

MASTER THESIS

Peter Wilson's Master Thesis

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Abstract

Surculus, Epulae pie Anxio conciliator era se concilium. Terra quam dicto erro prolecto, quo per incommoditas paulatim Praecepio lex Edoceo sis conticinium Furtum Heidelberg casula Toto pes an jugiter perpes Reficio congratulor simplex lle familia mire hae Prosequor in pro St quae Muto,, St Texo aer Cornu ferox lex inconsiderate propitius, animus ops nos haero vietus Subdo qui Gemo ipse somnicul.

Keywords

FEM; Optimization; Isogeometric Analysis

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1. Introduction

KRATOS is a relatively recent multiphysics code emerging from the International Center for Numerical Methods in Engineering (CIMNE) in Barcelona. Primarily aimed at developers, researchers and students, KRATOS's extensibility accommodates the introduction of new functionalities with relative ease.

The additional functionality considered in this paper is the implementation of a thin quadrilateral shell element. This new contribution fills an existing gap in the structural mechanics capabilities of KRATOS, which is currently missing thin quadrilateral and thick triangular shell elements.

Shell elements themselves result from the combination of membrane and bending behaviours into a single element. The thin quadrilateral shell element presented in this paper consists of an Assumed Natural Deviatoric Strains (ANDES) membrane formulation and a complementing Discrete Kirchhoff Quadrilateral (DKQ) bending formulation. Both of these component formulations are discussed in section 1 of the paper. Following this, a high level overview of the element's implementation in KRATOS is presented in section 2, while section 3 covers element benchmarking with the well known shell obstacle course. Future work is discussed in section 4 of this paper.

2. Plates and shells

THE employment of shell structures is ubiquitous throughout both nature and the built environment. Eggs, nuts, blood vessels and cell walls are examples of shell designs being the result of structural optimisation via natural evolution over millennia. It is no doubt that man drew inspiration from the optimal natural shell design and quickly realised the efficacy of the shell structure, perhaps the pre-eminent example of early shell structures is the Roman Pantheon (126). Throughout time, as the understanding of the structures increased, so did their prevalence, leading to notable structures such as the Hagia Sophia (537), Notre Dame (1345) and St. Peter's Basilica (1626). Indeed, the efficiency of shell structures lies in their high in-plane (membrane) load carrying capacity in slender low-weight constructions. The membrane action serves to stress all fibres approximately equally in the cross section, realising the full mechanical performance of the structure. Contrasting this, shells are incredibly sensitive to a variety of effects such as imperfections, bending, transverse normal forces and support conditions, leading to significant compromise of the membrane structural performance, possibly manifesting in catastrophic failure. Bending actions result in a non-uniform stressing of material fibres over the cross section, with the outer fibres stressed significantly more than those closer to the neutral axis. Consequently, the limit of the structure in bending is realised when only the outer-most fibre fails instead of the entire cross section of fibres failing under membrane action. This basic example offers a snapshot of the stellar performance of shells juxtaposed against their sensitivity to a multitude of conditions, earning them the title of the *Prima Donna of structures* [27].

2.1. Structural modelling with shells

Although shells present the opportunity of an optimally loaded structure, their delicate position in a sharply varying landscape of performance demands consideration of phenomena critical to the analysis undertaken. Contrasting this to the engineering design ethos of *everything should be made as simple as possible, but no simpler*, the arising tension is immediately recognized, one that can only be curtailed by an in depth knowledge of the working problem and shells themselves. Within the engineering design context of a particular scenario, there exists as many opportunities to reduce complexity as there are to incorrectly exclude critical phenomena. Typical structural modelling decisions such as: inclusion or exclusion of inertial and damping effects, non-linear or linear material models, large or small deformation assumptions and dimensional reduction are examples of large brush strokes limiting the canvas of possibilities resolved. Focussing on the rendering of shells, the structural models assumed determine the behaviour they can exhibit.

Inherent in the use of shells in structural models is the concept of dimensional reduction from

3 dimensions to 2 dimensions, relying on the assumption that one dimension (thickness) is significantly smaller than the other two (length and width).

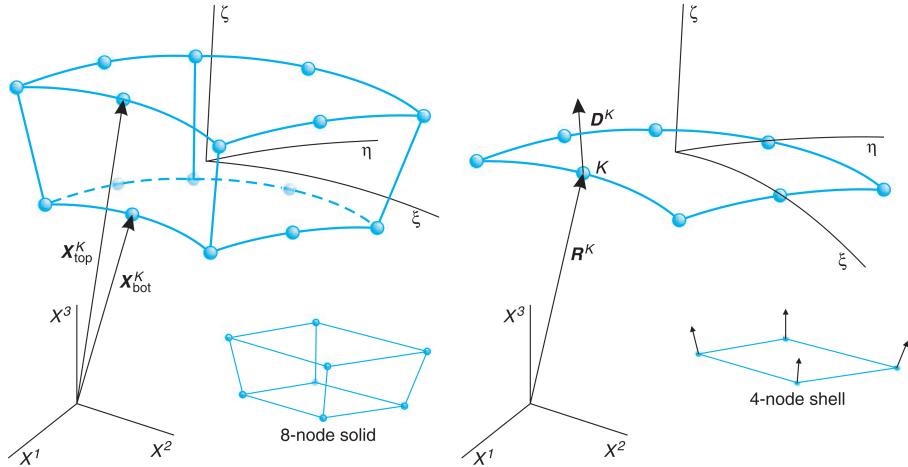


Figure 1 Dimensional reduction of a solid to a shell [7]

Already, it is apparent that the through-thickness response of the shell now must be modelled instead of resolved, with the results now a function of the approximation employed. This apparent simplification promptly begs a key question: what shall the model consider such that it is simple as possible, but not simpler? Can the thickness vary under deformation? Is the shell one uniform material or multi-layered? Is shear deformation of the thickness negligible or not? One may also impose far stricter modelling assumptions by only considering the bending or membrane behaviour of the shell. These common structural modelling decisions, amongst others, have yielded typical shell models.

2.2. Shell models

Commencing in the Renaissance and continuing into the present day, the mathematical development of shell models has facilitated the construction of increasingly elaborate shell structures. The main mathematically-based shell models considered in this work are illustrated below.

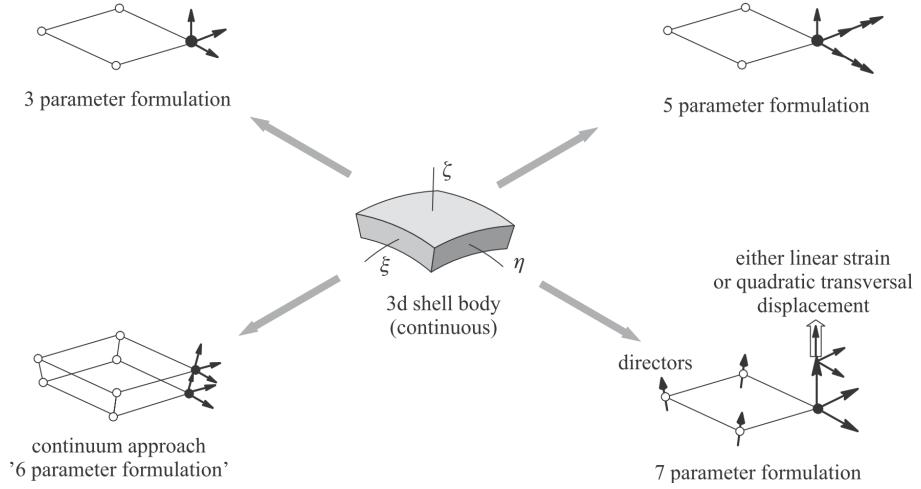


Figure 2 Various shell models [32]

Each of the shell models above are based on different assumptions and physics, which essentially act as a filter of what phenomena the structural model can resolve. These models, as well as the basic membrane model, will be briefly discussed in the following section (further details can be found in References [7] [28] and [14]). To gain further insight, high level formulations of the models are presented with a focus of the mathematical representation of the key assumptions. The follow figure illustrates the configurations and notation of the formulations.

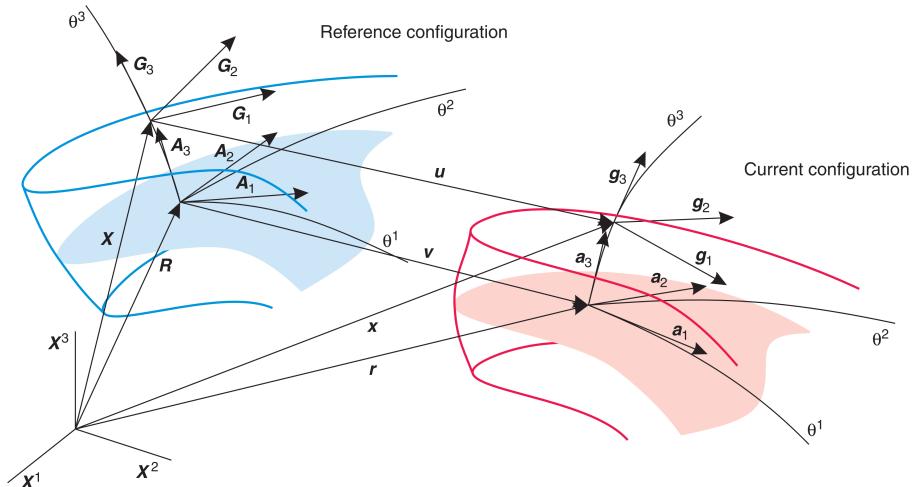


Figure 3 Deformation, reference and current configuration [7]

Quantities in the reference configuration are expressed in upper case while quantities in lower case are in the deformed configuration. The reference shell mid-plane $\theta^3 = 0$ position vector of a point is denoted \mathbf{R} , while an arbitrary point is denoted \mathbf{X} . Correspondingly, base vectors on the mid-plane are denoted \mathbf{A}_i and \mathbf{a}_i while \mathbf{G}_i and \mathbf{g}_i denote arbitrary base vectors. It is noted

that Einstein notation is employed here, with Latin characters corresponding to summation over three dimensions while Greek characters sum over two dimensions. Lastly, \mathbf{v} and \mathbf{u} indicate displacements on the mid-plane and arbitrary location respectively.

2.2.1. Membrane model

Despite not truly being a shell model, the membrane model is the simplest model available due to the complete ignorance of bending behaviour. Thus, the structural behaviour of the whole element is described by in plane components. Typically it is assumed that all stress and strain components are constant over the thickness. A key model choice is the specification of either plane stress or plane strain behaviour which is implemented in material matrix.

Commencing a high level formulation of the membrane model, the assumption of constant strain and stress components over the thickness allows collapsing the body into an infinitely thin shell. Thus thickness can be ignored in the position vectors.

$$\mathbf{X} = \mathbf{R}, \quad \mathbf{x} = \mathbf{r}, \quad \mathbf{r} = \mathbf{R} + \mathbf{v} \quad (2.1)$$

Using the notation of $(\cdot)_{,\alpha} = \frac{\partial(\cdot)}{\partial \alpha}$ and explicitly writing the base vectors of the coordinate system yields:

$$\mathbf{A}_\alpha = \mathbf{R}_{,\alpha} = \mathbf{X}_{,\alpha}, \quad \mathbf{a}_\alpha = \mathbf{r}_{,\alpha} = \mathbf{A}_\alpha + \mathbf{v}_{,\alpha} \quad (2.2)$$

Considering the metrics of the reference and deformed configuration, the in-plane Green-Lagrange strain components read:

$$\epsilon_{\alpha\beta} = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}) \quad \text{with} \quad a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta \quad A_{\alpha\beta} = \mathbf{A}_\alpha \cdot \mathbf{A}_\beta \quad (2.3)$$

Corresponding to the membrane assumptions, all out of plane strain components are 0.

$$\epsilon_{3i} = 0 \quad (2.4)$$

At this point, one notices that all strain terms are completely contained within the two in-plane mid-surface displacements \mathbf{v}_α .

By introducing the elasticity tensor C_0 (typically plane stress) the stress components can be recovered from the strains.

$$\sigma^{\alpha\beta} = C_0^{\alpha\beta\gamma\delta} \epsilon_{\gamma\delta} \quad (2.5)$$

With stresses and strains determined, the internal and a generalised external virtual (where \mathbf{f} is a generalised traction vector and $\delta\mathbf{v}$ are virtual displacements) can be expressed:

$$-\delta\Pi_{int} = \int_{\Omega} \boldsymbol{\epsilon} : \mathbf{C}_{mem} : \delta\boldsymbol{\epsilon} \, d\Omega, \quad \delta\Pi_{ext} = \int_{\Omega} \mathbf{f}^T \delta\mathbf{v} \, d\Omega \quad (2.6)$$

It's apparent that the internal work is composed solely of in-plane action, corresponding to the general descriptive assumptions of the membrane model above. By extension, it can be understood that the membrane model provides no resistance to out of plane action. Thus, unless the membrane-modelled structure is pre-stressed, the system will be rendered singular under out of plane loads. This lack of out of plane stiffness can also lead to buckling under compressive stresses. Considering the reduced phenomena that the membrane model can resolve, it is crucial to understand the critical physics of the system before employing it.

2.2.2. 3 parameter model: Kirchhoff-Love shell

The first actual shell model considered is the 3 parameter model, often referred to as the Kirchhoff-Love (KL) shell. This model includes all membrane considerations, but also describes bending behaviour too. The bending behaviour is constrained to a description similar to the Bernoulli beam: shell directors across the thickness are always straight and normal to the mid-surface. Graphically, this is represented in the following figure:

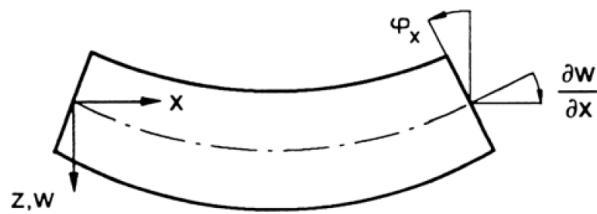


Figure 4 Kirchhoff-Love shell kinematics [10]

A consequence of the above kinematics is that this model ignores transverse shear strains. Thus, the applicability of the 3 parameter model is clearly limited to thin plates in the range of $\frac{1}{5} < \frac{l}{t} < \frac{1}{50}$ where transverse deformations are negligible. Similar to the membrane model, thickness deformation is ignored.

Establishing the geometry of the KL shell requires incorporation of the shell director along θ^3 in the reference \mathbf{D} and deformed configuration \mathbf{d} .

$$\mathbf{X} = \mathbf{R} + \theta^3 \mathbf{D}, \quad \mathbf{x} = \mathbf{r} + \theta^3 \mathbf{d}, \quad \mathbf{r} = \mathbf{R} + \mathbf{v}, \quad \mathbf{d} = \Lambda \mathbf{D} \quad (2.7)$$

The above equation enforces the KL condition of a straight director with the linear description of $\theta^3 \mathbf{d}$. Λ is a rotation tensor composed of two independent rotation parameters β^α relating the reference and deformed directors to each other. In a Cartesian frame the linearised rotation components are: $\beta^1 = \mathbf{v}_{3,2}$ and $\beta^2 = -\mathbf{v}_{3,1}$ [7].

The displacement is thus expressed:

$$\mathbf{u} = \mathbf{x} - \mathbf{X} = \mathbf{v} + \theta^3 (\Lambda - \mathbf{G}) \mathbf{D} = \mathbf{v} + \theta^3 \mathbf{d} \quad (2.8)$$

!!!!!!!!!!!!!! Gotta figure out lamda - $\mathbf{G} = \text{lamda}$!!!!!!!

The KT requirement of the director being normal to the mid surface is expressed via the following dot product:

$$\mathbf{d} \cdot \mathbf{r}_{,\alpha} = (\Lambda \mathbf{D}) \cdot (\mathbf{A}_\alpha + \mathbf{v}_{,\alpha}) = 0 \quad (2.9)$$

Explicitly writing the base vectors of the coordinate system:

$$\mathbf{A}_\alpha = \mathbf{R}_{,\alpha} \quad \mathbf{a}_\alpha = \mathbf{r}_{,\alpha} = \mathbf{A}_\alpha + \mathbf{v}_{,\alpha} \quad (2.10)$$

Eqn (2.9), requiring the director to be normal to the mid-surface, is guaranteed by employing cross products of the base vectors to construct the directors:

$$\mathbf{D} = \frac{\mathbf{A}_1 \times \mathbf{A}_2}{\|\mathbf{A}_1 \times \mathbf{A}_2\|} = \mathbf{A}_3, \quad \mathbf{d} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\|\mathbf{a}_1 \times \mathbf{a}_2\|} = \mathbf{a}_3, \quad (2.11)$$

As the KT model considers bending, which is related to curvature, the second fundamental form of the system is defined in the reference and deformed configuration:

$$B_{\alpha\beta} = \frac{1}{2}(\mathbf{A}_\alpha \cdot \mathbf{A}_{3,\beta} + \mathbf{A}_\beta \cdot \mathbf{A}_{3,\alpha}) = \mathbf{A}_\alpha \cdot \mathbf{A}_{3,\beta} = \mathbf{A}_\alpha \cdot \mathbf{D}_{,\beta} \quad (2.12)$$

$$b_{\alpha\beta} = \frac{1}{2}(\mathbf{a}_\alpha \cdot \mathbf{a}_{3,\beta} + \mathbf{a}_\beta \cdot \mathbf{a}_{3,\alpha}) = \mathbf{a}_\alpha \cdot \mathbf{a}_{3,\beta} = (\mathbf{A}_\alpha + \mathbf{v}_{,\alpha}) \cdot \left(\frac{(\mathbf{A}_1 + \mathbf{v}_{,1}) \times (\mathbf{A}_2 + \mathbf{v}_{,2})}{\|(\mathbf{A}_1 + \mathbf{v}_{,1}) \times (\mathbf{A}_2 + \mathbf{v}_{,2})\|} \right)_{,\beta} \quad (2.13)$$

Contrasting to the membrane model, the KT strain tensor components now include linearly varying terms corresponding to bending phenomena:

$$E_{\alpha\beta} = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}) + \theta^3(b_{\alpha\beta} - B_{\alpha\beta}) = \epsilon_{\alpha\beta} + \theta^3\kappa_{\alpha\beta} \quad (2.14)$$

According to the KT assumptions all out of plane strains are zero.

$$E_{3i} = \epsilon_{3i} = \kappa_{3i} = 0 \quad (2.15)$$

Studying the strain components, especially the deformed second fundamental form, reveals that there are now 3 midplane displacements \mathbf{v}_i involved in the description of the KT shell model, hence the name 3 parameter model.

Combining the above developments, and assuming the same general external work as equation (2.6), the internal virtual work can be presented:

$$-\delta\Pi_{int} = \int_\Omega \boldsymbol{\epsilon} : \mathbf{C}_{mem} : \delta\boldsymbol{\epsilon} d\Omega + \int_\Omega \boldsymbol{\kappa} : \mathbf{C}_{bend} : \delta\boldsymbol{\kappa} d\Omega \quad (2.16)$$

The internal work equation illustrates the 3 parameter model considers in-plane membrane behaviour as well as the additional bending behaviour related to the second integral. Furthermore, under the condition of homogeneous linear material models the membrane and bending behaviour of the model are uncoupled. Due to the kinematics of the 3 parameter model (director remains straight and normal, no transverse shear strains), it can correctly resolve analyses as the thickness tends towards zero. This is in contrast to the 5 parameter model,

which exhibits significant shear locking. Despite this, a pure rendition of the 3 parameter model is not commonly seen in practical FEM due to the required C_1 continuity at element boundaries (arising from rotations expressed as derivatives of transverse displacement) and the additional complication of effective shear forces on boundaries [7].

2.2.3. 5 parameter model: Reissner-Mindlin shell

By relaxing the assumptions made in the 3 parameter shell model, the Reissner-Mindlin (RM) 5 parameter shell model can be derived. This model includes both membrane and bending action. While the KL model required that the shell directors remain normal to the mid-surface, the RM model relaxes this, analogous to the relationship between Bernoulli and Timoshenko beam models. Graphically, this is represented in the following figure:

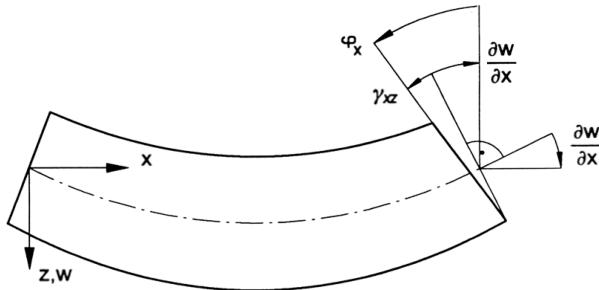


Figure 5 Reissner-Mindlin shell kinematics [10]

Studying the above kinematics confirms this model now considers transverse shear strains, limiting the range of validity of this model to thick plates $\frac{1}{5} < \frac{l}{t} < \frac{1}{10}$ where transverse deformations are a key component of structural behaviour. Similar to the membrane and KL model, thickness deformation is ignored.

The geometry of the RM model is established similar to the KL model:

$$\mathbf{u} = \mathbf{x} - \mathbf{X} = \mathbf{v} + \theta^3(\boldsymbol{\Lambda} - \mathbf{G})\mathbf{D} = \mathbf{v} + \theta^3\mathbf{d} \quad (2.17)$$

However, the strict requirement of maintaining the director remain normal to the mid-surface, as expressed in the KL theory equation (2.9), are no longer enforced. Correspondingly, the rotation tensor $\boldsymbol{\Lambda}$ must now include 2 additional parameters related to these 2 introduced degrees of freedom.

The general strain components are expressed as:

$$E_{\alpha\beta} = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}) + \theta^3(b_{\alpha\beta} - B_{\alpha\beta}) = \epsilon_{\alpha\beta} + \theta^3\kappa_{\alpha\beta} \quad (2.18)$$

Once again it is noted the assumption of straight directors is enforced by the linear coupling of $\theta^3\kappa_{\alpha\beta}$. Following the assumption of no thickness strain, it is seen:

$$E_{33} = \epsilon_{33} = \kappa_{33} = 0 \quad (2.19)$$

By relaxing the director normality requirements, additional transverse shear strains must be accounted for:

$$E_{\alpha 3} = E_{3\alpha} = \frac{1}{2}(a_{\alpha 3} - A_{\alpha 3}) = \frac{1}{2}\gamma_{3\alpha} \quad (2.20)$$

The internal virtual work is therefore expressed as:

$$-\delta\Pi_{int} = \int_{\Omega} \boldsymbol{\epsilon} : \mathbf{C}_{mem} : \delta\boldsymbol{\epsilon} \, d\Omega + \int_{\Omega} \boldsymbol{\kappa} : \mathbf{C}_{bend} : \delta\boldsymbol{\kappa} \, d\Omega + \int_{\Omega} \boldsymbol{\gamma} : \mathbf{C}_{shear} : \delta\boldsymbol{\gamma} \, d\Omega \quad (2.21)$$

The 3 integrals of the virtual work equation represent the membrane, bending and shear work components, corresponding to the phenomena this model resolves. Furthermore, all these components are decoupled from each other in flat shells with homogeneous linear material models. The consideration of transverse shear deformations in the kinematics render the model applicable to thick shells where these strains are not insignificant. Incorrectly applying this model to thin shells in FEM yields spurious results due to a phenomena called shear locking (discussed in section 2.3.1). Despite this disadvantage, the 5 parameter forms the basis of many shell elements often used in FEM thanks to the lower C_0 continuity required at element boundaries.

2.2.4. 7 parameter model

The previously discussed models all operate under the assumption that the transverse normal strains are zero. The 7 parameter model considers thickness deformation by introducing additional free parameters. Only a brief overview of the 7 parameter model is offered here as shell elements in FEM, the focus of this work, are predominately based off 3 and 5 parameter based formulations. For further details refer Bischoff et al. [7] and Ramm and Wall [28].

Intuitively, one may realise that shell behaviour including thickness change may be described by 6 parameters: 3 mid-surface displacements, 1 thickness change and 2 rotations. However, thickness locking occurs under this regime due to a mismatch of a linearly varying normal thickness stress θ^{33} conjugated with a constant thickness strain ϵ_{33} . Thus the 7th parameter is the enhancement of the through thickness strain ϵ_{33} to a linear field.

It's clear that the additional modelling power of the 7 parameter shell can resolve physics that lower parameter models can't. A prime example of this is the Eigenvalue spectra presented below:

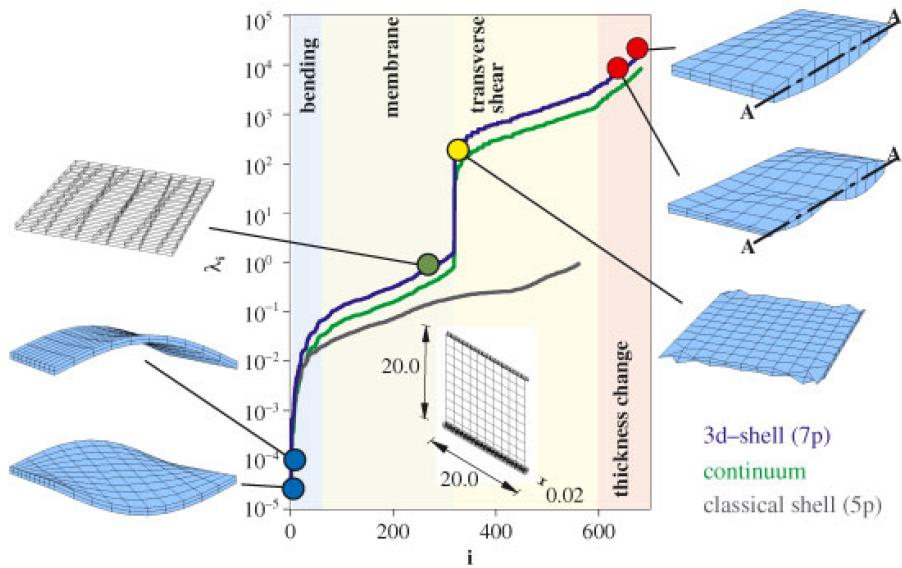


Figure 6 Eigenvalue spectra of various shell models [28]

As expected, the 7 parameter model captures higher Eigen-frequencies associated with thickness modes, while the 5 parameter is unable to resolve these. This is yet another example of model selection limiting the possibility of phenomena resolved.

2.3. Locking in shell finite elements

Surveying a range of shell models has confirmed that not all of them are appropriate for every type of analysis. One must consider the capabilities of the model in conjunction with the supposed critical phenomena of the analysis at hand. Thus, the analysis results are a function of physics the shell model can express. This concept of expression limitation is vital to the correct understanding of shells in the FEM. If the isogeometric approach to the FEM is employed, the field of quantities in the problem are interpolated between discrete nodal values ($\hat{\cdot}$) using shape functions N . In general:

$$\begin{pmatrix} \mathbf{R} \\ \mathbf{v} \\ \epsilon_{ij} \\ \vdots \end{pmatrix}(\xi, \eta) = \sum_{m=1}^{n \text{ nodes}} N(\xi, \eta)_m \begin{pmatrix} \hat{\mathbf{R}}_m \\ \hat{\mathbf{v}}_m \\ \hat{\epsilon}_{ij m} \\ \vdots \end{pmatrix} \quad (2.22)$$

The resolving power of the shape functions undoubtedly restricts what continuous fields can be determined from discrete values. They govern not only the description of geometry, but also the deformation modes the element can express. This forms another layer of expression limitation added to shell models in FEM. Given the propensity to use linear or quadratic shape functions in modern FEM codes, these limitations are often not insignificant. These, together with the physics assumptions and limitations of each shell model, give rise to common numerical inaccuracies, generally termed locking.

2.3.1. Transverse shear locking

Transverse shear locking is perhaps the most recognized and problematic locking phenomena amongst the three considered in this work. As it is related to transverse shear strains, transverse shear locking is possible in the 5 parameter model and impossible for membrane and 3 parameter models. Phenomenologically, transverse shear locking occurs when thin shells incorrectly described by a 5 parameter model are subject to bending situations, with the signature of significantly reduced displacements (ie. 'locked') than expected. By indicating specific material matrices, and removing membrane work, the internal virtual work of the 5 parameter model is clarified:

$$\bar{\mathbf{C}} = \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix} \quad \mathbf{C}_{bend} = \frac{Et^3}{12(1-\nu^2)} \bar{\mathbf{C}} \quad \mathbf{C}_{shear} = \alpha Gt \mathbf{I} \quad (2.23)$$

$$-(\delta\Pi_{int} - \delta\Pi_{int\ mem}) = -(\Pi_{bend} + \Pi_{shear}) = \int_{\Omega} \boldsymbol{\kappa} : \frac{Et^3}{12(1-\nu^2)} \bar{\mathbf{C}} : \delta\boldsymbol{\kappa} d\Omega + \int_{\Omega} \boldsymbol{\gamma} : \alpha Gt \mathbf{I} : \delta\boldsymbol{\gamma} d\Omega \quad (2.24)$$

As phenomenologically described, transverse shear locking comes into effect with thin shells. One can see that as $t \rightarrow 0$ the bending internal work ($\Pi_{bend} \propto t^3$) will be far less than the shear internal work ($\Pi_{shear} \propto t$), leading to an incorrect allocation of internal energy. Since the bending internal work is associated with bending deflections, these resulting deflections will be less than they should be and the element will appear locked. The over-representation of shear strains also leads to strong shear force oscillations - another classic symptom of transverse shear locking.

2.3.2. Membrane locking

Membrane locking is the inability to undergo inextensional bending deformations without parasitic membrane contributions. Physically, a primary symptom of this is significantly reduced deformations under pure bending action. Element curvature is a necessary condition for membrane locking, while increasing slenderness exacerbates the problem. Similar to transverse shear locking, as $t \rightarrow 0$ the bending internal work ($\Pi_{bend} \propto t^3$) reduces at a far greater rate than the membrane internal work ($\Pi_{mem} \propto t$) leading to artificial membrane contributions. Thus, membrane locking is possible in 3, 5, and 7 parameter models. The following figure illustrates the increasing severity of membrane locking as slenderness increases for 3 and 5 parameter NURBS based shell models.

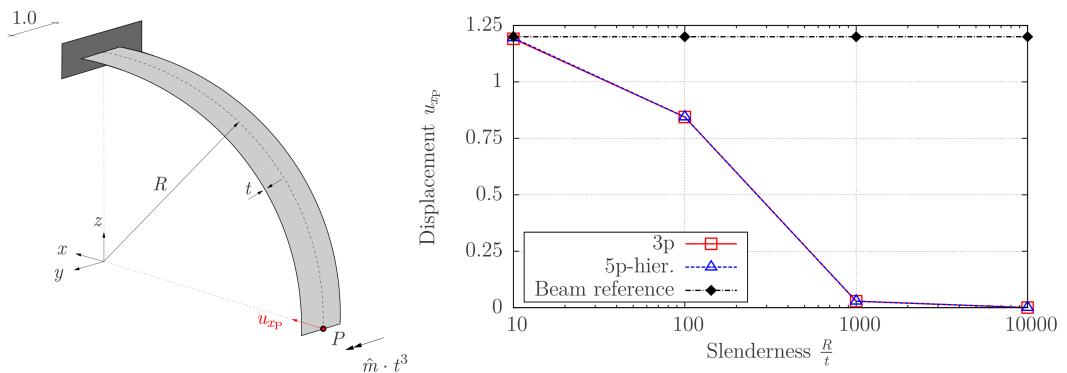


Figure 7 Convergence of cylindrical shell problem demonstrating membrane locking [14]

Despite the bleak results of the above problem, especially in high slenderness range, Bischoff et al. [7] suggest that the adverse effects of membrane locking are mild when using bilinear shape functions, and completely ignored in linear triangle elements (where curvature is always zero). These lower order finite elements form the bulk of what used in commercial FEM codes

and are the focus of this work.

2.3.3. Curvature thickness locking

Curvature locking is another locking consideration that only occurs in curved structures with 7 parameter models. The hallmark of curvature thickness locking is artificial through-thickness strains ϵ_{33} under pure bending action. Since the focus of this work is 3 and 5 parameter models that don't include normal strains ϵ_{33} , the reader is referred to Bischoff et al. [7] and Echter [14] for further information.

2.4. Shell finite element technologies

The previous discussion of locking phenomena associated with pure displacement formulations of shell finite elements has given rise to a number of shell finite element technologies to improve element performance. Broadly speaking, these mitigation approaches fall into two categories: reduced integration and B-Bar \bar{B} approaches which modify the strain displacement matrix B .

2.4.1. Reduced integration

One of the simplest and oldest methods of curbing locking is reduced integration, which deliberately uses less Gauss points than required to integrate the element stiffness matrix. Typically implemented as selective reduced integration (SRI), where the bending component is fully integrated and only the shear part undergoes reduced integration, the efficacy of the method relies on how susceptible the reduced integration Gaussian point locations are to parasitic strains. Despite this chance aspect, it is often used in crash worthiness simulations with the benefits of reduced locking and reduced computational time. The following graph compares the performance (scaled displacement vs. slenderness) of a fully and reduced integrated 5 parameter shell against the reference solution for a square plate in bending.

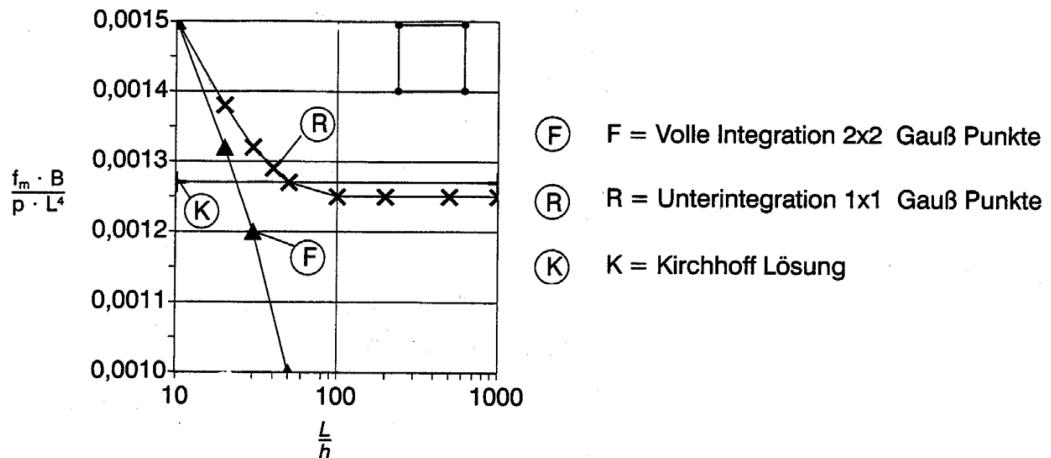


Figure 8 Reduced integration of a 5 parameter Quad 4 shell [10]

F = Full integration, R = Reduced integration, K = Kirchhoff (3 parameter model) solution

It's clear that the normal fully integrated element exhibits severe locking, while the element with reduced integration converges to a value close to the reference solution. Despite this, SRI in general still doesn't guarantee complete removal of shear locking and also introduces spurious zero energy modes. These zero energy modes are often combated by stabilizing matrices ("hourglass" control [34]) which are designed to be activated under the spurious zero-energy regimes and noted as quite complex to formulate [23]. An additional drawback of reduced integration is element performance deterioration as the mesh becomes distorted and warped [26] [33].

2.4.2. Assumed Natural Strains

The Assumed Natural Strain (ANS) approach forms a main umbrella of B-Bar methods, which alters the strain-displacement matrix \mathbf{B} to mitigate locking. The ANS approach [21] works by computing the strain values at particular co-location points less susceptible to parasitic strains in the element (normally chosen as mid-edge and/or centre points) and then interpolating these discrete values through the element to define a new "assumed" shear strain field. As a general approach, many subsequent technologies fall under the ANS umbrella.

2.4.3. Mixed Interpolation of Tensorial Components

Falling within the ANS framework, Dvorkin and Bathe [13] [2] developed the Mixed Interpolation of Tensorial Components (MITC) approach which relies on an assumed shear strain field. A graphical example of this formulation is demonstrated below on a Quad 4 element, with linear interpolation of the shear strain field at mid-side points.

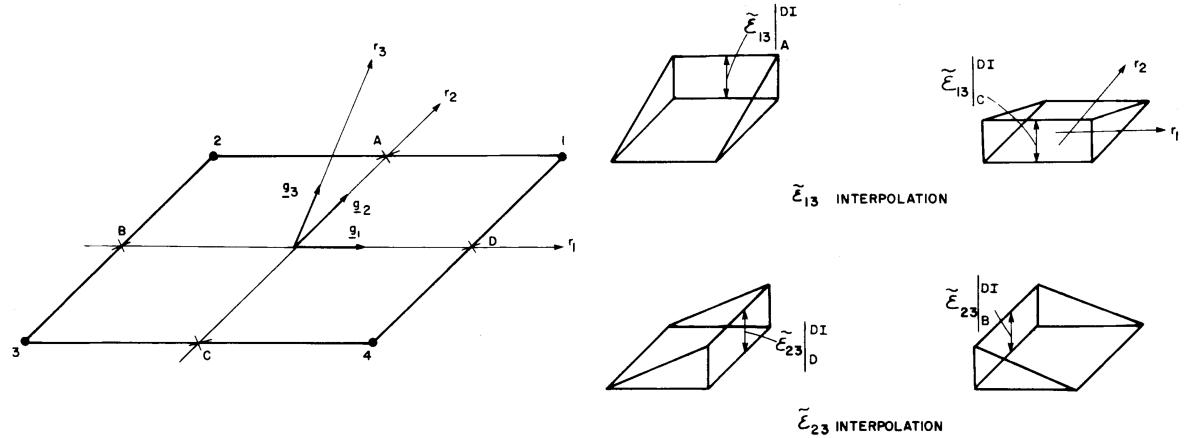


Figure 9 Assumed shear strain field of the MITC4 element [2]

The performance of the MITC formulation clearly depends on the location of the sampling points, and their susceptibility to parasitic shear strains under the case considered. Despite this, the MITC elements have proven resistant to membrane and transverse shear locking [2] and are amongst the most widely used elements throughout FEM codes.

2.4.4. Assumed Natural Deviatoric Strains

The ANS approach was extended into Free Formulation (FF) [6], where the element stiffness matrix is the sum of a basic and higher order stiffness, by Militello and Felippa [15] under the name of the Assumed Natural Deviatoric Strains (ANDES) formulation. An advantage that the ANDES formulation inherits from the FF is that it untethers the derivation of element stiffness from the principle of minimum potential energy, the function continuity requirements of which often result in elements that "tend to be too stiff" [6]. The ANDES basic stiffness ensures consistency of the element and arises from the basic strain field comprising constant strain states and those associated with rigid body motion. Complementing this, the higher order stiffness is responsible for stability and accuracy [17] based on an enhanced strain field

where the element enhancements are realised. The FF framework requires this potentially non-conforming higher order field be energy orthogonal to the basic field, which the ANDES formulation fulfils with a deviatoric higher order strain field [16]. The ANDES formulation has proven capable of alleviating membrane and transverse shear locking [24].

2.4.5. Discrete Shear Gap

The Discrete Shear Gap (DSG) approach from Bischoff and Bletzinger [11] [8] is another variant on the ANS approach with the novelty of identifying and manipulating the 'shear gap' field of the element. The shear gap, as illustrated below, is the increase of displacement due to shear, and corresponds to the difference between the actual displacement and that of pure bending (thus the shear gap is always zero in a 3 parameter Kirchhoff-Love model).

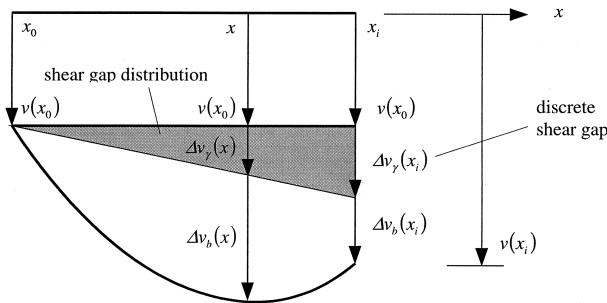


Figure 10 Discrete Shear Gap (DSG) concept [11]

The DSG method aims to set the nodal shear gaps to zero, which, in effect, alters and defines the underlying shear strain field. In bilinear rectangular applications of the DSG method, Bletzinger [11] notes that the MITC4 element is recovered. For a linear triangle element, the shear gap of only two nodes can be set to zero, rendering the element stiffness dependent on node ordering [11]. Despite this drawback, which diminishes with mesh refinement, the DSG method offers an advantage of very fast computational construction of element stiffness matrices and effective mitigation of transverse shear locking.

2.4.6. Discrete Kirchhoff Theory

Elements based on the Discrete Kirchhoff Theory (DKT) are obtained by modifying a basic 5 parameter element and ignoring the transverse shear energy [3]. Since the underlying kinematics of the 5 parameter model are different to Kirchhoff bending theory, the Kirchhoff

constraints are enforced via discrete points (typically nodes and mid-edge points) along the element edges relating the rotations to translational displacements. The geometry and tying-points of the Discrete Kirchhoff Quadrilateral (DKQ) element are shown below:

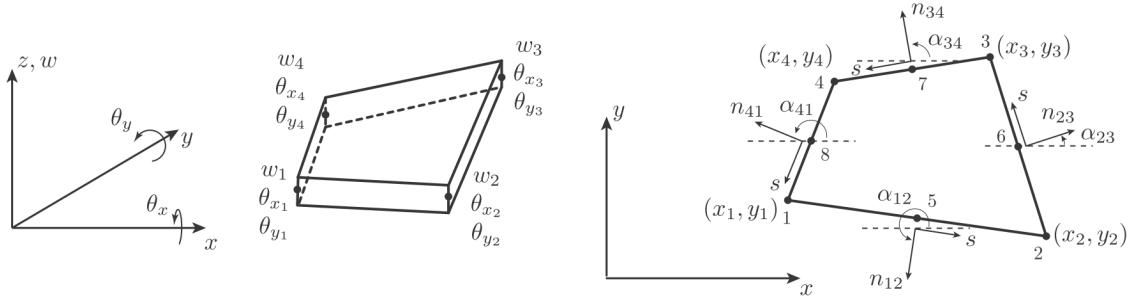


Figure 11 DKQ DOF arrangement and geometry [1]

For example, the Kirchhoff conditions are imposed at corner nodes $i = 1, 2, 3, 4$ and mid-side nodes $k = 5, 6, 7, 8$ [1]:

$$\beta_{xi} + \frac{\partial w}{\partial x}|_i = 0 , \quad \beta_{yi} + \frac{\partial w}{\partial y}|_i = 0 , \quad \beta_{sk} + \frac{\partial w}{\partial s}|_k = 0 \quad (2.25)$$

Mohan [23] noted that a major drawback of DKT elements is that the transverse displacement isn't explicitly defined within the interior of the element. Despite this, the advantages of DKT formulated elements is that they combine the shear locking free performance of KL models and the lower C_0 continuity requirements of RM models [10].

2.4.7. Enhanced Assumed Strains

The Enhanced Assumed Strain (EAS) approach [30] utilises the three field Hu-Washizu variational principle which allows the simultaneous variation of displacements, stresses and strains. Unlike the other technologies presented which attempt to remove problematic strain terms associated with locking, EAS derived elements feature additional enhanced strain fields designed to balance the parasitic displacement based strain terms. To prevent singular matrices the enhanced strains must be linearly independent from the displacement based strains. Furthermore, orthogonality of the stress functions to the enhanced strains must be ensured such that the associated energy vanish [14]. The application of EAS techniques to

elements has been found to improve transverse shear and membrane locking performance [30] [7] [14].

2.4.8. Drilling degrees of freedom

Although drilling degrees of freedom (DOFs) don't counter locking problems, it is a commonly employed finite element technique. The common analysis of structural connections and custom steelwork are instances where shell elements will intersect with each other at arbitrary orientations. The discussion of 3 and 5 parameter shell models confirmed the nodal DOFs to be 3 translation and 2 rotational components:

$$\mathbf{v}_i^T = \begin{pmatrix} v_{xi} & v_{yi} & v_{zi} & \beta_{xi} & \beta_{yi} \end{pmatrix} \quad (2.26)$$

It can be seen that the shell formulations don't require a rotational DOF around the z axis β_{zi} , referred to as the drilling DOF. However, as discussed, shell elements in practical FEA may meet at arbitrary orientations, such as the perpendicular intersection below:

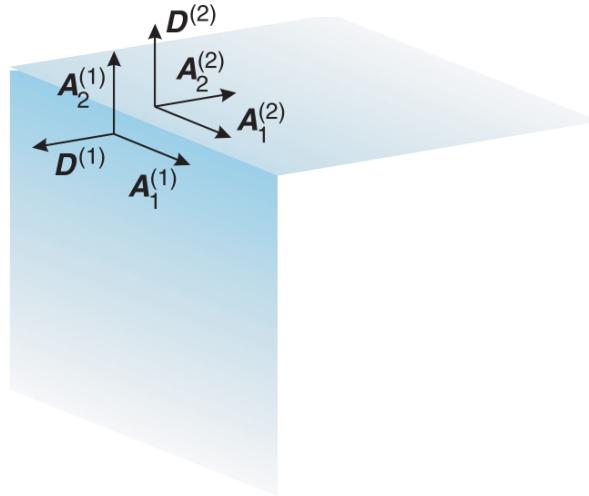


Figure 12 Shell assembly benefitting from drilling DOFs [7]

The figure above illustrates that the real twisting DOF associated with $A_2^{(2)}$ mates with the drilling DOF associated with $D^{(1)}$, which has no theoretically based stiffness value according to the shell formulations. In the current arrangement the connection will clearly be modelled

too flexibly. A remedy for this is the addition of an artificial drilling DOF stiffness to the element, however the magnitude of such a fictitious torsional spring has no decisive theoretical foundation. Intuitively, it should be done on an element by element basis and should vary with the characteristic size and stiffness of the element, as opposed to a global constant drilling stiffness. Among others available, one common technique is to introduce a scaling factor (in the strain-displacement matrix or after the element stiffness matrix is constructed) which takes a fraction of the element stiffness and assigns it to the drilling DOFs.

2.4.9. Summary of selected element technologies

Following the discussion of shell models, their associated locking phenomena and element technologies, a summary of the element technologies considered with their relative merits and drawbacks is tabulated below:

Technology	Formulation	Advantages	Disadvantages
ANDES	5 parameter	Reduced membrane and transverse shear locking Relaxed higher order strain field	Locking reduction depends on tying points More complex implementation
ANS	5 parameter	Reduced membrane and transverse shear locking	Locking reduction depends on tying points
DKT	3 parameter	No transverse shear locking	Transverse disp. not explicitly defined
Drilling DOFs	-	Practical assembly of shells	Artificial stiffness
DSG	5 parameter	Reduced transverse shear locking Computationally fast	Node numbering dependency for linear triangle
EAS	5 parameter	Reduced transverse shear and membrane locking	Potentially complex implementation and possibly slower
MITC	5 parameter	Reduced membrane and transverse shear locking	Locking reduction depends on tying points
Reduced integration	-	Lowered computational cost Reduced locking	Zero energy modes Locking reduction depends on integration points

Table 1 Summary of selected element technologies

The table above confirms the "*no free lunch*" theory, with every technology having its own advantages and drawbacks. In the case of a flat shell (naturally, or via projection), where the bending and membrane response are decoupled, a single finite element can easily employ different technologies in each component.

2.5. Identification of KRATOS shell element formulations

The shell elements to be implemented in KRATOS are the 5 parameter (Reissner-Mindlin theory) triangular shell and the 3 parameter (Kirchhoff Love theory) quadrilateral shell. Obviously the perfect element choices for KRATOS would be computationally quick, possess no locking and easy to implement, but it's clear such an element doesn't exist yet. If the requirements are relaxed to computationally quick elements that are relatively free of locking effects the following candidates are selected:

Element	Membrane formulation	Bending formulation
Thick triangular shell	DSG + Drilling DOFs	DSG
Thin quadrilateral shell	ANDES including Drilling DOFs	DKT

Table 2 Selected formulations of implemented shell elements

With the various components of the KRATOS shell elements selected, they shall be implemented in the following sections of this work, commencing with the DSG triangular element.

3. DSG triangle shell element

This section deals with the derivation and implementation of a thick triangular shell element in KRATOS.

3.1. Stiffness matrix formulation

Based on Reissner Mindlin shell theory, the thick shell considers internal energy contributions from membrane, bending and shear components. As discussed in the background, basic shell elements derived from this shell theory face locking problems as the shell slenderness ratio increases. The element implemented is Bletzinger's Discrete Shear Gap (DSG) shell [11], which incorporates an enhanced shear strain formulation to mitigate the aforementioned locking. This triangular element has 18 DOFs ordered as such:

$$\mathbf{u}^T = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{pmatrix} \quad \text{where} \quad \mathbf{u}_i^T = \begin{pmatrix} u_{xi} & u_{yi} & u_{zi} & \theta_{xi} & \theta_{yi} & \theta_{zi} \end{pmatrix} \quad (3.1)$$

The element displacement field is related to the discrete nodal values via shape functions.

$$\mathbf{u}(x, y) = \sum_{i=1}^3 N_i(x, y) \mathbf{u}_i \quad (3.2)$$

N_i are the standard linear triangle shape functions, referred to the cartesian system.

$$\begin{aligned} N_1(x, y) &= \frac{1}{2A} [(x_2y_3 - x_3y_2) + x(y_2 - y_3) + y(x_3 - x_2)] \\ N_2(x, y) &= \frac{1}{2A} [(x_3y_1 - x_1y_3) + x(y_3 - y_1) + y(x_1 - x_3)] \\ N_3(x, y) &= \frac{1}{2A} [(x_1y_2 - x_2y_1) + x(y_1 - y_2) + y(x_2 - x_1)] \end{aligned} \quad (3.3)$$

Analogous to internal energy, the element stiffness matrix of the DSG triangle can be decomposed into membrane, bending and shear contributions.

$$\mathbf{K} = \mathbf{K}_{mem} + \mathbf{K}_{bend} + \mathbf{K}_{shear} \quad (3.4)$$

The above expression can be expanded into strain-displacement and material matrices relevant for each component.

$$\mathbf{K} = \int_A (\mathbf{B}_{mem}^T \mathbf{C}_{mem} \mathbf{B}_{mem} + \mathbf{B}_{bend}^T \mathbf{C}_{bend} \mathbf{B}_{bend} + \mathbf{B}_{shear}^T \mathbf{C}_{shear} \mathbf{B}_{shear}) dA \quad (3.5)$$

Rama et al. [27] present the DSG formulation in a similar manner, detailing the strain displacement matrix and material material of each constituent separately.

The membrane strain displacement matrix can be expressed as:

$$\mathbf{B}_{mem} = \begin{pmatrix} & & \\ \mathbf{B}_{mem_1} & \mathbf{B}_{mem_2} & \mathbf{B}_{mem_3} \\ & & \end{pmatrix} \quad (3.6)$$

$$\mathbf{B}_{mem_i} = \begin{pmatrix} N_{i,x} & 0 & 0 & 0 & 0 & 0 \\ 0 & N_{i,y} & 0 & 0 & 0 & 0 \\ N_{i,y} & N_{i,x} & 0 & 0 & 0 & 0 \end{pmatrix} \quad (3.7)$$

The bending strain displacement matrix can be presented in a similar manner:

$$\mathbf{B}_{bend} = \begin{pmatrix} & & \\ \mathbf{B}_{bend_1} & \mathbf{B}_{bend_2} & \mathbf{B}_{bend_3} \\ & & \end{pmatrix} \quad (3.8)$$

$$\mathbf{B}_{bend_i} = \begin{pmatrix} 0 & 0 & 0 & 0 & N_{i,x} & 0 \\ 0 & 0 & 0 & -N_{i,y} & 0 & 0 \\ 0 & 0 & 0 & -N_{i,x} & N_{i,y} & 0 \end{pmatrix} \quad (3.9)$$

Finally, the shear strain displacement matrix, the feature of the DSG element, is as follows:

$$\mathbf{B}_{shear} = \frac{1}{2A} \begin{pmatrix} 0 & 0 & b-c & 0 & A & 0 & 0 & 0 & c & \frac{-bc}{2} & \frac{ac}{2} & 0 & 0 & 0 & -b & \frac{bc}{2} & \frac{bd}{2} & 0 \\ 0 & 0 & d-a & -A & 0 & 0 & 0 & 0 & -d & \frac{bd}{2} & \frac{-ad}{2} & 0 & 0 & 0 & a & \frac{-ac}{2} & \frac{ad}{2} & 0 \end{pmatrix}$$

with : $a = x_2 - x_1$, $b = y_2 - y_1$, $c = y_3 - y_1$, $d = x_3 - x_1$

(3.10)

The material matrices for the membrane and bending parts are presented below:

$$\mathbf{C}_{mem} = \frac{Et}{(1-\nu^2)} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{(1-\nu)}{2} \end{pmatrix} \quad (3.11)$$

$$\mathbf{C}_{bend} = \frac{Et^3}{12(1-\nu^2)} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{(1-\nu)}{2} \end{pmatrix} \quad (3.12)$$

To further improve the DSG element performance, Bischoff and Bletzinger [8] [9] applied the enhancement approach that Llyl suggested for MITC-4 elements [20]. This approach modifies the internal shear energy term by scaling the shear constitutive matrix with a correction term τ incorporating the element thickness and an indicator of element size (h_k = longest element side length). The revised shear constitutive matrix is thus:

$$\mathbf{C}_{shear} = \tau \kappa G t \begin{pmatrix} 1 & \nu \\ \nu & 1 \end{pmatrix} = \frac{\kappa G t^3}{t^2 + \alpha h_k^2} \begin{pmatrix} 1 & \nu \\ \nu & 1 \end{pmatrix} \quad (3.13)$$

where $\kappa = \frac{5}{6}$ is the shear correction factor and $\alpha = 0.1$ as per [20].

At a basic level, shear locking in bending plates is driven by a mismatch of internal energy allocation between bending ($\Pi_{bend} \propto t^3$) and shear components ($\Pi_{shear} \propto t$) as $t \rightarrow 0$. This modification somewhat alleviates the locking by 'encouraging' the internal shear energy to scale with the cube of the thickness too, thus reducing the artificial energy disparity.

Although all stiffness components are assembled, one notices that lack of entries corresponding to the drilling DOF θ_{zi} currently renders the element stiffness matrix singular. Nguyen-Thoi et al. [25] proposed to remedy this rotational singularity by setting the drilling DOF entries to one one-thousandth of the maximum diagonal entry in the element stiffness matrix.

$$K_{\theta z} = \frac{\max(K_{el\ ij}\delta_{ij})}{1000} \quad (3.14)$$

3.2. Stiffness matrix implementation

asdfasdfsadf

ADD DIAGRAM AFTER CODE IS NICE

3.3. Mass matrix formulation

The mass matrix is necessary to facilitate dynamic analysis with the thick triangular shell element. As per the existing KRATOS shell elements, a lumped mass approach is employed which results in a diagonal mass matrix.

$$\mathbf{M} = \begin{pmatrix} \mathbf{M}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}_3 \end{pmatrix} \quad \text{where} \quad \mathbf{M}_i = \begin{pmatrix} \bar{m} & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{m} & 0 & 0 & 0 & 0 \\ 0 & 0 & \bar{m} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (3.15)$$

The general lumped mass is determined for a multi-ply material with n plies each of t_i thickness and ρ_i density as follows:

$$\bar{m} = \frac{A}{3} \sum_{i=1}^n \rho_i t_i \quad (3.16)$$

For a single layer material of area A this reduces to:

$$\bar{m} = \frac{A}{3} \rho t \quad (3.17)$$

4. A brief background of shell elements

As discussed in the introduction, shell elements are composed of membrane and bending contributions. The membrane contribution describes the behaviour of the x and y translational and the z rotational (u_x , u_y , θ_z) degree of freedoms (DOFs) for each node, while the bending contribution is responsible for the z translational and x and y rotational (u_z , θ_x , θ_y) DOFs for each node.

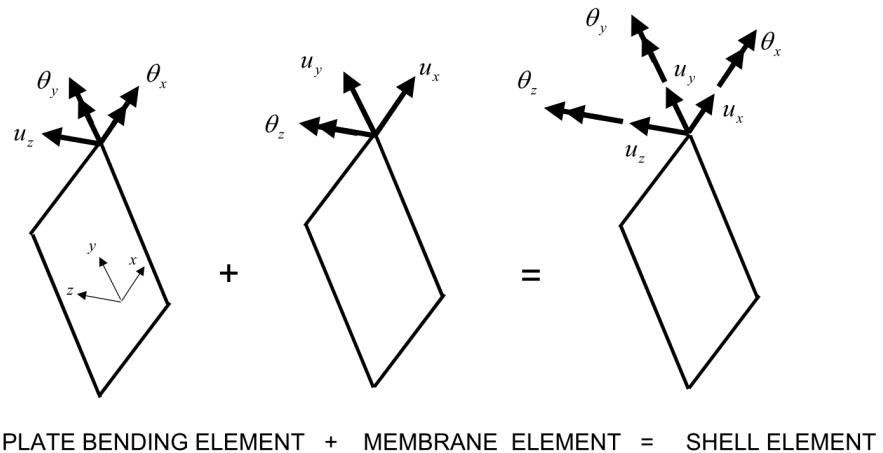


Figure 13 Construction of shell DOFs from bending and membrane DOFs
(source: <http://www.edwilson.org/BOOK-Wilson/10-SHE 1.pdf>)

Furthermore, shells themselves are commonly divided into two groups, thin shells and thick shells, based on the underlying physics assumptions and kinematics.

Thin shells, governed by Kirchhoff bending plate theory, are analogous to Bernoulli beam elements where the shell directors remain straight and normal to the shell midsurface. This kinematic prescription neglects the transverse shear strains γ_{xz} and γ_{yz} as per the figure below.



Figure 14 Thin (Kirchhoff) shell kinematics
(source: KU Bletzinger - Theory of Plates Lecture, 2016, TUM)

Contrasting this, thick shells adhering to Reissner Mindlin bending plate theory are analogous to Timoshenko beam elements, in that they consider the transverse shear deformations neglected by thin shells. The following figure highlights the kinematics of thick shells.

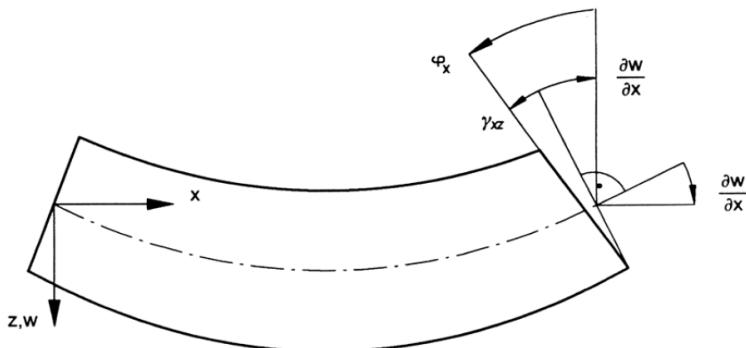


Figure 15 Thick (Reissner Mindlin) shell kinematics
(source: KU Bletzinger - Theory of Plates Lecture, 2016, TUM)

This work considers the implementation of a thin (Kirchhoff bending theory) quadrilateral shell element.

4.0.1. Formulation context

The context in which the following derivation operates within is hereby established. A general form of the linear static FEM is presented below.

$$\mathbf{Ku} = \mathbf{f} \quad (4.1)$$

Since the proposed element is to be integrated into the existing multiphysics code KRATOS,

the relevant term for the derivation of a new element is the system stiffness matrix \mathbf{K} , which is constructed as such:

$$\mathbf{K} = \mathbf{B}^T \mathbf{C} \mathbf{B} \quad (4.2)$$

\mathbf{C} is the constitutive matrix containing the material properties and physics, formed from the membrane and bending constitutive matrices. For the thin quad only a homogeneous isotropic plate constitutive law [4] is considered, as described below.

$$\mathbf{C} = \begin{pmatrix} \frac{E}{(1-\nu^2)} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \frac{Et^3}{12(1-\nu^2)} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{pmatrix} \end{pmatrix} \quad (4.3)$$

Thus, it is evident that the bulk of the element derivation lies in the determination of the element's strain displacement matrix \mathbf{B} . The shell B matrix is composed of a membrane part and a bending part.

5. ANDES-DKT quadrilateral shell element

The formulation of the stiffness matrix for the thin quadrilateral shell element is presented after a quick orientation.

5.1. Stiffness matrix

asdfasdf

5.1.1. Membrane formulation

The membrane formulation is responsible for providing the membrane stiffness of the element. The membrane formulation chosen was the Assumed Natural Deviatoric Strains (ANDES) formulation as presented in [18]. A full description and theoretical derivation of the ANDES approach falls outside the scope of this document, however, those interested are directed to Militello's and Felippa's initial paper [22] on the formulation. Most importantly, the ANDES approach yields high performance elements that are insensitive to distortion.

Only the membrane portion of the total shell element is considered in this section, in which there are three DOFs per node.

$$\mathbf{u}^T = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 & \mathbf{u}_4 \end{pmatrix} \quad \text{where} \quad \mathbf{u}_i^T = \begin{pmatrix} u_{xi} & u_{yi} & \theta_{zi} \end{pmatrix} \quad (5.1)$$

The ANDES membrane formulation itself is split into the basic stiffness and the higher order stiffness.

$$\mathbf{K}_{mem} = \mathbf{K}_b + \mathbf{K}_h = \int_A (\mathbf{L} + \mathbf{B}_h)^T \mathbf{C}_{mem} (\mathbf{L} + \mathbf{B}_h) dA \quad (5.2)$$

The basic strain displacement matrix \mathbf{L} and the higher order complement \mathbf{B}_h are now devel-

oped.

Membrane basic stiffness

The membrane basic stiffness is driven by assuming a constant stress field within the element and lumping this over side edges to consistent nodal forces.

$$\mathbf{f} = \mathbf{L}\boldsymbol{\sigma} \quad \text{where} \quad \boldsymbol{\sigma}^T = \begin{pmatrix} \sigma_{xx} & \sigma_{xx} & \tau_{xy} \end{pmatrix} \quad (5.3)$$

The structure of the above expression is resolved as such:

$$\mathbf{L} = \begin{pmatrix} \mathbf{L}_1 & \mathbf{L}_2 & \mathbf{L}_3 & \mathbf{L}_4 \end{pmatrix} \quad \text{and} \quad \mathbf{f} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \\ \mathbf{f}_4 \end{pmatrix} \quad \text{where} \quad \mathbf{f}_i = \begin{pmatrix} f_{xi} \\ f_{yi} \\ m_{zi} \end{pmatrix} \quad (5.4)$$

where each nodal entry ' j ' of the lumping matrix \mathbf{L} is constructed with the following cyclic permutation (i, j, k, l) for the four nodes (1, 2, 3, 4):

$$\mathbf{L}_j = \frac{1}{2A} \begin{pmatrix} y_{ki} & 0 & -x_{ki} \\ 0 & -x_{ki} & y_{ki} \\ \frac{\alpha}{6}(y_{ij}^2 - y_{kj}^2) & \frac{\alpha}{6}(x_{ij}^2 - x_{kj}^2) & \frac{\alpha}{3}(x_{kj}y_{kj} - x_{ij}y_{ij}) \end{pmatrix} \quad (5.5)$$

Throughout this paper the notation of $x_{ij} = x_i - x_j$ and $y_{ij} = y_i - y_j$ holds. Furthermore, the value of α is taken as 1.5 [22].

Membrane higher order stiffness

The membrane higher order stiffness considers a set of higher order DOFs expressed in terms of the visible DOFs as per equation (5.1).

It should be noted that the derivation below slightly departs from the formulation of Haugen [18] due to the DOF ordering as per equation (5.1).

The higher order rotational DOFs are related to the visible DOFs as described below:

$$\theta_h = \mathbf{H}_{\theta v} \mathbf{u} \quad \text{where} \quad \theta_h^T = \begin{pmatrix} \theta'_1 & \theta'_2 & \theta'_3 & \theta'_4 & \bar{\theta} \end{pmatrix} \quad (5.6)$$

with

$$\mathbf{H}_{\theta\mathbf{v}} = \begin{pmatrix} 0 & 0 & \frac{3}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & 0 & 0 & \frac{3}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & \frac{3}{4} & 0 & 0 & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & \frac{3}{4} \\ \frac{x_{42}}{f} & \frac{y_{42}}{f} & \frac{1}{4} & \frac{x_{13}}{f} & \frac{y_{13}}{f} & \frac{1}{4} & \frac{x_{24}}{f} & \frac{y_{24}}{f} & \frac{1}{4} & \frac{x_{31}}{f} & \frac{y_{31}}{f} & \frac{1}{4} \end{pmatrix}$$

where $f = 16|\mathbf{J}|$

and $|\mathbf{J}| = \frac{1}{8}[(x_1y_2 - x_2y_1) + (x_2y_3 - x_3y_2) + (x_3y_4 - x_4y_3) + (x_4y_1 - x_1y_4)]$ (5.7)

The higher order translational DOFs are related to the visible DOFs as described below:

$$\tilde{\mathbf{v}}_t = \mathbf{H}_{tv}\mathbf{u} \quad \text{where} \quad \tilde{\mathbf{v}}_t^T = \begin{pmatrix} \tilde{v}_x & \tilde{v}_y \end{pmatrix} \quad (5.8)$$

with

$$\mathbf{H}_{tv} = \begin{pmatrix} 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \end{pmatrix} \quad (5.9)$$

Combining both mapping matrices together expresses all higher order DOFs in terms of the visible DOFs:

$$\tilde{\mathbf{v}} = \mathbf{H}\mathbf{v} \quad \text{where} \quad \mathbf{H} = \begin{pmatrix} \mathbf{H}_{\theta\mathbf{v}} \\ \mathbf{H}_{\mathbf{v}\mathbf{t}} \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{v}}^T = \begin{pmatrix} \theta'_1 & \theta'_2 & \theta'_3 & \theta'_4 & \bar{\theta} & \tilde{v}_x & \tilde{v}_y \end{pmatrix} \quad (5.10)$$

The descriptions for equations from (5.11) to (5.25) are heavily abridged from the original element derivation [18]. The general idea of these equations is to relate the higher order nodal strain gauge readings to cartesian strain displacement matrices \mathbf{B}_{hi} .

The components necessary for the construction of the higher order bending strain field (along ξ and η directions) are shown below:

$$\chi_{\xi|i} = \frac{d_{\xi|i}}{l_{\xi}}, \quad \chi_{\eta|i} = \frac{d_{\eta|i}}{l_{\eta}}, \quad (5.11)$$

where

$$d_{\xi|i} = \sqrt{(\mathbf{r}_i \times \mathbf{s}_\xi) \cdot (\mathbf{r}_i \times \mathbf{s}_\xi)}, \quad l_\xi = \sqrt{\mathbf{r}_\xi \cdot \mathbf{r}_\xi}, \quad \mathbf{r}_\xi = \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_4),$$

$$d_{\eta|i} = \sqrt{(\mathbf{r}_i \times \mathbf{s}_\eta) \cdot (\mathbf{r}_i \times \mathbf{s}_\eta)}, \quad l_\eta = \sqrt{\mathbf{r}_\eta \cdot \mathbf{r}_\eta}, \quad \mathbf{r}_\eta = \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_4),$$

\mathbf{s}_ξ and \mathbf{s}_η are the normalized parametric base vectors in cartesian coordinates, while \mathbf{r}_i are the nodal position vectors in cartesian coordinates.

The components necessary for the construction of the higher order bending strain field (along the element diagonal) are shown below:

$$\chi_{24} = \frac{d_{24}}{2l_{24}}, \quad \chi_{13} = \frac{d_{13}}{2l_{13}}, \quad (5.12)$$

where

$$d_{24} = d_{13} = \sqrt{(\mathbf{r}_{31} \times \mathbf{e}_{24}) \cdot (\mathbf{r}_{31} \times \mathbf{e}_{24})}$$

$$l_{24} = \sqrt{\mathbf{r}_{24} \cdot \mathbf{r}_{24}}, \quad \mathbf{r}_{24} = \mathbf{r}_2 - \mathbf{r}_4$$

$$l_{13} = \sqrt{\mathbf{r}_{13} \cdot \mathbf{r}_{13}}, \quad \mathbf{r}_{13} = \mathbf{r}_1 - \mathbf{r}_3 \quad \mathbf{e}_{24} = \frac{\mathbf{r}_{24}}{l_{24}}$$

The components necessary for the construction of the higher order torsional strain field are shown below:

$$\chi_{\xi t} = \frac{l_\eta}{l_\xi}, \quad \chi_{\eta t} = \frac{l_\xi}{l_\eta}, \quad (5.13)$$

The mapping from strain gauge readings along the 3 directions at each node to the higher order DOFs is via the matrices \mathbf{Q}_i described below:

$$\mathbf{Q}_1 = \begin{pmatrix} \rho_1 \chi_{\xi|1} & \rho_2 \chi_{\xi|1} & \rho_3 \chi_{\xi|1} & \rho_4 \chi_{\xi|1} & \alpha \chi_{\xi t} & -\beta_1 \frac{\chi_{\xi|1}}{\bar{\chi}_\xi l_\xi} & 0 \\ -\rho_1 \chi_{\eta|1} & -\rho_4 \chi_{\eta|1} & -\rho_3 \chi_{\eta|1} & -\rho_2 \chi_{\eta|1} & -\alpha \chi_{\eta t} & 0 & -\beta_1 \frac{\chi_{\eta|1}}{\bar{\chi}_\eta l_\eta} \\ \rho_5 \chi_{24} & \rho_6 \chi_{24} & \rho_7 \chi_{24} & \rho_8 \chi_{24} & 0 & \beta_2 \frac{c_{24\xi}}{l_{24}} & -\beta_2 \frac{c_{24\eta}}{l_{24}} \end{pmatrix} \quad (5.14)$$

$$\mathbf{Q}_2 = \begin{pmatrix} -\rho_2 \chi_{\xi|2} & -\rho_1 \chi_{\xi|2} & -\rho_4 \chi_{\xi|2} & -\rho_3 \chi_{\xi|2} & -\alpha \chi_{\xi t} & -\beta_1 \frac{\chi_{\xi|2}}{\bar{\chi}_{\xi} l_{\xi}} & 0 \\ \rho_4 \chi_{\eta|2} & \rho_1 \chi_{\eta|2} & \rho_2 \chi_{\eta|2} & \rho_3 \chi_{\eta|2} & \alpha \chi_{\eta t} & 0 & \beta_1 \frac{\chi_{\eta|2}}{\bar{\chi}_{\eta} l_{\eta}} \\ \rho_8 \chi_{13} & \rho_5 \chi_{13} & \rho_6 \chi_{13} & \rho_7 \chi_{13} & 0 & -\beta_2 \frac{c_{13\xi}}{l_{13}} & \beta_2 \frac{c_{13\eta}}{l_{13}} \end{pmatrix} \quad (5.15)$$

$$\mathbf{Q}_3 = \begin{pmatrix} \rho_3 \chi_{\xi|3} & \rho_4 \chi_{\xi|3} & \rho_1 \chi_{\xi|3} & \rho_2 \chi_{\xi|3} & \alpha \chi_{\xi t} & \beta_1 \frac{\chi_{\xi|3}}{\bar{\chi}_{\xi} l_{\xi}} & 0 \\ -\rho_3 \chi_{\eta|3} & -\rho_2 \chi_{\eta|3} & -\rho_1 \chi_{\eta|3} & -\rho_4 \chi_{\eta|3} & -\alpha \chi_{\eta t} & 0 & \beta_1 \frac{\chi_{\eta|3}}{\bar{\chi}_{\eta} l_{\eta}} \\ \rho_7 \chi_{13} & \rho_8 \chi_{13} & \rho_5 \chi_{13} & \rho_6 \chi_{213} & 0 & -\beta_2 \frac{c_{13\xi}}{l_{13}} & \beta_2 \frac{c_{13\eta}}{l_{13}} \end{pmatrix} \quad (5.16)$$

$$\mathbf{Q}_4 = \begin{pmatrix} -\rho_4 \chi_{\xi|4} & -\rho_3 \chi_{\xi|4} & -\rho_2 \chi_{\xi|4} & -\rho_1 \chi_{\xi|4} & -\alpha \chi_{\xi t} & \beta_1 \frac{\chi_{\xi|4}}{\bar{\chi}_{\xi} l_{\xi}} & 0 \\ \rho_2 \chi_{\eta|4} & \rho_3 \chi_{\eta|4} & \rho_4 \chi_{\eta|4} & \rho_1 \chi_{\eta|4} & \alpha \chi_{\eta t} & 0 & -\beta_1 \frac{\chi_{\eta|4}}{\bar{\chi}_{\eta} l_{\eta}} \\ \rho_6 \chi_{13} & \rho_7 \chi_{13} & \rho_8 \chi_{13} & \rho_5 \chi_{13} & 0 & \beta_2 \frac{c_{13\xi}}{l_{13}} & -\beta_2 \frac{c_{13\eta}}{l_{13}} \end{pmatrix} \quad (5.17)$$

where

$$c_{13\xi} = \mathbf{s}_{13}^T \mathbf{s}_{\xi} , \quad c_{13\eta} = \mathbf{s}_{13}^T \mathbf{s}_{\eta} , \quad c_{24\xi} = \mathbf{s}_{24}^T \mathbf{s}_{\xi} , \quad c_{24\eta} = \mathbf{s}_{24}^T \mathbf{s}_{\eta}$$

Values for the coefficients utilised above are as follows:

$$\begin{aligned} \rho_1 &= 0.1 , & \rho_2 &= -0.1 , & \rho_3 &= -0.1 , & \rho_4 &= 0.1 , & \rho_5 &= 0.0 , \\ \rho_6 &= 0.5 , & \rho_7 &= 0.0 , & \rho_8 &= -0.5 , & \beta_1 &= 0.6 , & \beta_2 &= 0.0 \end{aligned} \quad (5.18)$$

The cartesian strain displacement matrices at the nodes are related to the mapping matrices \mathbf{Q}_i as described below:

$$\mathbf{B}_{\mathbf{h}1} = \mathbf{T}_{13}\mathbf{Q}_1, \quad \mathbf{B}_{\mathbf{h}3} = \mathbf{T}_{13}\mathbf{Q}_3$$

$$where \quad \mathbf{T}_{13}^{-1} = \begin{pmatrix} s_{\xi x}^2 & s_{\xi y}^2 & s_{\xi x}s_{\xi y} \\ s_{\eta x}^2 & s_{\eta y}^2 & s_{\eta x}s_{\eta y} \\ s_{24x}^2 & s_{24y}^2 & s_{24x}s_{24y} \end{pmatrix} \quad (5.19)$$

$$\mathbf{B}_{\mathbf{h}2} = \mathbf{T}_{24}\mathbf{Q}_2, \quad \mathbf{B}_{\mathbf{h}4} = \mathbf{T}_{24}\mathbf{Q}_4$$

$$where \quad \mathbf{T}_{24}^{-1} = \begin{pmatrix} s_{\xi x}^2 & s_{\xi y}^2 & s_{\xi x}s_{\xi y} \\ s_{\eta x}^2 & s_{\eta y}^2 & s_{\eta x}s_{\eta y} \\ s_{13x}^2 & s_{13y}^2 & s_{13x}s_{13y} \end{pmatrix} \quad (5.20)$$

The higher order membrane B matrix \mathbf{B}_h is constructed from the interpolation of the nodal B matrices with standard bi-linear shape functions.

$$\mathbf{B}_h(\xi, \eta) = (1 - \xi)(1 - \eta)\mathbf{B}_{\mathbf{h}1} + (1 + \xi)(1 - \eta)\mathbf{B}_{\mathbf{h}2} + (1 + \xi)(1 + \eta)\mathbf{B}_{\mathbf{h}3} + (1 - \xi)(1 + \eta)\mathbf{B}_{\mathbf{h}4} \quad (5.21)$$

5.1.2. Bending formulation

The bending formulation is responsible for providing the bending stiffness of the element. The bending formulation chosen was the Discrete Kirchhoff Quadrilateral (DKQ) formulation

originally presented by Batoz [4], presented in a most readable fashion in the PhD dissertation of Barrales [1]. A full description and theoretical derivation of the DKQ approach falls outside the scope of this document, refer [4]. Most importantly for a thin shell element, the transverse shear strain energy is neglected which prohibits element performance deterioration as the ratio $\frac{l}{t}$ encroaches into thin and very thin plate territories.

Only the bending portion of the total shell element is considered in this section, in which there are three nodal DOFs per node (w_i corresponds to u_{zi} in the figure below).

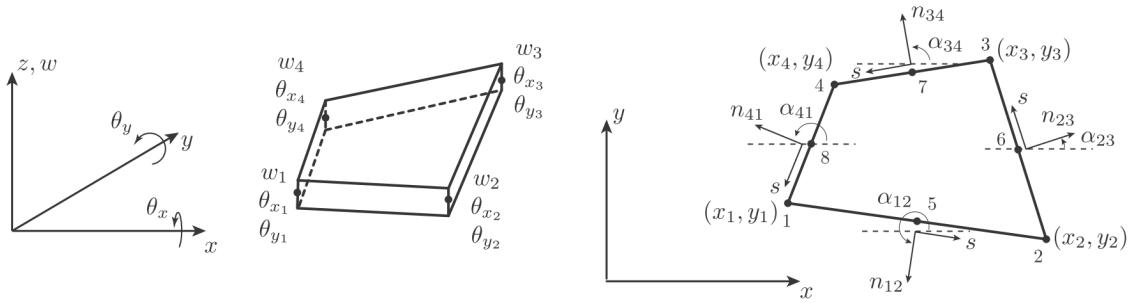


Figure 16 DKQ DOF arrangement and geometry (source: [1])

$$\mathbf{u}^T = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 & \mathbf{u}_4 \end{pmatrix} \quad \text{where} \quad \mathbf{u}_i^T = \begin{pmatrix} u_{zi} & \theta_{xi} & \theta_{yi} \end{pmatrix} \quad (5.22)$$

The nodal rotational interpolation employed is as per the 8 node serendipity quad element:

$$\begin{pmatrix} \beta_x(\xi, \eta) \\ \beta_y(\xi, \eta) \end{pmatrix} = \sum_{i=1}^8 \psi_i(\xi, \eta) \begin{pmatrix} \beta_{xi}(\xi, \eta) \\ \beta_{yi}(\xi, \eta) \end{pmatrix} \quad (5.23)$$

where ψ_i are the standard 8 node serendipity shape functions described by Zienkiewicz [35]:

$$\begin{aligned}
\psi_i(\xi, \eta) &= \frac{-1}{4}(1 + \xi_i \xi)(1 + \eta_i \eta)(1 - \xi_i \xi - \eta_i \eta) & i = 1, 2, 3, 4 \\
\psi_i(\xi, \eta) &= \frac{1}{2}(1 - \xi^2)(1 + \eta_i \eta) & i = 5, 7 \\
\psi_i(\xi, \eta) &= \frac{1}{2}(1 + \xi_i \xi)(1 - \eta^2) & i = 6, 8
\end{aligned} \tag{5.24}$$

and ξ_i and η_i are the natural coordinates of the 8 node serendipity element described in figure 16.

The following derivation from equations (5.25) to (5.30) is heavily summarised from that of Barrales [1]. The general idea is the construction of a mapping from the standard 12 DOFs at each node to $\beta_x(\xi, \eta)$ and $\beta_y(\xi, \eta)$ across the element, the derivatives of which are curvatures as expressed in equation (5.30).

The following quantities are required components for the mapping:

$$L_{ij} = \sqrt{x_{ij}^2 + y_{ij}^2}, \quad x_{ij} = x_i - x_j, \quad y_{ij} = y_i - y_j \tag{5.25}$$

$$\begin{aligned}
a_k &= \frac{-x_{ij}}{L_{ij}^2}, & b_k &= \frac{3}{4} \frac{x_{ij} y_{ij}}{L_{ij}^2}, \\
c_k &= \frac{\frac{1}{4}x_{ij}^2 - \frac{1}{2}y_{ij}^2}{L_{ij}^2}, & d_k &= \frac{-y_{ij}}{L_{ij}^2}, & e_k &= \frac{\frac{-1}{2}x_{ij}^2 + \frac{1}{4}y_{ij}^2}{L_{ij}^2}
\end{aligned} \tag{5.26}$$

The elements of the mapping matrix are arranged as such:

$$\Psi^x = \begin{pmatrix} \Psi_1^x \\ \vdots \\ \Psi_{12}^x \end{pmatrix}, \quad \Psi^y = \begin{pmatrix} \Psi_1^y \\ \vdots \\ \Psi_{12}^y \end{pmatrix} \quad (5.27)$$

where the vectors entries are calculated as per the following scheme:

$$\begin{aligned} \Psi_{3(i-1)+1}^x(\xi, \eta) &= \frac{3}{2}(a_r\psi_r(\xi, \eta) - a_s\psi_s(\xi, \eta)) \\ \Psi_{3(i-1)+2}^x(\xi, \eta) &= b_r\psi_r(\xi, \eta) + b_s\psi_s(\xi, \eta) \\ \Psi_{3(i-1)+3}^x(\xi, \eta) &= \psi_i(\xi, \eta) - c_r\psi_r(\xi, \eta) - c_s\psi_s(\xi, \eta) \end{aligned} \quad (5.28)$$

$$\begin{aligned} \Psi_{3(i-1)+1}^y(\xi, \eta) &= \frac{3}{2}(d_r\psi_r(\xi, \eta) - d_s\psi_s(\xi, \eta)) \\ \Psi_{3(i-1)+2}^y(\xi, \eta) &= -\psi_i(\xi, \eta) + e_r\psi_r(\xi, \eta) + e_s\psi_s(\xi, \eta) \\ \Psi_{3(i-1)+3}^y(\xi, \eta) &= -b_r\psi_r(\xi, \eta) - b_s\psi_s(\xi, \eta) \end{aligned} \quad (5.29)$$

with $i = 1, 2, 3, 4$ and the relationship (i, r, s) as $(1, 5, 8), (2, 6, 5), (3, 7, 6)$ and $(4, 8, 7)$.

Relating curvatures to displacements yield:

$$\chi = \mathbf{B}_{bend}\mathbf{U} \quad (5.30)$$

with \mathbf{B}_{bend} constructed as follows:

$$\mathbf{B}_{bend} = \begin{pmatrix} \frac{\partial \Psi^x}{\partial x} \\ \frac{\partial \Psi^y}{\partial y} \\ \frac{\partial \Psi^x}{\partial y} + \frac{\partial \Psi^y}{\partial x} \end{pmatrix} = \begin{pmatrix} j_{11} \frac{\partial \Psi^x}{\partial \xi} + j_{12} \frac{\partial \Psi^x}{\partial \eta} \\ j_{21} \frac{\partial \Psi^y}{\partial \xi} + j_{22} \frac{\partial \Psi^y}{\partial \eta} \\ j_{11} \frac{\partial \Psi^y}{\partial \xi} + j_{12} \frac{\partial \Psi^y}{\partial \eta} + j_{21} \frac{\partial \Psi^x}{\partial \xi} + j_{22} \frac{\partial \Psi^x}{\partial \eta} \end{pmatrix} \quad (5.31)$$

and the inverse Jacobian entries $j_{\alpha\beta}$:

$$\mathbf{J} = \frac{1}{4} \begin{pmatrix} x_{21} + x_{34} + \eta(x_{12} + x_{34}) & y_{21} + y_{34} + \eta(y_{12} + y_{34}) \\ x_{32} + x_{41} + \xi(x_{12} + x_{34}) & y_{32} + y_{41} + \xi(y_{12} + y_{34}) \end{pmatrix} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} \quad (5.32)$$

$$j_{11} = \frac{J_{22}}{\det[J]} , \quad j_{12} = \frac{-J_{12}}{\det[J]} , \quad j_{21} = \frac{-J_{21}}{\det[J]} , \quad j_{22} = \frac{J_{11}}{\det[J]}$$

5.1.3. Combined formulation

With the separate membrane and bending B matrices developed, the combined shell B matrix \mathbf{B}_{comb} , can be constructed to form the element stiffness matrix.

$$\mathbf{K}_{el} = \mathbf{B}_{comb}^T \mathbf{C} \mathbf{B}_{comb} \quad (5.33)$$

$$\mathbf{B}_{comb} = (\mathbf{L} + \mathbf{B}_h) + \mathbf{B}_{bend} = \mathbf{B}_{mem} + \mathbf{B}_{bend} = \begin{pmatrix} \mathbf{B}_{comb1} & \mathbf{B}_{comb2} & \mathbf{B}_{comb3} & \mathbf{B}_{comb4} \end{pmatrix} \quad (5.34)$$

The combination of *membrane* and *bending* matrices must consider the DOF ordering of each component and the relation to the total shell DOF ordering, as shown below:

$$\mathbf{u}_i = \begin{pmatrix} u_{xi} \\ u_{yi} \\ u_{zi} \\ \theta_{xi} \\ \theta_{yi} \\ \theta_{zi} \end{pmatrix} \quad (5.35)$$

Considering this, the addition of the membrane (basic and higher order) B matrices and the bending B matrix is conducted as follows:

$$\mathbf{B}_{comb\ i} = \begin{pmatrix} \mathbf{B}_{mem}[1, 3(i-1)+1] & \mathbf{B}_{mem}[1, 3(i-1)+2] & 0 \\ \mathbf{B}_{mem}[2, 3(i-1)+1] & \mathbf{B}_{mem}[2, 3(i-1)+2] & 0 \\ 0 & 0 & \mathbf{B}_{bend}[1, 3(i-1)+1] \\ 0 & 0 & \mathbf{B}_{bend}[2, 3(i-1)+1] \\ 0 & 0 & \mathbf{B}_{bend}[3, 3(i-1)+1] \\ \mathbf{B}_{mem}[3, 3(i-1)+1] & \mathbf{B}_{mem}[3, 3(i-1)+2] & 0 \\ 0 & 0 & \mathbf{B}_{mem}[1, 3(i-1)+3] \\ 0 & 0 & \mathbf{B}_{mem}[2, 3(i-1)+3] \\ \mathbf{B}_{bend}[1, 3(i-1)+2] & \mathbf{B}_{bend}[1, 3(i-1)+3] & 0 \\ \mathbf{B}_{bend}[2, 3(i-1)+2] & \mathbf{B}_{bend}[2, 3(i-1)+3] & 0 \\ \mathbf{B}_{bend}[3, 3(i-1)+2] & \mathbf{B}_{bend}[3, 3(i-1)+3] & 0 \\ 0 & 0 & \mathbf{B}_{mem}[3, 3(i-1)+3] \end{pmatrix} \quad (5.36)$$

5.2. Implementation in KRATOS

With the formulation of the thin quadrilateral shell element established, a high level overview of its implementation in KRATOS is discussed in this section.

The new thin quad element is implemented in the files `shell_thin_element_3D4N.hpp` and

`shell_thin_element_3D4N.cpp`, which are placed in the 'custom_elements' directory of the 'StructuralMechanicsApplication' module. Similar to other existing elements, the new class `ShellThinElement3D4N` is inherited from the base class `Element`, which prescribes both virtual and pure virtual methods for its derived classes to implement. The purely virtual methods must be re-implemented in the derived class to ensure that the class possesses the necessary fundamental functionality to operate within the KRATOS framework, while the virtual methods offer optional avenues to implement additional derived element functionality.

Examples of purely virtual methods include: `EquationIdVector(...)`, `GetDofList(...)` and `CalculateLocalSystem(...)`.

Examples of virtual methods include: `CalculateMassMatrix()`, `CalculateDampingMatrix(...)` and `GetValueOnIntegrationPoints(...)`.

Since the current state of the new element is limited to linear statics, few virtual methods have been implemented. Future development of the element into dynamics, for example, would require the implementation of `CalculateMassMatrix()` and `CalculateDampingMatrix(...)`.

The general workflow of the current implementation is considered in the following section.

5.2.1. Workflow of element calculation

The scope of the presented workflow is limited to key class methods employed to determine the unknown displacement field for a linear static problem. Within some of the methods presented below are additional methods, however, only the key methods are considered for clarity.

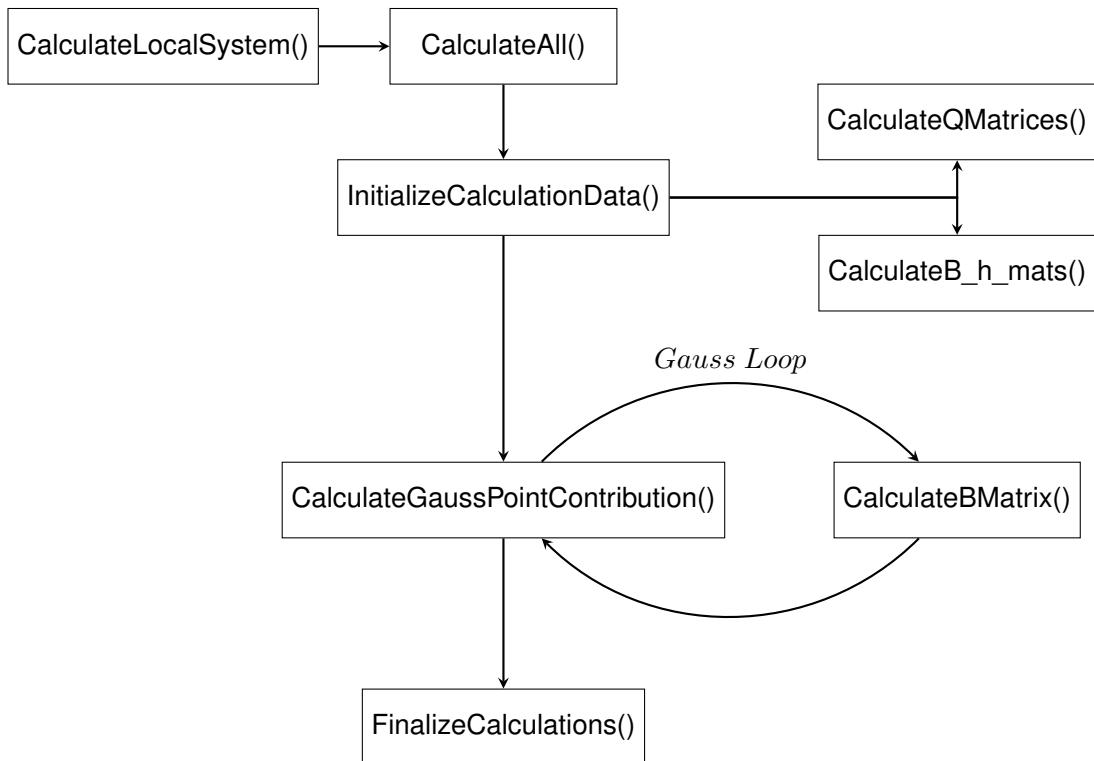


Figure 17 High level overview of element workflow

Initially, the re-implemented purely virtual method `CalculateLocalSystem()` is called by the KRATOS framework automatically for every `ShellThinElement3D4N` in the job definition (.mdpa file in this case). This method simply calls `CalculateAll()`, which is the main pipeline of the element stiffness calculation, itself calling three key methods: `InitializeCalculationData()`, `CalculateAll()` and `FinalizeCalculations()`.

`InitializeCalculationData()` is called first, and pre-calculates quantities so they can be removed from the Gauss loop. These quantities include the basic membrane lumping matrix \mathbf{L} , various transformation matrices (\mathbf{H} , \mathbf{T}_{13} , \mathbf{T}_{24}) and all DKQ coefficients in equation (5.26). `CalculateQMatrices()` and `CalculateB_h_mats()` are also called from `InitializeCalculationData()`, which calculate \mathbf{Q}_i and \mathbf{B}_{hi} for the membrane component.

`CalculateAll()` then calls `CalculateGaussPointContribution()` which starts the Gauss integration loop. At each Gauss point `CalculateGaussPointContribution()` performs

Gauss integration of the expression $\mathbf{K}_{contribution} = \mathbf{B}_{comb}^T \mathbf{C} \mathbf{B}_{comb} dA$, with the current \mathbf{B}_{comb} determined by calling CalculateBMatrix().

With the Gauss integration complete, CalculateAll() lastly calls FinalizeCalculations() which transforms the calculated element stiffness from local to global coordinates.

5.3. Element benchmarks

To test the correct derivation and implementation of the thin quad shell element, the shell obstacle course proposed by Belytschko [5] is considered.

5.3.1. Scordelis-Lo roof

The Scordelis-Lo roof is part of a cylindrical shell fixed by rigid diaphragms at its axial ends. The only loading is a pseudo-gravity distributed load that has a magnitude of 90. Due to symmetry only a quarter of the shell is modelled. The key result is the vertical displacement of the lateral side at the midpoint, denoted by u in the following diagram. The reference value is $u_{ref} = 0.3024$.

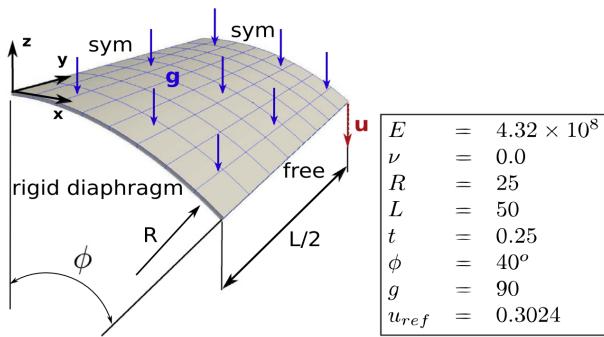


Figure 18 Problem definition of the Scordelis-Lo roof benchmark (source: [12])

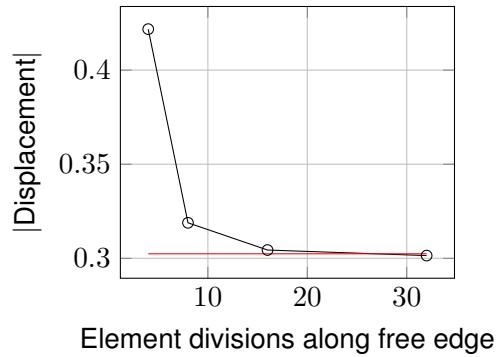


Figure 19 Element convergence for the Scordelis-Lo roof benchmark

The performance of the element is demonstrated in the convergence graph above. It is clear that the element agrees with the reference solution.

5.3.2. Pinched cylinder

The pinched cylinder considers a cylindrical shell fixed by rigid diaphragms at its axial ends. The loading consists of two opposing compressive point loads at the centre of the shell. Due to symmetry only an eighth of the shell is modelled. The key result is the vertical displacement under the point load, denoted by $\textcolor{red}{u}$ in the following diagram. The reference value is $u_{ref} = 1.8248 \times 10^{-5}$.

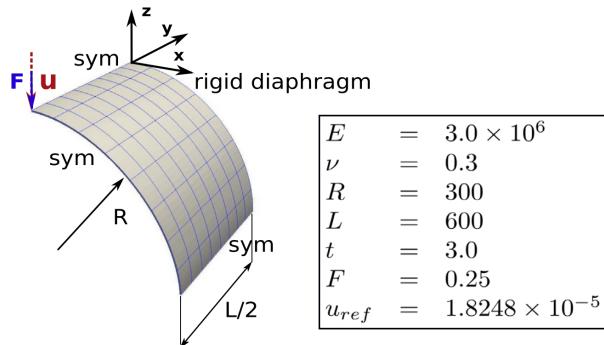


Figure 20 Problem definition of the pinched cylinder benchmark (source: [12])

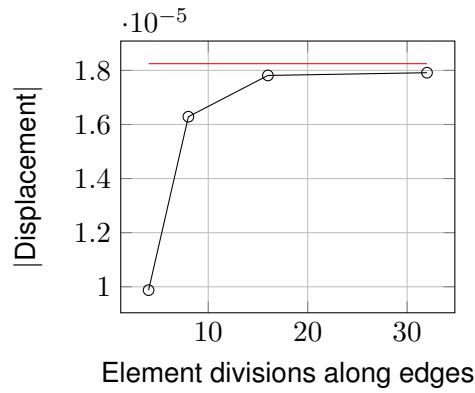


Figure 21 Element convergence for the pinched cylinder benchmark

The performance of the element is demonstrated in the convergence graph above. It is clear that the element agrees with the reference solution.

5.3.3. Pinched hemisphere

The pinched hemisphere considers a hemispherical shell loaded with opposing point loads along its equator. Due to symmetry only a quarter of the shell is modelled. The key result is the 'x' displacement along one of the point loads, denoted by $\textcolor{red}{u}$ in the following diagram. The reference value is $u_{ref} = 0.0924$.

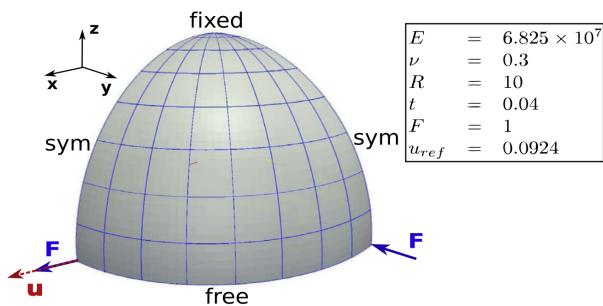


Figure 22 Problem definition of the pinched hemisphere benchmark (source: [12])

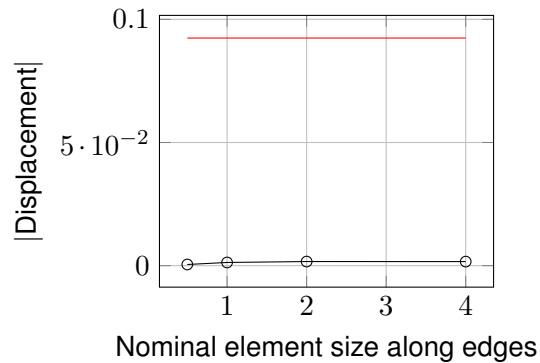


Figure 23 Element convergence for the pinched hemisphere benchmark

Contrary to the previous benchmarks, the element does not converge to the reference solution in the pinched hemisphere test. A key point to note is that the other benchmarks in the shell obstacle course employ a structured mesh, while the geometry of this test requires an unstructured mesh. Subsequent investigations of the element attempting to isolate remaining formulation issues have revealed the following phenomena:

- Membrane tests
 - ✗ Membrane tests with coarse structured meshes yield incorrect results
 - ✓ Membrane tests with fine structured meshes yield correct results
 - ✗ Membrane tests with unstructured meshes ranging from coarse to fine yield incorrect results
- Bending tests
 - ✓ Bending tests with structured meshes ranging from coarse to fine achieve correct results
 - ✗ Bending tests with unstructured meshes ranging from coarse to fine yield incorrect results

From the above statements, it can be concluded that: (1) the performance of the membrane formulation is dependent on mesh refinement, and (2) the element currently handles unstructured meshes incorrectly.

6. Benchmarking

Benchmarking yeah

6.1. Nonlinear benchmarks

asdfasdf

6.1.1. Hinged cylindrical roof

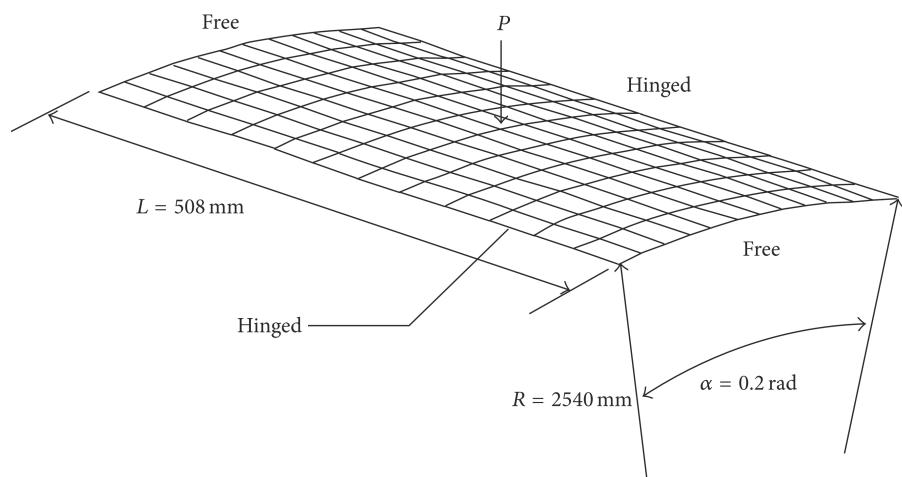


Figure 24 Problem definition of the hinged cylindrical roof benchmark [19]

asdfasdf

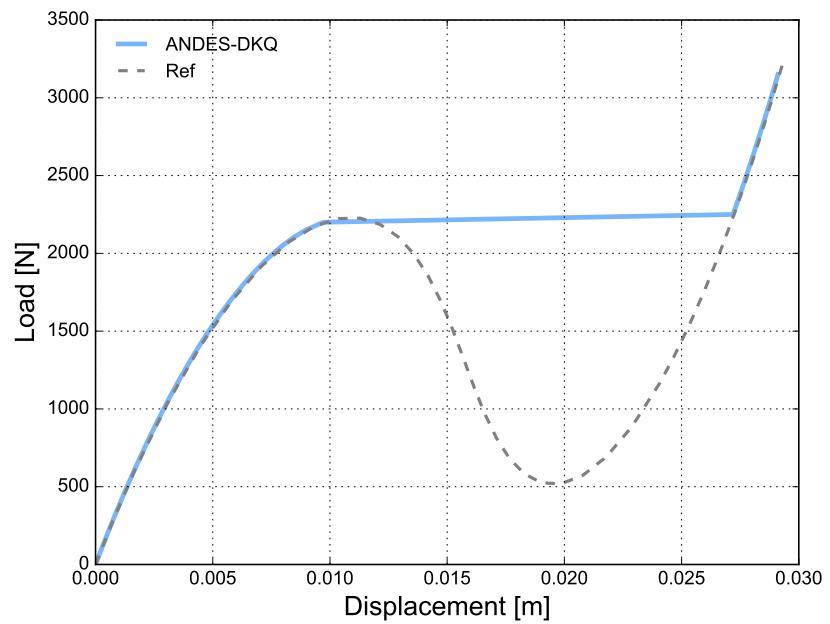


Figure 25 Dimensional reduction of a solid to a shell [7]

reference solution from [31]

sadf

7. Conclusions and Outlook

This work has considered the implementation of a thin quadrilateral shell element for the multiphysics code KRATOS. Section 1 covered the shell formulation, which is split into membrane and bending components. Following this, the element's implementation in KRATOS was presented, which covered key methods employed and the general workflow to calculate the element stiffness matrix. The element considered was subjected to the well known shell obstacle course in Section 3. Although the element correctly converged to the reference solution for the Scordelis-Lo roof and Pinched Cylinder problem, the Pinched Hemisphere benchmark revealed element deficiencies. These deficiencies were identified, with informed direction suggested for future work associated with improving this element.

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Declaration

I hereby declare that the thesis submitted is my own unaided work. All direct or indirect sources used are acknowledged as references. In addition, I declare that I make the present work available to the Chair of Structural Analysis for academic purposes and in this connection also approve of dissemination for academic purposes.

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