UCRL-CONF-206641

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

SIMULATION OF GEOMATERIALS USING CONTINUUM DAMAGE MODELS ON AN EULERIAN GRID

Ilya Lomov, Tarabay H. Antoun

September 20, 2004

11th International Conference on Fracture
Turin, Italy
March 20, 2005 through March 25, 2005

Disclaimer

SIMULATION OF GEOMATERIALS USING CONTINUUM DAMAGE MODELS ON AN EULERIAN GRID

I. LOMOV, AND T.H. ANTOUN
Lawrence Livermore National Laboratory, Livermore, CA 94550, USA, lomov1@llnl.gov

ABSTRACT

Abstract. A new continuum model for directional tensile failure has been developed that can simulate weakening and void formation due to directional tensile failure. The model is developed within the context of a properly invariant nonlinear thermomechanical theory. A second order damage tensor is introduced which allows simulation of weakening to tension applied in one direction, without weakening to subsequent tension applied in perpendicular directions. This damage tensor can be advected using standard methods in computer codes. Porosity is used as an isotropic measure of volumetric void strain and its evolution is influenced by tensile failure. The rate of dissipation due to directional tensile failure takes a particularly simple form, which can be analyzed easily. Specifically, the model can be combined with general constitutive equations for porous compaction and dilation, as well as viscoplasticity. A robust non-iterative numerical scheme for integrating these evolution equations is proposed. This constitutive model has been implemented into an Eulerian shock wave code with adaptive mesh refinement. A comparison of experimental results and computational simulations of spherical wave propagation in Danby marble was made. The experiment consisted of a 2-cm-diameter explosive charge detonated in the center of a cylindrical rock sample. Radial particle velocity histories were recorded at several concentric locations in the sample. An extensively damaged region near the charge cavity and two networks of cracks were evident in the specimen after the test. The first network consists of radial cracks emanating form the cavity and extending about halfway through the specimen. The second network consists of circumferential cracks occurring in a relatively narrow band that extends from the outer boundary of the radially cracked region toward the free surface. The calculations indicated load-induced anisotropy such as was observed in the experiment

1. INTRODUCTION

In this paper a continuum model and numerical method are presented for modeling large-deformation flows with directional tensile failure. A number of continuum damage models have been developed for Lagrangian codes, but problems frequently involve deformations too severe to be handled by the same Lagrangian mesh during entire calculation. The present work uses an Eulerian high-order Godunov scheme since it is easy to couple it with adaptive mesh refinement algorithms. Unfortunately, it is often difficult or impossible to implement complex constitutive models in Eulerian codes. The constitutive model described here is thermodynamically consistent [1] and can be implemented in a straightforward manner. Constitutive models for tensile failure and damage typically include a reduced yield strength, a reduced elastic modulus and an evolving void strain. The model presented in this paper focuses mainly on the latter. A comprehensive model for porous elastic-viscoplastic material with tensile failure that is applicable to shock problems had been recorded in [2] and addresses other phenomena. Porosity is used as an isotropic measure of volumetric void strain and its evolution is influenced by tensile failure. Furthermore, instead of introducing a void strain tensor, the inelastic effects of directional void opening and closing are modeled by introducing their effects directly on the rate of evolution of elastic deformation.

The main objective of a constitutive model for directional tensile failure, like the one developed in this paper, is to model the fact that although a brittle material (like rock) can fail in one direction it may retain virgin strength to tensile failure in a perpendicular direction. From the mathematical point of view it is always possible to propose evolution equations for internal state variables that ensure maximum dissipation. However, such constitutive assumptions can be difficult to interpret physically. Therefore, a major challenge in the development of a theory of directional tensile failure is to develop a theoretical structure that is amenable to the analysis of physically based constitutive assumptions and is amenable to the development of a robust integration scheme and an implementation to a general computer code.

2. CONSTITUTIVE MODEL

In contrast with standard approaches to plasticity which introduce measures of inelastic deformation through evolution equations, the approach taken here is to propose evolution equations directly for elastic deformation measures [2]. Specifically, within the context of the proposed model it is convenient to introduce a measure of elastic deformation as a symmetric, invertible, positive definite tensor $\mathbf{B}_e$ which is determined by integrating the evolution equation

$$\dot{\mathbf{B}}_e = \mathbf{L}\mathbf{B}_e + \mathbf{B}_e\mathbf{L}^T - J_e^{2/3}\mathbf{A} \ , \tag{1}$$

where J_e is a pure measure of elastic dilatation $J_e^2 = \det(\mathbf{B}_e)$, $\mathbf{L}$ denotes the velocity gradient and a superposed dot denotes material time differentiation. The tensor $\mathbf{A}$ includes the inelastic effects of the rate of plastic deformation as well as that due to directional tensile failure. Moreover it is possible to define $\mathbf{B}_e'$ as a unimodular tensor which is a pure measure of elastic distortional deformation

$$\mathbf{B}_e' = J_e^{-2/3}\,\mathbf{B}_e \ , \quad \det(\mathbf{B}_e') = 1 \ . \tag{2}$$

It can be shown that J_e and $\mathbf{B}_e'$ are determined by the evolution equations

$$\dot{J}_e / J_e = \mathbf{D} \bullet \mathbf{I} - 1/2\ \mathbf{A} \bullet \mathbf{B}_e'^{-1}, \quad \dot{\mathbf{B}}_e' = \mathbf{L}\mathbf{B}_e' + \mathbf{B}_e'\mathbf{L}^T - \frac{2}{3}\ (\mathbf{D} \bullet \mathbf{I})\ \mathbf{B}_e' - \left[\mathbf{A} - \frac{1}{3}\ (\mathbf{A} \bullet \mathbf{B}_e'^{-1})\ \mathbf{B}_e'\right], \tag{3a,b}$$

where $\mathbf{D}$ is the symmetric part of the velocity gradient. For porous materials it is common to introduce the current value ϕ of porosity, its reference value Φ, and the reference density ρ_{s0} of the solid matrix, such that

$$J_e = \left[\frac{1-\phi}{1-\Phi}\right] J \ , \quad \rho_0 = (1-\Phi)\rho_{s0} \ , \quad \rho = (1-\phi)J_e^{-1}\rho_{s0} \ , \tag{4}$$

The Helmholtz free energy ψ is assumed to be a function of the variables J_e, $\mathbf{B}_e'$, and temperature θ. However, since ψ must remain unaltered under superposed rigid body motions it follows that it can be a function of $\mathbf{B}_e'$ only through its two independent invariants $\alpha_1 = \mathbf{B}_e' \bullet \mathbf{I}$, $\alpha_2 = \mathbf{B}_e' \bullet \mathbf{B}_e'$. For simplicity, ψ is taken to be independent of α_2 so that it takes the form $\psi = \psi(J_e,\alpha_1,\theta)$.

Constitutive equations are required to satisfy statements of the second law of thermodynamics which include the condition that heat flows from hot to cold, and the condition that the material dissipation is nonnegative:

$$\rho\theta\xi' = \mathbf{T} \bullet \mathbf{D} - \rho(\dot{\psi} + \eta\dot{\theta}) \geq 0. \tag{5}$$

For the model under consideration, the Cauchy stress $\mathbf{T}$ and the entropy η are given in the hyperelastic forms:

$$\mathbf{T} = -\,p\,\mathbf{I} + \mathbf{T}', \ \eta = -\frac{\partial\psi}{\partial\theta}\ , \ p = (1-\phi)\,p_s, \ \mathbf{T}' = (1-\phi)\mathbf{T}_s',$$

$$p_s = -\,\rho_{s0}\frac{\partial\psi}{\partial J_e}\ , \mathbf{T}_s' = 2J_e^{-1}\rho_{s0}\frac{\partial\psi}{\partial\alpha_1}\mathbf{B}_e'', \tag{6}$$

where p is the pressure, $\mathbf{T}'$ is the deviatoric part of the stress, $\mathbf{B}_e''$ is the deviatoric part of $\mathbf{B}_e'$ and p_s and $\mathbf{T}_s'$ are the pressure and deviatoric stress of the solid matrix, respectively.

Next, the inelastic deformation tensor $\mathbf{A}$ is separated into a part $\mathbf{A}_p$ associated with viscoplasticity and a part $\mathbf{A}_v$ associated with void formation (due to porosity and cracks) due to tensile failure

$$\mathbf{A} = \mathbf{A}_p + \mathbf{A}_v\ , \quad \mathbf{A}_p = \Gamma_p\left[\mathbf{B}_e' - \left\{\frac{3}{\mathbf{B}_e'^{-1}\bullet\mathbf{I}}\right\}\mathbf{I}\right]\ , \tag{7}$$

where the scalar Γ_p requires a constitutive equation. In order to propose a constitutive equation for $\mathbf{A}_v$ it is convenient to define $\mathbf{p}_i$ as the orthonormal right-handed set of eigenvectors of $\mathbf{B}_e'$, so that

$$\mathbf{B}_e' = \beta_1\,(\mathbf{p}_1\otimes\mathbf{p}_1) + \beta_2\,(\mathbf{p}_2\otimes\mathbf{p}_2) + \beta_3\,(\mathbf{p}_3\otimes\mathbf{p}_3)\ , \tag{8}$$

where β_i are the eigenvalues of $\mathbf{B}_e'$. Thus, in view of the constitutive equations (6), the stress $\mathbf{T}$ can be written in its spectral form

$$\mathbf{T} = \sigma_1\,(\mathbf{p}_1\otimes\mathbf{p}_1) + \sigma_2\,(\mathbf{p}_2\otimes\mathbf{p}_2) + \sigma_3\,(\mathbf{p}_3\otimes\mathbf{p}_3)\ , \tag{9}$$

where σ_i are the principal stresses. Next, it is assumed that the rate of void formation tends to reduce these principal stresses so that $\mathbf{A}_v$ is specified in the form

$$\mathbf{A}_v = 2\left[\Gamma_{v1}\,\beta_1\,(\mathbf{p}_1\otimes\mathbf{p}_1) + \Gamma_{v2}\,\beta_2(\mathbf{p}_2\otimes\mathbf{p}_2) + \Gamma_{v3}\,\beta_3\ (\mathbf{p}_3\otimes\mathbf{p}_3)\right], \tag{10}$$

where the scalar functions Γ_{vi} require constitutive equations. For these constitutive assumptions the rate of material dissipation (5) reduces to [1]

$$\xi' = \xi_v' + \xi_d'\ , \ \rho\theta\xi_v' = \sigma_1\,\Gamma_{v1} + \sigma_2\,\Gamma_{v2} + \sigma_3\,\Gamma_{v3}\ , \tag{11}$$

where $\rho\theta\xi_v'$ is the dissipation of void formation and $\rho\theta\xi_d'$ is the dissipation of plastic distortional deformation, which is nonnegative if $\partial\psi/\partial\alpha_1$, and Γ_p are each non-negative [2]. The rate of change of porosity and the rate of elastic distortional deformation (3) can then be rewritten in the forms

$$\dot{\phi}/(1-\phi) \ = \Gamma_{v1} + \Gamma_{v2} + \Gamma_{v3},$$

$$\dot{\mathbf{B}}_e' = \mathbf{L}\mathbf{B}_e' + \mathbf{B}_e'\mathbf{L}^T - \frac{2}{3}(\mathbf{D}\bullet\mathbf{I})\mathbf{B}_e' - \mathbf{A}_p - 2\beta_1\Gamma_{v1}'(\mathbf{p}_1\otimes\mathbf{p}_1) - 2\beta_2\,\Gamma_{v2}'(\mathbf{p}_2\otimes\mathbf{p}_2) - 2\beta_3\,\Gamma_{v3}'\ (\mathbf{p}_3\otimes\mathbf{p}_3). \tag{12}$$

Next, it is convenient to introduce a symmetric tensor $\mathbf{\Delta}$, which is interpreted as the distribution of damage due to directional tensile failure. In particular, the damage Δ in a general direction $\mathbf{n}$ ($\mathbf{n}\bullet\mathbf{n}$ =1) and the damage Δ_i in the principal directions of stress $\mathbf{p}_i$ are defined by

$$\Delta = \left\langle \mathbf{\Delta}\bullet(\mathbf{n}\otimes\mathbf{n})\right\rangle\ , \quad \Delta_i = \left\langle \mathbf{\Delta}\bullet(\mathbf{p}_i\otimes\mathbf{p}_i)\right\rangle \quad \text{(no sum on i)}\ , \tag{13}$$

where $\langle x\rangle$ represents the Macauley brackets $\langle x\rangle = 1/2\left[x + |x|\right]$. Thus, the principal directions of $\mathbf{\Delta}$ represent normals to potential weak planes, with the weakest plane being normal to the principal direction associated with the largest principal value of $\mathbf{\Delta}$. In this sense, $\mathbf{\Delta}$ acts like a structural tensor which characterizes the directionality of tensile failure.

3. NUMERICAL SCHEME

The Eulerian framework of adaptive mesh refinement (AMR) [3] is a relatively mature technique for dynamically applying high numerical resolution to those parts of a problem domain that require it, while solving less sensitive regions on less expensive, coarser computational grids. In combination, Eulerian Godunov methods with AMR have been proven to produce highly accurate and efficient solutions to shock capturing problems. The method used here is based on some modifications of the single-phase high-order Godunov method. The multidimensional equations are solved by using an operator splitting technique.

Here, it is of interest to compute large-deformation flows in problems consisting of multiple resolved phases. The algorithm used here treats the propagation of surfaces in space in terms of an equivalent evolution of volume fractions. The approach to modeling multimaterial cells is similar to that in [4]. Specifically, material properties are multiply-valued in a cell, but the velocity and stress are single valued. In order to use the single-fluid solver it is necessary to define an effective single phase for the mixed cells and to update material volume fractions based on self-consistent cell thermodynamics [4].

Many source terms for viscoplastic materials with damage are very non-linear and consequently require special numerical methods appropriate for solutions of stiff equations. Often, it is possible to simplify the numerical procedure by defining the "target" value of a parameter and then solve a relaxation equation implicitly based on the "trial" value and the target value of the parameter. This approach was used to find appropriate values for Γ_{vj} in (12) based on an acoustic approximation. In this case it is possible to form a system of linear equations,

$$\sigma_i^{n+1} = \sigma_i^* - C_{ij}\,\Gamma_{fj} \quad i,j=1,2,3 \tag{15}$$

where C_{ij} is a matrix dependent on elastic coefficients and σ_i^* is a "trial" stress. The specific values of C_{ij} depend on whether or not there is an active failure process in specific directions. Consequently, the solution is obtained by guessing a branch of the solution (based on the values of Γ_{fi} associated with estimates of the stresses σ_i), then using the appropriate values of C_{ij} to solve (15) for the updated values σ_i^{n+1}. The solution is considered to be correct if the updated values of Γ_{fi} correspond to the same branch that is being checked.

4. SPHERICAL WAVE EXPERIMENT

In the experiment, a 2-cm-diameter EL-506D (Detasheet) explosive charge weighing 6 g was detonated at the center of an instrumented 27-cm-diameter, 27-cm-long cylindrical block of marble [5]. The velocity histories at few ranges are shown in Fig. 1. The letters 'a' and 'b' following the gage number are used to distinguish the two gage arrays on opposite sides of the charge.

At early times, the recorded velocity histories are characterized by a sharp rise to peak followed by an outward motion that lasts for about 10 μs. This early-time response is reproducible, as indicated by the nearly identical records from the gage arrays on either side of the charge. The Danby marble specimen of the present study was severely cracked, as shown in Fig. 2. In addition to the extensively damaged region near the charge cavity, two distinct networks of cracks can be seen in each half of the specimen. The first network consists of numerous cracks emanating from the charge boundary and extending radially outward toward the free surface of the specimen. These radial cracks extend throughout the gaged region of the specimen, and a few cracks propagate all the way to the free surface. The second network of cracks consists primarily of circumferential cracks and does not appear to be symmetric with respect to the center of the explosive charge. An additional crack that does not appear to be associated with either of the crack networks mentioned so far can be observed spanning the whole specimen surface. This crack follows the path of a pre-existing *in situ* joint in the rock.

5. NUMERICAL SIMULATIONS

The model was calibrated using laboratory data that included elastic properties, unconfined compressive strength, and a pressure dependent failure surface. Pressure-volume data from 1D strain wave propagation experiments were also used to calibrate the Mie-Grüneisen EOS used in the simulations. Material parameters that could not be determined from the aforementioned data were determined through an optimization process using the measured particle velocity histories shown earlier in Fig 1. As shown in the figure, the calibrated model is in good agreement with the data at early time, when the flow field can be reasonably viewed as spherically symmetric. At late time, reflected waves from the cylindrical boundary of the specimen converge toward the charge cavity and in so doing render the flow field three-dimensional. Also at late time, the sample response becomes anisotropic due to the interaction of the stress waves with pre-existing planes of weakness in the sample. These two phenomena cause a breakdown in the 2D axisymmetry assumption. For this reason no attempt was made to match the late time velocity histories.

The damage patterns computed with the calibrated model are shown in Fig. 3. The two halves of the figure show void volume fraction and crack patterns, both of which are indication of damage. The main difference between the two is that void volume fraction is reversible (i.e., voids can undergo recompaction under compression) whereas damage is irreversible, increasing under tension and remaining constant under compression.

These patterns look remarkably similar to the cracking patterns observed in the experiment. Like in the experiment, two crack networks are observed; the first consisting of radial cracks propagating away from the charge cavity toward the free surface, and the second consisting of

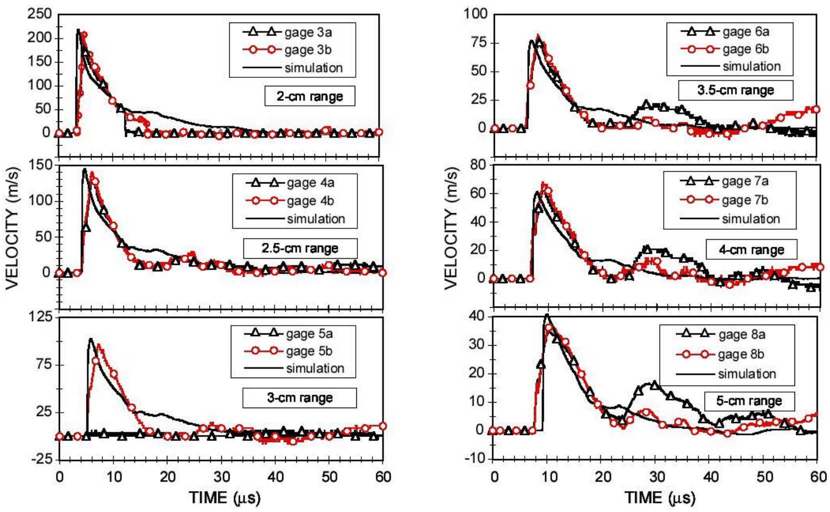

Figure 2. Measured and simulated particle velocity histories at 6 radii from the explosive charge.

rings of circumferential cracks caused by the reflected wave near the free surface of the specimen. The simulated circumferential cracks network is closer to the surface of the specimen than was observed experimentally. This is probably because in the simulation the reflected wave is spherically symmetric, and therefore more intense than its cylindrically symmetric counterpart in the experiment.

Fig. 3 also shows a near-source region dominated by bulking. Bulking porosity as high as 10% was computed in the near-source region. This form of isotropic scalar damage is related to plastic distortion under compression. It is different in nature from the radial and circumferential components of the directional damage variable.

The 2D simulations are in reasonably good agreement with the data indicating that our multidimensional cracking model is well suited for simulating directional damage within a continuum mechanics framework. To improve agreement with data, a 3D simulation is needed to properly account for specimen geometry, including preexisting joints, and for the complex wave interactions that take place during the later stages of the experiment.

Acknowledgements This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

References

[1] Rubin M.B., Lomov I.N. Mechanical and numerical modeling of a porous elastic-viscoplastic material with tensile failure. Submitted to Int. J. Solids Struct.

[2] Rubin M.B., Vorobiev O.Y., Glenn L.A. Mechanical and numerical modeling of a porous elastic-viscoplastic material with tensile failure. Int. J. Solids Struct, 37 (13), 1841-1871, 2000

[3] Berger M.J., Colella P. Local Adaptive Mesh Refinement for Shock Hydrodynamics. J Comput Phys, 82(1), 64-84,1989

[4] Miller G.H., Puckett E.G. A high-order Godunov method for multiple condensed phases Comput Phys, 128 (1), 134-164, 1996.

[5] Antoun, T.A., Curran, D.R., “Wave Propagation in Intact and Jointed Calcium Carbonate (CaCO3) Rock,” DNA Report No. DNA-TR-95-47, (1996).

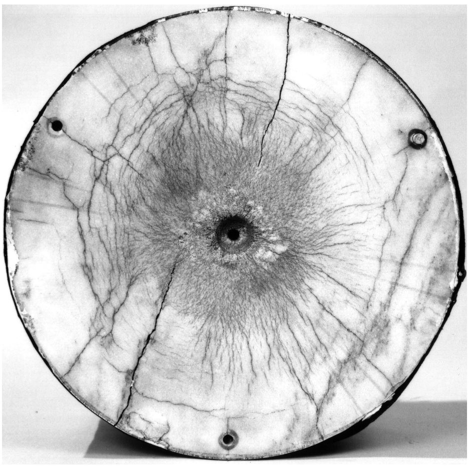

Figure 2. Observed damage at the midsection of the explosively loaded Danby marble specimen.

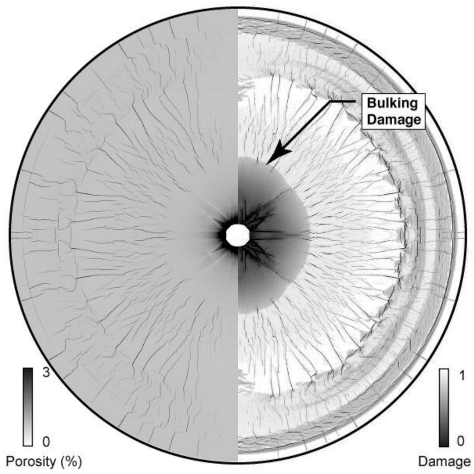

Figure 3. Void volume and directional damage from the 2D simulation of the spherical wave experiment.