Preprint
UCRL-JC-151087

Numerical Simulation of Damage using a Elastic-Viscoplastic Model with Directional Tensile Failure

I. Lomov, M. B. Rubin

This article was submitted to
7th International Conference on Mechanical and Physical Behavior of Materials Under Dynamic Loading, Porto, Portugal, September 8-12, 2003

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

March 17, 2003

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

I.Lomov, M.B.Rubin

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 number of simulations of complicated shock loading of different materials have been performed including problems of fracture of rock. These simulations show that directionality of damage can play a significant role in material failure.

1. INTRODUCTION

We present a continuum model and numerical method for modeling large-deformation flows with directional tensile failure. A number of continuum damage models was developed for Lagrangian codes, but problems frequently involve deformations too severe to be handled by the same Lagrangian mesh during entire calculation. Several Eulerian approaches on staggered grid were developed [1] which are capable to survive severe material distortion. We are using high-order Godunov scheme since it is easy to couple it with adaptive mesh refinement algorithms. On the other hand it is often difficult or impossible to implement complex constitutive models in Eulerian codes. The constitutive model described here combines a straightforward implementation and possibility of the thermodynamic analysis [2]. Constitutive models for tensile failure and damage typically include a reduced yield strength, a reduced elastic modulus 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 is recorded in [3] 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 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 the internal state variables that ensure maximum dissipation. However, such constitutive assumption may 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, to the development of a robust integration scheme and 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 [3]. 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 $J_e^2 = \det(\mathbf{B}_e)$ and $\mathbf{L}$ denotes the velocity gradient. 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

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

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

$$J_e = [\frac{1-}{1-}]\,J \ , \quad _0 = (1- \ ) \ _{s0} \ , \quad = (1- \ )J_e^{-1} \ _{s0} \ , \tag{4}$$

The Helmholtz free energy is assumed to be a function of the variables J_e, $\mathbf{B}_e'$, and temperature . However, since 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 $_1 = \mathbf{B}_e' \bullet \mathbf{I}$, $_2 = \mathbf{B}_e' \bullet \mathbf{B}_e'$. For simplicity, is taken to be independent of $_2$ so that it takes the form $=$ $(J_e, \ _1, \ )$.

Constitutive equations are required to satisfy statements of the second law of thermodynamics with include the condition that heat flows from hot to cold, and the condition that the material dissipation is nonnegative [4]:

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

It can be shown [3] that in order to satisfy the condition (5) the stress $\mathbf{T}$ and the entropy have to be given in the hyperelastic forms:

$$\mathbf{T} = -\,p\,\mathbf{I} + \mathbf{T}', \quad = -\frac{\partial}{\partial}, \ p = (1- \ )\,p_s, \ \mathbf{T}' = (1- \ )\mathbf{T}_s', \qquad p_s = - \ _{s0}\frac{\partial}{\partial J_e}, \ \mathbf{T}_s' = 2J_e^{-1} \ _{s0}\frac{\partial}{\partial \ _1}\mathbf{B}_e'',$$

where p is the pressure, $\mathbf{T}'$ is the deviatoric part of the stress, $\mathbf{B}_e''$ is the deviatoric part of $\mathbf{B}_e'$, 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 tensile failure

$$\mathbf{A} = \mathbf{A}_p + \mathbf{A}_v \ , \quad \mathbf{A}_p = \ _p [\mathbf{B}_e' - \{\frac{3}{\mathbf{B}_e'^{-1} \bullet \mathbf{I}}\}\mathbf{I}] \ , \tag{6}$$

where the scalar $_p$ 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

$$\mathbf{B}_e' = \ _1 (\mathbf{p}_1 \ \ \mathbf{p}_1) + \ _2 (\mathbf{p}_2 \ \ \mathbf{p}_2) + \ _3 (\mathbf{p}_3 \ \ \mathbf{p}_3) .$$

Thus, in view of the constitutive equations (21), the stress $\mathbf{T}$ can be written in its spectral form

$$\mathbf{T} = \ _1 (\mathbf{p}_1 \ \ \mathbf{p}_1) + \ _2 (\mathbf{p}_2 \ \ \mathbf{p}_2) + \ _3 (\mathbf{p}_3 \ \ \mathbf{p}_3) ,$$

where $_i$ 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

$$\mathbf{A}_v = 2 [\ _{v1} \ _1 (\mathbf{p}_1 \ \ \mathbf{p}_1) + \ _{v2} \ _2 (\mathbf{p}_2 \ \ \mathbf{p}_2) + \ _{v3} \ _3 (\mathbf{p}_3 \ \ \mathbf{p}_3)] ,$$

where the scalar functions $_{vi}$ require constitutive equations. The rate of dissipation reduces to [2]

$$' = \ _v' + \ _d' , \qquad _v' = \ _1 \ _{v1} + \ _2 \ _{v2} + \ _3 \ _{v3}$$

where $_v'$ is the dissipation of void formation and $_d'$ is the dissipation of plastic distortional deformation which is nonnegative if $\partial \quad \partial \ _1$ and $_p$ are each non-negative [3].

The rate of change of porosity and the rate of elastic distortional deformation (3) can be rewritten in the forms

$$\dot{} /(1- \quad = \ _{v1} + \ _{v2} + \ _{v3} ,$$

$$\dot{\mathbf{B}}_e' = \mathbf{L}\mathbf{B}_e' + \mathbf{B}_e'\mathbf{L}^T - \frac{2}{3}(\mathbf{D} \bullet \mathbf{I})\mathbf{B}_e' - \mathbf{A}_p - 2 \ _1 \ _{v1}'(\mathbf{p}_1 \ \ \mathbf{p}_1) - 2 \ _2 \ _{v2}'(\mathbf{p}_2 \ \ \mathbf{p}_2) - 2 \ _3 \ _{v3}'(\mathbf{p}_3 \ \ \mathbf{p}_3) . \tag{7}$$

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

$$= \triangle \bullet (\mathbf{n} \ \ \mathbf{n}) \ , \quad _i = \triangle \bullet (\mathbf{p}_i \ \ \mathbf{p}_i) \quad \text{(no sum on i)} \ ,$$

where x represent the Macauley brackets x $= 1/2[x + |x|]$. Thus, the principal directions of $\triangle$ represent normals to potential weak planes, with the weakest plane being normal to the principal direction associated with the largest principal value of $\triangle$. In this sense, $\triangle$ acts like a structural tensor to specify the directionality of tensile failure. Moreover, $\triangle$ is determined by the evolution equation

$$\dot{\triangle} = \mathbf{W}\triangle + \triangle\mathbf{W}^T + m \quad \mathbf{A} \ ,$$

$$\mathbf{A} \quad = [\frac{f1 \quad 1}{(1+ \ _1)^n} (\mathbf{p}_1 \ \ \mathbf{p}_1) + \frac{f2 \quad 2}{(1+ \ _2)^n} (\mathbf{p}_2 \ \ \mathbf{p}_2) + \frac{f3 \quad 3}{(1+ \ _3)^n} (\mathbf{p}_3 \ \ \mathbf{p}_3)] , \tag{8}$$

where m and n are material constants, $\mathbf{W}$ is the skew-symmetric part of the velocity gradient, and $\mathbf{A}$ determines the direction of increase in damage. This is one of simplest equations that allows for directional dependence of damage and remain properly invariant under superposed rigid body motions.

A specific constitutive equation for directional tensile failure is proposed in the form:

$$_{vi} = \ _{v0} [\frac{_i - 1 - \ _i \ T_f}{T_f} - \frac{_f}{a_f + \ _f} \frac{-(\ _i + 1 - \ _i \ T_f)}{T_f} (\ _i)^{n_f}] , \tag{9}$$

where $_{v0}$, T_f, a_f and n_f are non-negative material constants. It then follows that (9) predicts dilation for $_i$ greater than the tensile failure value $1 - \ _i \ T_f$ and it predicts compaction for $_i$ less than the compressive failure. Since $1 - \ _i T_f$ is non-negative, these functions automatically satisfy the restriction $'_v \geq 0$. The term $_f/(a_f + \ _f)$ eliminates further compaction when the failure porosity vanishes and the term $(\ _i)^{n_f}$ reduces compaction due to tensile failure in directions that have not been sufficiently damaged.

3. NUMERICAL SCHEME

Eulerian framework adaptive mesh refinement (AMR) [5] 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 obtain highly accurate and efficient solutions to shock capturing problems. Our method is based on some modifications of the single-phase high-order Godunov method. We present a brief summary of it. For solid mechanics, the governing equations consist of the laws of conservation of mass, momentum and energy, the equation (3b), and a number of equations in a form of

$$\frac{\ \ _i}{t} \qquad {}_i\mathbf{v} \qquad , \ , \ _1, \ldots, \ _n \ , \tag{10}$$

which represents a specific rheological equation $_i$ for history dependent parameters $_i$ (like porosity, plastic strain, etc.) The equations for viscoplasticity can be written in conservative form, required for finite-volume methods, only at additional cost (for example, consideration of the full nonsymmetric deformation tensor and complementary plastic deformation tensor) [6]. However, highly nonlinear behavior of shear stresses (like shear shock waves and rarefaction fans) is very rare and a divergent formulation does not have simple and clear physical meaning. While equations (7,8) are not written in conservative form (10), we update $\mathbf{B}'_e$ and Δ in the same way as other history dependent variables. The estimate for velocity gradient **L** is calculated by Riemann solver described below. So for each material we have a system of conservation laws

$$\frac{\mathbf{u}}{t} \qquad \mathbf{f}(\mathbf{u}) \qquad \mathbf{\Phi} \ \ \mathbf{u} \tag{11}$$

Our numerical scheme for single fluid cell is based on approach of Miller and Puckett [7] and Colella, etc. [8] with some modifications to take into account full stress tensor. We solve multidimensional equations by using operator splitting technique, in which we solve the one-dimensional equations for each direction:

$$2L \qquad L_1 L_2 L_3 S L_3 L_2 L_1 S \ ,$$

where L is full update operator, L_p is update of in p direction without using the right part of equation (11) and S is update with the right part of equation (11).

Each operator L_p is update of cell i from time step n to time step n+1 with fluxes computed at the cell egdes $(i \quad 1/2, i \quad 1/2)$ in p direction,

$$\mathbf{u}_i^{n\ \ 1} \qquad \mathbf{u}_i^n \qquad \frac{t}{x} \ \mathbf{f} \ \ \mathbf{u}_{i\ \ 1/2}^{n\ \ 1/2} \qquad \mathbf{f} \ \ \mathbf{u}_{i\ \ 1/2}^{n\ \ 1/2}$$

In order to construct time- and edge-centered states $\mathbf{u}_{i\ \ 1/2}^{n\ \ 1/2}$ we are using an upwind characteristic tracing method based on the quasilinear form of (11),

$$\frac{\mathbf{w}}{t} \quad \mathbf{C}\frac{\mathbf{w}}{x} \quad \boldsymbol{\Psi}\ \mathbf{w}\ , \quad \mathbf{w} \quad , \quad ,\mathbf{v},\mathbf{T}, \ _i \ ^T$$

The eigenvalue decomposition of the matrix **C** provides all necessary information to do upwind characteristic tracing following [7] and to solve the Riemann problem in an acoustic approximation. While the latter is an appropriate approximation for shear waves, we calculate longitudinal waves in a manner similar to [8] without compromising the quality of solution for strong shock waves and rarefaction fans.

We are concerned with computing large-deformation flows in problems consisting of multiple resolved phases. The algorithm described here treats the propagation of surfaces in space in terms of an equivalent evolution of volume fractions. Our approach to modeling multimaterial cells is similar to [7]. Material properties are multiply valued in a cell, but the velocity and stress are single valued. In order to use the single-fluid solver we need to define effective single phase for the mixed cells and update material volume fractions based on self-consistent cell thermodynamics [7]:

$$K \quad \frac{f}{K}^{\ 1} \ , \quad p \quad K \quad \frac{f\, p_a}{K}, \quad \frac{f}{t} \qquad f\,\mathbf{v} \quad \frac{f}{K} K \ \mathbf{v}$$

where f , p , K are the volume fraction, pressure and the bulk modulus of material . The averaging of the shear modulus G , the stress deviator $\mathbf{T}$, and calculation of velocity gradient $\mathbf{L}$ for specific material is done in a similar way,

$$1/G \qquad f\ /G\ , \quad \mathbf{T} \quad G \quad f\,\mathbf{T}\ /G\ , \quad \mathbf{L} \qquad \mathbf{L}G/G$$

Many source terms in (10) for viscoplastic materials with damage are very non-linear which leads to necessity to deal with numerical solutions of the stiff equations. When the constitutive model allow such a representation, it is possible to simplify the process by defining the "target" value for parameters and then solve a relaxation equation implicitly based on the "trial" value and the target value of parameters. We used this approach to find appropriate values for $_{vj}$ in (7) in acoustic approximation. In this case it is possible to form a system of linear equations,

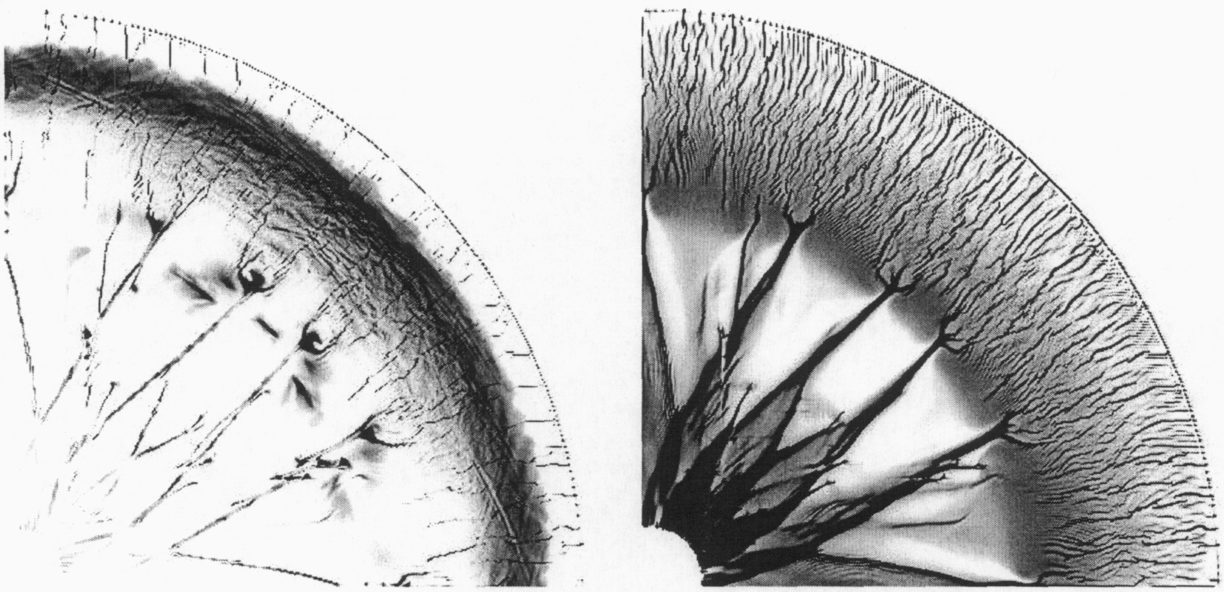
$$^{n+1}_{i} = \ ^{*}_{i} - C_{ij} \ _{fj} \quad i,j=1,2,3 \qquad (12)$$

where C_{ij} is a matrix dependent on elastic coefficients and $^{*}_{i}$ is a "trial" stress. C_{ij} depends on whether there is an active failure process in specific direction. So the solution is obtained by guessing a branch of the solution (based on the values of $_{fi}$ associated with estimates of the stresses $_i$), then using the appropriate values of C_{ij} solving (12) for the updated $^{n+1}_{i}$. The solution is considered to be correct if the updated values of $_{fi}$ correspond to the same branch that is being checked.

4. SIMULATION EXAMPLE

To test the present model and implementation of the numerical scheme simulations of explosion inside a marble cylinder were undertaken. We model marble as elastic-plastic material with constant shear modulus and pressure-dependent yield strength. We implemented a Mie-Grüneisen equation of state to represent volumetric response. We use an Eulerian computational mesh with 400x400 cells.

A damage map on the cross-section of the cylinder is shown in Figure 1. Time corresponds to approximately $2.5R/c_l$ (when the development of major damage features almost stopped), where R is the radius of the cylinder and c_l is longitudinal sound speed in marble. Figures 1a and 1b represent component $_{rr}$ and of the tensor field $\mathbf{\Delta}$. We can see distinctive features in the field due to the outward movement close to the source and spall induced damage in the $_{rr}$ field near the edges.



a) b)

Figure 1. Components of the damage tensor in the rock cylinder subjected to explosive loading

Acknowledgements

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

References

[1] Benson D.J. A mixture theory for contact in multi-material Eulerian formulations. Computer Methods in Applied Mechanics and Engineering, 140 (1-2), 59-86, 1997

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

[3] 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

[4] Rubin, M.B., An elastic-viscoplastic model for large deformation. Int. J. of Engng. Sci. 24, 1083-1095, 1986

[5] Berger M.J., Colella P. Local adaptive mesh refinement for shock hydrodynamics. J. Comput. Phys., 82(1), 64-84,1989

[6] Kondaurov V.I., Relaxation-type equations for viscoelastic media with finite deformations. PMM Journal Of Applied Mathematics And Mechanics, 49 (5): 608-615 1985

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

[8] Colella P., Glaz H. Efficient solution algorithms for the Riemann problem for real gases. J.Comput Phys, 59 (2), 264-289, 1985