Coupled thermomechanical analysis using isoparametric curved shell elements

Análise termomecânica acoplada usando elementos de shell curvos isoparamétricos

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ABSTRACT
This study focuses on the coupled thermo-mechanical formulation in isoparametric shell elements and its implementation in curved laminar structures. The formulation is based on the direct isoparametric formulation, specifically designed for flat and curved shell elements, and relies on the theory of degenerated solids. The research provides a comprehensive description of the coupled thermo-mechanical analysis, including the mechanical equilibrium equations, the interrelations between stress, temperature, displacement, deformation, and the conservation of thermal energy. It adopts a simultaneous approach to addressing the impacts of temperature and mechanical loads. The paper elaborates on various numerical examples that substantiate the formulation. These examples include simulations that encompass linear scenarios, which are then compared to analytical solutions and results derived from other numerical software. The examples highlighted include one-dimensional temperature diffusion, radial diffusion, and the thermal behavior of a cylindrical cover and a pipe under a linear temperature gradient. These simulations demonstrate the formulation’s capacity to accurately capture the interactions between temperature variations and structural displacements. They
also confirm the alignment of the proposed model with existing analytical and numerical solutions. In conclusion, the research provides a good framework for coupled thermo-mechanical analysis. The flexibility of the formulation is evidenced across different configurations and scenarios, accommodating various types of boundary conditions such as constant and linear temperature fields, distributed loads, and constraints on displacements and rotations. It effectively manages temperature flows across one, two, and three dimensions, highlighting its extensive applicability in the realm of structural analysis. This versatility underscores its broad applicability in the field of structural analysis.

**Keywords:** Coupled Thermomechanical Analysis. Finite Elements. Shell Elements. Transient Analysis.

RESUMO
Este estudo foca na formulação termomecânica acoplada em elementos de casca isoparamétricos e sua implementação em estruturas laminares curvas. A formulação é baseada na formulação isoparamétrica direta, projetada especificamente para elementos de casca planos e curvos, e se apoia na teoria de sólidos degenerados. A pesquisa fornece uma descrição abrangente da análise termomecânica acoplada, incluindo as equações de equilíbrio mecânico, as inter-relações entre tensão, temperatura, deslocamento, deformação e a conservação da energia térmica. Adota-se uma abordagem simultânea para tratar os impactos da temperatura e das cargas mecânicas. O estudo detalha vários exemplos numéricos que fundamentam a formulação. Esses exemplos incluem simulações que abrangem cenários lineares, os quais são então comparados a soluções analíticas e resultados derivados de outros softwares numéricos. Os exemplos destacados incluem difusão de temperatura unidimensional, difusão radial e o comportamento térmico de uma cobertura cilíndrica e de um tubo sob um gradiente de temperatura linear. Essas simulações demonstram a capacidade da formulação em capturar precisamente as interações entre variações de temperatura e deslocamentos estruturais. As análises também confirmam a alinhamento do modelo proposto com soluções analíticas e numéricas existentes. Em conclusão, a pesquisa fornece uma boa estrutura para análise termomecânica acoplada. A flexibilidade da formulação é evidenciada em diferentes configurações e cenários, acomodando vários tipos de condições de contorno, como campos de temperatura constantes e lineares, cargas distribuídas e restrições em deslocamentos e rotações. A formulação gerencia efetivamente os fluxos de temperatura em uma, duas e três dimensões, destacando sua aplicabilidade extensiva no âmbito da análise estrutural. Essa versatilidade sublinha sua ampla aplicabilidade no campo da análise estrutural.


RESUMEN
Este estudio se enfoca en la formulación termomecánica acoplada a elementos de conchas isoparamétricas y su implementación en estructuras laminares curvas. La formulación se basa en la formulación isoparamétrica directa,
diseñada específicamente para elementos de conchas planas y curvas, y se basa en la teoría de sólidos degenerados. La investigación proporciona una descripción completa del análisis termomecánico acoplado, incluyendo las ecuaciones de equilibrio mecánico, las interrelaciones entre voltaje, temperatura, desplazamiento, deformación y conservación de energía térmica. Se adopta un enfoque simultáneo para abordar los impactos de la temperatura y las cargas mecánicas. El estudio detalla varios ejemplos numéricos que sustentan la formulación. Estos ejemplos incluyen simulaciones que cubren escenarios lineales, que luego se comparan con soluciones analíticas y resultados derivados de otro software numérico. Los ejemplos incluyen la difusión de temperatura unidimensional, la difusión radial y el comportamiento térmico de una cubierta cilíndrica y un tubo bajo un gradiente de temperatura lineal. Estas simulaciones demuestran la capacidad de la formulación para capturar con precisión las interacciones entre las variaciones de temperatura y los desplazamientos estructurales. Los análisis también confirman la alineación del modelo propuesto con las soluciones analíticas y numéricas existentes. En conclusión, la investigación proporciona un buen marco para el análisis termomecánico acoplado. La flexibilidad de la formulación se pone de manifiesto en diferentes configuraciones y escenarios, que dan cabida a diversos tipos de condiciones de frontera, como los campos de temperatura constante y lineal, las cargas distribuidas y las restricciones a los desplazamientos y las rotaciones. La formulación gestiona eficazmente los flujos de temperatura en una, dos y tres dimensiones, destacando su amplia aplicabilidad en el marco del análisis estructural. Esta versatilidad subraya su amplia aplicabilidad en el campo del análisis estructural.


**1 INTRODUCTION**

Laminar structures with curved designs, where the thickness is minimal compared to their other dimensions, are increasingly employed across various sectors today. These applications range from cylindrical shed roofs and domes to silos and wind turbine towers. Within the realm of finite element analysis, these structures are often modelled using shell elements, which are differentiated into thin or thick categories based on their application. What sets these structures apart is their ability to efficiently distribute loads, predominantly through in-plane forces known as membrane stresses. This load-balancing capability allows shell structures to cover large areas effectively, using as little material as possible.
In the context of shell elements, one of the most well-known element formulations is referred to as the degenerated element formulation (Bathe and Dvorkin (1983), Yuan and Liang (1989), Koziy and Mirza (1997), Bucalem and Nóbrega (2000)). This formulation represents an eight-node quadratic element as a simplified version of a quadratic hexahedron, although there are other versions. It is based on isoparametric elements and offers significant advantages, as it aligns perfectly with the traditional structure of finite elements, using the same shape functions for both geometry and displacement fields.

It is worth noting that existing works on isoparametric shell elements often present long formulations to express the finite element equations. These complex formulations can represent implementation challenges, especially for newcomers.

The formulations related to curved shell elements involve complexities arising from multiple factors specific to these elements. Notably, geometry is a crucial factor; the presence of curvature increases the complexity involved both in the geometric characterization and in the deformation analysis. Moreover, the conversion of displacements and rotations, which entails transitioning from a global to a local space through curved coordinate systems, adds an extra layer of difficulty to the process. Additionally, the dynamics between membrane and bending stresses heighten the complexity. These aspects are typically addressed individually, which significantly amplifies the overall complexity of the formulations.

One the other hand, the change of the temperature field results in thermal stresses. The influence of this variation on the governing thermoelastic equations is represented through the constitutive law, see e.g. Hetnarski and Eslami (2009). The theory of thermoelasticity is based on the linear addition of thermal strains to mechanical stresses.

The change in temperature may represent severe loading conditions, as they can produce excessive deflections and/or high stresses in structures. Furthermore, non-uniform temperature fields create temperature gradients between the upper and interior surfaces of shells, produce changes in curvature, and therefore, rotations (Szilard, 2004).
Rezaiee-Pajand et al. (2019) mention the importance of thermomechanical analysis in shell-type structures for the design of pressure vessels, storage silos, ship hulls, as the thermal effect in these structures increases deformations and stresses. Furthermore, thermal analyses can be used for different industrial applications, flares, and wind turbine towers.

It is also noted that the scarcity of detailed formulations covering shell finite elements with temperature coupling makes it difficult to implement custom computational routines for the study of more complex engineering structures. For example, it is observed the lack of details in the formulations of internal force matrices for energy balance and in the incremental integration process over time.

This work aims to explore the thermomechanical effects on shell-type metallic structures through the application of isoparametric elements. The versatility of these elements enables them to accommodate a variety of isoparametric surface shapes, such as 3 and 6-node triangles, and 4, 8, and 12-node quadrilaterals, among others. We developed and implemented a coupled thermomechanical formulation capable of accurately modeling both the thermal and mechanical effects in isoparametric shell elements. To facilitate this, the article is structured into the following sections: Section 2 discusses the coupled thermomechanical formulation for its application in both solid and shell elements. Section 3 provides an overview of the isoparametric formulation adopted for the shell element's implementation. Section 4 presents four examples to validate and compare the formulations proposed in this study. Finally, Section 5 showcases the conclusions derived from the results obtained in the simulated examples.

2 COUPLED THERMOMECHANICAL ANALYSIS

Coupled thermomechanical analysis is an approach that considers, simultaneously, the effects of temperature and mechanical loads on a system. This analysis investigates how temperature changes influence the mechanical behavior of a structure and vice versa. In summary, coupled thermomechanical analysis allows predicting the behavior of materials and structures under variable...
temperature and load conditions. The following is the mathematical derivation for the computational implementation of coupled thermomechanical analysis.

2.1 MECHANICAL EQUILIBRIUM

The mechanical equilibrium is defined by:

\[ \nabla \dot{\sigma} + \dot{b} = 0 \]  

(1)

Where:

\( \dot{\sigma} \) is the rate of tensor stress
\( \dot{b} \) is the rate of body forces.

After, applying the virtual work principle (VWP) to Eq. (1), we can get to:

\[ \int u^* (\dot{\sigma} \cdot n) dS - \int \nabla u^* \cdot \dot{\sigma} dV + \int u^* \cdot \dot{b} dV = 0 \]  

(2)

Where:

\( u^* \) is the vector of virtual displacements components,
\( n \) is the vector normal to the surface,
\( dS \) is the area differential
\( V \) is the volume.

2.2 STRESS, TEMPERATURE, DISPLACEMENT, AND STRAIN RELATIONS

The temperature in a point is expressed as:

\[ \theta = T - T_0 \]  

(3)

where:
The current temperature \( T \) is the initial temperature both in Kelvin.

Thus:

\[
\dot{\theta} = \dot{T}
\]  

(4)

On the other hand, the total stress tensor that takes into account thermal effects is expressed by:

\[
\bar{\sigma} = \bar{D} : \varepsilon - \beta \dot{\delta}
\]  

(5)

Where:

- \( \bar{D} \) is the constitutive tensor,
- \( \varepsilon \) is the strain tensor,
- \( \delta \) is delta de Kronecker
- “:\:“ represents the double contraction operator.

Furthermore, the thermal stress \( \beta \) for 3D strain is given by the following equation:

\[
\beta = \frac{E \alpha}{1 - 2v}
\]  

(6)

where:

- \( \alpha \) is thermal expansion coefficient of the material,
- \( E \) is the Young's modulus
- \( v \) is the Poisson's ratio.

Meanwhile \( \ddot{\sigma} \) is given by:

\[
\ddot{\sigma} = \ddot{D} : \varepsilon - \beta \ddot{\delta}
\]  

(7)
Using matrix notation, we can rewrite the Eq. (7) as:

$$\sigma = -\beta \theta m + D \epsilon$$

(8)

Where:

$$m^T = \langle 1, 1, 1, 0, 0, 0 \rangle$$. For the case of plane stresses $\beta$ and $m^T$ are defined, respectively, as follows:

$$\beta = \frac{E \alpha}{1 - \nu}$$

(9)

$$m^T = \langle 1, 1, 0, 0, 0, 0 \rangle$$

(10)

2.3 FINITE ELEMENTS IN THE MECHANICAL EQUILIBRIUM EQUATION

Applying the VWP and the element discretization to Eq. (2), we have:

$$\int U^* N \cdot t \, dS - \int U^* B^T (D \epsilon - \beta \theta m) \, dV + \int U^* N \cdot b \, dV = 0$$

(11)

Where:

$U^*$ is a vector of virtual displacements,
$N$ is the vector with shape functions,
$t$ is represents surface tractions and
$B$ is deformation-displacement matrix.

Discarding the virtual displacements and after some mathematical manipulations, we obtain:

$$\int B^T D B \, dV \dot{U} - \int B^T \beta m N^T \, dV \dot{\theta} = \int N \cdot b \, dV + \int N \cdot t \, dS$$

(12)
Where:

\[ \hat{\epsilon} = B \hat{U}, \sigma = D \hat{\epsilon}, \hat{\theta} = N^T \hat{\theta} \] and:

\[ K = \int B^T D B \, dV \quad (13) \]

\[ C = -\int B^T \beta m N^T \, dV \quad (14) \]

\[ F = \int N \cdot \hat{b} \, dV + \int N \cdot \hat{t} \, dS \quad (15) \]

### 2.4 THERMAL ENERGY CONSERVATION

The thermal energy conservation equation is described by:

\[ \nabla \cdot q + \rho c_v \hat{\theta} + T \beta \epsilon_v = 0 \quad (16) \]

Where:

\[ q = -k \nabla \theta \] is the heat flux given by Fourier’s law,
\[ k \] is the diagonal 3x3 thermal conductivity matrix,
\[ \rho \] is the material density,
\[ c_v \] is the specific heat
\[ \epsilon_v \] is the volumetric strain.

Since the temperature variation is small when compared to the absolute ambient temperature, \( T \) can be approximated by the constant \( T_0 \). Applying an approach analogous to the VWP Eq. (16) we get:

\[ \theta^* \nabla q = \nabla (\theta^* \cdot q) - \nabla \theta^* \cdot q \quad (17) \]

Integrating over the domain and substituting Fourier’s law we obtain:

\[ \int \theta^* q \cdot n \, dV + \int \nabla \theta^* (-k \nabla \theta) \, dV = \int \theta^* \rho c_v \hat{\theta} \, dV + \int \theta^* T_0 \beta (m \cdot \hat{\epsilon}) \, dV = 0 \quad (18) \]

Where:
\( q \cdot n = q_0 \) represents the heat flux normal the domain boundary.

2.5 FINITE ELEMENTS IN THE THERMAL ENERGY CONSERVATION EQUATION

Eq. (16) can be rewritten by applying the Finite Element Method as:

\[
\int \theta^T B_\theta^T \frac{k}{T_0} B_\theta \, dV \theta + \int \theta^T N \frac{\rho c_v}{T_0} N^T \, dV \dot{\theta} + \int \theta^T N \beta m^T B \, dV \dot{U} + \int \theta^T N \frac{\dot{q}_\theta}{T_0} dS = 0
\]

(19)

Once again discarding the virtual temperature increments:

\[
- \int B_\theta^T \frac{k}{T_0} B_\theta \, dV \theta - \int N \frac{\rho c_v}{T_0} N^T \, dV \dot{\theta} - \int N \beta m^T B \, dV \dot{U} = \int N \frac{\dot{q}_\theta}{T_0} dS
\]

(20)

Where:

\[
H = - \int B_\theta^T \frac{k}{T_0} B_\theta \, dV
\]

(21)

\[
M = - \int N \frac{\rho c_v}{T_0} N^T \, dV
\]

(22)

\[
L = - \int N \beta m^T B \, dV = C^\nu
\]

(23)

\[
F_\theta = \int N \frac{\dot{q}_\theta}{T_0} dS
\]

(24)

In turn, the thermal deformation-displacement matrix \( B_\theta \) is given by temperature gradient \( \nabla \theta \), which is defined by:

\[
\nabla \theta = \begin{bmatrix} \frac{\partial \theta}{\partial x'} \\ \frac{\partial \theta}{\partial y'} \end{bmatrix}
\]

(25)

where:
\[
\frac{\partial \theta}{\partial x'} = \sum \frac{\partial N_i}{\partial x'} \theta_i 
\]  
(26)

\[
\frac{\partial \theta}{\partial y'} = \sum \frac{\partial N_i}{\partial y'} \theta_i 
\]  
(27)

Using matrix notation:

\[
\begin{pmatrix}
\frac{\partial \theta}{\partial x'} \\
\frac{\partial \theta}{\partial y'} 
\end{pmatrix} =
\begin{bmatrix}
\frac{\partial N_1}{\partial x'} & \frac{\partial N_2}{\partial x'} & \frac{\partial N_3}{\partial x'} & \frac{\partial N_4}{\partial x'} \\
\frac{\partial N_1}{\partial y'} & \frac{\partial N_2}{\partial y'} & \frac{\partial N_3}{\partial y'} & \frac{\partial N_4}{\partial y'}
\end{bmatrix}
\begin{pmatrix}
\theta_1 \\
\theta_2 \\
\theta_3 \\
\theta_4 
\end{pmatrix} 
\]  
(28)

Finally, we have:

\[
\begin{pmatrix}
\frac{\partial \theta}{\partial x'} \\
\frac{\partial \theta}{\partial y'} 
\end{pmatrix} =
B_{\theta}
\begin{pmatrix}
\theta_1 \\
\theta_2 \\
\theta_3 \\
\theta_4 
\end{pmatrix} 
\]  
(29)

2.6 INTERNAL FORCES AND INTERNAL ENERGY

After solving the system of equations for each load increment, it is necessary to compute the internal forces to get the corresponding increment’s residue. For this purpose, the internal forces vector in an element is given by:

\[
F_{int} = \int B^T D B \dot{U} dV - \int B^T \beta mN^T \dot{\theta} dV 
\]  
(30)

After substituting Eqs. (13) into (15), Eq. (30) can be rewritten, as:

\[
F_{int} = \int B^T \Delta \sigma dV - \int B^T \beta m\Delta \theta dV 
\]  
(31)

The internal heat energy in an element is obtained by the following equation:
\[
F_{q_{\text{int}}} = \int B_0^T \frac{k}{t_0} B_0 \theta dV - \int N \frac{\rho c_v}{t_0} N^T \dot{\theta} dV - \int N \beta m^T B \dot{\theta} dV \tag{32}
\]

After some simplifications, the increment of the internal energy is given by:

\[
F_{q_{\text{int}}} = - \int B_\theta^T \frac{q}{t_0} dV - \int N \frac{\rho c_v}{t_0} \Delta \theta dV - \int N \beta \Delta \epsilon_{\text{vol}} dV \tag{33}
\]

### 2.7 TIME INTEGRATION

Considering an incremental analysis the mechanical equilibrium and energy conservation equations, can be joined as:

\[
\begin{bmatrix} K & C \\ L & M \end{bmatrix} \begin{bmatrix} \Delta U \\ \Delta \theta \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & H \end{bmatrix} \begin{bmatrix} U \\ \theta \end{bmatrix} = \begin{bmatrix} F \\ F_\theta \end{bmatrix} \tag{34}
\]

Using a finite difference approximation for the time integration, we get:

\[
\begin{bmatrix} U \\ \theta \end{bmatrix}_{t + f \Delta t} = \begin{bmatrix} U \\ \theta \end{bmatrix}_t + f \left\{ \frac{\Delta U}{\Delta \theta} \right\} \tag{35}
\]

Thus:

\[
\begin{bmatrix} \Delta U \\ \Delta \theta \end{bmatrix}_{t + f \Delta t} = \frac{1}{\Delta t} \begin{bmatrix} \Delta U \\ \Delta \theta \end{bmatrix} \tag{36}
\]

Substituting Eq. (36) into Eq. (35) and then into Eq. (34), the final system of equations for a coupled increment analysis is given by:

\[
\begin{bmatrix} K & C \\ L & M + f \Delta t H \end{bmatrix} \begin{bmatrix} \Delta U \\ \Delta \theta \end{bmatrix} = \begin{bmatrix} \Delta F \\ \Delta F_\theta \end{bmatrix} + \begin{bmatrix} 0 \\ \Delta t \dot{\theta} \end{bmatrix} \tag{37}
\]

The solution over the entire time interval of interest is obtained by incrementing time and successively solving the system in Eq. (37). For implicit
integration, \( f \) should be greater than or equal to 0.5 and it is often convenient to select \( f=1 \) (see Booker and Small, 1974).

### 3 DEGENERATED ISOPARAMETRIC SHELL FINITE ELEMENT

A shell element with its respective degrees of freedom in local and global coordinates can be illustrated as shown in Figure (1).

Figure 1 – Local and global coordinates for shell elements.

Furthermore, it is possible to illustrate the displacement field according to Figure (2):

Figure 2 – Displacement field for isoparametric shell.

Calculating the relative displacements as functions of the local rotations, we have:
\[ u_{r'} = \frac{t}{2} \zeta \begin{pmatrix} \theta_{y'} \\ -\theta_{x'} \\ 0 \end{pmatrix} \] (38)

where \( t \) is the thickness of the shell.

Then the displacement field for a shell element can be expressed by:

\[
\begin{bmatrix}
    u_{x'} \\
    u_{y'} \\
    u_{z'}
\end{bmatrix} = \sum_{i=1}^{n} N_i \begin{bmatrix}
    u_{x'i} \\
    u_{y'i} \\
    u_{z'i}
\end{bmatrix} + \sum_{i=1}^{n} N_i \frac{t}{2} \zeta \begin{bmatrix}
    \theta_{y'i} \\
    -\theta_{x'i} \\
    0
\end{bmatrix}
\] (39)

In turn, the strain vector is given by:

\[
\varepsilon = \begin{bmatrix}
    \varepsilon_{x'} \\
    \varepsilon_{y'} \\
    \varepsilon_{z'} \\
    2\varepsilon_{y'}\varepsilon_{z'} \\
    2\varepsilon_{z'}\varepsilon_{x'} \\
    2\varepsilon_{x'}\varepsilon_{y'}
\end{bmatrix}^T
\] (40)

Putting the previous equation in the local reference:

\[
\begin{bmatrix}
    \varepsilon_{x'} \\
    \varepsilon_{y'} \\
    \varepsilon_{z'} \\
    2\varepsilon_{y'}\varepsilon_{z'} \\
    2\varepsilon_{z'}\varepsilon_{x'} \\
    2\varepsilon_{x'}\varepsilon_{y'}
\end{bmatrix}^T = \bar{B} \begin{bmatrix}
    u_{x'1} \\
    u_{y'1} \\
    u_{z'1} \\
    u_{\theta_{y'1}} \\
    u_{\theta_{x'1}}
\end{bmatrix}
\] (41)

Assuming that \( \bar{B} \) is composed by submatrices related to each node, the submatrix \( \bar{B}_i \) corresponding to node \( i \) is written as:

\[
\bar{B}_i = \begin{bmatrix}
    \frac{\partial N_i}{\partial x'} & 0 & 0 & 0 & \frac{\partial N_i}{\partial x'} t/2 \\
    0 & \frac{\partial N_i}{\partial y'} & 0 & -\frac{\partial N_i}{\partial y'} t/2 \zeta & 0 \\
    0 & 0 & \frac{\partial N_i}{\partial y'} & 0 & 0 \\
    0 & 0 & N_i & -N_i & 0 \\
    \frac{\partial N_i}{\partial y'} & 0 & 0 & \frac{\partial N_i}{\partial y'} t/2 \zeta & \frac{\partial N_i}{\partial y'} t/2 \zeta \\
\end{bmatrix}
\] (42)
To express this matrix in global coordinates, the following transformation is necessary:

\[ B_i = \bar{B}_i R_{\theta i} \]  

(43)

where \( R_{\theta i} \) is a rotation matrix formed by the direct cosines and expressed as:

\[
R_{\theta i} = \begin{bmatrix}
 l_x & l_y & l_z & 0 & 0 & 0 \\
 m_x & m_y & m_z & 0 & 0 & 0 \\
 n_x & n_y & n_z & 0 & 0 & 0 \\
 0 & 0 & 0 & l_{xi} & l_{yi} & l_{zi} \\
 0 & 0 & 0 & m_{xi} & m_{yi} & m_{zi}
\end{bmatrix}
\]  

(44)

Finally, we have:

\[
\begin{bmatrix}
\varepsilon_{x}' \\
\varepsilon_{y}' \\
\varepsilon_{z}' \\
2\varepsilon_{y}'\varepsilon_{z}' \\
2\varepsilon_{z}'\varepsilon_{x}' \\
2\varepsilon_{x}'\varepsilon_{y}'
\end{bmatrix} = \begin{bmatrix}
u_{x1} \\
u_{y1} \\
u_{z1} \\
u_{\theta x1} \\
u_{\theta y1} \\
u_{\theta z1} \\
\vdots \\
u_{xn} \\
\theta_{xn} \\
\theta_{yn} \\
\theta_{zn}
\end{bmatrix} \begin{bmatrix}
 l_x & l_y & l_z & 0 & 0 & 0 \\
 m_x & m_y & m_z & 0 & 0 & 0 \\
 n_x & n_y & n_z & 0 & 0 & 0 \\
 0 & 0 & 0 & l_{xi} & l_{yi} & l_{zi} \\
 0 & 0 & 0 & m_{xi} & m_{yi} & m_{zi}
\end{bmatrix}
\]  

(45)

Once the strain matrix \( B \) is derived, one can use a conventional finite element procedure, such as the virtual work method, to arrive at a more conventional form for the stiffness matrix of the shell element:

\[ K = \int B^T S D B \, dV \]  

(46)
Where:

\[ D \] is the constitutive matrix for plane stress conditions, excluding the row and column related to \( \sigma_{z'} \).

\[ S \] is introduced to improve the prediction of shear distribution in out-of-plane directions (\( \sigma_{x'z'} \) and \( \sigma_{y'z'} \)).

Matrix \( S \) is explicitly given by:

\[
S = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & \alpha_s & 0 & 0 \\
0 & 0 & 0 & \alpha_s & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}
\] (47)

with \( \alpha_s = 5/6 \). The matrix \( D \) is represented by:

\[
D = \begin{bmatrix}
\frac{E}{1-\nu^2} & \frac{E\nu}{1-\nu^2} & 0 & 0 & 0 \\
\frac{E\nu}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 & 0 & 0 \\
0 & 0 & \frac{E}{2(1+\nu)} & 0 & 0 \\
0 & 0 & 0 & \frac{E}{2(1+\nu)} & 0 \\
0 & 0 & 0 & 0 & \frac{E}{2(1+\nu)}
\end{bmatrix}
\] (48)

The numerical integration is performed as follows, using at least two layers of integration points in the normal direction to the shell.

\[
K \approx \sum_{i=1}^{n_ip} B_i^T S D B_i w_i \det f_i
\] (49)

### 4 NUMERICAL SIMULATIONS

This section presents a set of numerical examples to validate the formulation introduced for coupled thermomechanical analysis in shell elements. The simulations cover linear scenarios, with results rigorously compared to
analytical and numerical findings in the literature. Examples 1 to 2 examine temperature flow and deformations, particularly under linear elastic conditions in unidirectional and radial directions, respectively. The other two examples are models with finite element software with different boundary conditions and compared with the implementation proposed in this work. It is essential to note that all implementations, numerical simulations, and the presentation of curves and meshes were performed using the Amaru finite element library (see, for example, Durand and Silva (2021) and Durand et al. (2021)) available at https://github.com/NumSoftware/Amaru.

4.1 ONE-DIMENSIONAL TEMPERATURE FLOW

The first analysis aims to validate the coupled thermomechanical formulation with shell and bulk elements applied to one-dimensional temperature flow. The example in question was previously investigated by Carter and Booker (1989) and involves a plate made of a thermoelastic material with length $h$. Initially, the plate is at an absolute temperature $T_0$. The base of the structure is rigid and thermally insulated, as illustrated in Figure (3).

Figure 3 - One-dimensional thermomechanical problem.
Source: Prepared by the authors themselves.
In this study, the following condition was adopted: starting from \( t > 0 \), a temperature of \( \theta_0 = 100^\circ C \) is applied to the free surface. Furthermore, Carter and Booker (1989) presented the analytical solution for the displacement in \( z \) direction and the temperature profile along the plate, applying the thermal stress \( \beta \) in case of plane strain, according to the following equations:

\[
\bar{\theta} = \left( \frac{\theta_0}{s} \right) \frac{\cosh(\mu z)}{\cosh(\mu h)} \quad (50)
\]

\[
\bar{w} = \left( \frac{\theta_0}{\mu s} \right) \left( \frac{\beta}{\chi} \right) \frac{\cosh(\mu z)}{\cosh(\mu h)} \quad (51)
\]

where:

\[
\mu = \sqrt{\frac{sA}{\kappa_tM}} \quad (52)
\]

In Eqs. (50) and (51), \( \bar{\theta} \) and \( \bar{w} \) are Laplace transforms with respect to the variable \( s \), \( A \) and \( M \) correspond to adiabatic and isothermal conditions, and \( \kappa_t \) is the diffusivity coefficient. For isothermal conditions, \( M \) is represented by:

\[
M = \frac{E(1-v)}{(1+v)(1-2v)} \quad (53)
\]

On the other, \( A \) is calculated by the following equation:

\[
A = M + \frac{\beta^2 T_0}{\rho c_v} \quad (54)
\]

Finally, \( \kappa_t \) is obtained through:

\[
\kappa_t = \frac{k}{\rho c_v} \quad (55)
\]
In addition to the exact solution, the authors presented the numerical response. For this, the structure was discretized according to Fig. (4). In this work we discretized the same domain using 8-node bulk and shell elements.

![Figure 4 - Mesh discretization. Adapted from Carter and Booker (1989).](image)

Additionally, the authors used the ratio $A/M = 2$. Based on this premise, this study adopted the following material characteristics: $E = 200\, GPa$, $\nu = 0.3$, $c_v = 118.35 \times 10^3 \, J/ton/K$, $k = 50.2 \, W/m/K$, $\rho = 6.0 \, ton/m^3$ and $\alpha = 5.0 \times 10^{-5} K^{-1}$. Finally, for the analysis performed using the Amaru library, the same mesh used previously was applied, and the results obtained for the temperature field will be presented in Figure (5).

![Figure 5 – Temperature field of the plate for $t = 13547.80$ seconds.](image)
Figures (6) and (7) provide a comparison between the results of the analysis conducted by Carter and Booker (1989), the implementation in Amaru, and the analytical solution for the temperature and displacement fields, respectively, captured at different time intervals, expressed through the relationship $\kappa t/h^2$, where $t$ is the time.

Figure 6 - Temperature isochrones for one-dimensional flow. Analytical vs. numerical responses.

Figure 7 - Comparison of vertical displacement of the free surface versus time. Analytical vs. numerical responses.

Source: Prepared by the authors themselves.
With this, it is noted that the implementation of coupled thermomechanical analysis through Amaru obtained significant results for the study of one-dimensional temperature flow and vertical displacements. Figs. (6) and (7) highlight the findings of the transient analysis, presenting various simulated scenarios at different time intervals (0.01, 0.1, 0.5 and 1.0 time factors) with shell and bulk elements. It is observed that the results using plane-strain were close to those found in the literature. Furthermore, to facilitate a comparison with the results obtained from the shell element, it was imperative to simulate the bulk element using plane-stress, leading to a convergence in findings between the two analyses. Thus, it is concluded that the methodology employed demonstrated effectiveness in this type of investigation.

4.2 RADIAL TEMPERATURE FLOW

Another example proposed by Carter and Booker (1989) is an infinitely long cylinder with uniform initial temperature $T_0$, subjected to radial thermal flow, illustrated in Figure (8).

Figure 8 – Thermomechanical problem in a cylinder.

Source: Prepared by the authors themselves.

The analysis involves applying a temperature $\theta_0$ to the surface $r = a$, aiming to verify the thermal diffusion inside the structure. The analytical solution is described by:
\[
\beta \bar{\theta} = 2(M - A)R + S I_0(\mu r) \quad (56)
\]

\[
\bar{u} \overline{r} = R + \left( \frac{S}{M} \right) \left( \frac{I_0(\mu r)}{\mu r} \right) \quad (57)
\]

where:

\[
R = \left( \frac{G}{M} \right) \left( \frac{I_0(\mu m)}{\mu a} \right);
\]

\[
S = (A - G)\Omega;
\]

\[
\Omega = \beta \bar{\theta}_0 / \left[ (A - G)I_0(\mu a) + 2(M - A) \left( \frac{G}{M} \right) \left( \frac{I_0(\mu a)}{\mu a} \right) \right].
\]

It is important to note that \( I_0 \) presents the modified Bessel function of the first kind and order zero, \( u \) corresponds to the radial displacement, and \( G \) denotes the shear modulus. In their study, the authors employed the ratio \( A/M = 1.75 \). For this purpose, this work adopted the following material properties: \( E = 200GPa \), \( \nu = 0.3 \), \( c_v = 140.79 \cdot 10^3 J/ton/K \), \( k = 50.2W/m/K \), \( \rho = 6.0ton/m^3 \), and \( \alpha = 5.0 \cdot 10^{-5}K^{-1} \). Carter and Booker (1989) provided the exact solution and a numerical solution, and for the latter, a specific mesh discretization was used as shown in Figure (9).
The following figures display the analytical responses and the numerical results from this work and Carter and Booker (1989) for temperatures and radial displacements, respectively, adopting a temperature $\theta_0 = 200 \, ^\circ C$, at different time intervals, expressed through the relationship $\kappa t / a^2$, where $t$ is the time.
When examining the results illustrated in Fig. (10), it is observed that the temperature values attained were, overall, consistent with the numerical analysis referenced in the literature and aligned with the theoretical response using plane-strain. In Fig. (11), a congruence was observed in the three analyzed methodologies, where radial displacements closely approximated the analytically predicted values. Additionally, both figures demonstrate the transient response...
to the problem at hand, indicating that the coupled formulation also provided satisfactory performance for temperature flow and radial displacements. When plane-stress is considered, the results for both, shell and solid elements presented excellent agreement.

4.3 CYLINDRICAL ROOF UNDER TEMPERATURE EFFECT

In this example a cylindrical roof is analyzed. This model was attributed to Scordelis and Lo, it is subjected to a uniformly distributed load $q = 620.53kN/m^3$ in the z-direction. This example was selected to examine the increase in displacement resulting from temperature application, compared to the solution from a pure static analysis. Additionally, three meshes, 14x20 (280 elements), 28x40 (1120 elements), and 42x60 (2520 elements), were used for comparative analysis.

The roof is supported by two rigid walls, as shown in the figure, where the displacements in the x and z axes are both zero. The thickness of the roof is 6.25 mm. Additionally, a temperature field of $400^\circ C$ was applied. The material properties are defined as follows: $E = 2978.5 \, GPa$, $\nu = 0$, $c_v = 439.20 J/kgK$, $k = 54.108 \, W/mK$, $\rho = 7800 kg/m^3$ and $\alpha = 1.2 \cdot 10^{-5} K^{-1}$.

Figure 13 - Scordelis-Lo roof with applied temperature field.

Source: Prepared by the authors themselves.
Through the results observed in Fig. (14), it was verified that the curves of the numerical modeling in this work and in Abaqus converged for node P in the same manner and direction, however, a finer mesh discretization was required for Abaqus.

![Figure 14 - Scordelis-Lo Roof - Vertical displacement of point p over time.](image)

Source: Prepared by the authors themselves.

To observe the displacement field of the deformed structure and the temperature field, Figures (15) and (16) of the 42x60 mesh analysis was presented, respectively.

![Figure 15 - Scordelis-Lo Roof - Deformed Structure.](image)

Source: Prepared by the authors themselves.
4.4 PIPE UNDER PRESCRIBED TEMPERATURE

This analysis discusses the von Mises stress field for a tube subjected to a temperature field at its right end, as illustrated in Fig. (17). The tube is fixed at both ends while a temperature of $u_t = 80 + 0.1t$ is applied to the right side of the structure, as shown in Fig. (18), where $t$ is the time varying from 0 to 1200 seconds. The geometric properties of the pipe include a length ($L$) of 150 mm, a radius ($r$) of 25.4 mm, and a thickness of 2 mm. Mechanical and material properties are characterized by Young’s modulus of 200 GPa, a Poisson’s ratio $\nu = 0$, a yield stress $f_y = 243$ MPa, $c_v = 439.20 J/kgK$, $k = 54.108 W/mK$, $\rho = 7800 kg/m^3$ and $\alpha = 1.2 \cdot 10^{-5}K^{-1}$.

**Figure 16** - Scordelis-Lo Roof – Temperature field.

Source: Prepared by the authors themselves.

**Figure 17** – Pipe under prescribed temperature.

Source: Prepared by the authors themselves.
Figure (19) presents the von Mises stress $\sigma_{VM}$ distribution along the length $L$ of the tube using isoparametric Quad8 shell elements compared to the results obtained using solid Hex20 elements. Good agreement is observed for the stress field along the entire structure, except at the right end of the tube. Meanwhile, Fig. (20) displays the deformed mesh depicting the von Mises stress field. It can be observed that the maximum stress is located near the end where the temperature is applied.
Next, Figure (21) shows a comparison of the temperature along the length of the pipe, using Quad8 shell elements and Hex20 solid elements. An excellent agreement is observed. Furthermore, it is noted that at the left end the temperature reaches approximately 125 °C, while at the right end this value increases to 200 °C. Finally, Fig. (22) shows the temperature field for whole pipe with excellent agreement using shell and solid elements.

Source: Prepared by the authors themselves.
5 CONCLUSIONS

This research presents a coupled thermo-mechanical formulation applied to isoparametric shell elements through a series of numerical examples. The results demonstrate that this formulation efficiently captured the interaction between temperature and displacement in shell analysis. To assess the effectiveness of this method, we initially compared the outcomes with analytical solutions for plane strain, examining one-dimensional and radial temperature flows. The results were compared with analytical results when available. Also, the results obtained from shell elements were compared with numerical results using bulk solid elements under plane stress conditions the finite element software Abaqus.

For example, the comparative analysis with Hex20 solid elements with Abaqus, using an identical finite element configuration and the same discretization, indicated significant agreement in the results, both for stationary and transient analyses. Finally, a tube subjected to temperature loads is presented. It is found that coupled thermomechanical analysis converged to good results using Quad8 shell elements and Hex20 solid elements in terms of von Mises stress and temperature fields.

In conclusion, the methodology developed through this study proves to be a solid tool for coupled thermo-mechanical analysis. Its flexibility is demonstrated across various configurations and scenarios, accommodating different types of
boundary conditions (constant and linear temperature fields, distributed loads and restrictions on displacements and rotations), and handling temperature flows in one, two, and three dimensions. This versatility underscores its broad applicability in the field of structural analysis, both in academia for structural design courses and in the professional market. The study does have some limitations; for instance, it only addresses static and linear analysis. Therefore, as recommendations for future work, it is suggested to incorporate geometric nonlinearity to assess large displacements and structural instability, as well as dynamic analysis for studying seismic activities, wind loads, and other dynamic forces.

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