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Finite element procedure of initial shape determination for hyperelasticity

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Abstract. In the shape design of flexible structures. it is useful to predict the initial shape from the desirable large deformed shapes under some loading conditions. In this paper, we present a numerical procedure of an initial shape determination problem for hyperelastic materials which enables us to calculate an initial shape corresponding to the prescribed deformed shape and boundary condition. The present procedure is based on an Arbitrary Lagrangian-Eulerian (ALE) finite element method for hyperelasticity, in which arbitrary change of shapes in both the initial and deformed states can be treated by considering the variation of geometric mappings in the equilibrium equation. Then the determination problem of the initial shape can be formulated as a nonlinear problem to solve the unknown initial shape for the specified deformed shape that satisfies the equilibrium equation. The present approach can be implemented easily to the finite element method by employing the isoparametric hypothesis. Some basic numerical results are also given to characterize the present procedure.

Key words: initial shape determination; incompressible hyperelasticity; arbitrary Lagrangian-Eulerian; finite element method.

1. Introduction

Flexible or expansible materials such as rubber-like ones are often used under elastic large deformed states with severe stress concentration in the structures. In such situations, the initial shape of the structure or the shape to be manufactured should be designed so that large deformed shape under some loading conditions may be desirable. In the conventional design process of such structures, large deformation analyses in which the deformed shape is calculated from the given initial shape and boundary condition are performed successively for various initial shapes until some requirement for the deformed shape is satisfied. In more sophisticated ways to obtain an optimal initial shape, sensitivity with respect to design parameters is calculated simultaneously with the large deformation analysis (e.g., Kleiber and Hisada 1993).

An initial shape determination (or inverse shape) problem, in which the initial shape is solved from the prescribed deformed shape under the given boundary condition, may lead to an alternative approach in this kind of the design problem. In this paper, the initial shape determination problem of hyperelasticity, which is often employed in the computational mechanics to analyze this type of large deformation problems, is discussed and a numerical procedure for this problem is developed.

Hyperelasticity is characterized by the stored energy function expressed in terms of the de-

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formation mapping associating the initial configuration with the spatial one. Then the stresses can be uniquely determined through the stored energy density from the deformation gradient independently of strain histories, and hence the initial and spatial configuration can be interchanged in the representation of the equilibrium equation. By using this material property, Shield (Shield 1967) introduced the inverse motion in which the deformed shape is taken as the reference configuration and the initial shape is unknown variable and proposed a formulation of an initial shape determination problem recently, Govindjee, *et al.* (Govindjec and Mihalic 1995) extended this method by using the energy-momentum formulation and developed a finite element procedure of this problem.

In this work, we propose another approach of this problem by an arbitrary Lagrangian-Eulerian (ALE) kinematic description. The ALE formulation for hyperelasticity was originally developed by the authors to introduce arbitrary mesh motion in the finite element analysis of the large deformation problem (Yamada and Kikuchi 1993). In this formulation, a reference configuration that is independent of both the initial and deformed ones is introduced and arbitrary changes of shapes in both the initial and deformed state can be treated without loss of accuracy by considering the variation of geometric mappings in the equilibrium equation. Therefore the initial shape determination problem can be formulated as a problem to find the pair of the initial and deformed configurations that satisfy the equilibrium equation formulated by the ALE description. Further the present ALE description can be approximated easily by the finite element discretization based on the isoparametric hypothesis.

In this paper, our approach is applied to incompressible hyperelasticity that is a typical constitutive relation of rubber-like materials and a finite element procedure of the initial shape determination based on the ALE formulation is presented. Several numerical examples are also shown to characterize the present approach.

2. Variational formulation

2.1. Large deformation problem of incompressible hyperelasticity

For the purpose of formulating the boundary value problem of hyperelasticity, the Lagrangian description of motion is usually employed. In the Lagrangian description, the deformation is described by the deformation mapping ϕ, which is defined as the mapping from the initial configuration R_X to the deformed configuration R_y. By introducing the Lagrange multiplier p enforcing the incompressibility constraint, the boundary value problem can be formulated as the stationary problem of the following functional defined in terms of ϕ and p:

$$\Pi(\phi, p) = \int_{R_X} \{W(\widetilde{F}) - p(J-1)\}\, dX + \Pi^{ext}(\phi), \tag{1}$$

where W is the stored energy function of incompressible hyperelastic material; J is the Jaconbian of the deformation gradient, and equal to the ratio of current to initial volume; $\widetilde{F}$ is the normalized deformation gradient, in which the volumetric part of the deformation gradient F is eliminated multiplicatively as follows:

$$\widetilde{F}^a_A = J^{-1/3} F^a_A. \tag{2}$$

Further $\Pi^{ext}(\phi)$ is the potential energy of the external loads defined by

$$\Pi^{ext}(\phi) = -\int_{R_X} b_a \phi^a \, dX - \int_{\partial R_X^t} t_a \phi^a \, dS \,, \tag{3}$$

where b_a is the body force and t_a is the traction force defined on a part of boundary $\partial R_X^t \subset \partial R_X$.

Let η and ζ be the admissible variations of ϕ and p, respectively. By taking the first variation of the functional Eq. (1) with respect to ϕ and p, two variational equations can be given by

$$N^{eq}(\phi, p; \eta) = D_\phi \Pi(\phi, p) \cdot (\eta \circ \phi)$$

$$= \int_\Omega [\{\bar{\tau}^{ab}(\tilde{F}) - \frac{1}{3}\bar{\tau}^{cd}(\tilde{F}) g_{cd} g^{ab}\} \eta_{(a,b)} - pJG'(J) \eta^a |_a] \, dX + \Pi^{ext}(\eta) = 0, \tag{4}$$

$$N^{con}(\phi, p : \zeta) = D_p \Pi(\phi, p) \cdot \zeta = -\int_\Omega \zeta (J-1) \, dX = 0 \,, \tag{4}$$

where

$$\eta_{(a,b)} = \frac{1}{2}(\eta^c |_a g_{cb} + \eta^c |_b g_{ca}), \; \bar{\tau}^{ab}(\tilde{F}) = \left[2F_A^a F_B^b \frac{\partial W(F)}{\partial C_{AB}} \right]_{F=\tilde{F}} \,,$$

and '$|$' is used to designate the covariant derivative; $D_f \Pi(f)$ denotes the Fréchet derivative of $\Pi(f)$ with respect to f. Note that the first variation of $\Pi^{ext}(\phi)$ is $\Pi^{ext}(\eta)$. The Eqs. (4) and (5) are the weak forms of the equilibrium equation and the incompressibility contraint equation, respectively.

2.2. ALE formulation and initial shape determination

To formulate the determination problem of the initial shape, we employ an ALE description for hyperelasticity in which the deformation mapping can be represented exactly. To realize an ALE description, we introduce the reference configuration which is independent of both the initial and deformed configurations. We assume that the reference configuration R_z is connected with the initial configuration R_X and the deformed configuration R_y by the mapping χ and ψ, respectively (see Fig. 1). In this case, the deformation mapping ϕ can be expressed as the following composite mapping of χ and ψ:

$$\phi = \psi \circ \chi^{-1}. \tag{6}$$

Here, the mappings χ and ψ are one-to-one and onto.

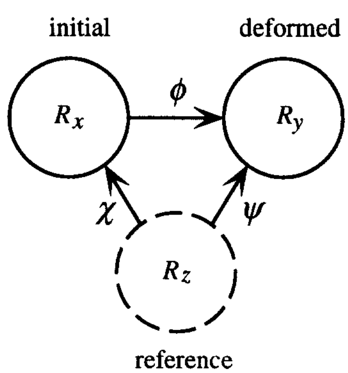


Fig. 1 Diagram of domains and mappings for ALE description.

In this case, the unknown function ϕ in the variational Eqs. (4) and (5) can be replaced by the function χ and ψ. Using χ and ψ, we can rewrite Eqs. (4) and (5) as follows:

$$N^{eq}(\phi, p; \eta) = N^{eq}(\chi, \psi, p; \eta) = 0, \tag{7}$$
$$N^{con}(\phi, p; \zeta) = N^{con}(\chi, \psi, p; \zeta) = 0. \tag{8}$$

Here, we assume that the pressure field p is defined in terms of the reference coordinates.

If ψ is fixed and χ is taken as an unknown variable, we have a formulation of the initial shape determination, in which the initial shape is calculated from the specified deformed configuration under certain loading condition. Now if χ is solved in this problem, the mapping ϕ composed of χ and ψ is determined uniquely. Thus the solvability of the initial shape determination problem based on the present formulation is similar to that of the large deformation problem.

To establish a numerical procedure to solve the variational Eqs. (7) and (8), which are nonlinear, we need to obtain the incremental forms of the variational equations calculated by the linearization with respect to increments of the unknown variables. Let U, v and q be the increments of χ, ψ and p, respectively. It is noted that U and v are respectively defined in the initial and current configuration, and q is defined in the reference configuration. By substituting $\{\chi + U\circ\chi,\ \psi + v\circ\psi,\ p+q\}$ for $\{\chi, \psi, p\}$ in Eqs. (7) and (8) and using Taylor's formula up to the first order terms of increments, the incremental variational equations can be shown to be

$$\begin{aligned}
&N^{eq}(\chi + U\circ\chi, \psi + v\circ\psi, p + q; \eta) \cong N^{eq}(\chi, \psi, p; \eta)\\
&+D_\chi N^{eq}(\chi, \psi, p; \eta)\cdot(U\circ\chi) + D_\psi N^{eq}(\chi, \psi, p; \eta)\cdot(v\circ\psi)\\
&+D_p N^{eq}(\chi, \psi, p; \eta)\cdot q = 0,
\end{aligned} \tag{9}$$

$$\begin{aligned}
&N^{con}(\chi + U\circ\chi, \psi + v\circ\psi, p + q; \zeta) \cong N^{con}(\chi, \psi, p; \zeta)\\
&+D_\chi N^{con}(\chi, \psi, p; \zeta)\cdot(U\circ\chi) + D_\psi N^{con}(\chi, \psi, p; \zeta)\cdot(v\circ\psi)\\
&+D_p N^{con}(\chi, \psi, p; \zeta)\cdot q = 0.
\end{aligned} \tag{10}$$

The Fréchet derivatives with respect to χ appearing in Eqs. (9) and (10) correspond to sensitivities related with the change of the initial configuration.

To evaluate Eqs. (9) and (10), we need to calculate the Fréchet derivatives of the stress with respect to χ. In the hyperelastic constitutive relation discussed here, the stresses can be uniquely determined through the stored energy density from the deformation gradient independently of the stress histories. Thus, suppose that the material is homogeneous in the whole domain, the Fréchet derivatives of the stress can be calculated from the Fréchet derivatives of the deformation gradient. Concrete forms of the Fréchet derivatives in the weak forms are expressed by

$$\begin{aligned}
D_\chi N^{eq}(\chi, \psi, p; \eta)\cdot(U\circ\chi) = &\int_{R_X}\Big[-c^{abcd}\big(\eta_{(a,b)} - \tfrac{1}{3}\eta^e|_e\, g_{ab}\big)\big(U^{\#}_{(c,d)} - \tfrac{1}{3}U^E|_E\, g_{cd}\big)\\
&+2\bar{\tau}^{ab}(\tilde{F})\big(\eta_{(a,b)} - \tfrac{1}{3}\eta^d|_d\, g_{ac}\big)U^{\#c}{}_{,b} + \tfrac{5}{3}\bar{\tau}^{ab}(\tilde{F})\big(\eta_{(a,b)} - \tfrac{1}{3}\eta^c|_c\, g_{ab}\big)U^A|_A\\
&+pJ^2G''(J)\eta^a|_a U^A|_A\Big]dX - \int_{R_X}\big(b_a\eta^a U^A|_A + b_{a,A}\eta^a U^A\big)\,dX\\
&-\int_{\partial R_X^t}\{t_a\eta^a(U^A|_A - U^A|_C(v^X)_A(v^X)_B G^{BC}) + t_{a,A}\eta^a U^A\}\,dS,
\end{aligned} \tag{11}$$

$$D_\psi N^{eq}(\chi, \psi, p; \eta)\cdot(v\circ\psi)$$

$$\int_{R_X}\Big[c^{abcd}\big(\eta_{(a,b)} - \tfrac{1}{3}\eta^e|_e\, g_{ab}\big)\big(v_{(c,d)} - \tfrac{1}{3}v^e|_e\, g_{cd}\big)$$

$$+\bar{\tau}^{ab}(\tilde{F})\{2(\eta^c|_a - \frac{1}{3}\eta^e|_e\,\delta_a^c)(v^d|_b - \frac{1}{3}v^f|_f\,\delta_b^d) - \eta^c|_a\,v^d|_b\}g_{cd}$$
$$-p\{JG'(J)+J^2G''(J)\}\eta^a|_a\,v^b|_b$$
$$+\left\{\frac{1}{3}\bar{\tau}^{ab}(\tilde{F})g_{cd} + pJG'(J)\right\}\eta^a|_b\,v^b|_a]dX, \tag{12}$$

$$D_pN^{eq}(\chi,\psi,p;\eta)\cdot q = -\int_{R_X} qJG'(J)\eta^a|_a dX, \tag{13}$$

$$D_\chi N^{con}(\chi,\psi,p;\zeta)\cdot(U\circ\chi) = -\int_{R_X}\zeta\{G(J)-JG'(J)\}U^A|_A dX, \tag{14}$$

$$D_\psi N^{con}(\chi,\psi,p;\zeta)\cdot(v\circ\psi) = -\int_{R_X}\zeta JG'(J)v^a|_a dX, \tag{15}$$

$$D_pN^{con}(\chi,\psi,p;\zeta)\cdot q = 0, \tag{16}$$

where

$$b_{a,A} = \frac{\partial b_a}{\partial X^A},\quad t_{a,A} = \frac{\partial t_a}{\partial X^A}.$$

The detail of the derivation of the above expressions can be found in our previous paper (Yamada and Kikuchi 1993).

By using the Eqs. (9) and (10), the linearized initial shape determination problem can be formulated as a problem to solve the following equations with U and q taken as unknown variables:

$$D_\chi N^{eq}(\chi,\psi,p;\eta)\cdot(U\circ\chi) + D_pN^{eq}(\chi,\psi,p;\eta)\cdot q$$
$$= -N^{eq}(\chi,\psi,p;\eta) - D_\psi N^{eq}(\chi,\psi,p;\eta)\cdot(v\circ\psi), \tag{17}$$

$$D_\chi N^{con}(\chi,\psi,p;\zeta)\cdot(U\circ\chi) + D_pN^{con}(\chi,\psi,p;\zeta)\cdot q$$
$$= -N^{con}(\chi,\psi,p;\zeta) - D_\psi N^{con}(\chi,\psi,p;\zeta)\cdot(v\circ\psi). \tag{18}$$

It is noted that v, the increment of the deformed configuration, is not zero necessarily. If v is specified appropriately, we can consider the initial shape determination problem for prescribed displacements as a loading condition.

3. Finite element discretization

To discretize geometry and kinematics by the finite element approximation for the present ALE formulation, we adopt the isoparametric hypothesis in which the initial and deformed configurations are described by using common interpolation functions defined in terms of the isoparametric coordinates. In this case, the isoparametric coordinates are identified with the coordinates of the reference domain R_z. Thus, the mapping from the parent element into the material configuration corresponds to the mapping χ, whereas the mapping from the parent element into the spatial configuration corresponds to the mapping ψ (see Fig. 1). In the conventional large deformation analysis by using the isoparametric element and the Lagrangian description, the mapping χ is fixed and the mapping ψ is taken as an unknown variable. On the other hand, in the present initial shape determination, the mapping χ is taken as an unknown variable, while ψ is fixed.

In this work, the plane strain problems are considered and the plane strain assumption is treated by imposing as zero the displacement component perpendicular to the plane. For a pressure/displacement mixed finite element, we employ the six node composite element, in which its displacement field is assumed to be piecewise linear by a combination of four linear triangle elements, and its pressure field is assumed to be constant over an element and discontinuous across element interfaces (Fig. 2). Note that this element satisfies the BB (or the uniform lifting) condition.

By implementing the present ALE formulation to such finite element discretization, the matrix form of variational Eqs. (7) and (8) can be derived as

$$N^{eq}(\chi, \psi, p; \eta) = \boldsymbol{\eta}^t (\boldsymbol{f}^{int} - \boldsymbol{f}^{ext}) = 0, \tag{19}$$

$$N^{con}(\chi, \psi, p; \zeta) = -\boldsymbol{\zeta}^t \boldsymbol{r} = 0, \tag{20}$$

Further, the Fréchet derivatives appearing in the incremental variational Eqs. (9) and (10) can be expressed as

$$\begin{aligned}
D_\chi N^{eq}(\chi, \psi, p; \eta) \cdot U \circ \chi &= \boldsymbol{\eta}^t \boldsymbol{K}^{AD} \boldsymbol{U}, \\
D_\psi N^{eq}(\chi, \psi, p; \eta) \cdot v \circ \psi &= \boldsymbol{\eta}^t \boldsymbol{K}^{LD} \boldsymbol{v}, \\
D_\chi N^{con}(\chi, \psi, p; \zeta) \cdot U \circ \chi &= \boldsymbol{\zeta}^t \boldsymbol{K}^{AP} \boldsymbol{U}, \\
D_\psi N^{con}(\chi, \psi, p; \zeta) \cdot v \circ \psi &= \boldsymbol{\zeta}^t \boldsymbol{K}^{LP} \boldsymbol{v}, \\
D_p N^{eq}(\chi, \psi, p; \eta) \cdot q &= \boldsymbol{\eta}^t (\boldsymbol{K}^{LP})^t \boldsymbol{q}, \\
D_p N^{con}(\chi, \psi, p; \zeta) \cdot q &= 0.
\end{aligned} \tag{21}$$

Finally by considering that admissible vectors $\boldsymbol{\eta}$ and $\boldsymbol{\zeta}$ are arbitrary, the matrix forms of the discretized incremental variational Eqs. (17) and (18) can be shown to be

$$\begin{bmatrix} \boldsymbol{K}^{AD} & (\boldsymbol{K}^{LP})^t \\ \boldsymbol{K}^{AP} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{U} \\ \boldsymbol{q} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}^{ext} - \boldsymbol{f}^{int} \\ \boldsymbol{r} \end{bmatrix} - \begin{bmatrix} \boldsymbol{K}^{LD} \\ \boldsymbol{K}^{LP} \end{bmatrix} [\boldsymbol{v}]. \tag{22}$$

By using Eq. (22) and applying the newton-Raphson method, an iterative procedure to solve the determination problem of the initial shape can be constructed. The iterations in this procedure are continued until the residual force vector appearing as the first term in the right hand side of Eq. (22) reaches the tolerance.

In the actual calculation of the initial shape determination, which involves geometrical nonlinearity, we cannot always obtain the required solution in one iterative process for the specified condition. Then we need to use an incremental procedure, in which an initial condition and a loading history are specified. For an initial condition, we can use the trivial solution in which the initial configuration is identical with the deformed one and the subjected force is zero. For a loading history, the increment of the external force f^{ext} can be specified. Then the initial shape that corresponds to the prescribed deformed shape for such a incremental external force can be calculated by the iterative procedure mentioned above. For another kind of a loading history, the in-

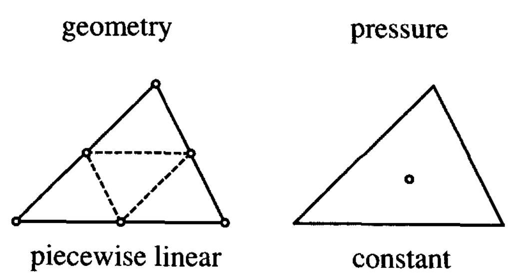


Fig. 2 Finite element.

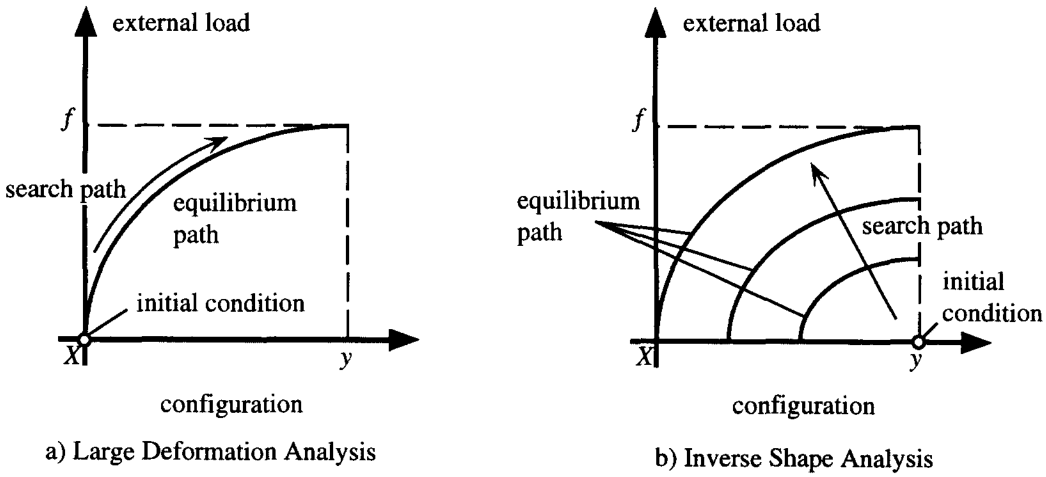


Fig. 3 Schematic diagrams of solution process.

crement of the deformed configuration, denoted by v in the Eq. (22), can be applied instead of the incremental external force. In this case, the initial shape can be successively calculated and the final initial shape is attained when the increasing deformed shape reaches the required state.

3.1. Remarks

In the large deformation analysis, numerical solutions of the deformed shape are sought along the equilibrium path. For the initial shape determination analysis presented here, numerical solutions of the initial shape are found among pairs of the initial and deformed shapes that satisfy the equilibrium equation under the prescribed boundary condition and are on the different e-quilibrium paths (see Fig. 3). Therefore the loading history that brings the equilibrium state from the calculated initial shape to the prescribed deformed one cannot be taken into account in the present initial shape determination. Further the loading history applied in the initial shape determination corresponds to neither the loading nor unloading path associated with the calculated initial shape and the prescribed deformed one.

4. Numerical examples

In the following numerical examples, Mooney-Rivlin's law is employed as the most popular constitutive relation for isotropic rubber-like materials. For this material modelling, the stored energy function W is described as

$$W(F) = W(I_1, I_2) = c_1(I_1 - 3) + c_2(I_2 - 3), \tag{4.1}$$

where I_1 and I_2 are the first and second invariants of the right Cauchy-Green deformation tensor, respectively; c_1 and c_2 are material constants, which are chosen: c_1=1.5, c_2=0.5.

4.1. Compression by uniform end shortening

An initial shape determination problem of a block subjected to uniform end shortening in the

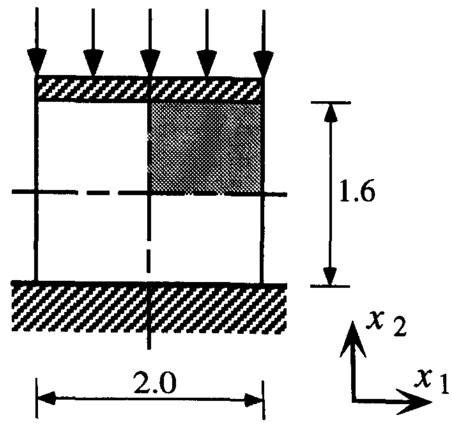


Fig. 4 Compression by uniform end shortening: definition of the problem.

plane strain is solved as the first example. Considered geometry and boundary conditions are depicted in Fig. 4. Only one quarter of the block indicated as a shaded part in Fig. 4 is considered by taking advantage of symmetric properties of the problem. Displacement in x_1-direction along the left edge and that in x_2-direction along the bottom edge are fixed owing to symmetric condition. Along the top edge, displacement in x_1-direction is fixed and uniform compressive displacement in x_2-direction is considered. The finite element mesh in the prescribed deformed configuration is shown in Fig. 5.

Fig. 6 indicates the initial shape for 20% compression in which the initial height is 2.0. It is confirmed that the deformed shape prescribed in the initial shape determination is identical with that obtained by the large deformation analysis with the initial shape calculated from the present approach. Fig. 7 shows the distribution of the stored energy density in the deformed state associated with the calculated initial shape. The distribution of the stored energy density corresponding to the square block subjected to the uniform end shortening is also depicted in Fig. 7. This result is calculated by the Updated Lagrangian procedure with the rezoning (Yamada 1993). It is observed that severe stress concentration occurs around the corner for the compressed square block. On the other hand, the stress concentration for the calculated initial shape is not so severe. Thus the present approach gives an initial shape designed better. Therefore the

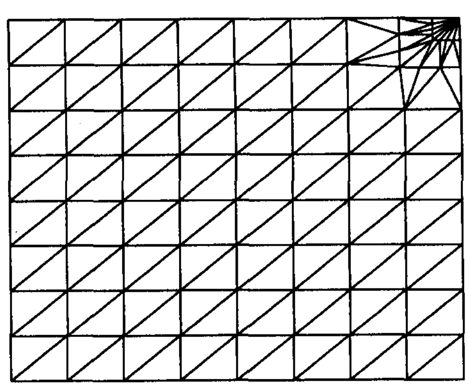


Fig. 5 Compression by uniform end shortening: finite element mesh.

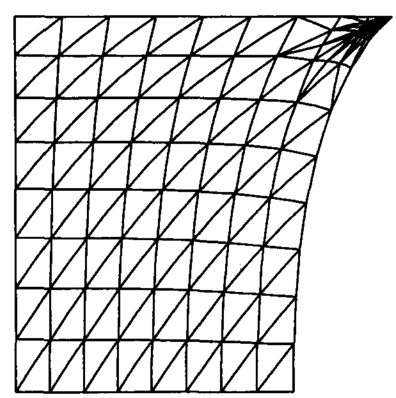
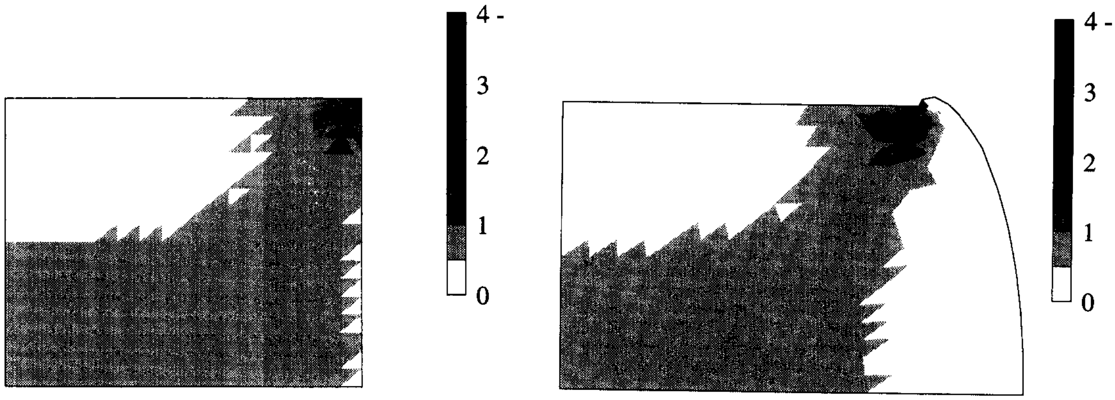


Fig. 6 Compression by uniform end shortening: calculated initial shape for 20% compression.



(a) Calculated Initial Shape (b) Square Initial Shape

Fig. 7 Compression by uniform end shortening: distribution of the stored energy density for 20% compression.

present approach is efficient to design the initial shape of the structure subjected to the large prescribed displacement.

4.2. Compression by uniform traction

The second example is an initial shape determination problem of a block subjected to uniform traction indicated in Fig. 8. Only a half of the block indicated as a shaded part in Fig. 8 is considered by taking advantage of symmetric properties of the problem. Displacement in x_1-direction along the left dege is fixed owing to symmetric condition. The displacement along the bottom edge are fixed in both the directions. Along the top edge, uniform compressive traction in x_2-direction is applied. The same finite element mesh in the deformed configuration as in the previous example shown in Fig. 5 is used.

Fig. 9 indicates the calculated initial shape for the traction f=1.0. The large deformation analysis is also performed by applying the uniform traction to the top edge of the calculated initial shape in Fig. 9. In this analysis, the incremental procedure with the traction increased monotonically is employed. The corresponding deformed shape for the traction f=1.0 is shown in Fig. 10. This deformed shape is quite different from the prescribed one in the initial shape determination. In other words, the deformed shape cannot reach the prescribed one from the calculated initial shape in the large de-

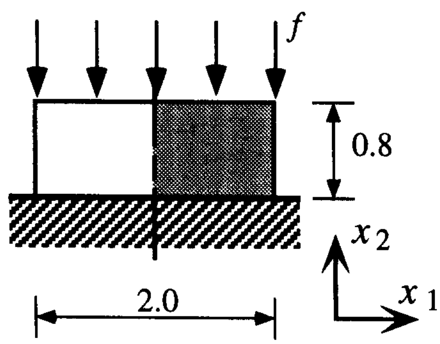


Fig. 8 Compression by uniform traction: definition of the problem.

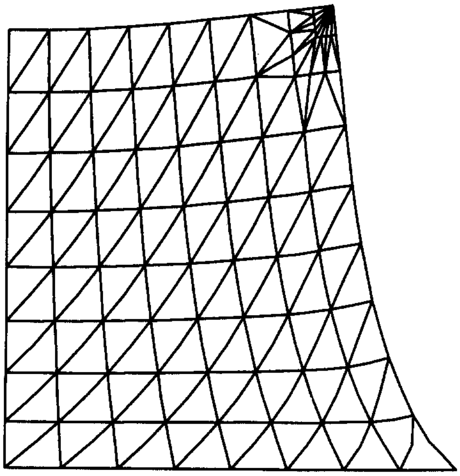


Fig. 9 Compression by uniform traction: calculated initial shape for f=1.0.

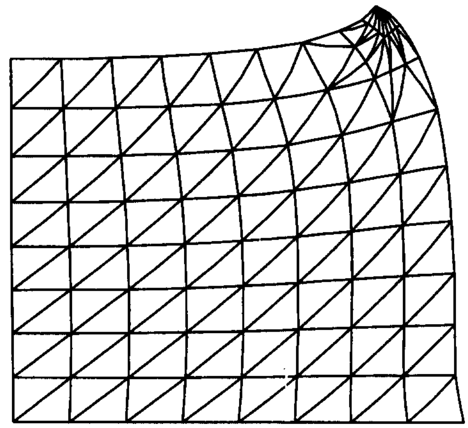


Fig. 10 Compression by uniform traction: deformed shape associated with the calculated initial shape and uniform traction f=1.0.

formation analysis. It is recalled that the equilibrium path cannot be considered in the present initial shape determination. These results show that the calculated initial shape is sought on the different loading path from the path corresponding to the uniform traction increased monotonically (see Fig. 11). However the pair of the calculated initial shape and the prescribed deformed one in the initial shape determination satisfies the governing equation and hence there may exist at least one loading path from such an initial shape to the deformed one.

5. Concluding remarks

A formulation of an initial shape determination based on an arbitrary Lagrangian-Eulerian description of motion and its finite element procedure have been presented for the large deformation problem of hyperelasticity. The initial shape that gives the specified deformed shape under the given loading condition can be calculated in the similar procedure to the large deformation analysis. In this procedure, the equilibrium path is not considered to obtain the initial

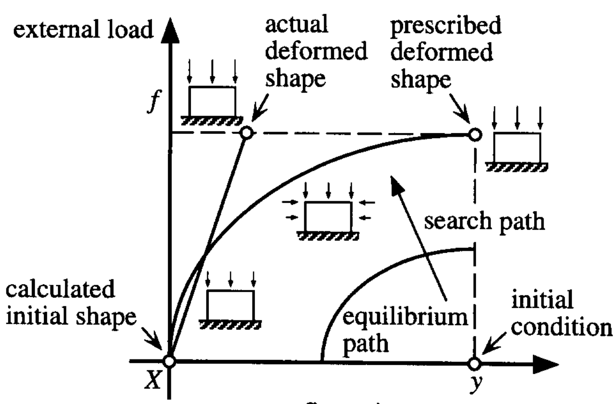


Fig. 11 Schematic diagram of unsuccessful initial shape determination.

shape and the deformed shape started from the calculated initial shape does not always reach the prescribed deformed shape in the large deformation analysis. To apply the present approach to practical problems, it is necessary to verify the deformed shape by performing the large deformation analysis with the obtained initial shape. We need further research to characterize the present initial shape determination problem.

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