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Drilling couples and refined constitutive equations in the resultant geometrically non-linear theory of elastic shells

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Abstract It is well known that distribution of displacements through the shell thickness is non-linear, in general. We introduce a modified polar decomposition of shell deformation gradient and a vector of deviation from the linear displacement distribution. When strains are assumed to be small, this allows one to propose an explicit definition of the drilling couples which is proportional to tangential components of the deviation vector. The consistent second approximation to the complementary energy density of the geometrically non-linear theory of isotropic elastic shells is constructed. From differentiation of the density we obtain the consistently refined constitutive equations for 2D surface stretch and bending measures. These equations are then inverted for stress resultants and stress couples. The second-order terms in these constitutive equations take consistent account of influence of undeformed midsurface curvatures. The drilling couples are explicitly expressed by the stress couples, undeformed midsurface curvatures, and amplitudes of quadratic part of displacement distribution through the thickness. The drilling couples are shown to be much smaller than the stress couples, and their influence on the stress and strain state of the shell is negligible. However, such very small drilling couples have to be admitted in non-linear analyses of irregular multi-shell structures, eg. shells with branches, intersections, or technological junctions. In such shell problems six 2D couple resultants are required to preserve the structure of the resultant shell theory at the junctions during entire deformation process.

Keywords: Drilling couple, Resultant shell theory, Geometrical non-linearity, Constitutive equations, Complementary energy, Second approximation

1 Introduction

Drilling couples M^α are two-dimensional (2D) stress couple fields which appear in the resultant non-linear model of a shell. Such shell model was initiated by Reissner (1974), developed in a number of papers for example by Chróścielewski et al. (1992, 1997), Ibrahimbegović (1997), Eremeyev and Pietraszkiewicz (2006, 2011), Pietraszkiewicz (2011), Birsan and Neff (2013), and summarized in monographs by Libai and Simmonds (1983,1998), Chróścielewski et al. (2004), and Eremeyev and Zubov

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(2008), where further references are given. The explicit original definition of M^{α} proposed in section 3 of this report reveals that the drilling couples are generated by non-linear part of tangential displacement distribution through the shell thickness. This is the reason why M^{α} do not appear in most popular non-linear shell models based on kinematic constraints “material fibres, which are normal to the undeformed shell base surface, remain straight during shell deformation” or their equivalents as well as in the Cosserat type models with one deformable director, see for example Naghdi (1972), Pietraszkiewicz (1979, 1989), Altenbach and Zhilin (1988), Simo and Fox (1989), Rubin (2000), Bischoff et al. (2004), Antman (2005), or Wiśniewski (2010). Also in all classical linear models of elastic shells the resultant 2D stress couple vector does not have the normal (drilling) component by definition, due to identification of deformed and undeformed shell geometries, see for example Love (1927), Gol’denveizer (1961), Naghdi (1963), Green and Zerna (1968), or Başar and Krätzig (2001).

In the non-linear resultant 2D shell model the local equilibrium equations are *exact implication* of the through-the-thickness integration of 3D equilibrium equations of non-linear continuum mechanics. Then the 2D virtual work identity allows one to construct *uniquely* the 2D shell kinematics consisting of the translation vector and rotation tensor fields (six independent components) as well as the corresponding twelve 2D strain measures work-conjugate to the twelve 2D resultant stress measures, all defined on the shell base surface. The resultant shell model naturally includes three parameters of finite rotation as independent field variables and two drilling stress couples with corresponding two work-conjugate drilling bendings. All these fields become necessary in analyses of irregular shells with folds, branchings and intersections (Chróścielewski et al. 1997, Konopińska and Pietraszkiewicz 2007), when connecting shell elements between themselves (Pietraszkiewicz and Konopińska 2011) and with beams, columns and stiffeners, as well as in two-dimensional formulation of singular phenomena such as phase transition (Eremeyev and Pietraszkiewicz 2004, 2011), crack propagation, dislocations (Eremeyev and Zubov 2008), wave motion, etc.

Yet, in almost all theoretical papers and numerical finite-element analyses of geometrically non-linear shell problems the simplest 2D constitutive equations of the classical linear theory of plates of Reissner (1944) type with only modest extensions have been used. Moreover, the constitutive equations for M^{α} are either proposed without derivation in the form analogous to that for shear stress resultants Q^{α} only with bending stiffness D and different correcting factor α_t, or are derived as for higher-order stress moments also denoted by M^{α} or $M^{\alpha 3}$ which meaning is different from the one of drilling couples as we understand them. In fact, we are not aware of any explicitly derived constitutive equations for the drilling couples M^{α} available in the literature.

In this paper we propose new explicit definition $(16)_2$ of the drilling couples for shells undergoing small strains. It reveals that the drilling couples appear as a result of through-the-thickness integration of tangential stresses cross-multiplied by non-linear part of displacement distribution in the shell space. This explicit result becomes possible when we apply after Pietraszkiewicz et al. (2006) the modified polar decomposition (10) of the shell deformation gradient and isolate in (9) the intrinsic deformation vector which describes the non-linear part of displacement distribution through the thickness.

In the resultant shell model 2D strain measures are defined only on the base surface, without any relation to 3D strain measures of non-linear elasticity. Thus, it is not possible to found our discussion here on the 3D strain energy density W as in many publications on elastic shells. Instead, we are forced here to begin our discussion of 2D constitutive equations from the 3D complementary energy density W_c.

Various forms of complementary energy in 3D nonlinear elasticity and associated variational principles following from that proposed by Fraeijs de Veubeke (1972) were discussed for example by Guo (1980), Atluri (1984), Reissner (1987), Ibrahimbegović (1993, 1995) or Wempner (1992). In some analogous 2D shell models constructed from 3D ones by thickness kinematic constraints or 3D-to-2D degeneration the drilling couples and bendings were not present, see for example Atluri (1983), Wempner (1986), Simo and Fox (1989) or Ibrahimbegović (1994). In some other analogous shell models the drilling couples and bendings were included, but the constitutive equations for them were taken in the form similar as for shear stress resultants, see for example Chróścielewski et al. (1992, 1997), Sansour and Bufler (1992) or Bischoff et al. (2004). The 2D drilling stress couples and drilling bendings do not appear by definition in complementary shell models formulated directly on the base surface, such as in Altenbach and Zhilin (1988), Valid (1989), Gao and Cheung (1990) or Gałka and Telega (1992).

Brief review of possible forms of W_c in non-linear elasticity given in section 4 indicates that even if W is convex, its dual W_c obtained by the Legendre transformation need not be unique. For an isotropic elastic material undergoing small strains Koiter (1976) proved that the complementary energy density $\mathrm{W}_c = \mathrm{W}_c(\mathbf{T})$, where $\mathbf{T}$ is the Jaumann stress tensor, is the unique quadratic function provided rotations of material elements are at most moderate. But under small strains $\mathbf{T} \simeq \mathbf{S}$, where $\mathbf{S}$ is the 2nd Piola-Kirchhoff stress tensor. In our discussion the effective part (27) of W_c containing only tangential $\mathrm{S}^{\varphi\psi}$ and transverse shear $\mathrm{S}^{\varphi 3}$ stresses acting on the shell cross section is used.

For isotropic elastic shells undergoing small strains John (1965) obtained concrete qualitative error estimates for stresses and their derivatives. In particular, the stresses $\mathrm{S}^{\varphi 3}$ were proved to be one order smaller than $\mathrm{S}^{\varphi\psi}$. To assure the consistent approximation to W_c^{eff}, distribution of $\mathrm{S}^{\varphi\psi}$ through the thickness should be approximated up to cubic terms, while for $\mathrm{S}^{\varphi 3}$ only quadratic distribution is appropriate. In section 5 such cubic approximation (41) of $\mathrm{S}^{\varphi\psi}$ is constructed by analogy to refined statically and kinematically admissible stress distributions of the linear Reissner type shell theory, which were given by Rychter (1988). Applying the system of error estimates proposed by Koiter (1966, 1980), the through-the-thickness integration of W_c^{eff} with refined stress distributions gives the 2D complementary energy density Σ_c^{eff} in the form of quadratic polynomial (47) of the 2D resultant stress measures. Two principal terms of (47) can be viewed as the consistent 1st approximation to the complementary energy density of the geometrically non-linear isotropic elastic shell. Such quadratic form of Σ_c^{eff} is energetically equivalent to the consistent 1st approximation to the elastic strain energy density of the shell, which within the classical linear theory of shells was proposed by Koiter (1960). The four secondary terms of (47) provide a consistent energetic refinement of the two principal terms. We call six quadratic terms of Σ_c^{eff} the consistent 2nd approximation to the complementary energy density of the geometrically non-linear isotropic elastic shells. This consistently refined form of Σ_c^{eff} is new in the literature. The corresponding refined constitutive equations (56) - (58) for 2D strain measures are then obtained by differentiation of Σ_c^{eff} with regard to appropriate resultant stress measures.

To make the results more readable, in section 6 we present them in orthogonal lines of principal curvatures. It is explicitly shown that the 8×8 matrix of coefficients in the constitutive equations for the surface stretches and bendings $E_{\alpha\beta}, K_{\alpha\beta}$ can be divided into two matrices 4×4 for which determinants are calculated. Determinant of the first matrix 4×4 is always positive, while of the second one is positive provided that the principal curvatures R_1, R_2 of the undeformed middle surface are not equal. In both cases we are able to solve the set of linear algebraic equations analytically and provide the consistently refined constitutive equations for physical components of the stress resultants and stress couples $N_{\alpha\beta}, M_{\alpha\beta}$ in terms of $E_{\alpha\beta}, K_{\alpha\beta}$ and R_1, R_2.

Finally, in section 7 we derive the constitutive equations (83) - (85) for the drilling couples M^{α} following from their definition $(16)_2$, the constitutive equations $(52)_2$ for $M^{\alpha\beta}$, and the quadratic part of displacement distribution through the shell thickness. The drilling couples are estimated to be very small quantities of negligible order in analyses of regular shells. However, in case of irregular multi-shells one has to keep these small resultant fields in order to preserve the structure of six-field shell theory at the junctions.

2 Notation and some exact shell relations

A shell is a three-dimensional (3D) solid body identified in a reference (undeformed) placement with a region B of the physical space. The shell boundary $\partial\mathrm{B}$ consists of three separable parts: the upper M^+ and lower M^- shell faces, and the lateral shell boundary surface $\partial\mathrm{B}^*$. The position vectors $\mathbf{x}$ and $\mathbf{y} = \chi(\mathbf{x})$ of any material particle in the reference and deformed placements, respectively, can conveniently be represented by

$$\mathbf{x} = \boldsymbol{x} + \xi \boldsymbol{n}, \quad \mathbf{y} = \boldsymbol{y}(\boldsymbol{x}) + \boldsymbol{\zeta}(\boldsymbol{x}, \xi). \tag{1}$$

Here $\boldsymbol{x}$ and $\boldsymbol{y}$ are position vectors of some shell base surface M and $N = \chi(M)$ in the reference and deformed placements, respectively, ξ is the distance from M along the unit normal vector $\boldsymbol{n}$ orienting M such that $\xi \in [-h^-, h^+]$, $h = h^- + h^+$ is the shell thickness, $\boldsymbol{\zeta}$ is a deviation vector of $\mathbf{y}$ from N, while χ and χ mean the 3D and 2D deformation functions, respectively. In what follows we use the convention that fields defined on the shell base surface are written by italic symbols, except in a few explicitly defined cases.

Geometry of B can be described in normal coordinates $(\theta^{\alpha}, \xi), \alpha = 1, 2,$ such that the corresponding base vectors of M and in B are given by (see Naghdi 1963, Pietraszkiewicz 1979)

$$\boldsymbol{a}_\alpha = \frac{\partial \mathbf{x}}{\partial \theta^\alpha} \equiv \mathbf{x},_\alpha, \quad \boldsymbol{a}^\beta \cdot \boldsymbol{a}_\alpha = \delta^\beta_\alpha, \quad \boldsymbol{n} = \frac{1}{2}\varepsilon^{\alpha\beta}\boldsymbol{a}_\alpha \times \boldsymbol{a}_\beta, \quad b^\alpha_\beta = -\boldsymbol{a}^\alpha \cdot \boldsymbol{n},_\beta,$$
$$\mathbf{g}_\varphi = \frac{\partial \mathbf{x}}{\partial \theta^\varphi} \equiv \mathbf{x},_\varphi = \mu^\alpha_\varphi \boldsymbol{a}_\alpha, \quad \mathbf{g}^\psi \cdot \mathbf{g}_\varphi = \delta^\psi_\varphi, \quad \mathbf{g}^\psi = (\mu^{-1})^\psi_\beta a^{\alpha\beta}\boldsymbol{a}_\alpha, \quad \mathbf{g}_3 = \mathbf{g}^3 = \boldsymbol{n}, \tag{2}$$
$$\mu^\alpha_\varphi = \delta^\alpha_\varphi - \xi b^\alpha_\varphi, \quad (\mu^{-1})^\psi_\beta = \frac{1}{\mu}\left[\delta^\psi_\beta + \xi(b^\psi_\beta - 2H\delta^\psi_\beta)\right], \quad \mu^\alpha_\varphi(\mu^{-1})^\varphi_\beta = \delta^\alpha_\beta,$$
$$\mu^\alpha_\varphi(\mu^{-1})^\psi_\alpha = \delta^\psi_\varphi, \quad \mu = 1 - 2\xi H + \xi^2 K,$$

where $\varepsilon^{\alpha\beta}$ are contravariant components of the permutation tensor $\boldsymbol{\varepsilon}$ on M, b^α_β are mixed components of the curvature tensor $\boldsymbol{b}$ of M, μ^α_φ and $(\mu^{-1})^\psi_\beta$ are geometric shifters, $H = \frac{1}{2}b^\alpha_\alpha$ is the mean curvature and $K = \det\left(b^\alpha_\beta\right)$ the Gaussian curvature of M.

Within the resultant non-linear theory of shells, formulated in the referential description and summarised by Libai and Simmonds (1998) and Chróścielewski et al. (2004), the respective 2D internal contact stress resultant $\boldsymbol{n}_\nu$ and stress couple $\boldsymbol{m}_\nu$ vectors, defined at the edge ∂R of an arbitrary part of the deformed base surface $R = \chi(P), P \subset M$, but measured per unit length of the undeformed edge ∂P having the outward unit normal vector $\boldsymbol{\nu}$, are defined by

$$\boldsymbol{n}_\nu = \int_-^+ \mathbf{P}\mathbf{n}^* \mu \mathrm{d}\xi = \boldsymbol{n}^\alpha \nu_\alpha, \quad \boldsymbol{n}^\alpha = \int_-^+ \mathbf{p}^\alpha \mu \mathrm{d}\xi, \quad \int_-^+ \equiv \int_{-h^-}^{+h^+},$$
$$\boldsymbol{m}_\nu = \int_-^+ \boldsymbol{\zeta} \times \mathbf{P}\mathbf{n}^* \mu \mathrm{d}\xi = \boldsymbol{m}^\alpha \nu_\alpha, \quad \boldsymbol{m}^\alpha = \int_-^+ \boldsymbol{\zeta} \times \mathbf{p}^\alpha \mu \mathrm{d}\xi. \tag{3}$$

Here $\mathbf{P} = \mathbf{p}^\varphi \otimes \mathbf{g}_\varphi + \mathbf{p}^3 \otimes \mathbf{g}_3$ is the Piola stress tensor in the shell space, $\mathbf{n}^* = \mathbf{g}^\alpha \nu_\alpha$ is the external normal to the reference shell orthogonal cross section $\partial \mathrm{P}^*$ (see Konopińska and Pietraszkiewicz 2007, (A.13)), $\mathbf{p}^\alpha = \delta^\alpha_\varphi \mathbf{p}^\varphi$ and $\nu_\alpha = \boldsymbol{\nu} \cdot \boldsymbol{a}_\alpha$. Then the resultant 2D equilibrium equations satisfied for any part $P \subset M$ are

$$\boldsymbol{n}^\alpha|_\alpha + \boldsymbol{f} = \mathbf{0}, \quad \boldsymbol{m}^\alpha|_\alpha + \boldsymbol{y},_\alpha \times \boldsymbol{n}^\alpha + \boldsymbol{c} = \mathbf{0}, \tag{4}$$

where $(\cdot)|_\alpha$ is the covariant derivative in the metric of M, while $\boldsymbol{f}$ and $\boldsymbol{c}$ are the external resultant surface force and couple vectors applied at N, but measured per unit area of M.

The resultant fields $\boldsymbol{n}^\alpha$ and $\boldsymbol{m}^\alpha$ require a unique 2D shell kinematics associated with the shell base surface M. As it was shown in Libai and Simmonds (1983, 1998), Chróścielewski et al. (1992, 2004), and Eremeyev and Pietraszkiewicz (2006), such 2D kinematics consists of the translation vector $\boldsymbol{u}$ and the proper orthogonal (rotation) tensor

$\boldsymbol{Q}$, both describing the gross deformation (work-averaged through the shell thickness) of the shell cross section, such that

$$\boldsymbol{y}=\boldsymbol{x}+\boldsymbol{u}, \quad \boldsymbol{t}_{\alpha}=\boldsymbol{Q}\boldsymbol{a}_{\alpha}, \quad \boldsymbol{t}=\boldsymbol{Q}\boldsymbol{n}, \tag{5}$$

where $\boldsymbol{t}_{\alpha}, \boldsymbol{t}$ are three directors attached to any point of $N=\chi(M)$.

The vectors $\boldsymbol{n}^{\alpha}, \boldsymbol{m}^{\alpha}$ and $\boldsymbol{f}, \boldsymbol{c}$ can naturally be expressed in components relative to the rotated base $\boldsymbol{t}_{\beta}, \boldsymbol{t}$ by

$$\begin{aligned} &\boldsymbol{n}^{\alpha}=N^{\alpha\beta}\boldsymbol{t}_{\beta}+Q^{\alpha}\boldsymbol{t}, \quad \boldsymbol{m}^{\alpha}=\boldsymbol{t}\times M^{\alpha\beta}\boldsymbol{t}_{\beta}+M^{\alpha}\boldsymbol{t}=\varepsilon_{\lambda\beta}M^{\alpha\lambda}\boldsymbol{t}^{\beta}+M^{\alpha}\boldsymbol{t}, \\ &\boldsymbol{f}=f^{\beta}\boldsymbol{t}_{\beta}+f\boldsymbol{t}, \quad \boldsymbol{c}=\boldsymbol{t}\times c^{\beta}\boldsymbol{t}_{\beta}+c\boldsymbol{t}=\varepsilon_{\lambda\beta}c^{\lambda}\boldsymbol{t}^{\beta}+c\boldsymbol{t}. \end{aligned} \tag{6}$$

The 2D components $M^{\alpha}=\boldsymbol{m}^{\alpha}\cdot\boldsymbol{t}$ are usually called the drilling couples.

The shell stretch $\boldsymbol{\varepsilon}_{\alpha}$ and bending $\boldsymbol{\kappa}_{\alpha}$ vectors associated with the 2D shell kinematics (5), which are work-conjugate to the respective stress resultant $\boldsymbol{n}^{\alpha}$ and stress couple $\boldsymbol{m}^{\alpha}$ vectors, are defined by

$$\begin{aligned} &\boldsymbol{\varepsilon}_{\alpha}=\boldsymbol{y}_{,\alpha}-\boldsymbol{t}_{\alpha}=\boldsymbol{u}_{,\alpha}+(\mathbf{1}-\boldsymbol{Q})\boldsymbol{a}_{\alpha}=E_{\alpha\beta}\boldsymbol{t}^{\beta}+E_{\alpha}\boldsymbol{t}, \\ &\boldsymbol{\kappa}_{\alpha}=\operatorname{ax}\left(\boldsymbol{Q}_{,\alpha}\boldsymbol{Q}^{T}\right)=\boldsymbol{t}\times K_{\alpha\beta}\boldsymbol{t}^{\beta}+K_{\alpha}\boldsymbol{t}=\varepsilon_{\lambda\beta}K_{\alpha}^{\cdot\lambda}\boldsymbol{t}^{\beta}+K_{\alpha}\boldsymbol{t}, \end{aligned} \tag{7}$$

where $\mathbf{1}$ is the metric tensor of 3D space and $\operatorname{ax}(\cdot)$ is the axial vector of a skew tensor $(\cdot)$. We call the 2D components $K_{\alpha}=\boldsymbol{\kappa}_{\alpha}\cdot\boldsymbol{t}$ the drilling bendings.

In the numerical analysis it is convenient to assume $\boldsymbol{a}_{\alpha}, \boldsymbol{n}$ to be orthonormal, so that $\boldsymbol{t}_{\alpha}, \boldsymbol{t}$ remain orthonormal during shell deformation.

3 Components of stress resultants and stress couples

Let $\mathbf{S}=\mathbf{F}^{-1}\mathbf{P}=\mathrm{S}^{ij}\mathbf{g}_{i}\otimes\mathbf{g}_{j}=\mathbf{S}^{T}$, $i=1,2,3$, be the 2nd Piola-Kirchhoff stress tensor, where $\mathbf{F}=\operatorname{Grad}\boldsymbol{\chi}=\bar{\mathbf{g}}_{i}\otimes\mathbf{g}^{i}$ is the 3D deformation gradient tensor in the shell space. In convected coordinates (θ^{α},ξ) we have $\mathbf{F}^{-1}=\mathbf{g}_{k}\otimes\bar{\mathbf{g}}^{k}$ and $\mathbf{P}=\mathbf{F}\mathbf{S}=\mathrm{S}^{ij}\bar{\mathbf{g}}_{i}\otimes\mathbf{g}_{j}$, see Pietraszkiewicz and Badur (1963). Thus, the components of $\mathbf{P}$ in the mixed tensor basis $\bar{\mathbf{g}}_{i}\otimes\mathbf{g}_{j}$ coincide with S^{ij}, although $\mathbf{S}\neq\mathbf{P}$. In terms of S^{ij} the 2D resultants $\boldsymbol{n}^{\alpha}$ and $\boldsymbol{m}^{\alpha}$ appearing in (3) take the form

$$\boldsymbol{n}^{\alpha}=\int_{-}^{+}\mathrm{S}^{\alpha i}\mathbf{F}\mathbf{g}_{i}\mu\,d\xi, \quad \boldsymbol{m}^{\alpha}=\int_{-}^{+}\boldsymbol{\zeta}\times\mathrm{S}^{\alpha i}\mathbf{F}\mathbf{g}_{i}\mu\,d\xi. \tag{8}$$

In shell theory an initially straight and normal material fiber described by $\mathbf{x} = \xi \boldsymbol{n}$ deforms into a generally spatially curved material fiber described in the deformed placement by the deviation vector $\boldsymbol{\zeta}$, see (1). For what follows it is convenient to utilize after Pietraszkiewicz et al. (2006) the intrinsic deformation vector $\mathbf{e}(\boldsymbol{x},\xi)$ defined by

$$\mathbf{e} = \boldsymbol{Q}^T \boldsymbol{\zeta} - \xi \boldsymbol{n} = \mathbf{e} = \mathrm{e}^\rho \mathbf{g}_\rho + \mathrm{e}\boldsymbol{n}, \tag{9}$$

where $\boldsymbol{Q}\mathbf{e}$ is a measure of deviation of the deformed curved material fiber, which initially has been straight $\xi \boldsymbol{n}$, from its approximately linear rotated shape $\xi \boldsymbol{Q}\boldsymbol{n}$, see Fig. 1. The representation (9) is purely formal and does not introduce any approximation.

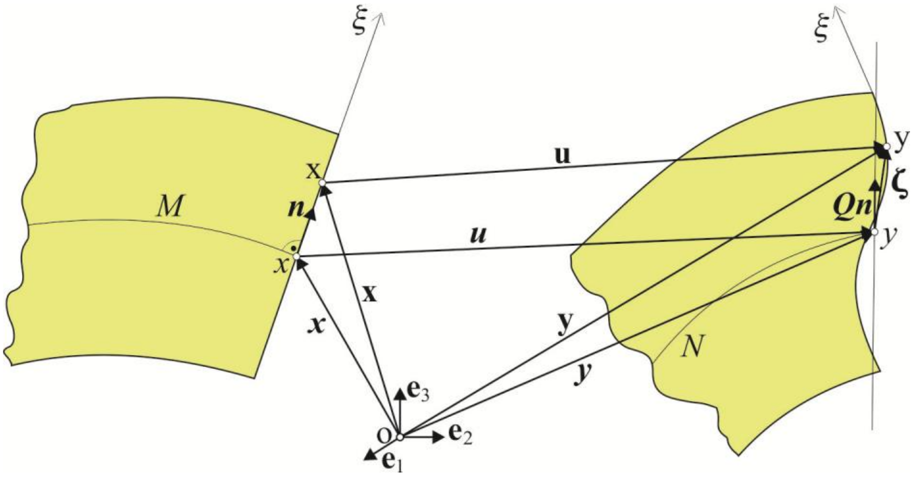

Figure 1. Deformation of the shell cross section

Since in this formulation of shell theory the rotational part of deformation is described by the tensor $\boldsymbol{Q}$, it is natural to apply here, in place of the usual polar decomposition $\mathbf{F} = \mathbf{R}\mathbf{U}$, the modified one in the form

$$\mathbf{F}(\boldsymbol{x},\xi) = \boldsymbol{Q}(\boldsymbol{x})\boldsymbol{\Lambda}(\boldsymbol{x},\xi) = \boldsymbol{Q}(\boldsymbol{x})[\mathbf{1} + \boldsymbol{\Theta}(\boldsymbol{x},\xi)]. \tag{10}$$

In (10) the modified stretch tensor $\boldsymbol{\Lambda}$ satisfies $\det \boldsymbol{\Lambda} > 0$, $\boldsymbol{\Lambda}^T \neq \boldsymbol{\Lambda}$, and the modified relative stretch tensor $\boldsymbol{\Theta}$ is also not symmetric, in general, $\boldsymbol{\Theta} = \Theta_{ij} \mathbf{g}^i \otimes \mathbf{g}^j \neq \boldsymbol{\Theta}^T$.

Let us introduce the referential stress resultant and stress couple vectors

$$\begin{aligned} \mathbf{n}^\alpha &= \boldsymbol{Q}^T \boldsymbol{n}^\alpha = \int_-^+ \mathrm{S}^{\alpha i} (\delta_i^k + \Theta_i^{\cdot k}) \mathbf{g}_k \mu \mathrm{d}\xi = N^{\alpha\beta} \boldsymbol{a}_\beta + Q^\alpha \boldsymbol{n}, \\ \mathbf{m}^\alpha &= \boldsymbol{Q}^T \boldsymbol{m}^\alpha = \int_-^+ (\xi \boldsymbol{n} + \mathbf{e}) \times \mathrm{S}^{\alpha i} (\delta_i^k + \Theta_i^{\cdot k}) \mathbf{g}_k \mu \mathrm{d}\xi = \varepsilon_{\lambda\mu} M^{\alpha\lambda} \boldsymbol{a}^\mu + M^\alpha \boldsymbol{n}. \end{aligned} \tag{11}$$

After some transformations the vector $\mathbf{m}^\alpha$ can also be given in the expanded form

$$\mathbf{m}^{\alpha}=\int_{-}^{+}\mathrm{S}^{\alpha i}\left\{\left[(\xi+\mathrm{e})(\delta_i^{\psi}+\Theta_i^{\cdot\psi})\mu_{\psi}^{\lambda}-\mathrm{e}^{\rho}(\delta_i^{3}+\Theta_i^{\cdot 3})\mu_{\rho}^{\lambda}\right]\varepsilon_{\lambda\mu}\boldsymbol{a}^{\mu}+\mathrm{e}^{\rho}(\delta_i^{\psi}+\Theta_i^{\cdot\psi})\varepsilon_{\gamma\lambda}\mu_{\rho}^{\gamma}\mu_{\psi}^{\lambda}\boldsymbol{n}\right\}\mu\mathrm{d}\xi\,. \tag{12}$$

The shell stress resultants and stress couples follow now from $(11)_1$ and (12) leading to

$$\begin{aligned} N^{\alpha\beta}&=\mathbf{n}^{\alpha}\cdot\boldsymbol{a}^{\beta}=\int_{-}^{+}\mathrm{S}^{\alpha i}(\delta_i^{\psi}+\Theta_i^{\cdot\psi})\mu_{\psi}^{\beta}\mu\mathrm{d}\xi\,,\\ Q^{\alpha}&=\mathbf{n}^{\alpha}\cdot\boldsymbol{n}=\int_{-}^{+}\mathrm{S}^{\alpha i}(\delta_i^{3}+\Theta_i^{\cdot 3})\mu\mathrm{d}\xi\,,\end{aligned} \tag{13}$$

$$\begin{aligned} M^{\alpha\beta}&=\mathbf{m}^{\alpha}\cdot\varepsilon^{\beta\gamma}\boldsymbol{a}_{\gamma}=\int_{-}^{+}\mathrm{S}^{\alpha i}\left[(\xi+\mathrm{e})(\delta_i^{\psi}+\Theta_i^{\cdot\psi})-\mathrm{e}^{\psi}(\delta_i^{3}+\Theta_i^{\cdot 3})\right]\mu_{\psi}^{\beta}\mu\mathrm{d}\xi\,,\\ M^{\alpha}&=\mathbf{m}^{\alpha}\cdot\boldsymbol{n}=\int_{-}^{+}\mathrm{S}^{\alpha i}\mathrm{e}^{\rho}(\delta_i^{\psi}+\Theta_i^{\cdot\psi})\varepsilon_{\gamma\beta}\mu_{\rho}^{\gamma}\mu_{\psi}^{\beta}\mu\mathrm{d}\xi\,.\end{aligned} \tag{14}$$

The relations (13) and (14) are *exact implications* of the through-the-thickness integration of an arbitrary stress distribution in the shell space.

Most shell models are constructed with the use of kinematic constraints "material fibres initially normal to the shell base surface remain straight during deformation process". In such shell models $\mathbf{e}\equiv\mathbf{0}$ and the drilling couples $(14)_2$ disappear by definition.

In the resultant geometrically non-linear shell theory the largest stretch in the shell space is assumed to be small, so that $\|\boldsymbol{\Theta}\|<<1$. Let us also assume here the length of intrinsic deformation vector $\mathbf{e}$ to be at least one order smaller as compared with *h*, so that $(|\mathbf{e}|/h)^2<<1$. In fact, we shall show in section 5 that in case of small elastic strains tangential components of $\mathbf{e}$ are of much smaller order. Then omitting the corresponding small terms with respect to the unity, we obtain

$$\begin{aligned} N^{\alpha\beta}&\simeq\int_{-}^{+}(\mathrm{S}^{\alpha\psi}+\mathrm{S}^{\alpha 3}\Theta_3^{\cdot\psi})\mu_{\psi}^{\beta}\mu\mathrm{d}\xi\simeq\int_{-}^{+}\mathrm{S}^{\alpha\psi}\mu_{\psi}^{\beta}\mu\mathrm{d}\xi,\\ Q^{\alpha}&\simeq\int_{-}^{+}(\mathrm{S}^{\alpha 3}+\mathrm{S}^{\alpha\psi}\Theta_{\psi}^{\cdot 3})\mu\mathrm{d}\xi\simeq\int_{-}^{+}\mathrm{S}^{\alpha 3}\mu\mathrm{d}\xi\,,\end{aligned} \tag{15}$$

$$\begin{aligned} M^{\alpha\beta}&\simeq\int_{-}^{+}\left[\mathrm{S}^{\alpha\psi}(\xi+\mathrm{e})+\mathrm{S}^{\alpha 3}(\xi\Theta_3^{\cdot\psi}-\mathrm{e}^{\psi})\right]\mu_{\psi}^{\beta}\mu\mathrm{d}\xi\simeq\int_{-}^{+}\mathrm{S}^{\alpha\psi}\mu_{\psi}^{\beta}\mu\xi\mathrm{d}\xi\,,\\ M^{\alpha}&\simeq\int_{-}^{+}(\mathrm{S}^{\alpha\psi}\mu_{\psi}^{\beta}\mu)\varepsilon_{\gamma\beta}\mu_{\rho}^{\gamma}\mathrm{e}^{\rho}\mathrm{d}\xi\,.\end{aligned} \tag{16}$$

The explicit definition $(16)_2$ of M^{α} have become possible because in (9) we have introduced explicitly the vector $\mathbf{e}$ and have applied the modified polar decomposition (10) of $\mathbf{F}$. The relation $(16)_2$ indicates that in the geometrically non-linear shell theory M^{α} can be established if $\mathrm{S}^{\alpha\psi}\mu_{\psi}^{\beta}\mu$ and e^{ρ} are known. We discuss this in more detail in section 7.

Libai and Simmonds (1983, 1998) introduced M^{α} implicitly as $\boldsymbol{M}^{\alpha}\cdot\boldsymbol{t}$ as well, but their resultant stress couple $\boldsymbol{M}^{\alpha}$ was defined relative to the deformed, non-material, weighted surface of mass of the shell, not relative to the deformed material shell base surface $N=\chi(M)$ as in this report. However, in some papers, see for example Naghdi (1972), Paimushin (1986), Bishoff et al. (2004) or Chróścielewski et al (2010), the 2D fields M^{α} or $M^{\alpha 3}$ are defined as the resultants of first moments of shear stresses $\int_{-}^{+} \mu S^{\alpha 3} \xi d\xi$. Such fields have other mechanical meaning than our drilling couples M^{α}.

4 3D complementary energy density

In non-linear elasticity the internal energy of the body is usually described by the stored energy density $\mathrm{W}=\mathrm{W}(\mathbf{F})$ per unit volume of B such that $\mathbf{P}=\partial \mathrm{W}/\partial \mathbf{F}$. In our approach the 2D vectorial stress measures (8) are the primary fields defined by direct through-the-thickness integration of the Piola stress tensor $\mathbf{P}$. Hence, for establishing 2D constitutive equations from their 3D form it is necessary to use the complementary energy density.

The first choice of such density $\mathrm{W}_c=\mathrm{W}_c(\mathbf{P})$, per unit volume of B, would be the one which is related to the strain energy density $\mathrm{W}(\mathbf{F})$ by the Legendre transformation

$$\mathrm{W}_c(\mathbf{P})=\mathbf{P}:\mathbf{F}-\mathrm{W}(\mathbf{F}) \ , \tag{17}$$

where $\mathbf{P}:\mathbf{F}=\operatorname{tr}(\mathbf{P}^T\mathbf{F})$. Existence of such $\mathrm{W}_c(\mathbf{P})$ crucially depends on whether the stress–strain relation $\mathbf{P}=\mathbf{P}(\mathbf{F})$ can be uniquely inverted to the form $\mathbf{F}=\mathbf{F}(\mathbf{P})$. Only then from (17) one could establish uniquely $\mathrm{W}_c(\mathbf{P})$ from which $\mathbf{F}=\partial \mathrm{W}_c/\partial \mathbf{P}$. Unfortunately, unique invertibility of the tensor function $\mathbf{P}=\mathbf{P}(\mathbf{F})$ is not assured, because the scalar-valued function $\mathrm{W}=\mathrm{W}(\mathbf{F})$ is not convex, in general. Only some special cases were discussed in several papers by Zubov, Koiter, Ogden, Gao, Shield, Wempner, and others. In particular, in the case of an isotropic elastic material Zubov (1976) proved that there are four different branches of such an inversion. But when the angle of rotation ϕ of principal axes of strain is such that $\cos\phi<1/3$, i.e. $\phi <\sim 70^{\circ}$, only one branch of the four is realized. In such a case the inverted tensor function $\mathbf{F}=\mathbf{F}(\mathbf{P})$ can be uniquely established, at least in principle, provided that the tensor $\mathbf{P}^T\mathbf{P}$ has distinct eigenvalues at any point of the body. Ogden (1977) independently confirmed that such a unique inversion is possible under the latter condition. These requirements suggest serious difficulties in constructing explicitly the unique function $\mathrm{W}_c(\mathbf{P})$.

For our purpose it is more convenient to use, after Koiter (1976), the stored energy density $\mathrm{W} = \bar{\mathrm{W}}(\boldsymbol{\varepsilon})$, where $\boldsymbol{\varepsilon} = \mathbf{U} - \mathbf{1} = \boldsymbol{\varepsilon}^T$ is the relative stretch tensor with the right stretch tensor $\mathbf{U} = \mathbf{U}^T$ following from the polar decomposition $\mathbf{F} = \mathbf{RU}$. Differentiating the density $\bar{\mathrm{W}}(\boldsymbol{\varepsilon})$ we obtain

$$\frac{\partial \bar{\mathrm{W}}}{\partial \boldsymbol{\varepsilon}} = \mathbf{T} = \frac{1}{2}\left(\mathbf{SU} + \mathbf{US}\right) = \mathrm{T}^{ij}\mathbf{g}_i \otimes \mathbf{g}_j \,, \tag{18}$$

where $\mathbf{T} = \mathbf{T}^T$ is the Jaumann stress tensor. But even in this case inversion of $\mathbf{T} = \mathbf{T}(\boldsymbol{\varepsilon})$ is still complex for anisotropic elastic materials, because then $\mathbf{T}$ and $\boldsymbol{\varepsilon}$ are not coaxial, in general. Only in the case of an isotropic elastic material, when $\mathbf{T}$ and $\boldsymbol{\varepsilon}$ become coaxial, one can invert in principle the stress-strain relation to $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{T})$, and applying the Legendre transformation one can construct explicitly $\bar{\mathrm{W}}_c(\mathbf{T})$ such that $\boldsymbol{\varepsilon} = \partial \bar{\mathrm{W}}_c / \partial \mathbf{T}$, provided that rotations of material elements are at most moderate, see Koiter (1976).

The elastic range of many engineering materials is restricted to *small strains* such that $\|\boldsymbol{\varepsilon}\| << 1$ and the constitutive equations are governed by the Hooke law. In such case $\bar{\mathrm{W}}(\boldsymbol{\varepsilon})$ becomes the positive definite, homogeneous, convex, quadratic function of the form

$$\bar{\mathrm{W}}(\boldsymbol{\varepsilon}) = \frac{1}{2}\mathrm{L}^{ijkl}\varepsilon_{ij}\varepsilon_{kl} \,, \quad \mathrm{L}^{ijkl} = \mathrm{L}^{jikl} = \mathrm{L}^{ijlk} = \mathrm{L}^{klij} \,, \tag{19}$$

where L^{ijkl} are components of the 4th-order tensor of elastic moduli. The linear constitutive equations $\mathrm{T}^{ij} = \partial \bar{\mathrm{W}} / \partial \varepsilon_{ij} = \mathrm{L}^{ijkl}\varepsilon_{kl}$ can now be easily inverted to obtain $\varepsilon_{ij} = \mathrm{K}_{ijkl}\mathrm{T}^{kl}$, where K_{ijkl} are components of the 4th-order tensor of elastic compliances, which satisfy the relation

$$\mathrm{K}_{ijkl}\mathrm{L}^{klpq} = \frac{1}{2}\left(\delta_i^p \delta_j^q + \delta_i^q \delta_j^p\right). \tag{20}$$

The corresponding complementary energy density follows from the Legendre transformation and takes the form

$$\bar{\mathrm{W}}_c(\mathbf{T}) = \mathbf{T} : \boldsymbol{\varepsilon}(\mathbf{T}) - \bar{\mathrm{W}}[\boldsymbol{\varepsilon}(\mathbf{T})] = \frac{1}{2}\mathrm{K}_{ijkl}\mathrm{T}^{ij}\mathrm{T}^{kl} \,. \tag{21}$$

It can easily be seen from (18) that within small strains $\mathbf{T} \simeq \mathbf{S}$, so that also their components $\mathrm{T}^{ij} \simeq \mathrm{S}^{ij}$ in the undeformed tensor base $\mathbf{g}_i \otimes \mathbf{g}_j$.

For an isotropic elastic material the 3D elastic moduli and compliances are

$$\mathrm{L}^{ijkl} = \frac{E}{2(1+\nu)}\left(\mathrm{g}^{ik}\mathrm{g}^{jl} + \mathrm{g}^{il}\mathrm{g}^{jk} + \frac{2\nu}{1-2\nu}\mathrm{g}^{ij}\mathrm{g}^{kl} \right) \tag{22}$$

$$\mathrm{K}_{ijkl}=\frac{1}{2E}\left[(1+\nu)\left(\mathrm{g}_{ik}\mathrm{g}_{jl}+\mathrm{g}_{il}\mathrm{g}_{jk}\right)-2\nu\mathrm{g}_{ij}\mathrm{g}_{kl}\right], \tag{23}$$

with E the Young modulus and ν the Poisson ratio.

The restriction to small elastic strains used in (19) and (21) does not reduce the non-linear elasticity to the linear theory of elasticity, because the rotational part of deformation $\mathbf{R}=\mathbf{F}\mathbf{U}^{-1}$ is still allowed to be moderate, see Koiter (1976).

Taking into account symmetries of K_{ijkl} and S^{ij}, the quadratic expression (21) can be written as the sum of four separate terms each representing a part of 3D complementary energy density calculated from the stresses $\mathrm{S}^{\varphi\psi}$, $\mathrm{S}^{\varphi 3}=\mathrm{S}^{3\varphi}$ and S^{33}, so that

$$\begin{aligned}\bar{\mathrm{W}}_c&=\frac{1}{2}\left[\mathrm{K}_{\varphi\psi\theta\sigma}\mathrm{S}^{\varphi\psi}\mathrm{S}^{\theta\sigma}+\mathrm{K}_{\varphi3\theta3}\left(\mathrm{S}^{\varphi3}+\mathrm{S}^{3\varphi}\right)\left(\mathrm{S}^{\theta3}+\mathrm{S}^{3\theta}\right)+2\mathrm{K}_{\varphi\psi33}\mathrm{S}^{\varphi\psi}\mathrm{S}^{33}+\mathrm{K}_{3333}\mathrm{S}^{33}\mathrm{S}^{33}\right]\\&=\frac{1}{2\mu^2}\Big[A_{\alpha\beta\lambda\mu}\mu^\alpha_\varphi\left(\mu\mathrm{S}^{\varphi\psi}\mu^\beta_\psi\right)\mu^\lambda_\theta\left(\mu\mathrm{S}^{\theta\sigma}\mu^\mu_\sigma\right)+4A_{\alpha3\lambda3}\mu^\alpha_\varphi\left(\mu\mathrm{S}^{\varphi3}\right)\mu^\lambda_\theta\left(\mu\mathrm{S}^{\theta3}\right)\\&\qquad+2A_{\alpha\beta33}\mu^\alpha_\varphi(\mu\mathrm{S}^{\varphi\psi}\mu^\beta_\psi)(\mu\mathrm{S}^{33})+A_{3333}(\mu\mathrm{S}^{33})(\mu\mathrm{S}^{33})\Big],\end{aligned} \tag{24}$$

where

$$\begin{aligned}&\mathrm{S}^{\alpha\psi}=\delta^\alpha_\varphi\mathrm{S}^{\varphi\psi}\ ,\quad \mathrm{K}_{\varphi\psi\theta\sigma}=A_{\alpha\beta\lambda\mu}\mu^\alpha_\varphi\mu^\beta_\psi\mu^\lambda_\theta\mu^\mu_\sigma\ ,\quad \mathrm{K}_{\varphi\psi33}=A_{\alpha\beta33}\mu^\alpha_\varphi\mu^\beta_\psi\ ,\\&\mathrm{S}^{\alpha3}=\delta^\alpha_\varphi\mathrm{S}^{\varphi3}\ ,\quad \mathrm{K}_{\varphi3\theta3}=A_{\alpha3\lambda3}\mu^\alpha_\varphi\mu^\lambda_\theta\ ,\quad \mathrm{K}_{3333}=A_{3333}\ .\end{aligned} \tag{25}$$

In particular, for an isotropic linearly elastic solid

$$\begin{aligned}&A_{\alpha\beta\lambda\mu}=\frac{1}{2E}\left[(1+\nu)\left(a_{\alpha\lambda}a_{\beta\mu}+a_{\alpha\mu}a_{\beta\lambda}\right)-2\nu a_{\alpha\beta}a_{\lambda\mu}\right],\quad A_{\alpha3\lambda3}=\frac{1+\nu}{2E}a_{\alpha\lambda}\ ,\\&A_{\alpha\beta33}=-\frac{\nu}{E}a_{\alpha\beta}\ ,\quad A_{3333}=\frac{1}{E}\ .\end{aligned} \tag{26}$$

However, definitions (13) - (16) of the resultant surface stress measures are given through the stress components $\mathrm{S}^{\alpha\psi}$, $\mathrm{S}^{\alpha3}$ alone, because only those stress components act on the shell cross section and their resultants enter the resultant shell equilibrium equations (4). The stress component S^{33} acts on the shell surfaces $\xi=\mathrm{const}$ parallel to the base surface M. Although S^{33} contributes to the 3D complementary energy density (24), it does not enter the resultant 2D equilibrium equations and does not contribute to the effective part $\bar{\mathrm{W}}_c^{eff}$ of $\bar{\mathrm{W}}_c$ associated with the resultants (13) - (16). Thus,

$$\bar{\mathrm{W}}_c^{eff}=\frac{1}{2\mu^2}\left[A_{\alpha\beta\lambda\mu}\mu^\alpha_\varphi\left(\mu\mathrm{S}^{\varphi\psi}\mu^\beta_\psi\right)\mu^\lambda_\theta\left(\mu\mathrm{S}^{\theta\sigma}\mu^\mu_\sigma\right)+4A_{\alpha3\lambda3}\mu^\alpha_\varphi\left(\mu\mathrm{S}^{\varphi3}\right)\mu^\lambda_\theta\left(\mu\mathrm{S}^{\theta3}\right)\right]. \tag{27}$$

This effective part of $\bar{\mathrm{W}}_c$ will be used to derive the constitutive equations of elastic shells.

Let us assume, for definiteness, that the base surface M is taken as the middle surface of the shell in the undeformed placement, that is $h^{-}=h^{+}=h/2$. This particular choice of M will considerably simplify all transformations given below. We also assume, for simplicity, that there are no surface forces applied at the upper and lower shell faces $M^{\pm}$, and no body forces applied in the internal shell space (otherwise these loads would appear explicitly in 2D constitutive equations, which we do not want). Then the exact reduction of 3D stress field to its 2D resultants defined by (15) and (16) means that to within bulk terms distribution of pseudo-stresses in the shell space can, in fact, be approximately represented up to cubic terms in the thickness direction according to

$$\begin{aligned}
&\mu S^{\alpha\psi}\mu_{\psi}^{\beta} \simeq \frac{1}{h}N^{\alpha\beta}+\frac{12}{h^{3}}M^{\alpha\beta}\xi+Q^{\alpha\beta}(\xi)+C^{\alpha\beta}(\xi)\,,\\
&\mu S^{\alpha 3} \simeq \frac{1}{h}Q^{\alpha} f(\xi), \quad f(\xi)=\frac{3}{2}\left(1-\frac{4\xi^{2}}{h^{2}}\right),
\end{aligned} \tag{28}$$

where $Q^{\alpha\beta}(\xi)$ are quadratic and $C^{\alpha\beta}(\xi)$ are cubic polynomials of ξ which should satisfy the relations

$$\begin{aligned}
&Q^{\alpha\beta}(-\xi)=Q^{\alpha\beta}(\xi)\,, \quad \int_{-}^{+}Q^{\alpha\beta}(\xi)d\xi=0\,, \quad \int_{-}^{+}\xi Q^{\alpha\beta}(\xi)d\xi=0\,,\\
&C^{\alpha\beta}(-\xi)=-C^{\alpha\beta}(\xi)\,, \quad \int_{-}^{+}C^{\alpha\beta}(\xi)d\xi=0\,, \quad \int_{-}^{+}\xi C^{\alpha\beta}(\xi)d\xi=0\,.
\end{aligned} \tag{29}$$

The approximately cubic tangential stress distribution $(28)_1$ with quadratic and cubic parts having properties (29) satisfy definitions $(15)_1$ for $N^{\alpha\beta}$ and $(16)_1$ for $M^{\alpha\beta}$. This distribution can be used to derive the approximate expressions for the drilling couples following from $(16)_2$.

Unfortunately, we are not aware of any discussion in the literature of possible forms of $Q^{\alpha\beta}(\xi)$ and $C^{\alpha\beta}(\xi)$ in the geometrically non-linear theory of elastic shells. Looking for suggestions as to appropriate forms of $Q^{\alpha\beta}(\xi)$ and $C^{\alpha\beta}(\xi)$, let us recall some results available in the linear shell theory.

5 The linear theory of shells

In the linear theory of shells not only strains in the shell space are small, but also translations and rotations are assumed to be small,

$$\varepsilon=\max_{x\in M}\left(\|\boldsymbol{u}\|,\|\boldsymbol{\psi}\|\right)<<1\,, \tag{30}$$

where $\boldsymbol{\psi} = \phi \boldsymbol{i}$ is the linearised rotation vector, with ϕ the angle of rotation about the rotation axis described by the eigenvector $\boldsymbol{i}$ of $\boldsymbol{Q}$, i.e. $\boldsymbol{Q}\boldsymbol{i} = +\boldsymbol{i}$.

In components we have

$$\boldsymbol{u} = u_\alpha \boldsymbol{a}^\alpha + w\boldsymbol{n}\,, \quad \boldsymbol{\psi} = \boldsymbol{n}\times(\psi_\alpha \boldsymbol{a}^\alpha) + \psi\boldsymbol{n} = \varepsilon^{\alpha\lambda}\psi_\alpha \boldsymbol{a}_\alpha + \psi\boldsymbol{n}\,. \tag{31}$$

Since for small rotations $\boldsymbol{Q} \simeq \mathbf{1} + \boldsymbol{\psi}\times\mathbf{1}$, following Chróścielewski et al. 2004, Chapter 2.8, we can linearize the kinematic relations (7) with regard to $\boldsymbol{u}$ and $\boldsymbol{\psi}$ to obtain

$$\begin{aligned} E_{\alpha\beta} &= \boldsymbol{u},_\alpha \cdot \boldsymbol{a}_\beta - \varepsilon_{\alpha\beta}\boldsymbol{\psi}\cdot\boldsymbol{n} = u_{\beta|\alpha} - b_{\alpha\beta}w - \varepsilon_{\alpha\beta}w\,, \\ E_\alpha &= \boldsymbol{u},_\alpha \cdot \boldsymbol{n} + \varepsilon_{\alpha\beta}\boldsymbol{\psi}\cdot\boldsymbol{a}^\beta = w,_\alpha + b_\alpha^\beta u_\beta + \psi_\alpha\,, \end{aligned} \tag{32}$$

$$\begin{aligned} K_{\alpha\beta} &= \boldsymbol{\psi},_\alpha \cdot \varepsilon_{\beta\lambda}\boldsymbol{a}^\lambda = \psi_{\beta|\alpha} - \varepsilon_{\beta\lambda}b_\alpha^\lambda \psi\,, \\ K_\alpha &= \boldsymbol{\psi},_\alpha \cdot \boldsymbol{n} = \psi,_\alpha - \varepsilon_{\lambda\beta}b_\alpha^\lambda \psi^\beta\,. \end{aligned} \tag{33}$$

Then linearization of component form of equilibrium equations (4) yields

$$\begin{aligned} &N^{\alpha\beta}|_\alpha - b_\alpha^\beta Q^\alpha + f^\beta = 0\,, \quad Q^\alpha|_\alpha + b_{\alpha\beta}N^{\alpha\beta} + f = 0\,, \\ &M^{\alpha\beta}|_\alpha + \varepsilon^{\lambda\beta}b_{\alpha\lambda}M^\alpha - Q^\beta + c^\beta = 0\,, \quad M^\alpha|_\alpha + \varepsilon_{\alpha\beta}(N^{\alpha\beta} - b_\lambda^\alpha M^{\lambda\beta}) + c = 0\,. \end{aligned} \tag{34}$$

Please note that within such resultant linear shell theory twelve linear kinematic relations (32) and (33) involve the drilling rotation ψ and the drilling bendings K_α while six linear equilibrium equations (34) include also the drilling couples M^α. This was explicitly shown already by Reissner (1974). In classical linear shell theories of Kirchhoff-Love and Timoshenko-Reissner types the components ψ, K_α and M^α do not appear in analogous shell relations, see for example Love (1927), Naghdi (1972), Basar and Kratzig (2001), Ciarlet (2005).

However, even within such extended six-field linear theory of shells we are not aware of any discussion on possible forms of $Q^{\alpha\beta}(\xi)$ and $C^{\alpha\beta}(\xi)$ available in the literature. Leaving such a discussion for future work, for the purpose of this report we shall use some results available for a simpler version of the linear shell theory.

Analysing accuracy of the linear Reissner-type shell theory, Rychter (1988) constructed consistently refined 3D displacement and stress fields in the shell as polynomials of 2D shell solutions. The refined 3D fields were then compared to unknown solutions of linear elasticity in energy norm using the hypersphere theorem of Prager and Synge (1947) (see also Synge 1957) and appropriate inequalities to obtain refined global error estimates. It was found, in particular, that the consistently refined kinematically admissible tangential components of 3D displacement field are (see Rychter 1988, Eqs. (26a), (27a,b,c,d))

$$\hat{\mathrm{u}}_\alpha(\theta^\kappa,\xi) \simeq u_\alpha(\theta^\kappa)+\xi\psi_\alpha(\theta^\kappa)+\left(\frac{4\xi^2}{h^2}-\frac{1}{3}\right)q_\alpha(\theta^\kappa)+\left(\frac{8\xi^3}{h^3}-\frac{6}{5}\frac{\xi}{h}\right)c_\alpha(\theta^\kappa)$$
$$q_\alpha=\frac{h}{4}D^{\lambda\mu}E_{(\lambda\mu)},_\alpha\,,\quad c_\alpha=\frac{h^3}{48}D^{\lambda\mu}K_{(\lambda\mu)},_\alpha-\frac{5}{24}hE_\alpha\,,\quad D^{\lambda\mu}=\left(L^{\lambda\mu 33}/L^{3333}\right)|_{\xi=0}=\frac{\nu}{1-\nu}a^{\lambda\mu}\,, \tag{35}$$

where symbols $\hat{u}_\alpha, x^\beta, t, \upsilon_\alpha, h, c_\alpha, d_\alpha, \bar{C}^{\lambda\mu}, \gamma_{(\alpha\beta)}, \gamma_{\alpha 3}, \kappa_{(\alpha\beta)}$ of Rychter (1988) have been changed here into the respective symbols $\hat{\mathrm{u}}_\alpha, \theta^\kappa, 2\xi/h, u_\alpha, 2h, q_\alpha, c_\alpha, D^{\lambda\mu}, E_{(\alpha\beta)}, E_\alpha, K_{(\alpha\beta)}$ used in this report. Within the consistent approximation (35) the 2D components $u_\alpha(\theta^\kappa)$ and $\psi_\alpha(\theta^\kappa)$ of the linear theory of shells of Reissner type can be interpreted through the kinematically admissible 3D components $\hat{\mathrm{u}}_\alpha(\theta^\kappa,\xi)$ of linear elasticity by

$$u_\alpha(\theta^\kappa)=\int_-^+\hat{\mathrm{u}}_\alpha(\theta^\kappa,\xi)d\xi\,,\quad \psi_\alpha(\theta^\kappa)=\int_-^+\hat{\mathrm{u}}_\alpha(\theta^\kappa,\xi)\xi d\xi\,. \tag{36}$$

The corresponding consistently refined statically admissible tangential pseudo-stresses of the linear shell theory of Reissner type take the form (see Rychter 1988, eqs. (30a), $(36)_2$)

$$\mu\bar{\sigma}^{\alpha\psi}\mu_\psi^\beta \simeq \frac{1}{h}N^{\alpha\beta}+\xi\frac{12}{h^3}M^{\alpha\beta}+H^{\alpha\beta\lambda\mu}\left[\left(\frac{4\xi^2}{h^2}-\frac{1}{3}\right)q_{(\lambda|\mu)}+\left(\frac{8\xi^3}{h^3}-\frac{6}{5}\frac{\xi}{h}\right)c_{(\lambda|\mu)}\right],$$
$$H^{\alpha\beta\lambda\mu}=\left(L^{\alpha\beta\lambda\mu}-L^{\alpha\beta 33}L^{33\lambda\mu}/L^{3333}\right)|_{\xi=0}=\frac{E}{2(1+\nu)}\left(a^{\alpha\lambda}a^{\beta\mu}+a^{\alpha\mu}a^{\beta\lambda}+\frac{2\nu}{1-\nu}a^{\alpha\beta}a^{\lambda\mu}\right) \tag{37}$$

where $\bar{\sigma}^{\alpha\psi}$ are statically admissible components of 3D symmetric stress tensor of linear elasticity. It is easy to check that the stress field $(37)_1$ is compatible with definitions $N^{\alpha\beta}$ and $M^{\alpha\beta}$ following from linearization of $(15)_1$ and $(16)_1$,

$$N^{\alpha\beta}=\int_-^+\bar{\sigma}^{\alpha\psi}\mu_\psi^\beta\mu d\xi\,,\quad M^{\alpha\beta}=\int_-^+\bar{\sigma}^{\alpha\psi}\mu_\psi^\beta\mu\xi d\xi\,. \tag{38}$$

The eqn. $(35)_1$ suggests that within the linear shell theory of Reissner type components $\mathrm{e}^\rho(\xi)$ of the intrinsic deviation vector **e** introduced in (9) can be consistently approximated by the following quadratic and cubic polynomials:

$$\mathrm{e}^\rho(\xi)\simeq k(\xi)q^\rho+g(\xi)c^\rho\,,\quad k(\xi)=\frac{4\xi^2}{h^2}-\frac{1}{3},\quad g(\xi)=\frac{8\xi^3}{h^3}-\frac{6}{5}\frac{\xi}{h}\,, \tag{39}$$

which satisfy the relations (29). In particular, the function $k(\xi)$ is even while $g(\xi)$ is odd with regards to ξ,

$$k(-\xi)=k(\xi)\,,\quad g(-\xi)=-g(\xi)\,. \tag{40}$$

Since orders of q^{ρ}, c^{ρ} following from $(35)_{2,3}$ seem to be very small, the values of M^{α} calculated from $(16)_2$ would be very small as well in the linear six-field shell model. This suggests that consistently refined 3D tangential displacement and stress fields $(35)_1$ and $(37)_1$, which are appropriate for the Reissner type linear shell model, should also be adequate for the resultant six-field linear shell model.

6 The geometrically non-linear theory of shells

The bulk distribution of $\mu \mathrm{S}^{\alpha\psi} \mu_{\psi}^{\beta}$ given in $(28)_1$ does contain only intrinsic resultant 2D variables. Thus, when strains are small everywhere in the shell space, the pseudo-stresses can still be refined by quadratic and cubic terms analogous to those appropriate for the Reissner type linear shell model in $(37)_1$,

$$\mu \mathrm{S}^{\alpha\psi} \mu_{\psi}^{\beta} \simeq \frac{1}{h} N^{\alpha\beta} + \xi \frac{12}{h^3} M^{\alpha\beta} + H^{\alpha\beta\lambda\mu} \left[k(\xi) q_{(\lambda|\mu)} + g(\xi) c_{(\lambda|\mu)} \right]. \tag{41}$$

For thin isotropic elastic shells undergoing small strains John (1965) obtained concrete quantitative error estimates for stresses and their derivatives in the case of vanishing surface and body forces. With additional physically motivated estimates proposed by Koiter (1960, 1966, 1980), we can estimate orders of some fields appearing in such small-strain shell theory as follows:

$$\begin{gathered} A_{\alpha\beta\lambda\mu} \sim \frac{1}{E}, \quad A_{\alpha 3\lambda 3} \sim \frac{\nu}{E}, \quad \mathrm{S}^{\varphi\psi} \sim E\eta, \quad \mathrm{S}^{\varphi 3} \sim E\eta\theta, \\ L = \min_{x \in M} \left(l, L_E, L_K \right), \quad \theta = \max_{x \subset M} \left(\frac{h}{L}, \frac{h}{d}, \sqrt{\frac{h}{R}}, \sqrt{\eta} \right), \quad \theta^2 << 1, \\ a_{\alpha\beta} \sim \delta_{\alpha}^{\beta} \sim 1, \quad b_{\alpha\beta} \sim b_{\alpha}^{\beta} \sim H \sim \frac{1}{R} \sim \frac{\theta^2}{h}, \quad K \sim \frac{1}{R^2} \sim \frac{\theta^4}{h^2}, \end{gathered} \tag{42}$$

where $\sim$ means "of the order of", l is the characteristic length of geometric patterns of *M*, L_E and L_K are the characteristic lengths of extensional and bending deformation patterns on *M*, respectively, d is the distance of internal shell points to the shell boundary $\partial \mathrm{B}$, and θ is the common small parameter.

Assuming that the stresses $\mathrm{S}^{\varphi\psi}$ entering definitions $(15)_1$ of $N^{\alpha\beta}$ and $(16)_1$ of $M^{\alpha\beta}$ are of the same order, from (28) and (42) we obtain the estimates

$$N^{\alpha\beta} \sim Eh\eta, \quad M^{\alpha\beta} \sim Eh^2\eta, \quad Q^{\alpha} \sim Eh\eta\theta. \tag{43}$$

We have assumed above (15) that in case of small strains $(|\mathbf{e}|/h)^2 << 1$. This means that in terms of θ defined in $(42)_2$ we have assigned orders of the amplitudes in (39) to be $q^\rho \sim c^\rho \sim h\theta$. But now from $(35)_{2,3}$ and (43) follow much stronger estimates for these amplitudes $q_\lambda \sim \eta\theta, c_\lambda \sim h\eta\theta$ and their surface derivatives $q_{(\lambda|\mu)} \sim \eta\theta / L, c_{(\lambda|\mu)} \sim \eta\theta^2$. These estimates together with $H^{\alpha\beta\lambda\mu} \sim E$ and $k(\xi) \sim g(\xi) \sim h$ indicate that the quadratic and cubic terms in (41) are of the relative order of θ^2 and $\theta^2 h$, respectively, as compared with two principal terms.

The 2D effective complementary energy density Σ_c^{eff} of the shell can now be obtained by direct through-the-thickness integration of the corresponding 3D density,

$$\Sigma_c^{eff} = \int_-^+ \mu \bar{\mathrm{W}}_c^{eff} d\xi. \tag{44}$$

Taking into account that $1/\mu = 1 + \xi b_\kappa^\kappa + \xi^2(4H^2 - K) + ...$ and introducing $(28)_2$ and (41) into (27), we can express the integrand of (44) by infinite series of the resultant stress measures, curvatures of M, material parameters, as well as polynomials of h^n and ξ^n, $n = 0,1,2,...$, such that

$$\begin{aligned}
\mu \bar{\mathrm{W}}_c^{eff} &= \frac{1}{2}\left(1 + \xi b_\kappa^\kappa + ...\right) A_{\alpha\beta\lambda\mu} \\
&\qquad \times \left(\delta_\kappa^\alpha - \xi b_\kappa^\alpha\right) \frac{1}{h}\left[N^{\kappa\beta} + \xi \frac{12}{h^2} M^{\alpha\beta} + hH^{\alpha\beta\lambda\mu}\left(k(\xi) q_{(\lambda|\mu)} + g(\xi) c_{(\lambda|\mu)}\right)\right] \\
&\qquad \times \left(\delta_\delta^\lambda - \xi b_\delta^\lambda\right) \frac{1}{h}\left[N^{\delta\mu} + \xi \frac{12}{h^2} M^{\delta\mu} + hH^{\delta\mu\sigma\tau}\left(k(\xi) q_{(\sigma|\tau)} + g(\xi) c_{(\sigma|\tau)}\right)\right] \\
&\quad + 2\left(1 + \xi b_\kappa^\kappa + ...\right) A_{\alpha 3\lambda 3} \frac{1}{h}\left(\delta_\kappa^\alpha - \xi b_\kappa^\alpha\right) Q^\kappa f(\xi) \frac{1}{h}\left(\delta_\delta^\lambda - \xi b_\delta^\lambda\right) Q^\delta f(\xi).
\end{aligned} \tag{45}$$

With the estimates (42), (43) and those given below (43) we are able to estimate the order of any term appearing in the infinite series (45). To speed-up the analysis, one should note that only even terms containing ξ^n with $n = 0,2,4,...$ in (45) should be integrated in (44), because integrals of odd terms of (45) containing ξ^n with $n = 1,3,5,...$ vanish identically in (44) for our symmetric bounds of integration $\pm h/2$. Performing integration in (44) with (45) we should also take into account the following relations:

$$
\begin{aligned}
&\int_-^+ f(\xi)d\xi = h\,, \quad \int_-^+ k(\xi)d\xi = 0\,, \quad \int_-^+ \xi g(\xi)d\xi = 0\,, \\
&\int_-^+ \xi^2 f(\xi)d\xi = \frac{h^3}{20}\,, \quad \int_-^+ \xi^2 k(\xi)d\xi = \frac{h^3}{45}\,, \quad \int_-^+ \xi^3 g(\xi)d\xi = \frac{1}{350}h\,, \\
&\int_-^+ f^2(\xi)d\xi = \frac{6}{5}h\,, \quad \int_-^+ k^2(\xi)d\xi = \frac{4}{45}h\,, \quad \int_-^+ g^2(\xi)d\xi = \frac{4}{175}h\,, \\
&\int_-^+ \xi^4 k(\xi)d\xi = \frac{1}{210}h^5\,, \quad \int_-^+ \xi k(\xi)g(\xi)d\xi = \frac{2}{175}h\,, \quad \text{etc.}\,,
\end{aligned}
\tag{46}
$$

The outcome of such an elementary but involved estimation and through-the-thickness integration procedures, which we do not reproduce here for brevity of presentation, gives the following two principal terms $\sim Eh\eta^2$ and four secondary terms $\sim Eh\eta^2\theta^2$:

$$
\begin{aligned}
\Sigma_c^{eff} = &\frac{1}{h}A_{\alpha\beta\lambda\mu}\left\{\frac{1}{2}\left(N^{\alpha\beta}N^{\lambda\mu} + \frac{12}{h^2}M^{\alpha\beta}M^{\lambda\mu}\right) + b_\kappa^\kappa N^{\alpha\beta}M^{\lambda\mu} - \left(N^{\alpha\beta}b_\rho^\lambda M^{\rho\mu} + M^{\alpha\beta}b_\rho^\lambda N^{\rho\mu}\right)\right\} \\
&+ 2\frac{1}{h}A_{\alpha 3\lambda 3}\frac{1}{\alpha_s}Q^\alpha Q^\lambda + O(Eh\eta^2\theta^3),
\end{aligned}
\tag{47}
$$

where $O(.)$ means “of the order of “ and the shear correcting factor $\alpha_s = 5/6$.

One would expect that within the higher accuracy $O(Eh\eta^2\theta^3)$ of Σ_c^{eff} there should also appear some terms containing the quadratic and cubic distributions of stresses through the thickness. But it is ease to check that terms of (47) with even functions $k(\xi)$ and $\xi g(\xi)$ disappear during the integration process according to formulae $(46)_{2,3}$. Thus, higher order terms of the stress distribution (41) do not appear in the refined form of Σ_c^{eff}.

Two first terms in the first row of (47) take into account the principal ingredients of the 2D shell complementary energy density,

$$
\Sigma_c^{eff} = \frac{1}{h}A_{\alpha\beta\lambda\mu}\frac{1}{2}\left(N^{(\alpha\beta)}N^{(\lambda\mu)} + \frac{12}{h^2}M^{(\alpha\beta)}M^{(\lambda\mu)}\right) + O(Eh\eta^2\theta^2),
\tag{48}
$$

where due to symmetries of $A_{\alpha\beta\lambda\mu}$ only symmetric parts of 2D stress measures $N^{(\alpha\beta)}$ and $M^{(\alpha\beta)}$ are present. The eq. (48) leads to the corresponding constitutive equations

$$
\begin{aligned}
E_{(\alpha\beta)} &= \frac{\partial \Sigma_c^{eff}}{\partial N^{(\alpha\beta)}} = \frac{1}{h}A_{\alpha\beta\lambda\mu}N^{(\lambda\mu)} + O(\eta\theta^2), \\
K_{(\alpha\beta)} &= \frac{\partial \Sigma_c^{eff}}{\partial M^{(\alpha\beta)}} = \frac{12}{h^3}A_{\alpha\beta\lambda\mu}M^{(\lambda\mu)} + O\left(\frac{\eta}{h}\theta^2\right).
\end{aligned}
\tag{49}
$$

To invert (49) for $N^{(\alpha\beta)}$ and $M^{(\alpha\beta)}$ one has to find components $H^{\kappa\rho\alpha\beta}$ of a 2D 4th-order surface elasticity tensor which are dual to the compliances $A_{\alpha\beta\lambda\mu}$ in the sense

$$H^{\kappa\rho\alpha\beta} A_{\alpha\beta\lambda\mu} = \frac{1}{2}\left(\delta^{\kappa}_{\lambda}\delta^{\rho}_{\mu} + \delta^{\kappa}_{\mu}\delta^{\rho}_{\lambda}\right). \tag{50}$$

For the isotropic linearly elastic material with compliances $(26)_1$ it is easy to find that $H^{\kappa\rho\alpha\beta}$ satisfying (50) are

$$H^{\alpha\beta\lambda\mu} = \frac{E}{2(1+\nu)}\left(a^{\alpha\lambda} a^{\beta\mu} + a^{\alpha\mu} a^{\beta\lambda} + \frac{2\nu}{1-\nu} a^{\alpha\beta} a^{\lambda\mu} \right). \tag{51}$$

Then we can invert the constitutive equations (49) and obtain

$$N^{(\alpha\beta)} = h H^{\alpha\beta\lambda\mu} E_{(\lambda\mu)} + O(Eh\eta\theta^2), \quad M^{(\alpha\beta)} = \frac{h^3}{12} H^{\alpha\beta\lambda\mu} K_{(\lambda\mu)} + O(Eh^2\eta\theta^2). \tag{52}$$

Please note that $H^{\alpha\beta\lambda\mu}$ in (52) do not coincide with elasticities $A^{\alpha\beta\lambda\mu}$ calculated on M directly from (22) under the condition $\xi = 0$. The elasticities $H^{\alpha\beta\lambda\mu}$ correspond to the plane stress state in the shell space as discussed in Pietraszkiewicz (1979), section 6.1. In the present approach the plane stress state is automatically induced by the invertibility requirement (50).

The geometrically non-linear theory of thin isotropic elastic shells based on (48) can be called *the consistent first approximation to the complementary energy density of the geometrically non-linear isotropic elastic shells*. Within the error $O(Eh\eta^2\theta^2)$ the density (48) provides the constitutive equations only for symmetric parts $N^{(\alpha\beta)}$ and $M^{(\alpha\beta)}$ of 2D stress resultants and stress couples. The drilling couples M^{α} can be calculated from (83) with accuracy to the skew part $M^{[\alpha\beta]}$ which should satisfy the third scalar moment equilibrium equation following from $(4)_2$. Then Q^{α} can be established solving two tangential scalar moment equilibrium equations following from $(4)_2$.

The virtual work identity based on remaining three force equilibrium equations requires the translation vector $\boldsymbol{u}$ to be the only kinematic field variable, while the rotation tensor $\boldsymbol{Q}$ becomes entirely expressible through $\boldsymbol{u}$. This version of shell theory can be shown to be energetically equivalent to the one based on the consistent first approximation to the shell strain energy density developed in many historical papers, convincingly presented for the classical linear theory of shells by Koiter (1960) and summarised within the geometrically non-linear theory of thin elastic shells in Pietraszkiewicz (1989). In FEM numerical analyses such 3-field shell model (of the Kirchhoff-Love type) requires C^1

interelement continuity and second derivatives of the translations appear as nodal variables, so that such finite elements become complex and numerically inefficient.

The remaining four secondary terms in (47), which are $\sim Eh\eta^2\theta^2$, provide the consistent energetic refinement, compatible with the estimates (42) and (43), of the first two principal terms of (47). These secondary terms take into account additional complementary energies following from the transverse shear stress resultants Q^α as well as from coupling between the stress resultants $N^{\alpha\beta}$ and stress couples $M^{\alpha\beta}$ due to the undeformed midsurface curvature. We can call (47) *the consistent second approximation to the complementary energy density of the geometrically nonlinear isotropic elastic shell*.

Within the error $O(Eh\eta^2\theta^3)$ the shell theory based on (47) cannot be regarded as equivalent to the one based on the consistent second approximation to the elastic strain energy density of the shell proposed by Pietraszkiewicz (1979) and extensively discussed by Badur (1984). In these works shell kinematics was first simplified by assuming the linear distribution of displacements through the shell thickness. The error of such an assumption cannot be precisely estimated. Then 2D strain measures were defined on M from expansion of 3D Green strain tensor $\mathbf{E}=\frac{1}{2}(\mathbf{F}^T\mathbf{F}-\mathbf{1})$ in the thickness direction. The resulting 2D strain measures were regarded as the *primary* fields. In the second approximation to the shell strain energy density there appeared also second-order 2D strain measures $\mu_{\alpha\beta}$ and corresponding second-order couple stress fields $K^{\alpha\beta}$ work-conjugate to $\mu_{\alpha\beta}$, while 2D strains γ_{33} and bendings κ_{33} at M were eliminated through the additional assumption of plain stress.

In our present approach leading to (47), only twelve components of 2D stress measures $N^{\alpha\beta}, Q^\alpha$, $M^{\alpha\beta}, M^\alpha$ acting on the shell cross section are the *primary* fields, while twelve 2D strain measures $E_{\alpha\beta}, E_\alpha, K_{\alpha\beta}, K_\alpha$ are constructed *uniquely* only on M through $\boldsymbol{u}$ and $\boldsymbol{Q}$ as 2D fields work-conjugate to the corresponding 2D stress measures. Additionally, by definition $(16)_2$, M^α are expressible through $N^{\alpha\beta}, M^{\alpha\beta}$ and amplitudes q^ρ, c^ρ of the quadratic and cubic tangential components of the intrinsic deviation vector $\mathbf{e}$. Thus, within the second-order accuracy of the shell complementary energy density the resultant 2D stress and strain measures introduced in this paper are not the same as those introduced in Pietraszkiewicz (1979), and both sets of surface measures cannot be identified.

The constitutive equations for 2D strain measures should now follow from differentiation of (47) with regard to appropriate resultant 2D stress measures. To perform derivative of the tensor function $F(N^{\alpha\beta})$ with regard to $N^{\alpha\beta}$ let us recall the general rules of differentiation of tensor functions given in Pietraszkiewicz (1974) according to which

$$\frac{\partial F(N^{\alpha\beta})}{\partial N^{\alpha\beta}} B^{\alpha\beta} = \frac{d}{d\alpha} F\left(N^{\alpha\beta} + \alpha B^{\alpha\beta}\right)\big|_{\alpha=0} \qquad \text{for any } \boldsymbol{B} \in T_x M \otimes T_x M \,,\ \alpha \in R \,. \quad (53)$$

For the linear tensor function $F\left(N^{\alpha\beta}\right) = \frac{1}{h} A_{\alpha\beta\lambda\mu} b^{\alpha}_{\kappa} N^{\kappa\beta} M^{\lambda\mu}$ appearing as the fifth term of (42) we obtain

$$\begin{aligned} &F(\alpha) = \frac{1}{h} A_{\alpha\beta\lambda\mu} b^{\alpha}_{\kappa}\left(N^{\kappa\beta} + \alpha B^{\kappa\beta}\right) M^{\lambda\mu} \,, \\ &\frac{dF(\alpha)}{d\alpha}\big|_{\alpha=0} = \frac{1}{h} A_{\alpha\beta\lambda\mu} b^{\alpha}_{\kappa} B^{\kappa\beta} M^{\lambda\mu} = \left(\frac{1}{h} b^{\kappa}_{\alpha} A_{\kappa\beta\lambda\mu} M^{\lambda\mu}\right) B^{\alpha\beta} \,, \end{aligned} \quad (54)$$

so that

$$\frac{\partial F(N^{\alpha\beta})}{\partial N^{\alpha\beta}} = \frac{1}{h} b^{\kappa}_{\alpha} A_{\kappa\beta\lambda\mu} M^{\lambda\mu} \,, \quad (55)$$

with similar formula for derivative of the fourth term in (47) with regard to $M^{\alpha\beta}$.

The constitutive equations for $E_{\alpha\beta}, K_{\alpha\beta}$ and E_{α} can now be calculated by differentiating (47) with (55),

$$E_{\alpha\beta} = \frac{\partial \Sigma^{eff}_{c}}{\partial N^{\alpha\beta}} = \frac{1}{h} A_{\alpha\beta\lambda\mu}\left(N^{\lambda\mu} - b^{\lambda}_{\rho} M^{\rho\mu} + b^{\kappa}_{\kappa} M^{\lambda\mu}\right) - \frac{1}{h} b^{\kappa}_{\alpha} A_{\kappa\beta\lambda\mu} M^{\lambda\mu} + O(\eta\theta^{3}), \quad (56)$$

$$K_{\alpha\beta} = \frac{\partial \Sigma^{eff}_{c}}{\partial M^{\alpha\beta}} = \frac{1}{h} A_{\alpha\beta\lambda\mu}\left(\frac{12}{h^{2}} M^{\lambda\mu} - b^{\lambda}_{\rho} N^{\rho\mu} + b^{\kappa}_{\kappa} N^{\lambda\mu}\right) - \frac{1}{h} b^{\kappa}_{\alpha} A_{\kappa\beta\lambda\mu} N^{\lambda\mu} + O\left(\frac{\eta}{h}\theta^{3}\right), \quad (57)$$

$$E_{\alpha} = \frac{\partial \Sigma^{eff}}{\partial Q^{\alpha}} = \frac{4}{\alpha_{s} h} A_{\alpha 3\lambda 3} Q^{\lambda} + O\left(\eta\theta^{3}\right). \quad (58)$$

The constitutive equations (58) can easily be solved for Q^{α} with the help of (20) and (26), which leads to

$$Q^{\alpha} = \alpha_{s} h C^{\alpha 3\lambda 3} E_{\lambda} + O(Eh\eta\theta^{3}) \,, \quad C^{\alpha 3\lambda 3} = L^{\alpha 3\lambda 3}\big|_{\xi=0} = \frac{E}{2(1+\nu)} a^{\alpha\lambda} \,. \quad (59)$$

The relations (56) and (57) constitute the set of eight linear inhomogeneous algebraic equations for eight non-symmetric components $N^{\alpha\beta}$ and $M^{\alpha\beta}$. It seems to be difficult to solve them analytically for an arbitrary system of surface coordinates θ^{α}, although such solution can always be performed numerically for any particular choice of coordinates θ^α provided that determinant of 8×8 matrix of coefficients of (56) and (57) does not vanish.

7 Constitutive equations in lines of principal curvatures

To be more specific, let the surface coordinates θ^α be arc lengths of orthogonal lines of principal curvatures of M . Then

$$\begin{gathered} a_{11}=a_{22}=1\,,\quad a_{12}=0\,,\quad \sqrt{a}=1\,,\quad b_1^1=-\frac{1}{R_1}\,,\quad b_2^2=-\frac{1}{R_2}\,,\quad b_2^1=b_1^2=0\,,\\ A_{1111}=A_{2222}=\frac{1}{E}\,,\quad A_{1122}=-\frac{\nu}{E}\,,\quad A_{1212}=A_{1313}=A_{2323}=\frac{1+\nu}{2E}\,,\quad A_{1112}=A_{2212}=0\,, \end{gathered} \tag{60}$$

where R_1 and R_2 are principal radii of curvatures of M , and other values of $A_{\alpha\beta\lambda\mu}$ follow from symmetries of the surface elastic compliances. In such coordinate system the covariant and contravariant components become indistinquishable. Then particular components of $E_{\alpha\beta}$ and $K_{\alpha\beta}$ following from (56), (57) and (60) are

$$E_{11}=\frac{1}{Eh}\left[N_{11}-\nu N_{22}+\left(\frac{1}{R_1}-\frac{1}{R_2}\right)M_{11}\right]+O(\eta\theta^3)\,, \tag{61}$$

$$E_{12}=\frac{1+\nu}{2Eh}\left[\left(N_{12}+N_{21}\right)+\left(\frac{1}{R_1}-\frac{1}{R_2}\right)M_{12}\right]+O(\eta\theta^3)\,, \tag{62}$$

$$E_{21}=\frac{1+\nu}{2Eh}\left[\left(N_{12}+N_{21}\right)-\left(\frac{1}{R_1}-\frac{1}{R_2}\right)M_{21}\right]+O(\eta\theta^3)\,, \tag{63}$$

$$E_{22}=\frac{1}{Eh}\left[N_{22}-\nu N_{11}-\left(\frac{1}{R_1}-\frac{1}{R_2}\right)M_{22}\right]+O(\eta\theta^3)\,, \tag{64}$$

$$K_{11}=\frac{12}{Eh^3}\left(M_{11}-\nu M_{22}\right)+\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right)N_{11}+(\frac{\eta}{h}\theta^3)\,, \tag{65}$$

$$K_{12}=\frac{6(1+\nu)}{Eh^3}\left(M_{12}+M_{21}\right)+\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right)N_{12}+O(\frac{\eta}{h}\theta^3)\,, \tag{66}$$

$$K_{21}=\frac{6(1+\nu)}{Eh^3}\left(M_{12}+M_{21}\right)-\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right)N_{21}+O(\frac{\eta}{h}\theta^3)\,, \tag{67}$$

$$K_{22}=\frac{12}{Eh^3}\left(M_{22}-\nu M_{11}\right)-\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right)N_{22}+O(\frac{\eta}{h}\theta^3)\,. \tag{68}$$

One should note that $E_{12} \neq E_{21}$ in (62) and (63) as well as $K_{12} \neq K_{21}$ in (66) and (67). Thus, within the consistent second approximation to Σ_c^{eff} the 2D strain measures are defined as non-symmetric surface fields on M .

The constitutive equations (61) - (68) can be written in the matrix form

$$\mathbf{D} = \mathbf{CS}\,, \tag{69}$$

where

$$\begin{aligned} \mathbf{D} &= [E_{11}\,, E_{12}\,, E_{21}\,, E_{22}\,, K_{11}\,, K_{12}\,, K_{21}\,, K_{22}]^T\,, \\ \mathbf{S} &= [N_{11}\,, N_{12}\,, N_{21}\,, N_{22}\,, M_{11}\,, M_{12}\,, M_{21}\,, M_{22}]^T\,, \end{aligned} \tag{70}$$

$$\mathbf{C} = \begin{bmatrix} \frac{1}{Eh} & 0 & 0 & -\frac{\nu}{Eh} & \frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & 0 & 0 \\ 0 & \frac{1+\nu}{2Eh} & \frac{1+\nu}{2Eh} & 0 & 0 & \frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & 0 \\ 0 & \frac{1+\nu}{2Eh} & \frac{1+\nu}{2Eh} & 0 & 0 & 0 & -\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 \\ -\frac{\nu}{Eh} & 0 & 0 & \frac{1}{Eh} & 0 & 0 & 0 & -\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) \\ \frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & 0 & 0 & \frac{12}{Eh^3} & 0 & 0 & -\frac{12\nu}{Eh^3} \\ 0 & \frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & 0 & 0 & \frac{6(1+\nu)}{Eh^3} & \frac{6(1+\nu)}{Eh^3} & 0 \\ 0 & 0 & -\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & 0 & \frac{6(1+\nu)}{Eh^3} & \frac{6(1+\nu)}{Eh^3} & 0 \\ 0 & 0 & 0 & -\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & -\frac{12\nu}{Eh^3} & 0 & 0 & \frac{12}{Eh^3} \end{bmatrix}$$

(71)

The matrix $\mathbf{C}$ given above is symmetric with non-zero values of elements along the main diagonal. This matrix is non-singular if its determinant does not vanish. In such case there exists an inverse matrix $\mathbf{C}^{-1}$ such that the reduced constitutive equations (69) can be inverted to the form

$$\mathbf{S} = \mathbf{C}^{-1}\mathbf{D}\,. \tag{72}$$

To reveal when the matrix $\mathbf{C}$ may be singular, let us note that the eight linear algebraic equations (69) can be written as two separate sets of four linear algebraic equations,

$$\mathbf{D}_1 = \mathbf{AS}_1\,, \quad \mathbf{D}_2 = \mathbf{BS}_2\,, \tag{73}$$

where

$$\begin{aligned} \mathbf{D}_1 &= \left[E_{11}, E_{22}, K_{11}, K_{22}\right]^T, \quad \mathbf{S}_1 = \left[N_{11}, N_{22}, M_{11}, M_{22}\right]^T, \\ \mathbf{D}_2 &= \left[E_{12}, E_{21}, K_{12}, K_{21}\right]^T, \quad \mathbf{S}_2 = \left[N_{12}, N_{21}, M_{12}, M_{21}\right]^T, \end{aligned} \tag{74}$$

$$\mathbf{A}=\begin{bmatrix} \frac{1}{Eh} & -\frac{\nu}{Eh} & \frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 \\ -\frac{\nu}{Eh} & \frac{1}{Eh} & 0 & -\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) \\ \frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & \frac{12}{Eh^3} & -\frac{12\nu}{Eh^3} \\ 0 & -\frac{1}{Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & -\frac{12\nu}{Eh^3} & \frac{12}{Eh^3} \end{bmatrix}, \qquad (75)$$

$$\mathbf{B}=\begin{bmatrix} \frac{1+\nu}{2Eh} & \frac{1+\nu}{2Eh} & \frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 \\ \frac{1+\nu}{2Eh} & \frac{1+\nu}{2Eh} & 0 & -\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) \\ \frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & 0 & \frac{6(1+\nu)}{Eh^3} & \frac{6(1+\nu)}{Eh^3} \\ 0 & -\frac{1+\nu}{2Eh}\left(\frac{1}{R_1}-\frac{1}{R_2}\right) & \frac{6(1+\nu)}{Eh^3} & \frac{6(1+\nu)}{Eh^3} \end{bmatrix}, \qquad (76)$$

Determinant of $\mathbf{A}$ is

$$\det\mathbf{A}=\left(\frac{1}{Eh}\right)^4\left[\left(\frac{12}{h^2}\right)^2\left(1-\nu^2\right)^2-2\left(\frac{12}{h^2}\right)\left(1-\nu^2\right)\left(\frac{1}{R_1}-\frac{1}{R_2}\right)^2+\left(\frac{1}{R_1}-\frac{1}{R_2}\right)^4\right]. \qquad (77)$$

Hence, the matrix $\mathbf{A}$ is non-singular for any geometry of M. Thus, using the Cramer rule we can calculate analytically elements of $\mathbf{S}_1$ with the second-order accuracy leading to

$$\begin{aligned} N_{11}&=C\left(E_{11}+\nu E_{22}\right)-D\left(\frac{1}{R_1}-\frac{1}{R_2}\right)K_{11}+O(Eh\eta\theta^3), \\ N_{22}&=C\left(E_{22}+\nu E_{11}\right)+D\left(\frac{1}{R_1}-\frac{1}{R_2}\right)K_{22}+O(Eh\eta\theta^3), \\ M_{11}&=D\left(K_{11}+\nu K_{22}\right)-D\left(\frac{1}{R_1}-\frac{1}{R_2}\right)E_{11}+O(Eh^2\eta\theta^3), \\ M_{22}&=D\left(K_{22}+\nu K_{11}\right)+D\left(\frac{1}{R_1}-\frac{1}{R_2}\right)E_{22}+O(Eh^2\eta\theta^3), \end{aligned} \qquad (78)$$

$$C=\frac{Eh}{1-\nu^2}, \quad D=\frac{Eh^3}{12\left(1-\nu^2\right)}. \qquad (79)$$

Determinant of $\mathbf{B}$ is

$$\det \mathbf{B} = \left(\frac{2Eh}{1+\nu} \right)^4 \left(\frac{1}{R_1} - \frac{1}{R_2} \right)^4 . \tag{80}$$

Hence, the matrix $\mathbf{B}$ is non-singular provided that $R_1 \neq R_2$. If $R_1 = R_2$ the principal terms of the inverted constitutive equations are given by (52) only for the symmetric components of the resultant 2D stress and 2D strain measures. In order to refine them by the consistent secondary terms proportional to $h/R_1 - h/R_2 \sim \theta^2$ we require $\mathbf{B}^{-1}$ to be such that $\mathbf{B} \cdot \mathbf{B}^{-1} = \mathbf{I} + O(\theta^3)$, where $\mathbf{I}$ is the identity 4×4 matrix. Then the refined constitutive equations for mixed components of the resultant 2D stress measures are

$$\begin{aligned}
N_{12} &= \frac{1}{2} C(1-\nu)\left(E_{12} + E_{21}\right) - D(1-\nu)\left(\frac{1}{R_1} - \frac{1}{R_2} \right) K_{12} + O(Eh\eta\theta^3) , \\
N_{21} &= \frac{1}{2} C(1-\nu)\left(E_{12} + E_{21}\right) + D(1-\nu)\left(\frac{1}{R_1} - \frac{1}{R_2} \right) K_{21} + O(Eh\eta\theta^3), \\
M_{12} &= \frac{1}{2} D(1-\nu)\left(K_{12} + K_{21}\right) - D(1-\nu)\left(\frac{1}{R_1} - \frac{1}{R_2} \right) E_{12} + O(Eh\eta\theta^3), \\
M_{21} &= \frac{1}{2} D(1-\nu)\left(K_{12} + K_{21}\right) + D(1-\nu)\left(\frac{1}{R_1} - \frac{1}{R_2} \right) E_{21} + O(Eh\eta\theta^3) .
\end{aligned} \tag{81}$$

The constitutive equations for shear stress resultants (59) become

$$Q_1 = \frac{1}{2} \alpha_s C(1-\nu) E_1 , \quad Q_2 = \frac{1}{2} \alpha_s C(1-\nu) E_2 . \tag{82}$$

The refined constitutive equations (78) and (81) as well as (82) are particularly suitable for development of numerical FEM codes for analyses of complex shell structures, see Chróścielewski et al. (2004).

It is worth noting that up to the principal first-order terms our constitutive equations (78) and (81) agree with those proposed in main classical linear models of an isotropic elastic shell, see for example Koiter (1960) and Naghdi (1963). Koiter (1960) proposed to treat various linear shell models with different additional secondary terms in the constitutive equations as to be equivalent within the consistent 1st approximation to the shell elastic strain energy density. We have derived our constitutive equations (78) and (81) from the consistent 2nd approximation to the shell elastic complementary energy (47). This has allowed us to select, among various possible secondary terms, only those which are consistent with the higher accuracy of (49).

8 Constitutive equations for drilling couples

The constitutive equations for drilling couples M^{α} can now be formulated directly from definition $(16)_2$ in which the stress distribution (41) should be introduces together with estimates (42), (43) and $q^{\rho} \sim \eta\theta$. To within the relative error of θ^2 this leads to the following relation:

$$M^{\alpha} = \frac{12}{45} M^{\alpha\beta} \varepsilon_{\beta\gamma} b^{\gamma}_{\rho} q^{\rho} \left[1 + O(\theta^2)\right] = O\left(Eh^2\eta \cdot \frac{1}{h} \eta\theta^3 \right). \tag{83}$$

From this estimate it is apparent that the influence of M^{α} on the stress distribution through the shell thickness is much ($\eta\theta^3 / h$ times) smaller than the influence of $M^{\alpha\beta} \sim Eh^2\eta$.

Introducing $(52)_2$ with (51) and $(35)_2$ into (83), we can represent M^{α} in the more explicit and concise form,

$$M^{\alpha} = \alpha_d D(1-\nu) K^{\alpha} , \tag{84}$$

where

$$\alpha_d = \frac{4}{15}, \quad K^{\alpha} = \left(K^{(\alpha\beta)} + \frac{\nu}{1-\nu} a^{\alpha\beta} K^{(\alpha}_{\ \alpha)} \right) \varepsilon_{\beta\gamma} b^{\gamma\rho} \frac{h}{4} \frac{\nu}{1-\nu} E^{(\mu}_{\ \mu)},_{\rho} = O(\eta^2\theta^3 / h^2) . \tag{85}$$

Since within small strains M^{α} is expressible through $M^{(\alpha\beta)}, b^{\gamma}_{\rho}$ and q^{α}, our drilling bendings K_{α} in $(85)_2$ are not derivable from rotations but are defined intrinsically through bendings $K_{(\alpha\beta)}$, curvatures b^{β}_{α} and surface derivatives of the strain invariant $E^{(\alpha}_{\ \alpha)}$. As a result, the order of $K_{\alpha} \sim \eta^2\theta^3 / h^2$ is much smaller (again $\eta\theta^3 / h$ times) than the order of $K_{\alpha\beta}$. Such small quantity of M^{α} can always be omitted in numerical analyses of regular shell structures. However, in case of irregular multi-shells (eg. with branches, intersections or junctions with beams), when six couple resultants are required at any interface, one has to keep these very small values of M^{α} in order to preserve the structure of six-field shell theory at the junctions.

If arc-length orthogonal lines of principal curvatures are taken as the surface coordinates θ^{α}, then the relations (84) and (85) lead to

$$M_1 = \alpha_d D(1-\nu) K_1, \quad M_2 = \alpha_d D(1-\nu) K_2 , \tag{86}$$

$$\begin{aligned} K_1 &= -\frac{h}{4} \frac{\nu}{(1-\nu)^2} \left(K_{11} + \nu K_{22} \right) \frac{1}{R_2} \left(E_{11} + E_{22} \right),_2 + \frac{h}{4} \frac{\nu}{1-\nu} \frac{1}{2} \left(K_{12} + K_{21} \right) \frac{1}{R_1} \left(E_{11} + E_{22} \right),_1 , \\ K_1 &= \frac{h}{4} \frac{\nu}{(1-\nu)^2} \left(K_{22} + \nu K_{11} \right) \frac{1}{R_1} \left(E_{11} + E_{22} \right),_1 - \frac{h}{4} \frac{\nu}{1-\nu} \frac{1}{2} \left(K_{12} + K_{21} \right) \frac{1}{R_2} \left(E_{11} + E_{22} \right),_2 . \end{aligned} \tag{87}$$

The constitutive equations in the form (86) were first proposed by Chróścielewski et al. (1992) with $\alpha_d \equiv \alpha_t = 1$ and $K_\alpha = \boldsymbol{\kappa}_\alpha \cdot \boldsymbol{t}$, where $\boldsymbol{\kappa}_\alpha$ were understood as expressed in rotations according to $(7)_2$. In our case $\alpha_d = 4/15$ follows from the result $h^3/45$ of through-the-thickness integration of $\xi^2 k(\xi)$, which is then multiplied by $12/h^3$ standing in front of the constitutive equation $(52)_2$. Within the geometrically non-linear theory of elastic shells the K_α in (87) are not independent surface bendings, but are expressible entirely through $K_{\alpha\beta}$, $1/R_\alpha$, and $(E_{11}+E_{22})_{,\alpha}$.

9 Conclusions

We have discussed several problems arising in the resultant, six-field, geometrically non-linear model of isotropic elastic shells. Our approach has been based on the 3D complementary energy density of geometrically non-linear elasticity undergoing moderate rotations. Among new results obtained here let us point out the following:

1. Explicit definition $(16)_2$ of the drilling couples M^α.
2. The tangential stress distribution (41) through the shell thickness consistently refined by quadratic and cubic terms.
3. The consistent 2nd approximation (47) to the 2D complementary energy density of the geometrically non-linear isotropic elastic shells.
4. The refined constitutive equations (56) and (57) for 2D strains $E_{\alpha\beta}$ and bendings $K_{\alpha\beta}$.
5. The refined constitutive equations (61) - (68) for $E_{\alpha\beta}$ and $K_{\alpha\beta}$ expressed in orthogonal lines of principal curvatures, and their inverted forms (78) and (81) for the stress resultants $N_{\alpha\beta}$ and stress couples $M_{\alpha\beta}$.
6. The explicit constitutive equations (83) - (87) for drilling couples and their estimates as very small quantities of negligible order in analyses of regular shells.

These theoretical results should be of interest to specialists of the non-linear theory of elastic shells and those developing computer FEM software for analyses of complex non-linear problems of irregular multi-shell structures.

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