SEMINARIO DE ANALISIS NUMERICO

EDITADO POR F. MICHAVILA

UNIVERSIDAD POLITECNICA DE MADRID 1985/86
COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING

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The mathematical formulation of large deformation problems entailing thermo-mechanical coupling is introduced at the onset of the paper. Then, a numerical strategy is proposed for their solution based on a Lagrangian finite-difference procedure and an explicit integration scheme. Also, a methodology is presented for automatic rezoning of the mesh when required. Finally, some examples are given to clarify the application of the proposed procedures to real problems.

1. INTRODUCTION

The motivation for the work presented here is the need to model processes where large strains and thermo-mechanical coupling are clearly present. Any numerical procedure attempting to simulate such processes must account accurately for the large local strains and rotations (geometrical non-linearities). It must also deal accurately with material behaviour up to those large strains (constitutive non-linearities). The mechanical equations must be solved simultaneously with the thermal equations, as the two are coupled in both directions. Finally, the procedure selected must be able to cope with localisation effects, including physical instabilities. To all these constraints, the necessity of predicting the transient, as opposed to steady-state, response of the material must be added in the present case.

The above requirements imply that a time-marching procedure should be used in conjunction with an incremental formulation referred to an updated Lagrangian frame. The very large geometrical non-linearities are otherwise practically impossible to handle.

The time integration could be explicit or implicit. The former has the advantages of simplicity and generality at the price of imposing a small integration timestep. The latter allows larger timesteps, but becomes less convenient as the non-linearities sharpen or wave propagation effects dominate. Further, convergence may be affected by problem characteristics and difficulties may arise when dealing with real physical instabilities (mainly adiabatic shear banding, buckling and necking).

Here, an explicit scheme has been selected. The small timestep forced by stability requirements has only moderate consequences. It is obviously of little significance in short duration problems. On the other hand, long problems are often quasi-static. This frequently allows contracting the timescale.

2. THEORY

The solution of the thermo-mechanical equations uses here a central finite-difference discretisation. The Lagrangian mesh is based on constant-strain tetrahedrons. Strictly speaking, a mixed discretisation [1] of space is used. The deviatoric part of the tensors is referred to a mesh of
constant-strain tetrahedrons, while their volumetric counterparts relate to a mesh of larger elements, each comprising typically three tetrahedrons. This avoids both hourglassing and artificial stiffening during plastic flow. The problem is advanced in time with an explicit central difference operator.

This combination offers a simple and efficient algorithm [2] and has proved very successful for non-linear mechanical analysis, both dynamic (e.g. [3] - [7]) and quasi-static (e.g. [8] - [10]). The method is extended here to encompass coupled thermo-mechanical processes. Three sources of coupling between thermal and mechanical phenomena are considered:

- thermal expansion
- thermal-dependent material behaviour (e.g. lower stiffness, lower yield, lower hardening index, higher rate sensitivity, etc., as temperature increases)
- heat generation from plastic deformation and friction.

As mentioned earlier, a rate-type formulation is employed in which variables are referred to an updated Lagrangian frame. As a function of the velocity and temperature fields, the rate of deformation tensor $\mathbf{d}_{ij}$ at a point may be expressed as:

$$\mathbf{d}_{ij} = 0.5 (\dot{\mathbf{u}}_{i,j} + \dot{\mathbf{u}}_{j,i}) + \beta \dot{T} \delta_{ij} \tag{1}$$

where $\dot{\mathbf{u}}_i$ is the velocity field
$\beta$ is the coefficient of thermal expansion
$T$ is the temperature
$\delta_{ij}$ is the Kronecker delta
commas indicate spatial derivatives
dots indicate material time derivatives.

Elastic-plastic constitutive laws are implemented using hypo-elastic predictions and a radial return method. The hypo-elastic prediction takes the form:

$$\Delta \mathbf{c}_{ij} = \lambda \dot{\mathbf{d}}_{ik} \delta_{ij} + 2\mu \dot{\mathbf{d}}_{ij} \tag{2}$$

where $\Delta \mathbf{c}_{ij}$ is the Jaumann rate of Cauchy stress
$\lambda, \mu$ are the Lame elastic constants.

The deviatoric components of the new stresses are then scaled back to the current yield surface, resulting in an associative flow rule. The yield surface site is given by Von Mises criterion including strain-rate and temperature dependence:

$$Y = Y_0(\bar{\dot{\varepsilon}}_p) (1 + B|\dot{T}|^m) T^q \tag{3}$$
where \( Y_0 \) is the reference quasi-static hardening law

\[
\dot{\varepsilon} = \frac{2}{3} \left( \frac{\partial P}{\partial e^p} \right)_{ijkl}^{1/2} \text{ is the effective plastic strain}
\]

\[\dot{\varepsilon} \] is the effective strain rate

\( B, m \) and \( q \) are material constants.

As the integration requires a small timestep for stability, the process is incrementally linear, obviating the need for substepping or iterations. Large strains and displacements are accurately recovered in this fashion.

The momentum equations are formulated with lumped masses. Integrated on a small space domain around each grid node, they can be expressed as:

\[
\ddot{u}_i = \frac{\int_{S_i} n_j ds + Mf_i + F_i}{M} \tag{4}
\]

Here \( M \) is the mass assigned to each node

\( S \) is the external surface around the corresponding region

\( n_j \) is the normal at each point of this surface

\( f_i \) are body forces per unit mass

\( F_i \) are external intensive forces.

The operation of the above equations is implemented in the fashion shown in Figure 1.a. Each time the cycle is completed, time increases by one integration timestep. Figure 1.b describes the thermal computational cycle.

An energy balance equation is needed to predict temperature variations. When integrated over a small volume \( V \), that equation takes the form:

\[
\dot{T} = \frac{\int_{S_i} k T_i n_j ds + \int_{V} s_{ij} \dot{\varepsilon}^{P} \dot{e}_{ij} dv + \dot{Q} V}{\rho C_p V} \tag{5}
\]

where \( k \) is the isotropic thermal conductivity

\( s_{ij} \) is the deviatoric stress tensor

\( \rho \) is the mass density

\( \dot{Q} \) is the heat power source per unit mass

\( C_p \) is the specific heat.

3. APPLICATION

In order to test the formulation, experiments were carried out on 6063 Aluminium alloy. They covered several orders of magnitude of strain rates, as well as temperatures ranging from 25°C to 450°C. Simple as well as complex test configurations were used.
The test configuration of the problem presented here is shown in Figure 2. The 6063 workpiece is initially a right circular cylinder, unstrained, and at 25°C. The workpiece is compressed axially between a low-friction flat rigid platen and a rough rigid steel block. The block is provided with a square hole through which the alloy can extrude. The distance between the indenting block and platen is decreased by one third (5mm) uniformly over 16msec. The problem is essentially static, as the loading time is much greater than the highest eigenperiod of the system.

The mechanical material properties were determined in calibration experiments. At 25°C, the material was found to behave as an elastic non-ideally plastic solid. Its elastic behaviour was described with a Young's modulus $E = 69.7$ GPa and a Poisson's ratio $\nu = 0.3$. A von Mises yield locus was assumed. Hardening was found to be represented by a power-law with a coefficient of 195MPa and a hardening index $\eta=2$. Due to the type of loading, the decision of which kind of hardening (isotropic or kinematic) is used is of little importance. Since isotropic hardening is simpler, it was selected for representing the material. No rate sensitivity was noticeable.

It is worth mentioning that, at 450°C, the constitutive description was found to be very different. No strain hardening was evident while rate sensitivity became all important. However, the above description could be maintained in the present case as temperatures never exceeded 100°C.

For similar reasons, the thermal properties, obtained from the literature, could be considered independent of temperature. The values adopted were a thermal conductivity $k = 174$ W/m°K, a specific heat $C = 9003$ J/kg°K and a coefficient of thermal expansion $a = 23.4 \times 10^{-6}$°K⁻¹.

As the mechanical problem is independent of the timescale, time can be contracted with two provisos: a) that the contraction is not so large that a non-existent dynamic character is triggered (i.e. inertia forces must remain negligible), b) that the thermal conductivity is suitably scaled. The computational timescale could then be contracted to complete the test in 0.1msec.

4. RESULTS AND DISCUSSION

The two symmetries allow restricting the model to one quarter of the workpiece. The mesh used, shown in Figure 3, consists of 6072 tetrahedrons and 1355 nodes. Each hexahedron in the figure is actually decomposed into six tetrahedrons. The shaded area corresponds to the contact with the block.

Contours of equal effective stress have been drawn on the deformed mesh after an indentation of 5mm (Figure 4). Contour 1 corresponds to 80MPa, from which they proceed in increments of 40MPa. This distribution was confirmed experimentally by microhardness testing on sectioned workpieces.

Temperature predictions are not shown but were made and compared with the trace of a thermocouple embedded in the workpiece. They too showed reasonably good agreement.

Of greater interest are the predictions of geometrical changes. Under pressure from the indentor, the workpiece curls up losing contact with the bottom platen over part of its initial area of contact. Figure 5 presents comparisons of various geometrical dimensions: a) the elevation of the top point in the workpiece and the elevation of the point on the bottom surface which separates most from the bottom platen; b) the elevation of the top of the extrude; c) the bottom diameter normal to the loading block; and d) the bottom diameter parallel to the loading block. As can be seen, all predictions are excellent except for that concerning the evolution of the bottom diameter parallel to the loading block. This is a consequence of the moderate misrepresentation involved in assuming a frictionless contact with the bottom platen.

The evolution of the indentation load is also presented here (Fig. 6). As can be seen, the comparison between numerical and experimental load-displacement results is not perfect but could be considered adequate.
Because of the absence of hardening, deformations are more localised and extrusion enhanced at higher temperatures. As a consequence, the problem cannot be handled without incorporating procedures to rezone the Lagrangian mesh. Such procedures are discussed in the following sections.

5. REZONING

The integration timestep is a function of the smallest dimension of a tetrahedron whilst discretisation errors are related to the size of the largest dimension. Therefore, in problems with very large distortions, the timestep becomes progressively smaller, whilst the discretisation errors tend to increase. The analysis thereby gets more and more inefficient and might eventually break down altogether due to the inability of the mesh to comply kinematically with the displacement field imposed by the boundary conditions. Hence, in order to continue a problem to a satisfactory stage, and to do so economically in terms of computer time, it becomes necessary to rezone the mesh at intervals.

The rezoning of distorted meshes appears to be not uncommon in fluid flow-related calculations [11-17], but its application to stress analysis situations, particularly three-dimensional ones, seems to be rather limited. Bertholf and coworkers [17] mention the use of rezoning in two-dimensional impact analysis but no mathematical details are given. The rezoning techniques reported in this paper are a modification of those proposed by Giuliani [18].

A new mesh may be produced in two ways:

(a) by optimising nodal locations without modifying the mesh topology;

(b) by generating a completely new mesh.

The second procedure enables the user to change the number of elements in the discretisation, but needs recourse to a preprocessor. The first technique maintains the same number of elements and therefore the problem size does not alter. Thus, it is easier to automate this technique within the computational procedure and this is the method adopted here. Rezoning of the deformed mesh is automatically triggered when the current integration timestep, which is recalculated at specified intervals, drops below a user-controlled fraction of the initial integration timestep or of the timestep computed after the last rezoning.

The rezoning procedure consists of two major operations:

(i) the optimal relocation of nodal grid-points;

(ii) the assignment of values to nodal and centroid variables in the new mesh.

Certain features, such as the external shape of the deformed body, the separation between material types, etc., must be retained unaltered when constructing the new mesh. Thus, not all nodes can be freely relocated. Nodes are classified into one of the following four categories:

(i) Kept nodes: These are nodes whose coordinates are not altered by rezoning.

(ii) Nodes on kept lines. These are nodes which are rezoned only along the curve defined in space by a string of nodes. Each node is relocated along the tangent to the string at that location and at equal distances from the two adjacent nodes on the kept line.

(iii) Nodes on kept surfaces. Each node is rezoned only within the tangent plane to the kept surface at that point and
re-located such that the shape of the surface triangles surrounding the point is optimised. This optimisation is not trivial and the details are given in Appendix I.

(iv) Internal nodes: The procedure followed for optimising the location of internal nodes is identical to that in two dimensions and the details can be found in Giuliani [18]. Basically it attempts to minimise the "squeeze" and "distortion" of the tetrahedrons surrounding each internal node in the mesh (Appendix I defines "squeeze" and "distortion"). The minimisation conditions provide the three components of the optimum position of each node.

Once the new mesh has been produced, there remains the problem of mapping all the field variables from the old deformed mesh to the new. Ideally, all mesh variables would be determined upon rezoning by simple application of local conservation conditions. In practice, however, there are more conservation conditions than variables and some choices must be made.

Amongst the nodal variables, mass and momentum constitute the most important parameters. The lumping of the mass of a zone onto its surrounding nodes is conducted as it would be at the onset of calculations: one quarter onto each node. However, the zonal mass is slightly more complicated to obtain because material densities have been affected by volumetric straining. The mass of the zone $M_z$ is

$$M_z = \rho_0 \exp(-\varkappa_k) \, V_z$$  \hspace{1cm} (6)

where $\rho_0$ is the initial density of the material

$\varkappa_k$ is the interpolated volumetric strain

$V_z$ is the current volume.

The procedure used for interpolating velocities is based on the smoothness of the momentum field. A new node will fall within some old tetrahedron (with some minor special considerations for boundaries). The velocity vector, $v_i^N$, of the new node, $N$, is computed as:

$$v_i^N = \frac{\sum_{\alpha} \frac{M^\alpha v^\alpha}{r^\alpha} \cdot i}{\sum_{\alpha} \frac{M^\alpha}{r^\alpha}}$$  \hspace{1cm} (7)

where $\alpha$ refers to each of the four nodes of the old zone

$M^\alpha$ is the nodal mass

$r^\alpha$ represents the distance between nodes $N$ and $\alpha$.

Stresses, strains, plastic strains and temperatures are some of the zonal variables which require similar treatment. The interpolation procedure used is again based on the smoothness of the respective fields. Consider a new zone, $z$, to which variables need to be assigned. Consider further the old node, $N$, closest to the new zone's centroid. The interpolation used is that shown below for the stress tensor:
COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING

\[
\sigma^2 = \frac{\sum_{a} \frac{\sigma^2}{V^2}}{\sum_{ij} \frac{\sigma^2}{i^2}}
\]

where \( \sigma_e \) refers to the old zones surrounding node \( N \)

\( V^2 \) is the volume of zone \( a \)

\( i^2 \) are the distances between the centroids of old zone and new zone \( Z \).

A check is kept on the rezoning procedure by monitoring the total momentum of the system before and after rezoning. In the tests performed to date, momentum appears to be conserved satisfactorily and the differences are negligible. Runs performed include several hundred rezoning operations in the same analysis.

1. APPLICATION OF REZONING

The test considered here has the same configuration of the one described earlier. It consisted of a right circular cylinder of Aluminium 6063 alloy being slowly compressed between a stationary rigid platen and a rigid block, both of them rough. The steel block was again provided with a square hole through which the Aluminium could extrude (Fig. 2). The test was conducted at a temperature of 425°C and the velocity of the block with respect to the platen was maintained constant during the test at 2mm/sec.

Due to the slow rate of loading, the test could be assumed to be running under isothermal conditions, so no thermal coupling was needed in the simulation. In cases of fast loading, in which temperature increases are not negligible, a fully coupled thermo-mechanical analysis is essential as shown in an earlier section.

From the results of calibration tests, the material at 425°C was modelled as an elastic, non-ideally plastic solid, with a Von Misses yield criterion. The Young's modulus was taken as 1.78GPa and Poisson's ratio as 0.3. The rate-dependent hardening behaviour was represented by:

\[
\sigma = \sigma_{yo} (1 + B\dot{\gamma})^{m}
\]

where \( \sigma_{yo} = 11.0MPa \) is the yield stress of the alloy at 450°C for zero strain-rate

\( B, m \) are material constants, having the values 6.16 and 0.719, respectively

\( \dot{\gamma} \) is the current yield stress.

The same procedures for contraction of the timescale described in the previous example were implemented in this case. In the numerical analysis, the alloy was compressed at 10m/sec.

The analysis was stopped at an indentation of 4.8mm and the mesh was rezoned once during this period. The comparison of workpiece dimensions between experimental and numerical results is shown in Fig. 7. As can be seen, the numerical results agree reasonably closely with the measured values. The computed elevation of the highest point in the extrude differs qualitatively from the experimental behaviour, but the actual displacements are very small when compared to the overall changes and therefore of little importance. The under-prediction of the amount of extrusion is probably due to the coarse mesh in the area of back extrusion.
The load-indentation curves from the experiment and the numerical analysis are shown in Fig. 8 and, again, show good agreement overall. The departure between the two curves at larger indentations could possibly be decreased by more frequent rezoning. The mesh was rezoned at an indentation just greater than 3mm and the perturbations arising from this manifest themselves in the oscillations displayed by the load-indentation curve at this time. The oscillatory behaviour quickly dies down and the trend following rezoning is consistent with earlier observations.

The contours of effective stress at an indentation of 4.8mm are shown in Fig. 9 on two mutually orthogonal planes. Fig. 10 shows the deformed shape of the mesh at 4.8mm. Since rezoning has already taken place, relative nodal positions must not therefore be taken to represent any measure of straining.

7. CONCLUSIONS

The equations governing the thermal and mechanical behaviour of solids undergoing large three-dimensional deformations have been embodied in the computer program PR3D.

Validation tests result in reasonably good comparisons of predictions and measurements, thus indicating that the numerical procedures and material behaviour implemented do indeed describe well the behaviour of the deforming solid. The very large deformations arising in processes such as extrusion can be handled by rezoning the distorted mesh at intervals. The rezoning facility is automated within the numerical procedure and is codified in the program PR3D. The experimental validations reported indicate that the methodology is suitable for analysis of three-dimensional problems involving large deformations.

The results obtained here could probably be improved further by using a more refined discretisation in areas of high gradients and by more frequent rezoning. More recent work than that reported here makes much greater use of the rezoning facilities and will be the subject of future publications.

APPENDIX I

OPTIMISATION OF KEPT SURFACES

Consider a node on the kept surface S and one of the surrounding triangles IJK. Let \( \mathbf{a} \) and \( \mathbf{b} \) be two mutually perpendicular unit vectors on the tangent plane to S at point I. The problem is to find a displacement vector \( \mathbf{d} \) contained in the plane which optimises the position of node I. Clearly, this vector can be expressed:

\[
\mathbf{d}_I = \mathbf{a} \mathbf{d}_a + \mathbf{b} \mathbf{d}_b
\]

where \( \mathbf{a} \) and \( \mathbf{b} \) are the two parameters sought.

When the node I is displaced by \( \mathbf{d}_I \), the new area, \( a \), of the IJK triangle can be written:

\[
a = \frac{-p \mathbf{d}_I + a'}{2}
\]

\[(A2)\]
where \( p_i = (x_{i+1}^J - x_{i+1}^K) - (x_{i+2}^J - x_{i+2}^K) \), an expression in which the
index additions are their equivalence classes mod_3.

\( x_j^i \) is the coordinate vector of node J

\( a \) is the triangle area before displacing node I

\[ a' = \frac{1}{2} p_i x_i + u \]

where the term \( u \) is

\[ u = \sum_{\alpha=1}^{3} x_j^\alpha (x_{\alpha+1}^K - x_{\alpha+2}^K) \] with index additions as above

On triangle \( IJK \), the base JK can be defined by vector \( v_i = x^K_j - x^J_i \) with
length \( b = \|v_i\| \).

Its height is clearly \( h = 2a/b \). The total area of the triangles around node is:

\[ A = \sum_{N} a' \]  \hspace{1cm} (A3)

and the perimeter of the line enclosing those triangles is:

\[ B = \sum_{N} b \]  \hspace{1cm} (A4)

This allows computing a mean height and base of the triangles:

\[ \bar{h} = \frac{2A}{B} \]

\[ \bar{E} = \frac{B}{N} \]  \hspace{1cm} (A5)

If the triangle \( IJK \) were isosceles, node I would have been at position T:

\[ x_i^T = x_i^K + \frac{2a}{b} (v_{ij_1} - v_{ij_2} - v_{ij_3}) \]  \hspace{1cm} (A6)

where \( x_i^K = \frac{1}{2} (x_i^J + x_i^K) \)

The distance, \( d \), from point T to node I is a measure of distortion while
the difference \( h - \bar{h} \) measures squeeze. Therefore, the criterion proposed by
Giuliani [18] is the minimisation of:

\[ G = \sum_{N} \left( \frac{h - \bar{h}}{\bar{h}} \right) + \sum_{N} \left( \frac{2d}{\bar{E}} \right)^2 \]  \hspace{1cm} (A7)

which, for the present case must be entered with the following expressions
for \( h \) and \( d \):
COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING

\[ h = \frac{1}{b} [P_k (1^\alpha \sigma_k + 1^\beta \sigma_k) + 2a'] \]  \hspace{1cm} (A8)

\[ d = |n_1| \]  \hspace{1cm} (A9)

where \( n_1 = x_1 + 1^\alpha a_1 + 1^\beta \beta_1 - x_1 \frac{P_k (1^\alpha \sigma_k + 1^\beta \sigma_k) + 2a'}{b} (v_j a_j \beta_1 - v_j \beta_j a_1) \)

The minimisation of \( G \) leads to the determination of \( 1^\alpha \) and \( 1^\beta \)

\[ 1^\alpha = \frac{S_1 S_{22} - S_{12} S_2}{S_{11} S_{22} - S_{12}^2} \hspace{1cm} (A10) \]

\[ 1^\beta = \frac{S_{11} S_2 - S_1 S_{12}}{S_{11} S_{22} - S_{12}^2} \]

where

\[ S_{11} = \sum_{N} R_1 P'_a \sigma^2 + \sum_{N} R_2 A_i A_i \]

\[ S_{12} = \sum_{N} R_1 P'_a \sigma \beta + \sum_{N} R_2 A_i B_i \]

\[ S_{22} = \sum_{N} R_1 \beta^2 + \sum_{N} R_2 B_i B_i \]

\[ S_1 = \Sigma R_1 Q \sigma \sigma \]

\[ S_2 = \Sigma R_1 Q \sigma \beta + \Sigma R_2 C_i A_i \]

\( P'_a = P_{a_i} / b \)

\( P'_\beta = P_{\beta_i} / b \)

\( A_i = a_i - P'_a \omega_i \)

\( B_i = \beta_i - P'_\beta \omega_i \)

\( C_i = x_i^T - x_i \omega_i - 2a' \)

\( \omega_i = v_j a_j \beta_1 - v_j \beta_j a_1 \)

\( R_1 = (B/2A)^2 \)

\( R_2 = (2N/B)^2 \)
REFERENCES


7. MAINI, Y.N.T. and WILKINS, M. - Two and Three-Dimensional Analysis of Penetration and Perforation, 6th International Conference in Fracture, New Delhi, India, 4-10 December 1984.


COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING


FIGURES

Figure 1. Mechanical and Thermal Computational Cycles
Coupled thermo-mechanical calculations using rezoning

Figure 4. Deformations and effective stress contours at 5mm indentation

Figure 5. Comparison of geometrical predictions
COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING

Figure 2. Experimental Setup

Figure 3. Mesh Idealisation Used in the Analysis
COUPLED THERMO-MECHANICAL CALCULATIONS USING REZONING

Figure 6. Computed and Measured Load-Indentation Relationships

Figure 7. Comparisons of Experimental Observations and Numerical Predictions
Figure 8. Comparison of Force-Indentation Curves

Figure 9. Contours of Effective Stress at 4.8mm Indentation in MPa
Figure 10. Deformed Shape after Rezoning at 4.8mm