NEW NONLINEAR HIGHER ORDER SHEAR DEFORMATION SHELL ELEMENT FOR METAL FORMING AND CRASHWORTHINESS ANALYSIS: PART I. FORMULATION AND FINITE ELEMENT EQUATIONS

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ABSTRACT

This work presents the finite element formulation of a higher order shear deformation shell element for nonlinear dynamic analysis with explicit time integration scheme. A corotational approach is combined with the velocity strain equations of a general third order theory in the formulation of a four-noded quadrilateral element with selectively reduced integration. A bilinear isoparametric formulation is utilized in the shell plane resulting in 9 degrees of freedom per node. The formulation requires C^0 continuity for the nodal variables. The finite element implementation of the new element in a general explicit finite element code is described in details, including boundary conditions and nodal mass calculation. A simple formula for the explicit time integration critical time step of the higher order element is developed. The described element is capable of correctly representing the through thickness distribution of the transverse shear, which makes it suitable for composite and sandwich shells analysis. In addition, the developed shell can be used for better representation of plastic flow through thickness in isotropic materials. It has been added to the element library of the nonlinear explicit finite element code DYNA3D. Its performance has been evaluated through a series of standard shell verification test problems, which show great promise for many applications. The results are presented in Part II of the present work.

Key words: nonlinear higher order shear deformation shell element, explicit finite element analysis, corotational formulation, refined shell theory, critical integration time step

INTRODUCTION

Creating new and improve existing analysis theories and formulations for plate and shell structures has been an active research area for decades. The specific geometric properties of plates and shells have been exploited to create numerous two-dimensional analysis formulations, which, in general, have provided significant simplifications and improved the analysis efficiency compared to the 3-D continuum mechanics solution approach. The

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simplest and oldest of these shell analysis formulations are based on the Love-Kirchhoff hypothesis and are well known as classic theories. One of their basic characteristics is neglecting the transverse shear deformation effects, which results in underpredicting of deflections and stresses, and overpredicting buckling loads and natural frequencies. Nevertheless, their accuracy is usually very good when the analysis involves thin homogeneous shells of conventional structural materials like metals. However, "unconventional" composite or sandwich shells are more and more often replacing these "conventional" shells. Their numerous advantages compared to metal shells like improved strength, stiffness, durability, cost, etc., as well as the technological advancements in their production have made composite and sandwich shells the preferred choice in many engineering structures. These shells differ significantly from metal shells: they are neither thin, nor homogeneous, and the neglected transverse shear plays a very important role in their behavior patterns. All this has made their analysis based on the classical shell theories inadequate and has invoked the development of more complicated and powerful analysis formulations, considering the transverse shear deformation effects. Most of the earlier developed approaches to composite and sandwich shell analysis are based on the Reissner [1]–Mindlin [2] type first order shear deformation theories. These theories assume that normals, which are initially straight and perpendicular to the reference surface, remain straight but are not necessarily perpendicular to the reference surface after the loading is applied. Hrabok and Hrudy [3], Ha [4], Burton and Noor [5], Zenkert [6], and the extensive review by Noor et al. [7], just to name a few, have described and referenced many of these theories. The major disadvantage of the first order theories is that although they account for the transverse shear they cannot correctly represent its through thickness distribution. As a result the traction conditions at the shell surfaces are violated. They also require shear correction coefficients to correct the corresponding strain energy terms and these coefficients are problem dependent and are not always easy to determine. As the shell thickness decreases these theories tend to experience shear locking. The displacement based formulations of the first order shear deformation theories represent the in-plane shell displacements as linear functions of the thickness coordinate, and the transverse displacements are assumed constant through the shell thickness. To overcome some of the disadvantages of the first order theories, the through thickness distributions of the displacement functions are assumed to be higher order polynomials of the thickness coordinate, resulting in a higher order shear deformation theory. Different authors have assumed quadratic, cubic, or higher degree polynomials. Higher order theories have been systematically described and referenced by Pandya and Kant [8], Reddy [9], Ha [4], Noor et al. [7], and others. An important holdback for the finite element implementation of the higher order theories is the fact that most of them require C^1 continuity of the nodal variables. This restricts their implementation into isoparametric shell elements with bilinear in-plane shape functions. The C^1 continuity requirement has been overcome in some higher order shear deformation theories, which only require C^0 continuity (see Kant and Kommineni [10]) and thus allow the use of bilinear isoparametric formulation.

The progress of the finite element formulations for shells follows the shell theory development. Starting with shell elements based on classical shell theories in earlier years, the bulk of shell elements at present utilize a first order shear deformation formulation. These first order shear deformable shell elements inherit both the advantages and disadvantages of the corresponding theoretical formulation. While in most cases they are capable of producing good results for the overall shell behavior, they cannot give accurate results for the transverse shear and transverse normal strains and stresses in composite and sandwich shells, which are very important in strength and failure analyses of these types of shell structures. To be able to better represent the strain and stress distribution through the shell thickness a shell element based on a higher order shell theory has to be utilized. Although higher order theories have been known, developed, and discussed for quite a while, their finite element implementation is presently quite limited. The main reasons for this are probably the widely spread notions

that their implementation is too complicated and their usage will extensively decrease the analysis computational efficiency. One aim of the present work is to oppose these notions by describing a simple and efficient finite element implementation of higher order shear deformation theories for explicit finite element analysis.

Explicit finite element analysis has already proven its efficiency and reliability in nonlinear dynamics of shells through its implementation in different research and commercial codes like DYNA3D [11], LS-DYNA [12], and ABAQUS/Explicit [13] to name just a few. Its performance is strongly dependent upon the accuracy and efficiency of the shell elements it utilizes. Elements based on first order shear deformation theory (e.g. see Hughes and Liu [14], Belytschko et al. [15, 16, 17]) have been widely implemented and developed since the 1980's. They were, and still seem to be considered the perfect combination of accuracy and computational efficiency, and still are the major workhorse in most codes. A decade or so ago it seemed that anything more complicated would be too heavy for the existent computational hardware and would result in an inefficient analysis. Nowadays, due to the fast growing computational power this has changed. It seems worthwhile to invest time and effort in changing shell element formulations in direction of improving their accuracy if this could be achieved without too much complication in the analysis formulation and its implementation. In the present work the very efficient corotational approach used in the Belytschko-Lin-Tsay [15] shell element is combined with a general third order shear deformation theory [18, 9, 19] in the formulation of a bilinear four-noded quadrilateral element with selectively reduced integration. The approach uses the velocity – rate of deformation relations. An isoparametric formulation with bilinear shape functions is utilized resulting in 9 degrees of freedom (DOF) per node. The new element is capable of correctly representing the through thickness distribution of the transverse shear. It is applicable to problems involving large displacements, and rotations. Its finite element implementation in a general explicit finite element code is described in details in Part I, including boundary conditions, nodal mass calculation, and a critical integration time step formula for the higher order element. The element formulation has been coded in the nonlinear explicit finite element code DYNA3D and results from standard verification tests are presented in Part II of the present work. The element proved to fit quite well in the explicit time integration scheme and provide an excellent overall performance.

THEORETICAL FORMULATION

The present third order shear deformation formulation follows the ideas of the well known displacement based higher order theories described in many investigations and generalized by one of the pioneers in that area – J.N. Reddy [9, 18]. The formulation is cast here using a corotational description, Cauchy stress, and rate of deformation (or velocity strain). This approach was first developed by Belytschko et al. [15] in the formulation of their first order shear deformation shell element.

The transformation matrix between the global and a local coordinate system is defined by

$$[\mathbf{T}] = [\mathbf{e}_1 \quad \mathbf{e}_2 \quad \mathbf{e}_3]^T, \tag{1}$$

where $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$, are the unit vectors of the local corotational coordinate system $\hat{x}\hat{y}\hat{z}$. This coordinate system is defined from the current geometry and configuration of the element and rotates with it in space. The unit vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ remain tangent to the shell midsurface, and $\boldsymbol{e}_3 = \boldsymbol{e}_1 \times \boldsymbol{e}_2$ is normal to the midsurface. For each in-plane integration point with natural coordinates ξ and η two vectors tangent to the midsurface are defined:

$$\mathbf{t}_1 = \left[\frac{\partial x}{\partial \xi} \quad \frac{\partial y}{\partial \xi} \quad \frac{\partial z}{\partial \xi}\right]\Bigg|_{\xi,\eta} ; \; \mathbf{t}_2 = \left[\frac{\partial x}{\partial \eta} \quad \frac{\partial y}{\partial \eta} \quad \frac{\partial z}{\partial \eta}\right]\Bigg|_{\xi,\eta} . \tag{2}$$

Then the vectors of the corotational coordinate system can be defined as

$$\mathbf{e}_1 \equiv \mathbf{t}_1; \quad \mathbf{e}_3 = \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\|\mathbf{t}_1 \times \mathbf{t}_2\|}; \quad \mathbf{e}_2 = \mathbf{e}_3 \times \mathbf{e}_1 . \tag{3}$$

This choice of coordinate system combined with the use of the rate of deformation and its conjugate Cauchy stress proves very efficient due to the fact that most material constitutive models are usually expressed through these two work conjugate tensors. No additional transformations need to be performed in applying the constitutive relations. Furthermore, by using a corotational approach the stress and strain tensor objectivity is preserved without the need of any special treatment. Note that in some formulations in order to deal with the frame invariance issues special stress rates (e.g. Jaumann or Green-Naghdi stress rates) have to be calculated and transformed at each analysis step. In addition, the use of velocity strain makes the present approach directly applicable to problems where the motion is path dependent, as is the case in plasticity.

Although a 4-point selectively reduced integration in the shell plane is utilized in the present work, the corotational system is defined only for the shell center point for the sake of simplicity. The defined in this manner corotational system is used for all 4 integration points for determining the fully integrated quantities, as well as for the single integration point for the underintegrated quantities. This will limit the use of the formulated elements to small strain problems, in particular shear strains must be limited. However, their accuracy will not be significantly affected for most practical problems.

Following the notation of Belytschko et al. [15] all quantities expressed in the element local coordinate system, in terms of the base vectors $\boldsymbol{e}_i$, will be denoted by a hat ($\hat{\cdot}$). The velocities of all points of the shell are defined through the velocities of the reference surface, which is the shell midsurface. The velocity components of an arbitrary point with thickness coordinate $\hat{z}$ in the local coordinate directions are defined as

$$\begin{aligned} \hat{v}_x &= \hat{v}_x^m + \hat{\theta}_y \hat{z} + \hat{\varphi}_y \hat{z}^2 + \hat{\psi}_y \hat{z}^3 \\ \hat{v}_y &= \hat{v}_y^m - \hat{\theta}_x \hat{z} - \hat{\varphi}_x \hat{z}^2 - \hat{\psi}_x \hat{z}^3 , \\ \hat{v}_z &= \hat{v}_z^m \end{aligned} \tag{4.a}$$

where $\hat{v}_i^m$ is the translational velocity of the midsurface along local axis *i*, $i = \hat{x}, \hat{y}, \hat{z}$; $\hat{\theta}_i$ is the rotational velocity of the midsurface about *i* for $i = \hat{x}, \hat{y}$; $\hat{\varphi}_i$, and $\hat{\psi}_i$, $i = \hat{x}, \hat{y}$, are the higher order terms in the velocity expansion polynomials. Unlike the zero and first order terms in the polynomial expansion, it is hard to assign any good physical meaning to the higher order terms. However, since $\hat{v}_i^m$ and $\hat{\varphi}_i$ only cause membrane stresses they can be referred to as membrane terms, whereas $\hat{\theta}_i$ and $\hat{\psi}_i$, which cause bending stresses can be referred to as bending terms.

At this point, let us define the velocity vector, $\hat{\mathbf{v}}$**:**

$$\hat{\mathbf{v}} = \dot{\hat{\mathbf{x}}} = \begin{Bmatrix} \dot{\hat{x}} \\ \dot{\hat{y}} \\ \dot{\hat{z}} \end{Bmatrix} = \begin{Bmatrix} \hat{v}_x \\ \hat{v}_y \\ \hat{v}_z \end{Bmatrix}. \tag{5}$$

The velocity gradient, **L**, in the local coordinate system is defined as

$$\hat{\mathbf{L}} = \frac{\partial \hat{\mathbf{v}}}{\partial \hat{\mathbf{x}}} \text{ or } \hat{L}_{ij} = \frac{\partial \hat{v}_i}{\partial \hat{x}_j}. \tag{6}$$

Then, the velocity strain will be

$$\hat{\mathbf{d}} = \frac{1}{2}\left(\hat{\mathbf{L}} + \hat{\mathbf{L}}^T\right) \text{ or } \hat{d}_{ij} = \frac{1}{2}\left(\hat{L}_{ij} + \hat{L}_{ji}\right) = \frac{1}{2}\left(\frac{\partial \hat{v}_i}{\partial \hat{x}_j} + \frac{\partial \hat{v}_j}{\partial \hat{x}_i}\right). \tag{7}$$

Substituting (4.a) into (7) gives the following expressions for the velocity strain components:

$$\hat{d}_x = \frac{\partial \hat{v}_x^m}{\partial \hat{x}} + \hat{z}\frac{\partial \hat{\theta}_y}{\partial \hat{x}} + \hat{z}^2\frac{\partial \hat{\varphi}_y}{\partial \hat{x}} + \hat{z}^3\frac{\partial \hat{\psi}_y}{\partial \hat{x}}$$

$$\hat{d}_y = \frac{\partial \hat{v}_y^m}{\partial \hat{y}} - \hat{z}\frac{\partial \hat{\theta}_x}{\partial \hat{y}} - \hat{z}^2\frac{\partial \hat{\varphi}_x}{\partial \hat{y}} - \hat{z}^3\frac{\partial \hat{\psi}_x}{\partial \hat{y}}$$

$$2\hat{d}_{xy} = \left(\frac{\partial \hat{v}_y^m}{\partial \hat{x}} + \frac{\partial \hat{v}_x^m}{\partial \hat{y}}\right) + \hat{z}\left(\frac{\partial \hat{\theta}_y}{\partial \hat{y}} - \frac{\partial \hat{\theta}_x}{\partial \hat{x}}\right) + \hat{z}^2\left(\frac{\partial \hat{\varphi}_y}{\partial \hat{y}} - \frac{\partial \hat{\varphi}_x}{\partial \hat{x}}\right) + \hat{z}^3\left(\frac{\partial \hat{\psi}_y}{\partial \hat{y}} - \frac{\partial \hat{\psi}_x}{\partial \hat{x}}\right) \tag{8.a}$$

$$2\hat{d}_{yz} = \left(\frac{\partial \hat{v}_z^m}{\partial \hat{y}} - \theta_x\right) - 2\hat{z}\hat{\varphi}_x - 3\hat{z}^2\hat{\psi}_x$$

$$2\hat{d}_{xz} = \left(\frac{\partial \hat{v}_z^m}{\partial \hat{x}} + \theta_y\right) + 2\hat{z}\hat{\varphi}_y + 3\hat{z}^2\hat{\psi}_y$$

The above expressions for the velocity strain components, Eq. (8.a), can be combined with a plain stress approach. Furthermore, they allow additional simplification of the formulation: vanishing of the transverse shear stresses at the top and bottom shell surfaces yields $\hat{\varphi}_x = \hat{\varphi}_y = 0$. At that, the velocity field in (4.a) simplifies into

$$\begin{aligned} \hat{v}_x &= \hat{v}_x^m + \hat{\theta}_y\hat{z} + \hat{\psi}_y\hat{z}^3 \\ \hat{v}_y &= \hat{v}_y^m - \hat{\theta}_x\hat{z} - \hat{\psi}_x\hat{z}^3, \\ \hat{v}_z &= \hat{v}_z^m \end{aligned} \tag{4.b}$$

and the corresponding velocity strain relations become

$$\hat{d}_x = \frac{\partial \hat{v}_x^m}{\partial \hat{x}} + \hat{z}\frac{\partial \hat{\theta}_y}{\partial \hat{x}} + \hat{z}^3\frac{\partial \hat{\psi}_y}{\partial \hat{x}}$$

$$\hat{d}_y = \frac{\partial \hat{v}_y^m}{\partial \hat{y}} - \hat{z}\frac{\partial \hat{\theta}_x}{\partial \hat{y}} - \hat{z}^3\frac{\partial \hat{\psi}_x}{\partial \hat{y}}$$

$$2\hat{d}_{xy} = \left(\frac{\partial \hat{v}_y^m}{\partial \hat{x}} + \frac{\partial \hat{v}_x^m}{\partial \hat{y}} \right) + \hat{z} \left(\frac{\partial \hat{\theta}_y}{\partial \hat{y}} - \frac{\partial \hat{\theta}_x}{\partial \hat{x}} \right) + \hat{z}^3 \left(\frac{\partial \hat{\psi}_y}{\partial \hat{y}} - \frac{\partial \hat{\psi}_x}{\partial \hat{x}} \right), \qquad (8.b)$$

$$2\hat{d}_{yz} = \left(\frac{\partial \hat{v}_z^m}{\partial \hat{y}} - \theta_x \right) - 3\hat{z}^2 \hat{\psi}_x$$

$$2\hat{d}_{xz} = \left(\frac{\partial \hat{v}_z^m}{\partial \hat{x}} + \theta_y \right) + 3\hat{z}^2 \hat{\psi}_y$$

which requires only 7 DOF in local and 9 DOF in global coordinate systems. Any further reduction of variables based on the zero transverse shear stresses (e.g. see Averill and Reddy [19]) require C^1 continuity for the nodal variables. The bilinear isoparametric formulation herein utilized provides only C^0 continuity, therefore, no further reduction is possible.

The rate form of the constitutive law expressed in the corotational system is

$$\dot{\boldsymbol{\sigma}} = \mathbf{C}(t, \boldsymbol{\sigma}, \mathbf{d}, ...)\dot{\mathbf{d}}, \qquad (9)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{C}$ is the tensor of material moduli, which is a fourth order tensor and, in general, may depend upon time, *t*, stress, strain rate, back stress if plasticity is involved, etc. The components of the velocity strain, Eq. (8.a,b), can be directly used in the constitutive calculations to evaluate the corresponding stress tensor components. Since the corotational coordinate system rotates with the element, its axes almost exactly coincide with the element material axes (for a detailed reasoning of this see Section 2 of Belytschko et al. [15]) and there is no need for frame invariance corrections. This is probably one of the main factors defining the simplicity of the approach, and it is well known that in the finite element analysis simplicity usually transfers into computational efficiency.

FINITE ELEMENT EQUATIONS

Following the present notation, the finite element equations of motion are

$$\mathbf{M}\dot{\mathbf{v}} = \mathbf{f}^{ext} - \mathbf{f}^{int}, \qquad (10)$$

where $\mathbf{M}$ is the mass matrix, $\dot{\mathbf{v}}$ is the acceleration vector ($\mathbf{v}$ is the velocity vector defined in Eq. (5) in local coordinates), and $\mathbf{f}^{ext}$ and $\mathbf{f}^{int}$ are the vectors of the external and internal forces respectively. Typically, at each time step of an explicit time integration scheme, we solve for the unknown nodal accelerations and integrate them to get the nodal velocities and nodal displacements. The acceleration vector corresponding to the velocity field in (4.b) will be

$$\dot{\hat{\mathbf{v}}} = \begin{Bmatrix} \dot{\hat{\mathbf{v}}}^m \\ \dot{\hat{\boldsymbol{\theta}}} \\ \dot{\hat{\boldsymbol{\psi}}} \end{Bmatrix},$$

where

$$\hat{\mathbf{v}}^m = \begin{Bmatrix} \hat{v}_x^m \\ \hat{v}_y^m \\ \hat{v}_z^m \end{Bmatrix}; \quad \hat{\boldsymbol{\theta}} = \begin{Bmatrix} \hat{\theta}_x \\ \hat{\theta}_y \\ 0 \end{Bmatrix}; \quad \hat{\boldsymbol{\psi}} = \begin{Bmatrix} \hat{\psi}_x \\ \hat{\psi}_y \\ 0 \end{Bmatrix} \qquad (11)$$

are the vectors with the nodal DOF in the local coordinate system. In global coordinate system these vectors will be

$$\mathbf{v}^m = \begin{Bmatrix} v_x^m \\ v_y^m \\ v_z^m \end{Bmatrix}; \quad \boldsymbol{\theta} = \begin{Bmatrix} \theta_x \\ \theta_y \\ \theta_z \end{Bmatrix}; \quad \boldsymbol{\psi} = \begin{Bmatrix} \psi_x \\ \psi_y \\ \psi_z \end{Bmatrix} \tag{12}$$

and the transformation from global to local coordinate system is performed using the already defined transformation matrix:

$$\hat{\mathbf{v}}^{\mathbf{m}} = [\mathbf{T}]\mathbf{v}^m; \quad \hat{\boldsymbol{\theta}} = [\mathbf{T}]\boldsymbol{\theta}; \quad \hat{\boldsymbol{\psi}} = [\mathbf{T}]\boldsymbol{\psi} \tag{13}$$

Note that any projections in the local $\hat{z}$ direction for $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\psi}}$ are ignored when transferring the vectors from global to local coordinate system.

To be able to utilize this scheme we also need to define the internal and external force vectors, the mass matrix, and the boundary conditions applied to the solved system.

Internal Nodal Forces

The internal nodal force vectors for each node are assembled from the contribution of each adjacent element. For each element, the internal forces are distributed to its nodes. For the velocity field in (4.b), the internal force vector of node *I* of element *e* will be

$$\left(\mathbf{f}^{int}\right)_I^e = \begin{Bmatrix} \mathbf{f}_I^e \\ \mathbf{m}_I^e \\ \mathbf{q}_I^e \end{Bmatrix},$$

where

$$\mathbf{f}_I^e = \begin{Bmatrix} f_{xI}^e \\ f_{yI}^e \\ f_{zI}^e \end{Bmatrix}; \quad \mathbf{m}_I^e = \begin{Bmatrix} m_{xI}^e \\ m_{yI}^e \\ 0 \end{Bmatrix}; \quad \mathbf{q}_I^e = \begin{Bmatrix} q_{xI}^e \\ q_{yI}^e \\ 0 \end{Bmatrix}. \tag{14}$$

Here $\mathbf{f}_I^e$, $\mathbf{m}_I^e$, and $\mathbf{q}_I^e$ are the internal nodal forces, moments and the higher order force terms for node *I* of element *e*. They can be expressed using the principle of virtual power in local coordinates:

$$\left(\delta\hat{\mathbf{v}}_I^e\right)^T \hat{\mathbf{f}}_I^e + \left(\delta\hat{\boldsymbol{\theta}}_I^e\right)^T \hat{\mathbf{m}}_I^e + \left(\delta\hat{\boldsymbol{\psi}}_I^e\right)^T \hat{\mathbf{q}}_I^e = \int_{V^e} \delta\hat{\mathbf{d}}^T \hat{\boldsymbol{\sigma}}\, dV, \tag{15}$$

where $\hat{\mathbf{d}}$ and $\hat{\boldsymbol{\sigma}}$ are the plain stress velocity strain and stress tensors arranged as vectors:

$$\hat{\mathbf{d}} = \begin{bmatrix} \hat{d}_x & \hat{d}_y & 2\hat{d}_{xy} & 2\hat{d}_{yz} & 2\hat{d}_{xz} \end{bmatrix}^T; \quad \hat{\boldsymbol{\sigma}} = \begin{bmatrix} \hat{\sigma}_x & \hat{\sigma}_y & \hat{\sigma}_{xy} & \hat{\sigma}_{yz} & \hat{\sigma}_{xz} \end{bmatrix}^T. \tag{16}$$

According to the bilinear isoparametric formulation the midplane geometry and the components of the velocity field throughout the element midplane are expressed as

$$\begin{Bmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{Bmatrix} = N_I \begin{Bmatrix} \hat{x}_I \\ \hat{y}_I \\ \hat{z}_I \end{Bmatrix}$$

$$\begin{Bmatrix} \hat{v}_x^m \\ \hat{v}_y^m \\ \hat{v}_z^m \end{Bmatrix} = N_I \begin{Bmatrix} \hat{v}_{xI} \\ \hat{v}_{yI} \\ \hat{v}_{zI} \end{Bmatrix}; \quad \begin{Bmatrix} \hat{\theta}_x \\ \hat{\theta}_y \end{Bmatrix} = N_I \begin{Bmatrix} \hat{\theta}_{xI} \\ \hat{\theta}_{yI} \end{Bmatrix}; \quad \begin{Bmatrix} \hat{\psi}_x \\ \hat{\psi}_y \end{Bmatrix} = N_I \begin{Bmatrix} \hat{\psi}_{xI} \\ \hat{\psi}_{yI} \end{Bmatrix}, \tag{17}$$

where N_I is the I^{th} shape function; repeated subscript indices imply summation over that index; and for the 4-noded quadrilateral shell element the node number I varies from 1 to 4. Then the velocity strain components, Eq. (8.b), expressed through the nodal DOF will be

$$\begin{aligned} \hat{d}_x &= B_{1I}\hat{v}_{xI} + \hat{z}B_{1I}\hat{\theta}_{yI} + \hat{z}^3 B_{1I}\hat{\psi}_{yI} \\ \hat{d}_y &= B_{2I}\hat{v}_{yI} - \hat{z}B_{2I}\hat{\theta}_{xI} - \hat{z}^3 B_{2I}\hat{\psi}_{xI} \\ 2\hat{d}_{xy} &= \left(B_{1I}\hat{v}_{yI} + B_{2I}\hat{v}_{xI}\right) + \hat{z}\left(B_{2I}\hat{\theta}_{yI} - B_{1I}\hat{\theta}_{xI}\right) + \hat{z}^3\left(B_{2I}\hat{\psi}_{yI} - B_{1I}\hat{\psi}_{xI}\right) \\ 2\hat{d}_{yz} &= B_{2I}\hat{v}_{zI} - N_I\hat{\theta}_{xI} - 3N_I\hat{\psi}_{xI}\hat{z}^2 \\ 2\hat{d}_{xz} &= B_{1I}\hat{v}_{zI} + N_I\hat{\theta}_{yI} + 3N_I\hat{\psi}_{yI}\hat{z}^2, \qquad I = 1,\ldots,4. \end{aligned} \tag{18}$$

Here $B_{1I} = \dfrac{\partial N_I}{\partial \hat{x}}$ and $B_{2I} = \dfrac{\partial N_I}{\partial \hat{y}}$.

Now, plugging the velocity strain components, Eq. (18), into the velocity strain vector, Eq. (16), and substituting the velocity strain and the stress vectors, (16), into (15), and by using the arbitrariness of the variations, we get the following expressions for the nodal internal forces:

$$\begin{aligned} \hat{f}_{xI}^e &= \int_{V^e} \left(B_{1I}\hat{\sigma}_x + B_{2I}\hat{\sigma}_{xy}\right) dV \\ \hat{f}_{yI}^e &= \int_{V^e} \left(B_{2I}\hat{\sigma}_y + B_{1I}\hat{\sigma}_{xy}\right) dV \\ \hat{f}_{zI}^e &= \int_{V^e} \left(B_{1I}\hat{\sigma}_{xz} + B_{2I}\hat{\sigma}_{yz}\right) dV \\ \hat{m}_{xI}^e &= -\int_{V^e} \left(B_{2I}\hat{\sigma}_y\hat{z} + B_{1I}\hat{\sigma}_{xy}\hat{z} + N_I\hat{\sigma}_{yz}\right) dV \\ \hat{m}_{yI}^e &= \int_{V^e} \left(B_{1I}\hat{\sigma}_x\hat{z} + B_{2I}\hat{\sigma}_{xy}\hat{z} + N_I\hat{\sigma}_{xz}\right) dV \\ \hat{q}_{xI}^e &= -\int_{V^e} \left(B_{2I}\hat{\sigma}_y\hat{z}^3 + B_{1I}\hat{\sigma}_{xy}\hat{z}^3 + 3N_I\hat{\sigma}_{yz}\hat{z}^2\right) dV \\ \hat{q}_{yI}^e &= \int_{V^e} \left(B_{1I}\hat{\sigma}_x\hat{z}^3 + B_{2I}\hat{\sigma}_{xy}\hat{z}^3 + 3N_I\hat{\sigma}_{xz}\hat{z}^2\right) dV\,. \end{aligned} \tag{19}$$

The above integrals are evaluated over the element volume, V^e, and depending on the assumed numerical integration rule can be further simplified. For example, the first integral

$$\hat{f}_{xI}^{e} = \int_{V^e} \left(B_{1I}\hat{\sigma}_x + B_{2I}\hat{\sigma}_{xy} \right) dV = \int_{\hat{x}}\int_{\hat{y}} \left(B_{1I}\int_{\hat{z}} \hat{\sigma}_x d\hat{z} + B_{2I}\int_{\hat{z}} \hat{\sigma}_{xy} d\hat{z} \right) d\hat{x}d\hat{y} =$$
$$= \int_{\xi}\int_{\eta} \left(B_{1I}\int_{\hat{z}} \hat{\sigma}_x d\hat{z} + B_{2I}\int_{\hat{z}} \hat{\sigma}_{xy} d\hat{z} \right) |\mathbf{J}| \, d\xi d\eta \quad , \quad (20)$$

where $|\mathbf{J}|$ is the determinant of the element Jacobian matrix, and ξ and η are the isoparametric coordinates: $-1 \le \xi, \eta \le 1$. The integrals along $\hat{z}$ can be numerically evaluated depending on the through thickness integration rule, and the integrals along ξ and η – depending on the in-plane integration rule, and the integration type – full, selectively reduced, or uniformly reduced.

Nodal Mass Calculation

To calculate the shell element mass matrix, the procedure described by Hughes et al. [20] and implemented in DYNA3D and LS-DYNA for all shell elements (see Section 9.4 in [12]) is used. The procedure defines only translational and rotational masses for the 6 DOF per node shell elements; therefore, the masses corresponding to the higher order terms have to be additionally defined.

Since in explicit calculations a diagonal mass matrix is desirable the consistent mass matrix defined by

$$\mathbf{M} = \int_{V^e} \mathbf{N}^T \rho \mathbf{N} \, dV \quad (21)$$

cannot be directly used. Here **N** is the shape function matrix and ρ is the material density. To get a diagonal mass matrix, first, the translational nodal masses are calculated by distributing the total element mass evenly among the 4 element nodes. Then the rotational and higher order nodal masses are calculated by scaling the translational mass at the node by a factor α:

$$m_\theta = \alpha_\theta m_t \quad (22)$$
$$m_\psi = \alpha_\psi m_t \, .$$

Here m_t, m_θ, and m_ψ are the translational, rotational and the higher order nodal masses, and the factors α are defined as follows:

$$\alpha_\theta = \frac{m_\theta}{m_t} = \frac{\int_h z^2 dz}{\int_h dz}; \quad \alpha_\psi = \frac{m_\psi}{m_t} = \frac{\int_h z^6 dz}{\int_h dz}, \quad (23)$$

where h is the shell thickness. If the reference surface is the shell midsurface and A is the element area, then

$$m_t = \rho \frac{A}{4} h; \quad \alpha_\theta = \frac{h^2}{12}; \quad \alpha_\psi = \frac{h^6}{448}. \quad (24)$$

The nodal masses thus defined are used in the finite element equations of motion, Eq. (10): m_t is used in calculating the translational accelerations, $\dot{\hat{\mathbf{v}}}^m$; m_θ is used for the rotational accelerations, $\dot{\hat{\boldsymbol{\theta}}}$; and m_ψ is used for the higher order acceleration terms – $\dot{\hat{\boldsymbol{\psi}}}$. In this manner the total mass of the system is correctly represented. The mass lumping procedure described by Kant and Kommineni [10] in their higher order element formulation and based on the

original work of Hinton et al. [21] is similar and will result in the same mass matrix. In both procedures the translational mass components in the diagonal mass matrix sum up to the total mass of the structure.

Boundary and Loading Conditions

When the displacement based finite element formulation involves 6 DOF per node they all have a sound physical interpretation and so do their corresponding displacement boundary conditions. It is not so with the higher order formulation. Since the higher order terms cannot be related to a specific physical term in the displacement field, like translations and rotations for the lower order terms, it cannot be expected from the finite element user to be able to specify values for them at physically restricted boundaries. Therefore, it is probably best if the boundary conditions for the higher order terms were internally specified without the need for the user to specify them. Furthermore, this approach will presumably require least changes when implementing the higher order shell formulation in an existing finite element code. To illustrate how this can be done, let us consider the simple cases of a clamped and a simply supported edge. It is obvious that in a clamped edge all displacement components should be zero. So, in the finite element input the user would specify zero conditions for the translations and rotations, and the rest of the displacement components should also be zeroed out in the code. In the case of a simply supported edge translations are zeroed out and rotations are not restricted. In this case the higher order bending terms (corresponding to ψ_i) should be free. Based on the above considerations, an algorithm for applying the boundary conditions on the in-plane displacements would consist of the following rules:

- Whenever zero is specified for θ_x, also zero out ψ_x.
- Whenever zero is specified for θ_y, also zero out ψ_y.

This simple algorithm was applied in the finite element implementation of the present formulation and it seems to work quite well.

The formulation of the higher order shell element does not require any changes in the way the external loading is specified compared to the first order shear deformable shell elements for concentrated forces, distributed loading along the shell sides, and lateral pressure.

There are different approaches to treating the drilling DOF for shell elements, the simplest of which is to ignore the *z*-component of the rotational velocity in local coordinate system. This same approach can be directly applied to the present element. Since $\hat{\theta}_z$ is not used in the formulation any external loading corresponding to it can just be ignored.

CRITICAL TIME STEP

Due to the conditional stability of the explicit time integration scheme the time step calculation plays a very important role for its performance. Larger time steps decrease the computational effort for solving the problem, but if a certain limit called critical time step, Δt_{cr}, is exceeded the solution rapidly diverges. To be able to efficiently use the well-known expression for the critical time step

$$\Delta t_{cr} = \frac{2}{\omega_{\max}}, \tag{25}$$

a simple estimate of the highest natural frequency, ω_{max}, of the structure is required. Since ω_{max} of the structure is smaller than the highest natural frequency of the finite elements that constitute it, Eq. (25) can be transformed into

$$\Delta t_{cr} = \min\left\{\left(\Delta t_{cr}^{e}\right)_i\right\}, \quad \left(\Delta t_{cr}^{e}\right)_i = \frac{2}{\left(\omega_{\max}^{e}\right)_i}, \qquad i = 1,\ldots,\text{number of elements in the structure} \tag{26}$$

Here $\left(\Delta t_{cr}^{e}\right)_i$ and $\left(\omega_{\max}^{e}\right)_i$ are the critical time step and the highest natural frequency of the i^{-th} element.

Therefore, the problem of determining the critical time step consists of determining it on element level. At that, the highest natural frequency of the element has to be evaluated. For that purpose let us define the generalized eigenvalue problem for an element of an undamped system

$$\left(\left[\mathbf{K}^{e}\right] - \omega^2\left[\mathbf{M}^{e}\right]\right)\left\{\mathbf{u}^{e}\right\} = \left\{\mathbf{0}\right\}. \tag{27}$$

Solving this for ω for each element throughout the whole analysis duration is a rather tedious task that could render the whole explicit scheme inefficient. Furthermore, the element stiffness matrix, $\left[\mathbf{K}^{e}\right]$, is not readily available in a typical explicit analysis scheme. Therefore, different solutions have been developed for all currently utilized element types in the explicit finite element solvers. The general idea of all of them is to come up with an estimate of the value of ω_{max} based on the material properties and dimensions of the element. Usually a more or less coarse upper bound of ω_{max} is calculated and used in the critical time step relation, Eq. (26). Flanagan and Belytschko [22] applied Gerschgorin's theorem [23] in developing estimates for the highest natural frequencies of three-dimensional hexahedron and two-dimensional quadrilateral elements with a single quadrature point. This resulted in simple formulas for $\omega_{\max}^{e}$, which can be used in Eq. (26) to get an estimate for the element critical time step. The application of Gerschgorin's theorem and the Rayleigh quotient in determining the critical time step is described and analyzed by Kulak [24]. Simple formulas for time step calculation used in LS-DYNA can be found in Chapter 19 of [12]. Leech [25] started with the differential equation of equilibrium for the Kirchhoff shell to arrive at an estimate for its critical time step. His approach was later used by Tsui and Tong [26] to develop a time step estimate for the Mindlin type shells. They came up with a relatively simple formula for the critical time step, which was slightly modified and used by Kant and Mallikarjuna [27]. Due to the lack of an estimate for the critical time step of higher order shear deformable shell elements Kant and Kommineni [10] used this same formula as an initial estimate in the implementation of their higher order element. However, this formula is derived based on the differential equation of equilibrium of the first order Mindlin shell and therefore is not applicable to higher order shear deformable shells. It was checked with several test problems in the present study and in all cases it significantly overestimated the critical time step. It is obvious that with the introduction of the higher order elements in the explicit analysis simple and efficient estimate of the critical time step for these elements is needed. Such an estimate is herein developed for the proposed 4-noded quadrilateral element.

Let us start with the shell element implementing the velocity field in Eq. (4.b). It has 7 DOF per node in local coordinate system resulting in a total of 28 DOF per element and its mass and stiffness matrices have dimensions of 28×28. Since the ultimate goal is to develop a symbolic expression for the critical time step all computations have to be symbolically performed. Obviously, this is an impossible task for a shell element of general geometry. Therefore, we will derive the formulas for a rectangular plane element of sides with length *a* and *b* along the local *x* and *y* axes respectively. The *x* and *y* axes are in the shell plane, and the *z*-axis is normal to the shell, the coordinate system origin is at the shell center. The shell thickness is *h*. The material of the shell is homogeneous isotropic with density ρ and three-dimensional constitutive matrix

$$[\mathbf{C}] = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix}, \quad (28)$$

where E is the Young's modulus and ν is Poisson's ratio.
To be able to use the generalized eigenvalue problem, Eq. (27), we need to assemble the element mass and stiffness matrices. The element lumped diagonal mass matrix is

$$[\mathbf{M}^e] = \begin{bmatrix} [\mathbf{M}_n] & \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} \\ \mathbf{0}_{7\times7} & [\mathbf{M}_n] & \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} \\ \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} & [\mathbf{M}_n] & \mathbf{0}_{7\times7} \\ \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} & \mathbf{0}_{7\times7} & [\mathbf{M}_n] \end{bmatrix}, \quad (29)$$

where $\mathbf{0}_{n\times m}$ is an $n\times m$ matrix of zeros and $[\mathbf{M}_n]$ is the nodal diagonal mass matrix:

$$[\mathbf{M}_n] = \begin{bmatrix} [\mathbf{M}_t] & \mathbf{0}_{3\times2} & \mathbf{0}_{3\times2} \\ \mathbf{0}_{2\times3} & [\mathbf{M}_\theta] & \mathbf{0}_{2\times2} \\ \mathbf{0}_{2\times3} & \mathbf{0}_{2\times2} & [\mathbf{M}_\psi] \end{bmatrix}, \quad (30)$$

and $[\mathbf{M}_t] = m_t[\mathbf{I}]_{3\times3}$, $[\mathbf{M}_\theta] = m_\theta[\mathbf{I}]_{2\times2}$, and $[\mathbf{M}_\psi] = m_\psi[\mathbf{I}]_{2\times2}$. Here $[\mathbf{I}]_{n\times n}$ is the $n\times n$ identity matrix, $m_t = \frac{\rho hab}{4}$, and m_θ, and m_ψ are already defined in the nodal mass section of this paper.

The element stiffness matrix is

$$[\mathbf{K}^e] = \int_{V^e} [\mathbf{B}]^T [\mathbf{C}][\mathbf{B}] dV = \int_{-\frac{h}{2}}^{\frac{h}{2}} \int_{-\frac{b}{2}}^{\frac{b}{2}} \int_{-\frac{a}{2}}^{\frac{a}{2}} [\mathbf{B}]^T [\mathbf{C}][\mathbf{B}] dx dy dz, \quad (31)$$

where

$$[\mathbf{B}] = [\,[\mathbf{B}_1] \;\; [\mathbf{B}_2] \;\; [\mathbf{B}_3] \;\; [\mathbf{B}_4]\,]_{5\times28}, \quad (32)$$

and

$$\left[\mathbf{B}_I\right]=\begin{bmatrix} \frac{\partial N_I}{\partial x} & 0 & 0 & 0 & z\frac{\partial N_I}{\partial x} & 0 & z^3\frac{\partial N_I}{\partial x} \\ 0 & \frac{\partial N_I}{\partial y} & 0 & -z\frac{\partial N_I}{\partial y} & 0 & -z^3\frac{\partial N_I}{\partial y} & 0 \\ \frac{\partial N_I}{\partial y} & \frac{\partial N_I}{\partial x} & 0 & -z\frac{\partial N_I}{\partial x} & z\frac{\partial N_I}{\partial y} & -z^3\frac{\partial N_I}{\partial x} & z^3\frac{\partial N_I}{\partial y} \\ 0 & 0 & \frac{\partial N_I}{\partial y} & -N_I & 0 & -3z^2N_I & 0 \\ 0 & 0 & \frac{\partial N_I}{\partial x} & 0 & N_I & 0 & 3z^2N_I \end{bmatrix}. \tag{33}$$

Here I is the nodal number, I = 1, …, 4, and N_I are the element shape functions:

$$\begin{aligned} N_1 &= \frac{1}{ab}\left(\frac{a}{2}-x\right)\left(\frac{b}{2}-y\right); \quad N_3 = \frac{1}{ab}\left(\frac{a}{2}+x\right)\left(\frac{b}{2}+y\right) \\ N_2 &= \frac{1}{ab}\left(\frac{a}{2}+x\right)\left(\frac{b}{2}-y\right); \quad N_4 = \frac{1}{ab}\left(\frac{a}{2}-x\right)\left(\frac{b}{2}+y\right) \end{aligned}. \tag{34}$$

Although the element implementation is based on isoparametric representation, its use will only complicate the present calculations and therefore is avoided. The above shape functions are different than the isoparametric shape functions used in the element implementation.

Having thus defined the element mass and stiffness matrices let us transform the generalized eigenvalue problem, Eq. (27), into a standard eigenvalue problem. Following the approach described in Chapter 10.2.5 of Bathe [28], which results in a symmetric standard eigenvalue problem, we can represent the mass matrix by

$$\left[\mathbf{M}^e\right]=[\mathbf{S}][\mathbf{S}]^T, \tag{35}$$

where

$$S_{ij} = \begin{cases} \sqrt{M_{ij}} \ \ for\ i=j \\ 0 \ \ for\ i \neq j \end{cases}. \tag{36}$$

Note that $[\mathbf{S}]^T = [\mathbf{S}]$. Since [**S**] is a diagonal matrix it is very easy to express [**S**]$^{-1}$. Then the generalized eigenvalue problem, Eq. (27), can be transformed into the following standard eigenvalue problem:

$$\left(\left[\tilde{\mathbf{K}}^e\right]-\omega^2[\mathbf{I}]\right)\left\{\tilde{\mathbf{u}}^e\right\}=\{\mathbf{0}\}. \tag{37}$$

where $\left[\tilde{\mathbf{K}}^e\right]=[\mathbf{S}]^{-1}\left[\mathbf{K}^e\right][\mathbf{S}]^{-1}$ and $\left\{\tilde{\mathbf{u}}^e\right\}=[\mathbf{S}]\left\{\mathbf{u}^e\right\}$. The matrix $\left[\tilde{\mathbf{K}}^e\right]$ can be symbolically assembled using a mathematical symbolic processor. Then $\omega^e_{\max}$ will be its maximum eigenvalue. Although it seems impossible to generate the eigenvalues of a 28×28 symbolic matrix it is feasible to make an estimate of its maximum eigenvalue using matrix norms. Here the infinity norm and the Frobelius norm (see Chapter 7 of [23]) were used to generate expressions for the maximum eigenvalue estimate. The infinity norm resulted in a lesser estimate for $\omega^e_{\max}$. Since $\left[\tilde{\mathbf{K}}^e\right]$ is a symmetric matrix the 1-norm and the infinity norm will produce the same result. Note that using the infinity norm there is more than one expression that could possibly be the correct eigenvalue estimate. Therefore, several different

geometric and material properties were used, which resulted in the same expression for the estimate, which is as follows

$$\left(\omega_{\max}^{e}\right)^2 \le \frac{2E\left(5\sqrt{21}+63\right)}{5\rho h^2\left(1+\nu\right)}. \tag{38}$$

Then for the critical time step of the element we get

$$\Delta t_{cr} \ge 0.3412h\sqrt{\frac{\rho\left(1+\nu\right)}{E}}. \tag{39}$$

Note that since all eigenvalues of $\left[\tilde{\mathbf{K}}^{e}\right]$ are real, the infinity norm will produce the same result as with applying Gerschgorin's theorem to the eigenvalue problem, Eq. (37). Although the above formulas are developed for rectangular shell elements, they could probably be used for an element of arbitrary shape.

The performance of the above formulas for Δt_{cr}, Eq. (39), was checked with the higher order shell element defined herein and implemented into DYNA3D. Results are compared with the exact critical time step calculated by solving the eigenvalue problem with concrete values for each variable. They are presented in Table 1. As seen the results acquired with the simple formulas give an excellent estimate for the critical time step.

Table 1

Test Problem	Exact, μsec	Eq. (39), μsec	% of Exact
Problem 3	3.327	2.860	86.0
Problem 4	0.8404	0.7863	93.6
Problem 5	0.2612	0.2400	91.9
Problem 6	0.8386	0.7704	91.9

Note: The problems in table 1 are taken from part II of the present work.

CONCLUSIONS

The explicit time integration scheme in the finite element analysis requires small time steps, which results in a huge number of steps for a complete analysis. Therefore, the finite elements defined for that type of analysis must be simple and computationally efficient. The higher order shell element herein formulated is considered a further step in increasing the accuracy while preserving simplicity and efficiency in the shell formulations for nonlinear dynamic explicit analysis. Its improved accuracy is due to the higher order shear deformation theory used in its formulation, and the efficiency is due to the corotational approach utilized and the velocity gradient used. The theoretical formulation of the new shell element is presented here and the basics for its implementation in an explicit dynamic finite element code are described. A simple formula for the critical time step of the explicit time integration scheme for the higher order element is derived. Its performance proved excellent. The higher order shell element has been implemented into the explicit code DYNA3D and the results from standard verification tests carried out on the new element are presented in Part II of the present work. The developed element is capable of correctly representing the through thickness distribution of the transverse shear, which makes it suitable for composite and sandwich shell analysis. In addition, the developed shell can be used for better representation of plastic flow through the thickness of isotropic materials.

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