'$)

shown in Figure 3, is described by the following yield function

$$f\left(\underset{\approx}{\boldsymbol{\sigma}}\right) = \Gamma^2\left(\theta\right) J_2 - f_f^2\left(I_1\right) f_c^2\left(I_1, \varkappa\right) J_2 \tag{9}$$

where I_1, J_2, and θ are the first and second invariants and Lode angle of $\underset{\approx}{\boldsymbol{\sigma}}$, respectively. Γ, f_f, and f_c are functions representing the dependence of the yield function on θ, the shear response, and the cap response, respectively. $\varkappa$ is an internal state variable representing the evolution of the cap surface.

Depending on the choice of model parameters, Kayenta is capable of producing, among others, any of the following features

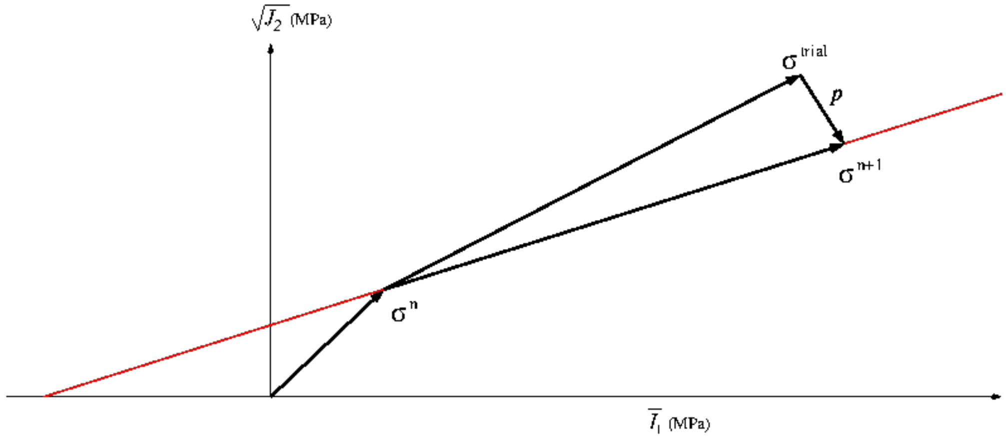
- Linear and nonlinear thermoelasticity.
- Von Mises and Tresca thermoplasticity.
- Linear and nonlinear, associative and nonassociative Drucker-Prager, Mohr-Coulomb, and Willam-Warnke plasticity.
- Rate-independent or strain-rate sensitive yield.
- Damage through the loss of stiffness and strength.
- Evolution of porosity.
- Pressure- and shear-dependent compaction (similar to p-α models during hydrostatic loading, but generalized to include shear effects in general loading).

Kayenta has been used in applications ranging from quasistatic loading of sandstone caprock during CO_2 sequestration, ductile fracture of metals, to brittle fracture of ceramic armor systems.

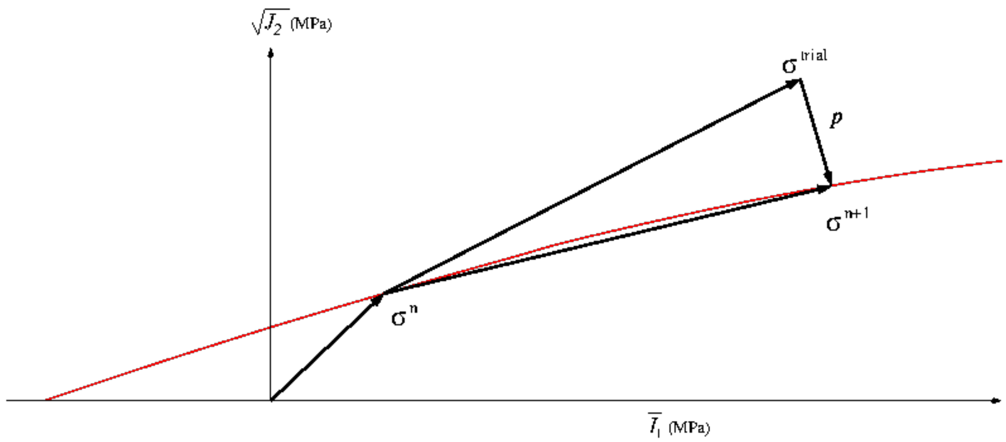
IV Coupling Equations of State with Inelastic Flow

As explained in Section II.A.1, if a material exhibits incompressible inelastic flow, the stress/strain relationship of Equation (6) is separable in to hydrostatic and deviatoric components. In this case, incorporating an equation of state response with the deviatoric response involves replacing the hydrostatic component $\kappa \dot{\varepsilon}_{\mathrm{v}} \underset{\approx}{\boldsymbol{\delta}}$ of Equation (10) with the pressure response p^{eos} from an arbitrary equation of state:

$$\dot{\underset{\approx}{\boldsymbol{\sigma}}} = -\dot{p}^{\mathrm{eos}} \underset{\approx}{\boldsymbol{\delta}} + 2\mu \left(\dot{\underset{\approx}{\boldsymbol{\gamma}}} - \dot{\lambda} \underset{\approx}{\boldsymbol{m}}' \right). \tag{10}$$



(a) Meridional view of the linear Drucker-Prager yield surface



(b) Meridional view of the nonlinear Drucker-Prager yield surface

Figure 2: Dilatant inelastic flow occurs in materials in which the shear strength increases with confining pressure. The simplest constitutive models to capture this type of behavior are the linear and nonlinear Drucker-Prager models shown.

For inelastically compressible materials, dilatant inelastic flow prohibits the decoupling of the hydrostatic and deviatoric responses, as in Equation (10). Instead, the material response is computed from the more general expression of Equation (6)

$$\dot{\underset{\approx}{\boldsymbol{\sigma}}} = -\dot{p}\underset{\approx}{\boldsymbol{\delta}} + 2\mu\left(\dot{\underset{\approx}{\boldsymbol{\gamma}}} - \dot{\lambda}\underset{\approx}{\boldsymbol{m}}'\right). \tag{11}$$

where we have substituted $\dot{p} = \kappa\dot{\varepsilon}_{\text{v}} - 1/3\dot{\lambda}\,\text{tr}\,\underset{\approx}{\boldsymbol{p}}$. Comparing Equations (10) and (11), if the hydrostatic/deviatoric coupling is neglected, discrepancies are seen to arise as p^{eos} deviates from p. Such an inconsistency leads to further inconsistencies in other material variables computed from the equation of state including the sound-speed, density, and ultimately, the stable timestep. We have found in Alegra that these iconsistencies ultimately manifest themselves in simulations that end prematurely due to unresolvably bad material states.

The approach adopted in Alegra to resolve the above consistencies is an iterative approach similar to the Alegra multi-material treatment [2], whereby the bulk modulus is given by

$$\kappa = \rho^{\star}{c_s}^2(u, \rho^{\star}), \tag{12}$$

where c_s is the energy and density dependent sound speed returned by the equation of state, and $\rho^{\star}$ is the "solid density" of the material. Using κ, the pressure is updated by

$$\dot{p} = \kappa\dot{\varepsilon}_{\text{v}} - \frac{1}{3}\dot{\lambda}\,\text{tr}\,\underset{\approx}{\boldsymbol{p}}, \tag{13}$$

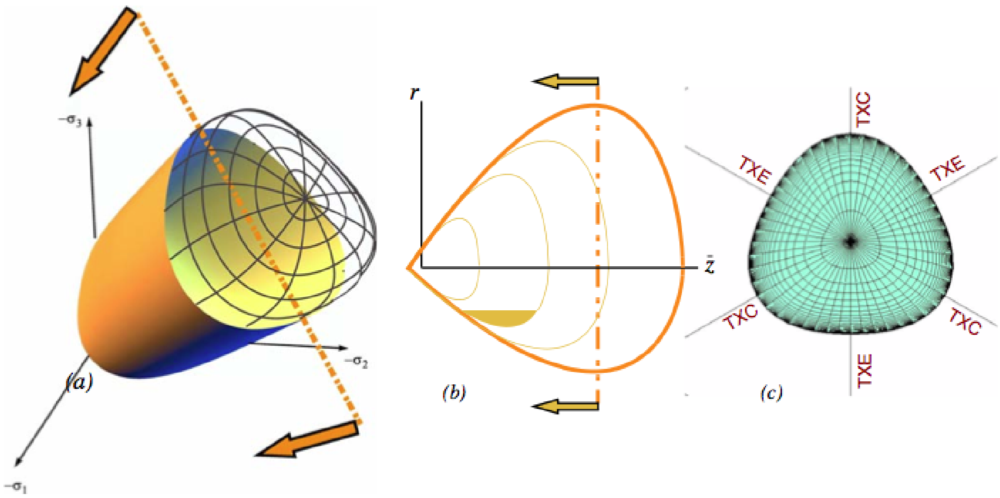


Figure 3: Kayenta continuous yield surface. (a) three-dimensional view in principal stress space with the high pressure cap shown as a wire frame, (b) the meridional side view with the cap shown on the more compressive right-hand side of the plot using cylindrical coordinates in which z points along the compressive [111] direction, and (c) the octahedral view, which corresponds to looking down the hydrostat (onto planes perpendicular to the [111] direction); an option is available for a pressure-varying octahedral profile.

and the solid density updated iteratively by

$$\rho_n^\star = \rho_{n-1}^\star + \frac{p - p_{n-1}^{\text{eos}}}{dp/d\rho^\star}. \tag{14}$$

Convergence is achieved when $p = p^{\text{eos}}$. In this way, the discrepancy between the mean response of the constitutive model and the pressure response of the equation of state is eliminated. The solid density $\rho^\star$ is interpreted as the density of the intact material absent the presence of void.

As an example of an inconsistency that can develop between the constitutive model and host finite element code, consider a case of pure shear of a single element of Kayenta material. During pure shear, the deformation is isochoric and pressure changes computed by the equation of state are small in comparison to changes in the mean stress computed from the constitutive model.

V Tensile Control in Shock-Hydrocode Simulations

Control of excessive tension for non-gaseous materials becomes necessary when the deformation of the material indicates expansion to an unphysical density. Generally, equation of state models will break down under such conditions unless specific action is taken to detect and mitigate the excessive tension. The physical observation for material under these conditions is fracture for solids and cavitation for liquids.

In the Alegra code, the method for controlling excessive tension involves limiting the pressure of the material to a relaxed value less tensile than would be indicated by the expansion of the element. This results in an increased density and, consequently, a decrease in material volume fraction to satisfy mass conservation. The difference in volume is taken up by an increase in the void volume fraction.

The density associated with the relaxed pressure is obtained using an iterative with pressure computed from the equation of state as a function of density and internal energy, $p^{\text{eos}} = p^{\text{eos}}(u, \rho)$.

Density iterations are estimated from $dp^{\text{eos}}/d\rho$ and evaluated until the pressure computed by the equation of state converges to the relaxed pressure. While other codes may use other approaches to controlling excessive expansion, this "Void Insertion" approach is used by Alegra. However, this void insertion method implicitly assumes that the pressure is only a function of the equation of state and is equivalent to the mean stress of the material. With the Kayenta material model, this assumption cannot be guaranteed, particularly for dilatant behavior. Thus, the standard tensile control in Alegra cannot be utilized with the Kayenta material model, or any other material in which dilatant inelastic flow is allowed. Instead, the following approach has been implemented to allow consistent response between the equation of state model and the tensile response computed in the Kayenta material model.

Returning to the assumption of the additive decomposition of the total strain in to elastic and inelastic parts, we further subdivide the inelastic strain rate in to parts due to plasticity and void expansion such that the elastic strain rate is now given by

$$\dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{e}} = \dot{\underset{\approx}{\boldsymbol{\varepsilon}}} - \dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{v}} - \dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{p}} \tag{15}$$

where $\dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{p}}$ is the strain rate due to plasticity and $\dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{v}}$ that due to void expansion. We assume that void expansion is a purely hydrostatic process so that its rate is given by

$$\dot{\underset{\approx}{\boldsymbol{\varepsilon}}}^{\mathrm{v}} = \dot{\zeta}\hat{\underset{\approx}{\boldsymbol{\delta}}} \tag{16}$$

where $\hat{\underset{\approx}{\boldsymbol{\delta}}}$ is the normalized second order identity tensor and $\dot{\zeta}$ the magnitude of the rate of void strain.

The onset of excessive tensile deformation is marked by $p > p^{\mathrm{spall}}$ where p^{spall} is the value of pressure at which spall is observed to occur. Analogous to computing $\dot{\lambda}$ such that the yield criterion is satisfied, $\dot{\zeta}$ is computed such that the spall criterion $p \leq p^{\mathrm{spall}}$:

$$p_{n+1} = p_n + \dot{p}_n\Delta t = p_n + 3\kappa\,\mathrm{tr}\left(\dot{\underset{\approx}{\boldsymbol{\varepsilon}}} - \dot{\zeta}\hat{\underset{\approx}{\boldsymbol{\delta}}} - \dot{\lambda}\underset{\approx}{\boldsymbol{m}}\right)\Delta t \geq p^{\mathrm{spall}},$$

thus, we compute $\dot{\zeta}$ by

$$\dot{\zeta} = \begin{cases} 0 & \text{if } p_{n+1} \geq p^{\mathrm{spall}} \\ \frac{1}{\sqrt{3}}\left(\dot{\varepsilon}_{\mathrm{v}} - \dot{\lambda}\,\mathrm{tr}\,\underset{\approx}{\boldsymbol{m}} - \frac{p^{\mathrm{spall}} - p_n}{3\kappa\Delta t}\right) & \text{if } p_{n+1} < p^{\mathrm{spall}} \end{cases} \tag{17}$$

Kayenta then returns both the updated stress $\underset{\approx}{\boldsymbol{\sigma}}$ *and* the magnitude of the void strain increment $\dot{\zeta}$ to Alegra and the material volume fraction adjusted such that mass is conserved.

Figure 4 depicts graphically the return of the trial stress to the yield surface and then to spall-cut plane.

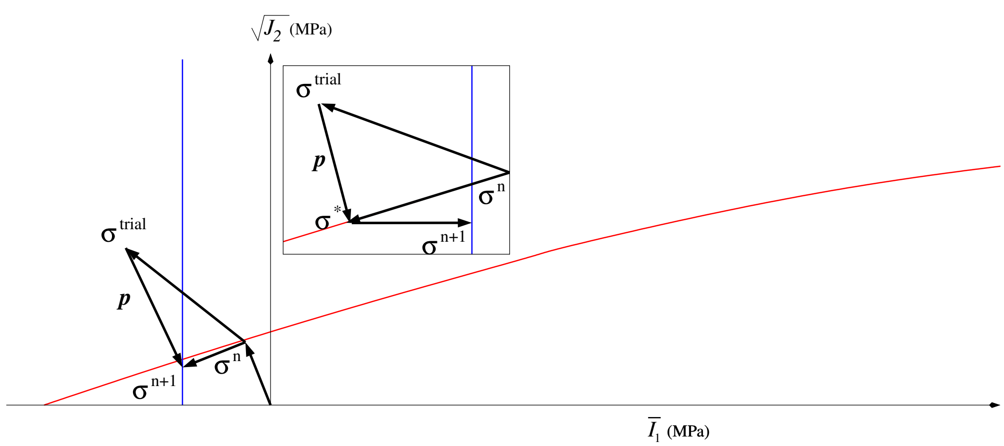


Figure 4: Return to the spall cut plane used for tensile control.

V.A Comparison of Density with/without Tensile Control

We now show the improved treatment of tensile states through a simulation designed to demonstrate the density and tensile control outlined in Sections IV and V. In this problem, a single element of Kayenta material is deformed in pure shear, upon reaching a critical value of shear strain the element is then deformed in tension along one of its diagonals, as shown in Figure 5. The path through stress space for the problem is also shown.

The density response of the material is shown in Figures 6(a) and 6(b). In Figure 6(a), the pressure and density update in the Kayenta material neglected the hydrostatic/deviatoric coupling. Upon reaching

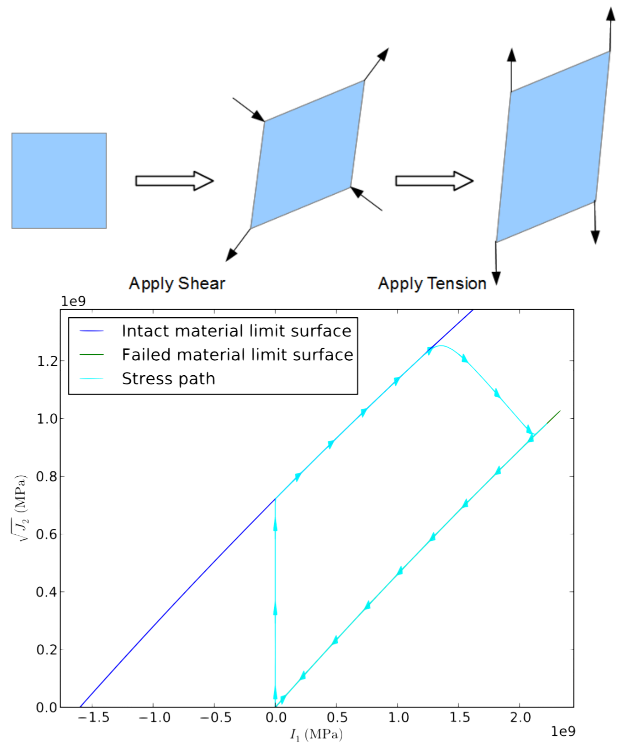
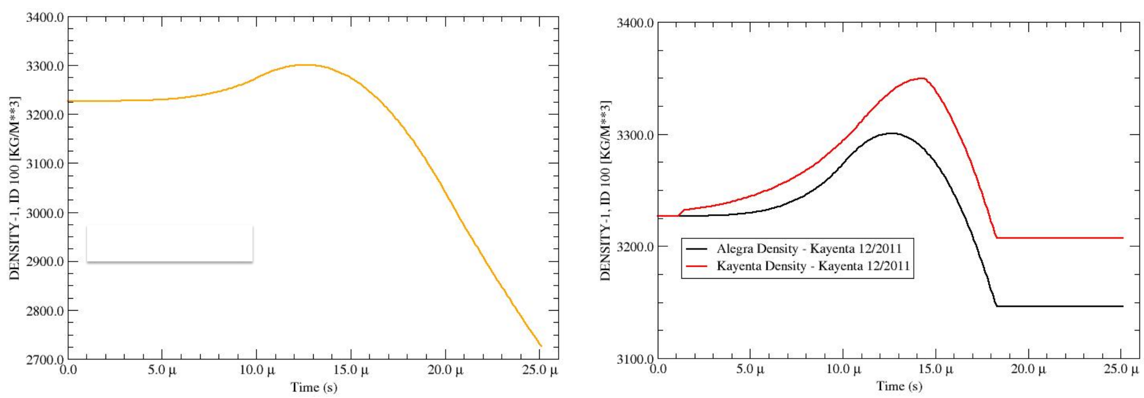


Figure 5: Prescribed deformation path for the described example problem.

excessive tensile states the density reduces to unphysical levels and the simulation eventually became unstable. There is no distinction between the element density and the solid density. In contrast, the pressure and density updates in Figure 6(b) adhered to the methods outlined in Sections IV and V. In this simulation, there is a clear dilineation between the solid density (upper curve) and the element density (lower curve). Upon reaching the tensile limit, void is accumulated in the element, evidenced by the near constant density in the right half of the figure.

VI Conclusion

Recent efforts coupling the hydrostatic equation of state response with the deviatoric material response in Alegra finite element code were described. The inseperability of the hydrostatic and deviatoric material responses in materials exhibiting dilatant inelastic flow were described. Unphysical material densities were shown to occur if the coupling is neglected. A new method of coupling the equation of state response and the deviatoric material was response was shown to resolve unphysical tensile states in a shock-hydrocode simulation, leading to more stable treatment of extreme tensile states common in the simulation of blast and penetration events.



(a) Density comparison without the density control described in Sections IV and V

(b) Density comparison with the density control described in Sections IV and V

Figure 6: Dilatant inelastic flow occurs in materials in which the shear strength increases with confining pressure. The simplest constitutive models to capture this type of behavior are the linear and nonlinear Drucker-Prager models shown.

A Notation, Terminology, and Nomenclature

I.A Tensor Notation

Tensors and tensors operations are given using a "direct" notation, whereby tensor order is indicated by the number of number of "under tildes" in each argument. For example, a first order tensor (vector) A is typset as $\underset{\sim}{\boldsymbol{A}}$, second order tensor A as $\underset{\approx}{\boldsymbol{A}}$, third order tesor A as $\underset{\approx\!\!\sim}{\boldsymbol{A}}$, etc. Tensor contractions are indicated by raised dots between tensor arguments, where the number of dots represents the order of contraction. For example, the "double dot" product of tensors $\underset{\approx\!\approx}{\mathbb{C}}$ and $\underset{\approx}{\boldsymbol{A}}$ would be given in indicial notation by

$$\underset{\approx}{\boldsymbol{B}} = \underset{\approx\!\approx}{\mathbb{C}} : \underset{\approx}{\boldsymbol{A}} = C_{ijkl} A_{kl} = B_{ij}$$

where the summation convention of repeated indices applies. Other operations are defined as used throughout the document.

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