A Conservative Time Integration Scheme for Dynamics of Elasto-damaged Thin Shells

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Abstract: Some aspects of the application of a conservative time integration scheme to the non-linear dynamics of elasto-damaged thin shells are presented. The main characteristic of the scheme is to be conservative, in the sense that it allows the time-discrete system to preserve the basic laws of continuum, namely the balance of the linear and angular momenta as well as the fulfillment of the second law of thermodynamic. Here the method is applied to thin shells under large displacements and rotations. The constitutive model adopted is built coupling the linear elastic model of De Saint Venant-Kirchhoff with a scalar damage function depending on the maximum value of a suitable strain measure attained through the deformation history.

keyword: shells, large deformations, non-linear dynamics, time integration algorithms

1 Introduction

The present paper deals with the application of the energy-momentum method to the non-linear dynamics of thin shells, made of materials with internal dissipation. The approach follows the method already applied to the elasto-damaged continuum dynamics in finite strains [Briseghella, Majorana and Pavan (1998); Briseghella, Majorana, Pavan (2000)]. The energy-momentum method is a time integration algorithm that has been formulated with respect to the rigid body [Simo and Wong (1991)], the continuum [Simo and Tarnow (1992)], the shells [Simo, Rifai and Fox (1992)] and rods [Simo, Tarnow, and Doblare (1995)] dynamics. The algorithm is an implicit scheme, defined as conservative because it ensures the fulfillment of the basic laws of continuum, i.e. the balance laws of linear and angular momentum and the balance of energy of the system. The conservation of the energy of the system leads to define the method as unconditionally stable. This means, for example, that for an elastic body subjected only to initial conditions (assigned configuration and velocity fields) and in absence of external loading the total energy of the system, discretised in time, represents a constant of the motion, that is what happens in the continuum system. This property is not preserved by other types of integration schemes such those belonging to the Newmark’s family if applied to non linear dynamics of elastic systems because the latter can ensure only the balance of the linear and angular momentum. Hence, this time integration scheme has been applied in particular to long term dynamics of elastic systems ensuring a similar description of the motion in contrast with solutions arising from other types of schemes.

The conservative character of the scheme if applied to a system with internal dissipation must be intended as the fulfillment of the Clausius-Duhem inequality in time in its discrete form. On the other side, for elastic systems the latter inequality leads simply to the equivalence between the rate of the stored energy function of the material and the internal power, i.e. the rate of work made by the internal forces.

The implementation here presented is strictly related to a quite standard approach as far as the parameterisation of the shell is concerned [Brank, Briseghella, Tonello and Damjanic (1998); Brank, Mamouri and Ibrahimbegovi (2003)]. The present approach is closed to these works especially as regards:

- the kinematics of the shell and in particular the description of the finite rotations and their updating in the discrete time system;
- the definition of the elastic constitutive model adopted as basis for the definition of the elasto-damage constitutive model;
- the general approach in the definition of the weak form, its discretisation and linearisation method.
On the contrary, the method is modified as regards the choice of the constitutive model. This fact has some consequences in terms of:

- definition of the internal forces and dissipation;
- method for the evaluation of the conservative algorithmic forms of the latter;
- specific aspects in the application of the Newton method adopted for the linearisation of the weak form.

The constitutive model adopted is chosen only to have an internal dissipation and it is not assumed to describe any real material behaviour. Hence the simplicity of the model has been favoured. The elasto-damage model is obtained starting from the definition of the De Saint Venant-Kirchhoff elastic model coupling the related stored energy function with a scalar damage function. The resulting constitutive model is similar to those proposed for the description of elastomeric materials, where the fraction of damage depends on the maximum value attained by an equivalent strain measure in the strain history of the material [Simo (1987)].

The space discretisation is made by using isoparametric four noded elements, in order to preserve the conservative character of the algorithm. Possible shear locking problems, arising in case of thin shells, are avoided through the adoption of the ‘assumed natural strain’ (ANS) approach [Dvorkin and Bathe (1984); Baar and Kintzel (2003)]. The weak form of the balance of momentum is linearised by using the Newton-Raphson method leading to a second order scheme. Some details on the calculation of the internal forces term of the weak form are given, together with the procedure adopted in order to get the algorithmic forms of stress and dissipation that lead to the conservative character of the time integration scheme.

Finally, the examples here reported show the properties of the time integration scheme adopted in terms of fulfilment of the balance laws of the linear and angular momentum, as well as of the discrete form of the Clausius-Duhem inequality, emphasizing the convergence properties.

2 Kinematics of shell

The reference configuration of the shell is defined by the \( \Omega \subseteq \mathbb{R}^3 \). The motion is the set of configurations given by

\[ \varphi(\Omega,t) : \mathbb{R}^3 \times [0,T] \rightarrow \mathbb{R}^3 \] where \([0,T]\) is the time interval of interest.

A point in the reference configuration of the shell is given by:

\[ \mathbf{X}(\xi^1,\xi^2,\xi) = \mathbf{X}(\xi^1,\xi^2) + \xi \mathbf{T} \] (1)

where \( \mathbf{X} \) is a point belonging to the mid surface of the shell. The unit vector \( \mathbf{T} \) is normal to the mid surface at the point \( \mathbf{X} \).

![Figure 1: Reference system of co-ordinate of the mid plane of the shell.](image)

The adopted system of co-ordinates \( \xi^1, \xi^2, \xi \) is defined with \( \xi^1, \xi^2 \) lying on the mid surface and \( \xi \) along \( \mathbf{T} \). The variable \( \xi \) assumes the values \( \xi \in [-h/2,+h/2] \) where \( h \) is the thickness of the shell. The points of the current, or deformed, configuration of the shell are defined by

\[ \mathbf{x}(\xi^1,\xi^2,\xi) = \mathbf{x}(\xi^1,\xi^2) + \xi \mathbf{t} \] (2)

with \( \mathbf{t} \) the unit vector. The unit vectors \( \mathbf{T} \) and \( \mathbf{t} \) are called the inextensible directors of the shell. A simple representation of the co-ordinate system in the reference configuration is shown in Figure 1. The displacements of a generic point of the shell \( \mathbf{U} \) and of a point belonging to its mid surface \( \mathbf{u} \) are defined as

\[ \mathbf{U} = \mathbf{x} - \mathbf{X}, \quad \mathbf{u} = \mathbf{x} - \mathbf{X} \] (3)

Adopting a lagrangian description [Suetake, Iura and Atluri (2001)] of the shell kinematics, the strains are described in terms of the Green-Lagrange tensor, defined by

\[ \mathbf{E} = \frac{1}{2} (\mathbf{g}_i \cdot \mathbf{g}_j - \mathbf{G}_i \cdot \mathbf{G}_j) \mathbf{G}^i \otimes \mathbf{G}^j \quad (i = 1, 2, 3) \] (4)
The terms \( G_i \) and \( g_i \) are the covariant components, while \( G^i \) are the contravariant components (dual basis of \( G_i \)) of the metric in the material and, respectively, the spatial reference systems. The covariant basis in the undeformed configuration is defined as

\[
G_\alpha = \frac{\partial X}{\partial \xi^\alpha}, \quad G_3 = \frac{\partial X}{\partial \xi} \quad (\alpha = 1, 2) \tag{5}
\]

while in the current reference systems one has

\[
g_\alpha = \frac{\partial \xi}{\partial \xi^\alpha}, \quad g_3 = \frac{\partial \xi}{\partial \xi} \quad (\alpha = 1, 2) \tag{6}
\]

According to the assumption made with the choice of the parameterisation represented by eq. (1) if the thickness \( h \) of the shell is small the components of the Green-Lagrange strain tensor are such that one obtains

\[
E_{ij} = E_{ij}^{(0)} + \xi E_{ij}^{(1)} + \xi^2 E_{ij}^{(2)} \quad (i = 1, 2, 3) \tag{7}
\]

With the assumption of a thin shell the terms of the second order in \( \xi \) can be neglected, while with relations (4), (5) and (6) at hands one obtains

\[
E_{\alpha 3}^{(0)} = E_{3\alpha}^{(0)} = \frac{1}{2} \left[ \partial X/\partial \xi^\alpha \cdot (t - T) + \partial u/\partial \xi^\alpha \cdot t \right] \tag{8}
\]

\[
E_{\alpha \beta}^{(0)} = \frac{1}{2} \left[ \partial X/\partial \xi^\alpha \cdot \partial u/\partial \xi^\beta \right. \\
\left. + \partial X/\partial \xi^\beta \cdot \partial u/\partial \xi^\alpha + \partial u/\partial \xi^\alpha \cdot \partial u/\partial \xi^\beta \right] \tag{9}
\]

\[
E_{\alpha \beta}^{(1)} = \frac{1}{2} \left[ \partial X/\partial \xi^\alpha \cdot \partial (t - T)/\partial \xi^\beta \\
+ \partial X/\partial \xi^\beta \cdot \partial (t - T)/\partial \xi^\alpha \\
+ \partial u/\partial \xi^\alpha \cdot \partial t/\partial \xi^\beta + \partial u/\partial \xi^\beta \cdot \partial t/\partial \xi^\alpha \right] \tag{10}
\]

Moreover the component \( E_{33} \) vanishes. Further assumptions are introduced in order to simplify the formulation of the shell structure. Covariant and contravariant components in the reference configuration, are approximated by their values in the mid plane of the shell \( M_0 \)

\[
A_j = G_j|_{\xi=0} \quad A^i = G^i|_{\xi=0} \quad (i = 1, 2, 3) \tag{11}
\]

This makes it possible to integrate the stress components through the thickness of the shell obtaining stress resultants. All the details about the indicated procedure can be found in [Brank, Briseghella, Tonello and Damanic (1998)]. The strain components can be identified as membrane, transverse shear and bending components

\[
e = \begin{bmatrix} E^{(0)}_{11} & E^{(0)}_{12} & 2E^{(0)}_{12} \\
E^{(0)}_{12} & E^{(0)}_{22} & 2E^{(0)}_{22} \end{bmatrix}^T \tag{12}
\]

\[
\gamma = \begin{bmatrix} 2E^{(0)}_{13} & E^{(0)}_{23} \end{bmatrix}^T \tag{13}
\]

\[
k = \begin{bmatrix} E^{(1)}_{11} & E^{(1)}_{12} & 2E^{(1)}_{12} \end{bmatrix}^T \tag{14}
\]

The inextensible directors of the shell mid-surface in the reference and current configurations are related through an orthogonal tensor, element of the not-commutative space of rotations SO(3):

\[
t = RT, \quad R \in SO(3) = \left\{ R : R^T = R^{-1}, \det R = 1 \right\} \tag{15}
\]

Every orthogonal tensor represents a finite rotation around a vector \( s \) (the axis of rotation). A skew-symmetric tensor \( S \)

\[
S \in so(3) = \left\{ S : S^T = -S \right\} \tag{16}
\]

can be associated to the vector \( s \) (which is called axial of \( S \)). The set \( so(3) \) is the space of infinitesimal rotations. The skew-symmetric tensor \( S \) is defined by the properties \( Ss = 0 \) and \( Sb = s \times b \), fulfilled for any vector \( b \). The tensors \( S \) give the rotation tensor \( R \) through the exponential map

\[
R = \exp[S] = I + (\sin ||s||/||s||) S \\
+ \left[ (1 - \cos ||s||)/||s||^2 \right] S^2 \tag{17}
\]

The main characteristic of the representation of \( R \) tensor through the exponential map (called also Rodrigues’ formula) is to result free from any singularity. This is particularly important if the system to be described undergoes large rotations (which is the case here considered). The velocity of a point of the shell mid plane (derivative with respect to time of \( x \)) will be indicated by \( \dot{x} \) and the angular velocity of the director \( t \) will result \( \omega = \dot{t} \times t \).
3 Constitutive model

The choice of the constitutive model is here motivated in order to obtain a material with internal dissipation. The definition of an elasto-damage model such as the one here presented has the advantage to lead to simple expressions of the internal forces as well as of the terms arising from the linearisation of the weak form. The elasto-damage constitutive model is defined starting from the elastic De Saint Venant-Kirchhoff constitutive model. The stored energy function is coupled in multiplicative way with a scalar damage function defining the Helmoltz free-energy function.

3.1 Elastic constitutive model

For the elastic De Saint Venant-Kirchhoff constitutive model the relation between the second Piola-Kirchhoff stress tensor and the Green-Lagrange strain tensor is given by

\[ S = H : E = \lambda tr[E]I + 2\mu E \] (18)

where \( \lambda \) and \( \mu \) are the Lamè’s elastic constants. In terms of components one has

\[ H_{ijkl} = \lambda G^{ij}G^{kl} + \mu \left( G^{ik}G^{jl} + G^{il}G^{jk} \right) \] (19)

Following the standard procedure in the case of thin shell, the stress component along the normal direction to the mid plane of the shell itself is assumed to be zero and a reduced material tensor can be deduced from eq. (19)

\[ C^{ijkl} = H_{ijkl} - \frac{H^{33kl}}{H^{3333}} (i j \neq 33, k l \neq 33) \] (20)

According to the approximation assumed for the components of the metric, the terms of the reduced four rank tensor (20) are constant through the thickness of the shell, thus the membrane, transverse shear and bending resultant stresses are defined as

\[ n = n^{\alpha \beta}A_{\alpha} \otimes A_{\beta} \] (21)

\[ q = n^{\alpha 3}A_{\alpha} \otimes T + n^{3\alpha}T \otimes A_3 \] (22)

\[ m = m^{\alpha \beta}A_{\alpha} \otimes A_{\beta} \] (23)

where the scalar components are given by

\[ n^{ij} = \int_{-h/2}^{+h/2} C^{ijkl}E_{kl}^{(0)} d\xi , i j \neq 33 , k l \neq 33 \] (24)

\[ m^{\alpha \beta} = \int_{-h/2}^{+h/2} C^{\alpha \beta \gamma \delta}E_{\gamma \delta}^{(1)}(\xi)^{2} d\xi \] (25)

On the basis of the simplifications assumed the stored energy function associated to the constitutive relation (18) results as the sum of three terms relating respectively to the membrane, transverse shear and bending components of the strain, which are not coupled. Adopting a matrix notation, the vector of the stress resultants \( r^T = [n^T, q^T, m^T] \) can be deduced from

\[ r = \frac{\partial W(\Gamma)}{\partial \Gamma} \] (26)

where the stored energy function is a quadratic form of the strain vector \( \Gamma^T = [\varepsilon^T, \gamma^T, \kappa^T] \)

\[ W(\Gamma) = \frac{1}{2} \Gamma^T \begin{bmatrix} C^n & 0 & 0 \\ 0 & C^q & 0 \\ 0 & 0 & C^m \end{bmatrix} \Gamma \] (27)

More details about the terms of the above matrix are given in appendix.

3.2 Elasto-damage constitutive model

Starting from the elastic model defined in the previous section, in particular with the stored energy function (27) at hand, the Helmoltz free energy function is defined as:

\[ \Psi = g(\Xi)W(\Gamma) \] (28)

where \( g \) is a not-growing damage function and \( W \) is the stored energy function of an undamaged material. The \( g \) function can be defined, for example, by

\[ g(\Xi) = b + a(1 - b) \left( 1 - e^{-\Xi/a} \right) \frac{1}{\Xi} \] (29)

where the constants \( a, b \) can assume the values \( a \in ]0, +\infty[ \) and \( b \in [0, 1] \) respectively. For a null value of \( \Xi \) the \( g \) function is equal to unit (undamaged material). For increasing values of \( \Xi \) the \( g \) function is decreasing to
the limit value of $b$ if $\Xi \to \infty$. Hence the parameter $b$ is related to the maximum damage, while $a$ affects the rate of the damage growing with $\Xi$. In the formulation here assumed the variable $\Xi$ represents an equivalent strain measure, based on the value of the stored energy function $W$ of the material supposed undamaged. The equivalent strain is defined as the maximum value attained in the strain history of the material:

$$\Xi = \max_{\tau \in (-\infty, t]} \sqrt{2W(\Gamma(\tau))}$$

(30)

The Clausius-Duhem inequality

$$-\dot{\Psi} + r^T \Gamma = D_{\text{int}} > 0$$

(31)

on the basis of the free energy function assumed leads to the expressions of the generalised stress resultants (components of the vector $r$)

$$n = g(\Xi) C^n e, \quad q = g(\Xi) C^q \gamma, \quad m = g(\Xi) C^m \kappa$$

(32)

and of the internal dissipation

$$D_{\text{int}} = \frac{W(\Gamma)}{\Xi} \frac{dW}{d\Xi} \left[ \frac{\partial W}{\partial \Gamma} \right]^T \Gamma \geq 0.$$  

(33)

The internal dissipation results not negative because of the assumption of a not growing damage function $g$. It is possible to define a damage surface by means of the equation

$$\phi(\Gamma, \Xi) = \sqrt{2W(\Gamma)} - \Xi = 0$$

(34)

the surface $\phi$ gives the admissible values of the variables $\Gamma$ and $\Xi$ that must satisfy the following inequality

$$\phi(\Gamma, \Xi) \leq 0$$

(35)

The previous inequality represents the damage criterion that can be re-assumed by the set of relations

$$\begin{cases} \dot{g}(\Xi) < 0 & \text{for } \phi = 0 \text{ and } [\partial \phi / \partial \Gamma]^T \Gamma > 0 \\ \dot{g}(\Xi) = 0 & \text{otherwise} \end{cases}$$

(36)

The set of relations (36) means that the growing of damage occurs for a loading path starting from the damage surface.

### 4 Balance equations

The following relation gives the total linear momentum of the system:

$$L(\Phi) = \frac{\int}{\Omega} \rho_0 (\dot{x} + \xi \dot{t}) \, d\Omega$$

(37)

where $\rho_0$ is the density in the reference configuration and the symbol $\Phi$ is used to indicate an element of the phase space represented by the pairs $(x, t)$. Integration through the thickness of the shell enables one to rewrite the equation (37) as

$$L(\Phi) = \int_{M_0} p \, dM_0$$

(38)

where the vector $p$ is the linear momentum of the mid surface of the shell resulting from:

$$p = \rho_0 h \dot{x}$$

(39)

With a similar procedure the total angular momentum of the shell

$$J(\Phi, \Phi) = \frac{\int}{\Omega} \rho_0 (x + \xi t) \times (\dot{x} + \xi \dot{t}) \, d\Omega$$

(40)

is obtained in the alternative form

$$J(\Phi, \Phi) = \int_{M_0} (x \times p + t \times \pi) \, dM_0$$

(41)

The vector $\pi$ is called director momentum. A comparison of the previous equations gives

$$\pi = \rho_0 \frac{h^3}{12} \dot{t}$$

(42)

Finally the kinetic and internal energy of the system are given by

$$K(\Phi) = \frac{1}{2} \int_{M_0} \left( \rho_0 h \dot{x} \cdot \dot{x} + \rho_0 \frac{h^3}{12} \dot{t} \cdot \dot{t} \right) \, dM_0$$

(43)

$$V_{\text{int}} = \int_{M_0} g(\Xi) W(\Gamma) \, dM_0$$

(44)
The basic laws of the continuum for a pure initial value problem, i.e. if the absence of external loading is supposed, are the conservation of the total linear momentum $\mathbf{L}$ and the total angular momentum $\mathbf{J}$ of the system

$$d\mathbf{L}(\Phi)/dt = 0 \quad d\mathbf{J}(\Phi,\Phi)/dt = 0$$  \hfill (45)

In addition the balance of energy must fulfil the following inequality

$$d\left[\mathbf{K}(\Phi) + V_{\text{int}}(\Phi)\right]/dt = D_{\text{int}} \geq 0$$  \hfill (46)

If the presence of a conservative loading is admitted the related term of potential must be included in the previous inequality

$$d\left[\mathbf{K}(\Phi) + V_{\text{int}}(\Phi) + V_{\text{ext}}(\Phi)\right]/dt = D_{\text{int}} \geq 0$$  \hfill (47)

The weak form of the balance of momentum of the shell can be written as

$$G_{\text{dyn}}(\Phi,\Phi,\partial \Phi) = G_{\text{ine}}(\Phi,\partial \Phi)
+ G_{\text{stat}}(\Phi,\partial \Phi) - G_{\text{ext}}(\partial \Phi)$$  \hfill (48)

in which the terms relating to the inertial forces, to the internal forces and to the external loading are given respectively by

$$G_{\text{ine}}(\Phi,\partial \Phi) = \int_{M_0} (\dot{\mathbf{p}} \cdot \partial \mathbf{u} + \dot{\mathbf{\pi}} \cdot \partial \mathbf{t}) dM_0$$ \hfill (49)

$$G_{\text{stat}}(\Phi,\partial \Phi) = \int_{M_0} (\mathbf{n} : \partial \mathbf{\varepsilon} + \mathbf{q} : \partial \mathbf{\gamma} + \mathbf{m} : \partial \mathbf{\kappa}) dM_0$$ \hfill (50)

$$G_{\text{ext}}(\partial \Phi) = -V_{\text{ext}}(\partial \Phi)$$ \hfill (51)

Equation (48) is completed by the initial conditions imposed on $\Phi$:

$$(\mathbf{x},\mathbf{t})|_{t=0} = (\mathbf{X},\mathbf{T}) \quad (\mathbf{p},\mathbf{\pi})|_{t=0} = (\mathbf{p}_0,\mathbf{\pi}_0)$$ \hfill (52)

The admissible variation of the elements of the phase space is obtained as directional derivative of $\Phi$. The variations $\partial \mathbf{t}$ are tangent to the mid plane of the shell. Because of the inextensible character of $\mathbf{t}$, its variation satisfies the properties $\partial \mathbf{t} \cdot \mathbf{t} = 0$, resulting tangent to the unit sphere defined by $\mathbf{t}$ itself.

The substitution in the weak form of particular test functions makes it possible to obtain the basic laws of balance represented by (45), (46) and (47). It is expected that a finite element formulation arising from the discretisation in time and space of the weak form let the balance laws to be fulfilled. This is what results from the procedure explained partially in the next sections.

5 Time integration scheme

In the present section some details about the application of the time integration scheme are presented. The total time interval of interest is divided in sub-intervals:

$$[0,T] = \bigcup_{n=0}^{N} [t_n,t_{n+1}]$$ \hfill (53)

Let the configuration (displacement and velocity fields) of the system at time $t_n$ is known. The problem of the integration in time is the evaluation of the unknown configuration of the system at time $t_{n+1}$. The value of displacements and velocities in a generic intermediate time step of the interval $[t_n, t_{n+1}]$ is given as linear combination of the values at the time instants $t_n$ and $t_{n+1}$. The mid time configuration can be written as

$$(\mathbf{x},\mathbf{t})_{n+1/2} = \frac{1}{2} \left[(\mathbf{x},\mathbf{t})_n + (\mathbf{x},\mathbf{t})_{n+1}\right]$$ \hfill (54)

$$(\mathbf{p},\mathbf{\pi})_{n+1/2} = \frac{1}{2} \left[(\mathbf{p},\mathbf{\pi})_n + (\mathbf{p},\mathbf{\pi})_{n+1}\right]$$ \hfill (55)

Defining the amplitude of the generic time step $\Delta t = t_{n+1} - t_n$, the components of (3.3) are given as follows

$$\mathbf{p}_{n+1/2} = A_{p_0} \frac{x_{n+1} - x_n}{\Delta t}$$ \hfill (56)

$$\mathbf{\pi}_{n+1/2} = I_{p_0} \frac{t_{n+1} - t_n}{\Delta t}$$ \hfill (57)

With the equations (56) to (59) at hand, the weak form of the balance can be discretised in time and evaluated in the mid configuration of the time step

$$\frac{1}{\Delta t} \int_{M_0} \left[\partial \mathbf{u} \cdot (\mathbf{p}_{n+1} - \mathbf{p}_n) + \partial \mathbf{t} \cdot (\mathbf{\pi}_{n+1} - \mathbf{\pi}_n)\right] dM_0\]

$$+ G_{\text{stat}}(\Phi_{n+1/2},\partial \Phi) - G_{\text{ext}}(\partial \Phi) = 0$$ \hfill (58)
The previous relation is obtained by using the following expressions of the rate of $p$ and $\pi$ in the mid configuration
\[ \dot{p}_{n+1/2} = \frac{p_{n+1} - p_n}{\Delta t} \] (59)
\[ \dot{\pi}_{n+1/2} = \frac{\pi_{n+1} - \pi_n}{\Delta t} \] (60)

The evaluation of the static term related to the internal force is of crucial importance to obtain the conservative character of the time integration scheme. The variation of the Green-Lagrange strain tensor is evaluated in the mid configuration giving:
\[ G_{stat} = \int_{M_0} \left( n \cdot \delta \epsilon_{n+1/2} q \cdot \delta \gamma_{n+1/2} + m \cdot \delta \kappa_{n+1/2} \right) dM_0 \] (61)

The components of generalised stresses $n$, $q$, $m$ are evaluated by means of a particular algorithmic form that is explained in what follows. To ensure the properties of conservation of the time integration scheme the generalised form of stress is computed by means of a particular algorithmic form. This makes it possible to fulfil the Clausius-Duhem inequality. It can be shown that assuming a linear elastic constitutive model the conservative algorithmic generalised components of stress are given by:
\[ n^{\alpha\beta} = \frac{1}{2} C^{\alpha\beta\gamma\delta} \left[ (E_{\gamma\delta}^{(0)})_{n+1} + (E_{\gamma\delta}^{(0)})_n \right] \] (62)
\[ q^{\alpha\gamma} = \frac{1}{2} C^{\alpha\beta\gamma\delta} \left[ (2E_{\gamma\delta}^{(0)})_{n+1} + (2E_{\gamma\delta}^{(0)})_n \right] \] (63)
\[ m^{\alpha\beta} = \frac{1}{2} C^{\alpha\beta\gamma\delta} \left[ (E_{\gamma\delta}^{(1)})_{n+1} + (E_{\gamma\delta}^{(1)})_n \right] \] (64)

In case of non-linear elastic or dissipative constitutive models the algorithmic forms of the stress components are obtained as follows. The mean value theorem is applied to the variation of the Helmholtz free-energy function (30) in the generic time step:
\[ \Psi_{n+1} - \Psi_n = \left[ \frac{\partial \Psi}{\partial \Gamma} \right]_{n+\beta}^T \cdot [\Gamma_{n+1} - \Gamma_{n+1}] \] (65)

The comparison of the previous equation with the discrete (in time) form of the Clausius-Duhem inequality enables one to define the algorithmic forms of the generalised components of stress and dissipation:
\[ [n, q, m]^T = \left[ g \frac{\partial W}{\partial \Gamma} \right]_{n+\beta}^T \] (66)
\[ \Delta D_{n+1} = -\frac{1}{2} \left[ W \frac{\partial g}{\partial \Gamma} \right]_{n+\beta}^T \cdot [\Gamma_{n+1} - \Gamma_{n+1}] \] (67)

The method can be modified in order to ensure a quadratic convergence of the scheme with $\Delta t$. This procedure is based on the property of the function
\[ \frac{1}{2} (\Psi_{n+\beta} - \Psi_{n-1}) \] (68)

that enables to apply the mean value theorem as
\[ \Psi_{n+1} - \Psi_n = \frac{1}{2} \left[ \left( \frac{\partial \Psi}{\partial \Gamma} \right)_{n+\beta} + \left( \frac{\partial \Psi}{\partial \Gamma} \right)_{n+1-\beta} \right] \] (69)

This procedure leads to the alternative algorithmic forms
\[ [n, q, m]^T = \frac{1}{2} \left[ \left( \frac{\partial W}{\partial \Gamma} \right)_{n+\beta} + \left( \frac{\partial W}{\partial \Gamma} \right)_{n+1-\beta} \right] \] (70)
\[ \Delta D_{n, n+1} = -\frac{1}{2} \left[ W \frac{\partial g}{\partial \Gamma} \right]_{n+\beta}^T \cdot [\Gamma_{n+1} - \Gamma_{n+1}] \] (71)

Note that eqns. (70), (71) and (72), (73) are equivalent as regards the properties of conservation in terms of energy. The scalar parameter $\beta$ defines in practice the conservative configuration and is deduced as solution of the following non linear equation (with reference to eq. (71)):
\[ h(\beta) = \Psi_{n+1} - \Psi_n - \frac{1}{2} \left[ \left( \frac{\partial \Psi}{\partial \Gamma} \right)_{n+\beta} + \left( \frac{\partial \Psi}{\partial \Gamma} \right)_{n+1-\beta} \right] \] (72)

The evaluation of the solution of eq. (74) is performed at each time step at the Gauss point level. If the Helmholtz free-energy function is regular and if convexity is
ensured, the solution can be obtained by means of the application of the Newton scheme. The procedure requires
the derivation of the function $h$, hence the definition of the second order derivative of the Helmoltz free-energy function
with respect to the strain:

$$\frac{\partial^2 \Psi (\Xi, \Gamma)}{\partial \Xi \partial \Gamma} = g (\Xi) \left[ \frac{\partial^2 W (\Gamma)}{\partial \Gamma \partial \Gamma} \right] + W (\Gamma) \left[ \frac{\partial^2 g (\Xi)}{\partial \Gamma \partial \Xi} \right]$$

$$+ 2 g' (\Xi) \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]^T \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]$$

and the second order derivative of the damage function $g$:

$$\frac{\partial^2 g (\Xi)}{\partial \Gamma \partial \Xi} = \left( g'' - \frac{g'}{2} + \frac{g'''}{6} \right) \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]^T \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]$$

$$+ \frac{g'}{2} \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]^T \left[ \frac{\partial W (\Gamma)}{\partial \Gamma} \right]$$

where the terms $g'$ and $g''$ represent the derivative of the function $g$ with respect to the equivalent strain $\Xi$. The
lack of convexity requires sometimes the adoption of an alternative method for the solution of the equation instead
of the Newton method. All the previous relations make it possible to write the semi-discrete form of the balance

$$\frac{1}{M_0} \int_{M_0} \delta \Phi^T \left[ \begin{array}{cc}
\mathbf{p}_{n+1} - \mathbf{p}_n & 0 \\
0 & \mathbf{\pi}_{n+1} - \mathbf{\pi}_n
\end{array} \right] dM_0$$

$$+ \int_{M_0} \mathbf{r}^T \left( \mathbf{B}_{n+1/2} \delta \Phi \right) dM_0$$

(75)

The symbol $\mathbf{r}$ in the second term of the previous equation represents the conservative algorithmic form of generalised stress, given by the relation (66) or (70). The evaluation of its components is made taking into account the values of the generalised stresses at time $t_n$ and $t_{n+1}$. The latter are very simple to be found by virtue of the particular definition of the Helmoltz free-energy function, resulting in:

$$\mathbf{n}_t = g (\Xi_t) \mathbf{C}^n \mathbf{e}_t \quad (t = t_n, t_{n+1})$$

$$\mathbf{q}_t = g (\Xi_t) \mathbf{C}^n \mathbf{q}_t \quad (t = t_n, t_{n+1})$$

$$\mathbf{m}_t = g (\Xi_t) \mathbf{C}^n \mathbf{m}_t \quad (t = t_n, t_{n+1})$$

Finally the matrix $\mathbf{B}_{n+1/2}$ is the strain operator that allows one to obtain the variation of the strain components on
the basis of the variation of configuration $\delta \Phi^T = [\delta \mathbf{u}, \delta \mathbf{i}]$. The matrix $\mathbf{B}$ can be split pointing out membrane, transverse and bending components

$$\delta \mathbf{e} = \mathbf{B}_{n+1/2}^{e} \delta \Phi$$

$$\delta \mathbf{y} = \mathbf{B}_{n+1/2}^{y} \delta \Phi$$

$$\delta \mathbf{k} = \mathbf{B}_{n+1/2}^{k} \delta \Phi$$

(79)

(80)

(81)

The configuration of the strain operator is simply given by a linear interpolation of the same operators evaluated
at the time $t_n$ and $t_{n+1}$.

$$\mathbf{B}_{n+1/2}^{(i)} = \frac{1}{2} \left[ \mathbf{B}_{n}^{(i)} + \mathbf{B}_{n+1}^{(i)} \right]$$

(82)

More details about the terms of the strain operator $\mathbf{B}$ are given in appendix. Note how the semi-discrete weak form (75) is depending only on the unknown configuration $\Phi_{n+1}$ at the current time.

6 Space discretisation

The basic aspect of the discretisation in space is here explained. In what follows the indexes relating to time are omitted for simplicity. Isoparametric four noded elements are adopted. The positions in the reference configuration and in the current configuration of a point belonging to the mid plane of a generic element are given by

$$\mathbf{x} (\xi^1, \xi^2) \bigg|_\Omega = \sum_{l=1}^{4} N^l (\xi^1, \xi^2) \mathbf{x}_l$$

$$\mathbf{X} (\xi^1, \xi^2) \bigg|_\Omega = \sum_{l=1}^{4} N^l (\xi^1, \xi^2) \mathbf{X}_l$$

(83)

(84)

where $N^l (\xi^1, \xi^2)$ are the usual bi-linear shape functions with $(\xi^1, \xi^2) \in [-1, +1] \times [-1, +1]$. In a similar way, the fields of the director of the shell and of the displacements,
as well as of the linear and angular momentum is given by the formulas:

\[ T(\xi^1, \xi^2) \big|_\Omega = \sum_{l=1}^{4} N^l(\xi^1, \xi^2) T_l \]  \hfill (85)

\[ t(\xi^1, \xi^2) \big|_\Omega = \sum_{l=1}^{4} N^l(\xi^1, \xi^2) t_l \]  \hfill (86)

In order to avoid a possible ‘locking’ given by the thin thickness of the shell elements the ANS method is here adopted. The field of transverse shear strains is assumed as varying linearly from the opposite edges of a generic element. In the mid point of every edge the shear strain components are given by

\[ 2E_{13}^{(0)} = \frac{1}{2} (1 - \xi^2) 2E_{13}^{(0)A} + \frac{1}{2} (1 + \xi^2) 2E_{13}^{(0)C} \] \hfill (87)

\[ 2E_{23}^{(0)} = \frac{1}{2} (1 - \xi^1) 2E_{23}^{(0)D} + \frac{1}{2} (1 + \xi^2) 2E_{23}^{(0)B} \] \hfill (88)

The points of the mid surface \( x^L \) with \( L = A, B, C, D \) are given by the following expressions

\[ x^L = \frac{1}{2} x(\xi_M^1, \xi_M^2) + \frac{1}{2} x(\xi_M^1, \xi_M^2) \] \hfill (89)

being \( \{L,M,N\} \in \{(A,1,2),(B,2,3),(C,3,4),(D,1,4)\} \). Finally, the interpolations of the necessary terms of the discretisation in space of the semi-discrete weak form, are given by:

\[ \delta u \big|_\Omega = \sum_{l=1}^{4} N^l \delta u_l \] \hfill (90)

\[ \delta t \big|_\Omega = \sum_{l=1}^{4} N^l \delta t_l \]

\[ \frac{\partial u}{\partial \xi^a} \bigg|_\Omega = \sum_{l=1}^{4} \frac{\partial N^l}{\partial \xi^a} u_l, \quad \frac{\partial t}{\partial \xi^a} \bigg|_\Omega = \sum_{l=1}^{4} \frac{\partial N^l}{\partial \xi^a} t_l \] \hfill (91)

\[ \frac{\partial \delta u}{\partial \xi^a} \bigg|_\Omega = \sum_{l=1}^{4} \frac{\partial N^l}{\partial \xi^a} \delta u_l, \quad \frac{\partial \delta t}{\partial \xi^a} \bigg|_\Omega = \sum_{l=1}^{4} \frac{\partial N^l}{\partial \xi^a} \delta t_l \] \hfill (92)

With the previous relations at hand, the full discrete weak form of the balance of momentum can be obtained by the (75).

### 7 Linearisation aspects

The full discrete form of the weak form of the balance of momentum consists of a system of equations which has nodal displacements and rotations (evaluated at the current time \( t_{n+1} \)) as unknown terms. The solution of the system is found by means of the application of the Newton-Raphson method. Hence the directional derivative

\[ DG_{din} \left( \Phi_n, \Phi_n^{(i)}, \delta \Phi \right) \cdot \Delta \Phi_n^{(i)} = -G_{din}^{(i)} \] \hfill (93)

must be evaluated in order to improve the trial solution until a specified norm results below the specified tolerance. The derivative leads to three terms usually known as inertial, material and geometric indicated by \( D_D \), \( D_M \) and \( D_G \) respectively.

\[ D_D G_{din} \cdot \Delta \Phi_n^{(i)} = \bigcup_{e=1}^{Nelem} \int_{\Omega_e} \frac{2A_{p_0}}{(\Delta t)^2} \Delta u_{n+1} \cdot \delta u \Delta t_{n+1} \] \hfill (94)

\[ D_M G_{din} \cdot \Delta \Phi_n^{(i)} = \bigcup_{e=1}^{Nelem} \int_{\Omega_e} r \cdot \left[ D (D \delta E) \cdot \Delta \Phi_n^{(i)} \right] d\Omega_e \] \hfill (95)

On the basis of the Helmholtz free-energy function defined in section 3 the derivative of the internal forces in the
previous term gives the following expression

\[
D_\Gamma = \frac{1}{2} \left[ \beta_0 \dot{g} \left( \Xi_{n+1} \right) + (1 - \beta_0) \dot{g} \left( \Xi_{n+1} \right) \right]
\cdot \mathbf{C} \mathbf{B}_{n+1} \Delta \mathbf{\Phi}_{n+1}
\]

\[
+ \frac{1}{2} \beta_0 \dot{g} \left( \Xi_{n+1} \right) \left[ \frac{\partial W (\mathbf{\Gamma})}{\partial \mathbf{\Gamma}} \right]_{n+1}^{T} \left[ \frac{\partial W (\mathbf{\Gamma})}{\partial \mathbf{\Gamma}} \right]_{n+1}
\cdot \mathbf{B}_{n+1} \Delta \mathbf{\Phi}_{n+1}
\]

\[
+ \left[ \frac{\partial W (\mathbf{\Gamma})}{\partial \mathbf{\Gamma}} \right]_{n+1}^{T} \left[ \frac{\partial W (\mathbf{\Gamma})}{\partial \mathbf{\Gamma}} \right]_{n+1} \mathbf{B}_{n+1} \Delta \mathbf{\Phi}_{n+1}
\]

(97)

where the coefficient \( \beta_0 \) is the value ensuring the conservative character of the algorithmic internal stresses, as previously explained.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure2.png}
\caption{Initial configuration of the arch and loading history.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure3.png}
\caption{Deformation sequence of the arch.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure4.png}
\caption{Time history of energies (normalised values).}
\end{figure}

\section{Examples}

The following examples show the main properties of the algorithm in terms of fulfilment of the balance laws, both as regard momenta and energy of the system. Attention is also focused on the convergence property of the scheme, resulting of the second order by a consistent linearisation of the vector of internal forces.
8.1 Dynamics of an arch

The thin arch represented in Figure 2 is subjected to an impulse by means of the application of an initial loading. The arch is hinged along the lines indicated as $n-n$ and $m-m$ respectively. The elasto-damage model presented in section 3 is assumed. The density is set to be $1 \times 10^{-6}$. The constants of Lamè are $\lambda = 28.6$ and $\mu = 7.2$, while the parameters of the damage function are $a = 1$ and $b = 0.3$. The thickness of the arch is set to be 2 while the other dimensions are indicated in Figure 2.

Under the effects of the initial loading the arch oscillates as depicted in the Figure 3 for the first oscillation. The time history of the kinetic, internal and dissipated energy is reported in the chart of Figure 4 together with the total energy, again for the first oscillation of the system. The total energy is here intended as the sum of the energy of the system, i.e. kinetic and free energy, plus the dissipated energy. The total energy increases in the first steps of the motion by virtue of the work of the external forces applied. After the external forces disappear, the total energy of the system is constant, while the amount of dissipated energy increases together with the amount of the deformation of the structure. The conservative configurations of the internal forces and dissipation have been calculated by means of equations (70) and (71). The parameter $\beta_0$ that defines this configuration is usually closed to 0.2 or 0.8. This fact is helpful in the application of the Newton method adopted for the evaluation of the solutions of equation $h(\beta) = 0$. The existence of a double solution is due to the symmetry of the function $h$. The use of the expressions (66) and (67) instead of (70) and (71) will give a unique solution.

8.2 Dynamics of a ring

The free ring described in Figure 5 is subjected to four nodal forces with a triangular impulse. The forces are applied in the four points indicated as $A_1, A_2, A_3, A_4$. Again an elasto-damage constitutive model is adopted. The Young’s modulus is set to be $2.0 \times 10^7$ and the Poisson ratio is 0.45. A density of 0.05 is assumed. The scalar damage function is defined setting the constants $a$ as 20 and $b$ as 0.3.

The motion of the ring after the initial loading disappears is characterised by the conservation of the total momentum as well as of the conservation of the angular momentum. The time history of the latter is described in the
chart of the Figure 6 for the three components relating to the co-ordinate system x,y,z. The behaviour of energy is similar to that obtained in the previous example. Here, however, the strains attained by the structure are quite small and the consequent dissipated energy is shown in the chart of Figure 7, since its value is largely lower than the amounts of kinetic and internal energies. Anyway, the presence of a non-linearity in the constitutive model enforces to adopt the conservative algorithmic form (70) and (71) in order to preserve exactly the respect of the balance of the energies of the system. The behaviour of the kinetic and internal energy and their sum with the dissipated part is finally shown in Figure 8.

The properties of convergence can be evaluated in Table 1. Here the euclidean norm of the residuals is reported for some time steps. The use of a consistent linearisation of the weak form leads to a second order convergence.

<table>
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<th>n° iter</th>
<th>step 3</th>
<th>step 19</th>
<th>step 29</th>
<th>step 50</th>
</tr>
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<tr>
<td>1</td>
<td>2.66E+00</td>
<td>1.46E+00</td>
<td>3.36E+00</td>
<td>2.09E+00</td>
</tr>
<tr>
<td>2</td>
<td>6.04E-01</td>
<td>4.97E-01</td>
<td>6.61E-01</td>
<td>4.82E-01</td>
</tr>
<tr>
<td>3</td>
<td>4.55E-03</td>
<td>2.64E-03</td>
<td>4.50E-03</td>
<td>1.37E-03</td>
</tr>
<tr>
<td>4</td>
<td>6.30E-08</td>
<td>1.71E-08</td>
<td>5.24E-08</td>
<td>3.88E-09</td>
</tr>
<tr>
<td>5</td>
<td>6.84E-12</td>
<td>1.57E-13</td>
<td>6.59E-13</td>
<td>2.57E-13</td>
</tr>
</tbody>
</table>

9 Conclusions

Some aspects of the implementation of the energy-momentum method in the non-linear dynamics of thin shells have been presented. A simple scalar elasto-damage constitutive model has been assumed, making it possible to evaluate the conservative characteristics of the time integration algorithm if applied to system with internal dissipation. The stability of the time integration scheme arising from the particular choice of algorithmic forms of the stresses and internal dissipation must be intended as the fulfilment of the discrete form in time of the Clausius-Duhem inequality. Although the constitutive model here adopted is not related to the behaviour of an actual material it can be modified in suitable way in order to describe the dynamics of real structures made of materials with internal dissipation and undergoing large deformations.

References


Appendix

The terms of the matrix of the stored energy function (27) are given by

\[
C^n = \frac{Eh}{1-v^2} \overline{C}, \quad C^q = \chi G h \overline{C}, \quad C^m = \frac{Eh^3}{12(1-v^2)} \overline{C}
\]

where the matrix \( \overline{C} \) and \( \overline{C} \) are given respectively by

\[
\overline{C} = \begin{bmatrix}
A^{11} & A^{12} \\
\text{symm.} & A^{22}
\end{bmatrix}
\]

and

\[
\overline{C} = \begin{bmatrix}
A^{11} A^{11} + (1-v) A^{12} & \cdots & A^{11} A^{12} \\
A^{12} A^{22} & \cdots & A^{12} A^{22} \\
\cdots & \cdots & \cdots \\
\frac{1}{2} A^{22} A^{11} & \cdots & \frac{1}{2} A^{22} A^{12}
\end{bmatrix}
\]

Here \( h \) is the thickness of the shell. The coefficients \( E, G, \nu, \) are the Young's modulus, the shear modulus and the Poisson's ratio. Finally \( \chi \) represents the shear factor. The expressions of the strain operators used in (79), (80) and (81) are given by