Two Finite Element Approximations of Nagdhi’s Shell Model in Cartesian Coordinates

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Abstract

We present a penalized version of Nagdhi’s model and a mixed formulation of the same model, in Cartesian coordinates for linearly elastic shells with little regularity, and finite element approximations thereof. Numerical tests are given that validate and illustrate our approach.

Résumé


1 Introduction

The purpose of this work is to approximate the solution of a formulation of Nagdhi’s shell model in Cartesian coordinates that is appropriate for linearly elastic shells that present curvature discontinuities. Our intent is to use finite elements of class $C^0$ and implement the approximation scheme as simply as possible using the general purpose, open source, 2D finite element package FreeFem++ (http://www.freefem.org).

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The formulation of Naghdi’s model used here was introduced in Blouza [6] and Blouza and Le Dret [8]. This formulation is based on the idea of using a local basis-free formulation in which the unknowns are described in Cartesian coordinates instead of with covariant or contravariant components as is usually done in shell theory, see for example [5]. This formulation is able to accommodate shells with a $W^{2,\infty}$-mid-surface, thus allowing for curvature discontinuities, as opposed to $C^3$ in the classical formalism, and makes for much simpler expressions. Even though it was proven to be well-posed and to be the natural limit of the classical formulation when a sequence of regular midsurfaces converges to a $W^{2,\infty}$-mid-surface in [8], the new formulation has not been used in a numerical setting to the best of our knowledge.

The literature on finite element approximation of two-dimensional shell models is huge. Let us just mention a few different approaches. Concerning conforming methods, the Ganev and Argyris triangles provide $P_4$ and $P_5$ interpolation with high order convergence in $O(h^4)$ when the solution is smooth enough. These elements were used for example to study the linear Koiter model for a $C^3$-shell in the classical covariant formulation, see [3]. This method was applied to approximate geometrically exact shell models in [11]. The Argyris element was also used in [16] for the numerical analysis of Koiter’s model for shells with little regularity in the Cartesian formulation proposed in [7]. Let us also mention the 3D shell element approach, see [12].

Still in the context of shells with little regularity, a non conforming DKT element was used in [17] to approximate a Koiter model similar to the one introduced in [7].

This article is organized as follows. We first briefly recall the geometry of the mid-surface and Naghdi shell formulation given in [6] and [8]. This formulation involves the infinitesimal rotation vector, a vector unknown that is tangent to the mid-surface. Such tangency cannot be implemented in a conforming way in finite element spaces (a problem that does not occur in the classical covariant formulation).

Therefore, in section 3, we introduce a penalized version of Naghdi’s model intended to approximate the above mentioned tangency. We prove the existence and uniqueness of the solution of the penalized model and establish its convergence to the solution of the original Naghdi problem when the penalization parameter tends to 0.

In section 4, we present a mixed formulation of Naghdi’s model in which the tangency condition is enforced by a Lagrange multiplier. We prove that the inf-sup condition is satisfied and that the mixed problem is well-posed and solves the original Naghdi problem.

Section 5 is devoted to the finite element discretization of both formulations. The numerical analysis of the penalized version is rather standard. On the con-
trary, the discrete inf-sup condition for the mixed formulation does not follow from usual arguments, in the sense of those found in the discussion of approximations of the Stokes problem for instance.

Finally, we present a few numerical tests in section 5. The method was implemented in FreeFem++, a high level, free software package that manages mesh generation and adaption, matrix assembly and linear system resolution automatically, and only requires as input the resolution domain, boundary conditions and bilinear and linear forms. Since FreeFem++ has macro expansion capabilities, the only input required from the user is the definition of the covariant vectors and of the partial derivatives of the normal vector as FreeFem++ functions. All the other geometrical and mechanical quantities are code-generated. We present results for the standard hyperbolic paraboloid benchmark and for the planar-cylindrical $W^{2,\infty}$ shell considered in [16]. We also show results for a $W^{2,\infty}$ roof constructed on a basket-handle arch profile.

2 Notation

Greek indices and exponents take their values in the set $\{1,2\}$ and Latin indices and exponents take their values in the set $\{1,2,3\}$. Unless otherwise specified, the summation convention for indices and exponents is assumed.

Let $(e_1, e_2, e_3)$ be the canonical orthonormal basis of the Euclidean space $\mathbb{R}^3$. We note $u \cdot v$ the inner product of $\mathbb{R}^3$, $|u| = \sqrt{u \cdot u}$ the associated Euclidean norm and $u \wedge v$ the vector product of $u$ and $v$.

Let $\omega$ be a domain of $\mathbb{R}^2$. We consider a shell whose midsurface is given by $S = \varphi(\bar{\omega})$ where $\varphi \in W^{2,\infty}(\omega; \mathbb{R}^3)$ is one-to-one mapping such that the two vectors

$$a_\alpha = \partial_\alpha \varphi$$

are linearly independent at each point $x \in \bar{\omega}$. We let

$$a_3 = \frac{a_1 \wedge a_2}{|a_1 \wedge a_2|}$$

be the unit normal vector on the midsurface at point $\varphi(x)$. The vectors $a_i$ define the local covariant basis at point $\varphi(x)$. The contravariant basis $a^i$ is defined by the relations $a_i \cdot a^j = \delta^j_i$ where $\delta^j_i$ is the Kronecker symbol. In particular $a_3(x) = a^3(x)$. Note that all these vectors are of class $W^{1,\infty}$. We let $a(x) = |a_1(x) \wedge a_2(x)|^2$ so that $\sqrt{a(x)}$ is the area element of the midsurface in the chart $\varphi$.

The first fundamental form of the surface is given in covariant components by

$$a_{\alpha\beta} = a_\alpha \cdot a_\beta.$$
Let \( u \in H^1(\omega; \mathbb{R}^3) \) be a midsurface displacement and \( r \in H^1(\omega; \mathbb{R}^3) \) a rotation of the normal vector (which is related to the actual infinitesimal rotation vector, see formula (15) below), i.e., \( H^1 \)-regular mappings from \( \omega \) into \( \mathbb{R}^3 \) such that \( r \) is tangent to the midsurface, given in covariant and Cartesian components by

\[
  u(x) = u_i(x) a^i(x) = u_i^c(x) e_i, \quad \text{where} \quad u_i = u \cdot a_i \quad \text{and} \quad u_i^c = u \cdot e_i,
\]

and

\[
  r(x) = r_\alpha(x) a^\alpha(x) = r_i^c(x) e_i \quad \text{with the same meaning.}
\]

Note that the tangency requirement is easily expressed in covariant coordinates, as it simply reads \( r_3 = 0 \), whereas it becomes

\[
  r_i^c(x) a^c_{3,i}(x) = 0 \quad \text{in} \quad \omega, \quad (1)
\]

in Cartesian coordinates.

Let \( a^{\alpha \beta \rho \sigma} \in L^\infty(\omega) \) be the elasticity tensor, which we assume to satisfy the usual symmetries and to be uniformly strictly positive. In the case of homogeneous, isotropic material with Young modulus \( E > 0 \) and Poisson coefficient \( 0 \leq \nu < 1/2 \), we have

\[
  a^{\alpha \beta \rho \sigma} = \frac{E}{2(1 + \nu)} (a^{\alpha \rho} a^{\beta \sigma} + a^{\alpha \sigma} a^{\beta \rho}) + \frac{E \nu}{1 - \nu^2} a^{\alpha \beta} a^{\rho \sigma},
\]

where \( a^{\alpha \beta} = a^\alpha \cdot a^\beta \) are the contravariant components of the first fundamental form. In this context, the covariant components of the change of metric tensor read

\[
  \gamma_{\alpha \beta}(u) = \frac{1}{2} (\partial_{\alpha} u \cdot a_\beta + \partial_\beta u \cdot a_\alpha), \quad (2)
\]

the covariant components of the change of transverse shear tensor read

\[
  \delta_{\alpha 3}(u, r) = \frac{1}{2} (\partial_{\alpha} u \cdot a_3 + r \cdot a_\alpha), \quad (3)
\]

and the covariant components of the change of curvature tensor read

\[
  \chi_{\alpha \beta}(u, r) = \frac{1}{2} (\partial_{\alpha} u \cdot \partial_\beta a_3 + \partial_\beta u \cdot \partial_{\alpha} a_3 + \partial_{\alpha} r \cdot a_\beta + \partial_\beta r \cdot a_\alpha). \quad (4)
\]

see [6] and [8]. Note that all these quantities make sense for shells with little regularity, and are easily expressed with the Cartesian coordinates of the unknowns and geometrical data. For instance, we have

\[
  \partial_{\alpha} u \cdot a_\beta = \partial_{\alpha} u^c_i a_{\beta,i} \quad \text{and} \quad \text{so on.}
\]
We assume that the boundary $\partial \omega$ of the chart domain is divided into two parts: $\gamma_0$ of strictly positive 1-dimensional measure on which the shell is clamped and a complementary part $\gamma_1$ on which the shell is subjected to applied tractions and moments.

Let us consider the function space, introduced in [6] and [8], which is appropriate in the context of shells with little regularity

$$\mathcal{V} = \left\{ (v, s) \in H^1(\omega; \mathbb{R}^3)^2; \ s \cdot a_3 = 0 \text{ in } \omega, v = s = 0 \text{ on } \gamma_0 \right\}. \quad (5)$$

This space is endowed with the natural Hilbert norm

$$\| (v, s) \|_\mathcal{V} = \left( \| v \|_{H^1(\omega; \mathbb{R}^3)}^2 + \| s \|_{H^1(\omega; \mathbb{R}^3)}^2 \right)^{1/2}. \quad (6)$$

The boundary conditions considered are hard clamping conditions on part of the boundary. Soft clamping, or simple support conditions correspond to $v = 0$ on $\gamma_0$. These conditions also work provided that $\varphi(\gamma_0)$ is not included in a straight line, see [8].

Let us now recall the problem formulation and the existence and uniqueness result in the space $\mathcal{V}$ for the linear Nagdhi model for shells with little regularity.

**Theorem 2.1** Let $f \in L^2(\omega; \mathbb{R}^3)$ be a given resultant force density, $N \in L^2(\gamma_1; \mathbb{R}^3)$ an applied traction density, $M \in L^2(\gamma_1, \mathbb{R}^3)$ an applied moment density such that $M \cdot a_3 = 0$ almost everywhere on $\gamma_1$, and $e > 0$ the thickness of the shell. Then there exists a unique solution to the following problem: Find $(u, r) \in \mathcal{V}$ such that

$$\forall (v, s) \in \mathcal{V}, \ a((u, r); (v, s)) = L((v, s)), \quad (7)$$

where

$$a((u, r); (v, s)) = \int_\omega \left\{ e a^{\alpha\beta\rho\sigma} \left[ \gamma_{\alpha\beta}(u) \gamma_{\rho\sigma}(v) + \frac{e^2}{12} \chi_{\alpha\beta}(u, r) \chi_{\rho\sigma}(v, s) \right] + e \frac{E}{1 + v} a^{\alpha\beta} \delta_{\alpha3}(u, r) \delta_{\beta3}(v, s) \right\} \sqrt{a} \, dx \quad (8)$$

and

$$L((v, s)) = \int_\omega f \cdot v \sqrt{a} \, dx + \int_{\gamma_1} (N \cdot v + M \cdot s) \, d\gamma. \quad (9)$$

**Proof.** See [6] and [8].

Here and in the sequel, we make use of the following notational device: arguments in a bilinear form are separated by a semicolon, whereas members of a couple are separated by a comma. This will help keep track of who does what, since our bilinear forms often apply to couples.
3 A penalized version of Nagdhi’s model

The purpose of the present work is to approximate the solution of equation (7) with a finite element method and to proceed in the simplest possible way (note that we do not concern ourselves with locking in the present paper, in this respect see [2], [13]). As the solution is in \( H^1 \), \( C^0 \)-Lagrange \( P_1 \) elements should be sufficient. However, we immediately encounter a problem since the tangency constraint \( s \cdot a_3 = 0 \) in \( \omega \) clearly cannot be implemented in a conforming way for a general shell.

We thus introduce a penalized Naghdi problem in which the unknowns still are the displacement \( u \) and rotation \( r \), elements of the space \( H^1(\omega; \mathbb{R}^3) \) without any orthogonality constraint on \( r \).

Let us introduce the relaxed function space

\[
X = \{(v, s) \in H^1(\omega; \mathbb{R}^3)^2; v = s = 0 \text{ on } \gamma_0\}
\] (10)

and equip it with the standard \( H^1 \) norm.

**Theorem 3.1** Let \( p \in \mathbb{R} \) such that \( 0 < p \leq 1 \). Let \( f \in L^2(\omega; \mathbb{R}^3) \), \( N \in L^2(\gamma_1; \mathbb{R}^3) \) and \( M \in L^2(\gamma_1, \mathbb{R}^3) \). Then there exists a unique solution to the following problem:

Find \((u_p, r_p) \in X\) such that

\[
\forall (v, s) \in X, \quad a((u_p, r_p); (v, s)) + \frac{1}{p} b(r_p \cdot a_3; s \cdot a_3) = L((v, s)),
\] (11)

where

\[
b(\lambda; \mu) = \int_\omega \partial_\lambda \lambda \partial_\mu \mu dx.
\] (12)

The proof is based on the following version of the infinitesimal rigid displacement lemma.

**Lemma 3.2** Let \((u, r) \in H^1(\omega; \mathbb{R}^3)^2\) and assume that \( \varphi \in W^{2, \infty}(\omega; \mathbb{R}^3) \).

i) If \( \gamma_{a\beta}(u) = 0 \), then there exists \( \psi \in L^2(\omega; \mathbb{R}^3) \) such that \( \partial_\alpha \mu = \psi \wedge a_\alpha \).

ii) If \( \delta_{a3}(u, r) = 0 \), then \( \partial_\alpha u \cdot a_3 = -r \cdot a_\alpha \in H^1(\omega) \).

iii) If, in addition to i) and ii), \( \chi_{a\beta}(u, r) = 0 \), then \( \psi \) is a constant vector in \( \mathbb{R}^3 \) and there exists \( c \in \mathbb{R}^3 \) such that

\[
u(x) = c + \psi \wedge \varphi(x),
\] (13)

and

\[
r(x) = \psi \wedge a_3(x) + (r(x) \cdot a_3(x))a_3(x).
\] (14)

**Proof.** The argument is exactly the same as in [8], except that we do not assume \( r \cdot a_3 = 0 \), hence the extra term in formula (14). \( \square \)
Remarks. 1) Note that the infinitesimal rotation vector $\psi$ is given by

$$
\psi = \varepsilon^{\alpha\beta}(\partial^\beta u \cdot a_3)a_\alpha + \varepsilon^{\alpha\beta}(\partial^\alpha u \cdot a_\beta)a_3
$$

where $\varepsilon^{11} = \varepsilon^{22} = 0$ and $\varepsilon^{12} = -\varepsilon^{21} = 1/|a_1 \wedge a_2|$.  

2) If $(v, s) \in \mathcal{X}$ are such that (13) and (14) are verified, then we have

$$
u = 0 \text{ and } r = (r \cdot a_3)a_3 \text{ a.e. in } \omega,$$

due to the boundary conditions.

We now are in a position to prove the ellipticity of the penalized bilinear form.

**Lemma 3.3** The bilinear form in (11) is $\mathcal{X}$-elliptic, uniformly with respect to $p$ for $0 < p \leq 1$.

**Proof.** The proof follows lines similar to those found in [8]. We nonetheless include it for the reader’s convenience. Let us set

$$
\|\| (v, s) \|\| = \left\{ \sum_{\alpha, \beta} \| \gamma_{\alpha\beta}(v) \|_{L^2}^2 + \| \chi_{\alpha\beta}(v, s) \|_{L^2}^2 + \sum_{\alpha} \| \delta_{\alpha 3}(v, s) \|_{L^2}^2 + \sum_{\alpha} \| \partial_{\alpha}(s \cdot a_3) \|_{L^2}^2 \right\}^{1/2}.
$$

As $p \leq 1$ and due to the positive definiteness of the elasticity tensor, there exists a constant $C > 0$ such that

$$
a((v, s); (v, s)) + \frac{1}{p} b(s \cdot a_3; s \cdot a_3) \geq C \|\| (v, s) \|\|^2.
$$

It thus suffices to prove that $\|\cdot\|$ is a norm equivalent to $\|\cdot\|_\mathcal{X}$. We use the standard contradiction argument. Let us thus suppose that there exists a sequence $(v_n, s_n) \in \mathcal{X}$ such that $\|\| (v_n, s_n) \|\|_\mathcal{X} = 1$ but $\|\| (v_n, s_n) \|\| \to 0$ when $n \to 0$. There exists a subsequence, still denoted $(v_n, s_n)$, and $(v, s) \in \mathcal{X}$ such that

$$
(v_n, s_n) \rightharpoonup (v, s), \gamma_{\alpha\beta}(v_n) \rightharpoonup \gamma_{\alpha\beta}(v), \chi_{\alpha\beta}(v_n, s_n) \rightharpoonup \chi_{\alpha\beta}(v, s),
$$

$$
\delta_{\alpha 3}(v_n, s_n) \rightharpoonup \delta_{\alpha 3}(v, s) \text{ and } \partial_{\alpha}(s_n \cdot a_3) \rightharpoonup \partial_{\alpha}(s \cdot a_3),
$$

weakly in their respective spaces. By Rellich’s theorem, we have

$$
(v_n, s_n) \to (v, s) \text{ strongly in } L^2(\omega; \mathbb{R}^3)^2.
$$
On the other hand, we have assumed that \( \| (v_n, s_n) \| \to 0 \) which implies that
\[
\gamma_{\alpha\beta}(v_n) \to 0, \chi_{\alpha\beta}(v_n, s_n) \to 0, \delta_{\alpha3}(v_n, s_n) \to 0 \quad \text{and} \quad \partial_\alpha (s_n \cdot a_3) \to 0
\] strongly in \( L^2(\omega) \). Therefore, we have
\[
\gamma_{\alpha\beta}(v) = \chi_{\alpha\beta}(v, s) = \delta_{\alpha3}(v, s) = \partial_\alpha (s \cdot a_3) = 0.
\]
By the infinitesimal rigid displacement lemma 3.2 and the boundary conditions, we first conclude that \( v = \psi = 0 \), see [8] for the details. Moreover, the Poincaré inequality and the boundary conditions applied to \( s \cdot a_3 \) imply that \( s \cdot a_3 = 0 \). The second part of lemma 3.2 then shows that \( s = 0 \) as well.

Let us now introduce the two-dimensional vector \( (w_n)_{\alpha} = v_n \cdot a_{\alpha} \). We have, \( w_n \to 0 \) in \( L^2(\omega; \mathbb{R}^2) \) strongly. Let us define \( 2e_{\alpha\beta}(w) = \partial_\alpha w_\beta + \partial_\beta w_\alpha \). It is easy to see that
\[
e_{\alpha\beta}(w_n) = \gamma_{\alpha\beta}(v_n) + \frac{1}{2} v_n \cdot (\partial_\beta a_\alpha + \partial_\alpha a_\beta) \to 0 \quad \text{strongly in } L^2(\omega).
\]
Then, by (17) and the two-dimensional Korn inequality, we deduce that
\[
w_n \to 0 \quad \text{strongly in } H^1(\omega; \mathbb{R}^2).
\]
Next we note that
\[
\partial_\rho v_n \cdot a_\alpha = \partial_\rho ((w_n)_{\alpha}) - v_n \cdot \partial_\rho a_\alpha \to 0 \quad \text{strongly in } L^2(\omega). \quad (18)
\]
Moreover, as \( s_n \to 0 \) strongly in \( L^2(\omega; \mathbb{R}^3) \), and \( \partial_\rho v_n \cdot a_3 = 2\delta_{\rho3}(v_n, s_n) - s_n \cdot a_\alpha \), we already know by (17) that
\[
\partial_\rho v_n \cdot a_3 \to 0 \quad \text{strongly in } L^2(\omega). \quad (19)
\]
We deduce that
\[
\partial_\rho v_n = (\partial_\rho v_n \cdot a_k) a_k \to 0 \quad \text{strongly in } L^2(\omega; \mathbb{R}^3),
\] by (18) and (19). It follows that \( v_n \to 0 \) strongly in \( H^1(\omega; \mathbb{R}^3) \).

Next, let \( (w'_n)_{\alpha} = s_n \cdot a_\alpha \). Clearly, \( w'_n \to 0 \) strongly in \( L^2(\omega, \mathbb{R}^2) \). On the other hand, since
\[
2e_{\alpha\beta}(w'_n) = 2\chi_{\alpha\beta}(v_n, s_n) - (\partial_\alpha v_n \cdot \partial_\beta a_3 + \partial_\beta v_n \cdot \partial_\alpha a_3) + s_n \cdot (\partial_\alpha a_\beta + \partial_\beta a_\alpha),
\]
we see by (17) that
\[
e_{\alpha\beta}(w'_n) \to 0 \quad \text{strongly in } L^2(\omega).
\]
Thus, again by the two-dimensional Korn inequality, we conclude that
\[ w_n' \rightharpoonup 0 \text{ strongly in } H^1(\omega; \mathbb{R}^2). \]
Moreover, the Poincaré inequality and the last convergence in (17) imply that
\[ s_n \cdot a_3 \rightharpoonup 0 \text{ strongly in } H^1(\omega). \]
Consequently, since 
\[ s_n = (s_n \cdot a_i) a_i, \]
it follows that 
\[ s_n \rightarrow 0 \text{ strongly in } H^1(\omega; \mathbb{R}^3). \]
Combining now the convergence of \( v_n \) and \( s_n \), we see that \( \| (v_n, s_n) \|_X \rightarrow 0 \), which contradicts the hypothesis and proves the lemma.

Proof of Theorem 3.1. Apply the Lax-Milgram lemma.

Remark. It is important to note that the original bilinear form \( a \) is not \( X \)-elliptic, indeed it does not even define a norm on the relaxed space. It is therefore necessary to add such terms as the extra terms \( \| \partial_\alpha (s \cdot a_3) \|_{L^2}^2 \) to recover ellipticity over the larger space. In the case of soft clamping, these extra terms are not sufficient, since \( (0, a_3) \) still belongs to the kernel of the penalized bilinear form. In this case, one should add the full \( H^1 \) norm of \( s \cdot a_3 \), i.e., use a penalization term of the form 
\[ b(r \cdot a_3; s \cdot a_3) = \int_\omega [(r \cdot a_3)(s \cdot a_3) + \partial_\alpha (r \cdot a_3)\partial_\alpha (s \cdot a_3)] \, dx. \]

It is now fairly classical that the penalization provides an approximation of the constrained problem.

Theorem 3.4 Let \( U = (u, r) \) and \( U_p = (u_p, r_p) \) respectively be the unique solutions of problems (7) and (11). Then
\[ \| r_p \cdot a_3 \|_{H^1(\omega)} \leq C_p, \] (20)
and
\[ \| U_p - U \|_X \leq C_p. \] (21)

Proof. Let \( L = L^2(\omega; \mathbb{R}^2) \) and \( \Psi: X \rightarrow L \) defined by \( U \mapsto \nabla (r \cdot a_3) \). Now, we have \( \mathcal{V} = \ker \Psi \) and \( b(r \cdot a_3; r \cdot a_3) = \langle \Psi(U), \Psi(U) \rangle_L \). It is known that if \( \Psi \) has closed range, then the following estimates hold true, [18],
\[ b(r_p \cdot a_3; r_p \cdot a_3) \leq C p^2 \text{ and } \| U_p - U \|_X \leq C p. \]
The first estimate gives estimate (20) and the second estimate is precisely estimate (21).

Let us thus check that \( \Psi \) has closed range. Let us consider a sequence \( U_n \in X \) such that \( \Psi(U_n) \rightarrow Z \) in \( L \). By the Poincaré inequality, it follows that \( r_n \cdot a_3 \) is bounded in \( H^1(\omega) \) and we can extract a weakly convergent subsequence such that \( r_n \cdot a_3 \rightharpoonup \zeta \) in \( H^1(\omega) \). Moreover, since \( r_n \cdot a_3 = 0 \) on \( \gamma_0 \) in the sense of traces, it follows that \( \zeta = 0 \) on \( \gamma_0 \) as well. In addition, clearly \( Z = \nabla \zeta \). We thus set \( U = (0, \zeta a_3) \in X \) and we see that \( \Psi(U) = Z \). □
Remark. Since we are aiming for simplicity of implementation, we have made no attempt to make the penalization term intrinsic. In fact, it does depend on the chart, whereas the other terms do not. This could arguably be considered to be a poor choice, especially if a chart was used that gave much more weight to one part of the shell compared to the rest. An intrinsic choice that obviously works is
\[ b'(r \cdot a_3; s \cdot a_3) = \int_{\omega} a^{\alpha \beta} \partial_\alpha (r \cdot a_3) \partial_\beta (s \cdot a_3) \sqrt{a} \, dx. \]
This penalization term has the same properties as our simple penalization term and does not suffer from the above mentioned drawback.

4 A mixed formulation of Naghdi’s model

Another way of imposing a constraint in a variational problem is to use a mixed formulation. We follow this route in this section. Naturally, mixed formulations for Naghdi’s model already exist of the displacement/stress type, but in the context of attempting to write down non locking formulations, see for instance [2]. In the present article, we are not concerned with locking issues but only with imposing the tangency of the rotation vector in Cartesian coordinates. Hence the mixed formulation will be relatively simple. In particular, it involves the same bilinear forms as those used in the penalization approach. Let us set \( M = H^1_{\gamma_0}(\omega) \).

Theorem 4.1 For all \( \rho \geq 0 \), the variational problem: Find \( (U, \lambda) \in X \times M \) such that

\[
\forall (V, \mu) \in X \times M, \begin{cases}
  a(U; V) + \rho b((r \cdot a_3); (s \cdot a_3)) + b((s \cdot a_3); \lambda) = L(V), \\
  b((r \cdot a_3); \mu) = 0,
\end{cases}
\]

has a unique solution, which is such that \( U \in \mathcal{V} \) is the solution of Naghdi’s problem (7).

Proof. The bilinear form \( a + \rho b \) is \( \mathcal{V}' \)-elliptic (and even \( X \)-elliptic for \( \rho > 0 \) by Lemma 3.3). In order to prove that problem (22) has a unique solution, we therefore just need to prove that \( b \) satisfies the inf-sup condition, see [15], [10]. Let thus

\[ \beta = \inf_{\mu \in M} \sup_{V \in X} \frac{b((s \cdot a_3); \mu)}{\| V \|_X \| \mu \|_M}, \]

and we want to show that \( \beta > 0 \). Let \( \mu \in M \setminus \{0\} \) be arbitrary. Since \( \mu \) vanishes on \( \gamma_0 \) and since \( a_3 \in W^{1,\infty}(\omega; \mathbb{R}^3) \), we clearly have \( V = (0, \mu a_3) \in X \) and \( \mu a_3 \cdot a_3 = \mu \). Therefore,

\[
\sup_{V \in X} \frac{b((s \cdot a_3); \mu)}{\| V \|_X} \geq \frac{\| \nabla \mu \|^2_{L^2(\omega; \mathbb{R}^2)}}{\| a_3 \otimes \nabla \mu + \mu \nabla a_3 \|^2_{L^2(\omega; \mathbb{M}^3)}}.
\]
so that 
\[ \beta \geq \inf_{\mu \in \mathcal{M}} \frac{\| \nabla \mu \|_{L^2(\omega; \mathbb{R}^2)}}{\| a_3 \otimes \nabla \mu + \mu \nabla a_3 \|_{L^2(\omega; \mathcal{M}_{32})}}. \]

It is quite clear that the left-hand side of the above inequality is strictly positive, since the denominator is basically a lower order perturbation of the numerator. Let us quickly show this by a contradiction argument. Assume thus that we are given a sequence \( \mu_n \in \mathcal{M} \) such that 
\[ \| \nabla \mu_n \|_{L^2(\omega; \mathbb{R}^2)} \to 0 \]
but 
\[ \| a_3 \otimes \nabla \mu_n + \mu_n \nabla a_3 \|_{L^2(\omega; \mathcal{M}_{32})} = 1. \]

Obviously, due to the boundary conditions and the Poincaré inequality, \( \mu_n \to 0 \) in \( H^1(\omega) \), hence \( a_3 \otimes \nabla \mu_n \to 0 \) in \( L^2 \) and \( \mu_n \nabla a_3 \to 0 \) in \( L^2 \) (recall that \( a_3 \in W^{1,\infty} \)), contradiction. Hence the inf-sup condition holds true and the mixed formulation has one and only one solution.

Let us now check that this solution corresponds to the usual Nagdhi problem. Taking \( \mu = r \cdot a_3 \) in the second equation, we see that \( U \in \mathcal{V} \). Then, taking \( V \in \mathcal{V} \) cancels all terms involving \( b \) in the first equation, hence the result. \( \square \)

Remarks. 1. We can also replace \( b \) by any scalar multiple of itself, and in the case of soft clamping, we must replace it by the full \( H^1 \) scalar product between \( s \cdot a_3 \) and \( \mu \). The lack of intrinsic character can be cured in the same way as for the penalization.

2. The Lagrange multiplier \( \lambda \) that enforces the tangency constraint \( r \cdot a_3 = 0 \) does not have a specific mechanical meaning, since the bilinear forms are pretty arbitrary. Note that when nonzero, \( r \cdot a_3 \) is sometimes called the pinching component or pinching strain, see [12]. Indeed, it corresponds to a change in length of the deformed normal fiber in the 3D Kirchhoff-Love displacement constructed from \( u \) and \( r \). It is thus conceivable that a mechanical meaning could be ascribed to such a Lagrange multiplier, but we do not pursue this line of reasoning here.

3. We may choose \( \rho = 0 \) or \( \rho > 0 \). In the latter case, we are adding a penalization term in the spirit of augmented Lagrangian methods, which can be tuned for the best numerical results. \( \square \)

5 The discrete formulations

5.1 Finite element discretization of the penalized problem

The penalized problem is a standard variational problem formulated in \( H^1 \). We thus propose to use a standard conforming finite element approximation.
Let thus $T_h$ be a regular affine family of triangulations which covers the domain $\omega$. The discrete space of admissible displacements and rotations is given by
\[ X_h = \{ (v,s) \in C^0(\omega; \mathbb{R}^3)^2, (v,s)|_K \in P_1(K), v = s = 0 \text{ on } \gamma_0 \}, \tag{23} \]
which is obviously contained in the continuous space $X$.

The discrete problem thus reads: Find $(u_{p,h}, r_{p,h}) \in X_h$ such that
\[ \forall (v,s) \in X_h, a((u_{p,h}, r_{p,h}); (v,s)) + \frac{1}{p} b(r_{p,h} \cdot \mathbf{a}_3; s \cdot \mathbf{a}_3) = L(v,s). \tag{24} \]
Naturally, this problem has a unique solution.

### 5.2 Convergence

By virtue of the classical properties of Galerkin approximation, we have the following convergence result.

**Theorem 5.1** There exists a sequence $h_p \to 0$ such that
\[ \| (u,r) - (u_{p,h}, r_{p,h}) \|_X \to 0 \quad \text{when} \quad p \to 0. \tag{25} \]

**Proof.** For each $p$, we have $u_{p,h} \to u_p$ when $h \to 0$ because this is a Galerkin approximation of a classical variational problem. We then appeal to Theorem 3.4 to construct a converging diagonal sequence. \qed

If the solution is assumed to have some regularity, the second step of the approximation may of course be controlled via an error estimate.

**Proposition 5.2** Assume that the solution $(u_p; r_p)$ of problem (11) belongs to $H^2(\omega, \mathbb{R}^3)^2$ for all $p$, then there exists a constant $C_p$ independent of $h$, such that
\[ \| (u_{p,h}, r_{p,h}) - (u_p, r_p) \|_X \leq C_p h \| (u_p, r_p) \|_{H^2}. \tag{26} \]

**Proof.** See [14] for example. \qed

**Remarks.** 1. Since we are mostly interested in shells with little regularity, otherwise classical formulations would apply, it is presumably not useful to look for higher order elements in the hope of improving the rate of convergence. Indeed, even without taking into account the penalization term, in the case of such a shell, the underlying system of PDEs has nonsmooth coefficients. It is therefore unclear whether elliptic regularity can be applied to yield even an $H^2$ regularity, let alone $H^{k+1}$ regularity with $k \geq 1$. Note however that, if the midsurface chart is smooth
and we want to use our formulation nonetheless for simplicity as compared to the classical approach, then elliptic regularity will apply.

2. We could also combine estimates (21) and (26), to obtain a global error estimate for the whole penalization/discretization process. To achieve this goal, we would need to estimate the constant $C_p$ in terms of $p$, which would probably include terms of the order of $p^{-1}$ due to the continuity constant of the bilinear form $a_p$, and the term $\| (u_p, r_p) \|_{H^2}$. The latter term could be evaluated by using Nirenberg’s translations method, but the technical aspects involved hardly seem worth the effort in this particular case, in view of the previous remark. In any case, it is reasonable to expect locking due to the penalization term. □

5.3 Finite element discretization of the mixed problem

The mixed problem is also a standard variational problem formulated in $H^1$. In order to prove the convergence of conforming finite element approximations, we only need to establish the uniform discrete inf-sup condition. As is often the case, the uniform discrete inf-sup condition turns out to be much harder to prove than its continuous counterpart and in our particular case, the arguments are rather non-standard. Let us treat the $P_1$ case, with zero boundary condition for the multiplier, for simplicity. In this case, we have

$$\mathcal{M}_h = \{ \mu_h \in C^0(\bar{\omega}), \mu_h|_K \in P_1(K), \mu_h = 0 \text{ on } \partial\omega \}.$$ 

**Theorem 5.3** For all $\rho \geq 0$, the variational problem: Find $(U_h, \lambda_h) \in \mathcal{X}_h \times \mathcal{M}_h$ such that

$$\forall (V_h, \mu_h) \in \mathcal{X}_h \times \mathcal{M}_h, \left\{ \begin{array}{l} a(U_h; V_h) + \rho b((r_h \cdot a_3); (s_h \cdot a_3)) + b((s_h \cdot a_3); \lambda_h) = L(V_h), \\ b((r_h \cdot a_3); \mu_h) = 0, \end{array} \right.$$ 

has a unique solution for $h$ small enough. Moreover

$$\| U - U_h \|_X + \| \lambda - \lambda_h \|_{\mathcal{M}} \to 0 \text{ when } h \to 0.$$ 

We first need a couple of geometrical results.

**Lemma 5.4** Let $\varphi$ be a $W^{2,\infty}$ chart. There exists a constant $C > 0$ such that for all $x, y$ in $\omega$,

$$|a_3(x) \cdot (a_3(x) - a_3(y))| \leq C\| x - y \|^2.$$ 

(28)
Proof. We adapt an argument of [1], Lemma 3.5. By our regularity hypothesis, the normal vector \( a_3 \) is Lipschitz on \( \omega \). Hence, for all \( x_0 \in \omega \), the function
\[
Z(x) = (a_3(x) - a_3(x_0)) \cdot a_3(x_0),
\]
is also Lipschitz. Therefore, by Rademacher’s theorem it is almost everywhere differentiable and we have
\[
\nabla Z(x) = \nabla a_3(x)^T a_3(x_0),
\]
for almost all \( x \in \omega \). Therefore, due to the identification between Lipschitz and \( W^{1,\infty} \) functions in a Lipschitz domain (see [1] for a proof), there exists a constant \( C_\omega \) depending only on \( \omega \) such that
\[
|Z(x)| = |Z(x) - Z(x_0)| \leq C_\omega \| \nabla a_3^T a_3(x_0) \|_{L^{\infty}(B(x_0, \|x-x_0\|)) \cap \omega; \mathbb{R}^2} \|x - x_0\|.
\]
Now, \( a_3 \) is a unit vector. Hence, at any point \( y \) of differentiability of \( a_3 \), \( a_3(y) \) is orthogonal to the image of \( \nabla a_3(y) \), that is to say \( \nabla a_3(y)^T a_3(y) = 0 \). Consequently, we have that, almost everywhere in \( \overline{B}(x_0, \|x-x_0\|) \cap \omega \),
\[
\nabla a_3(y)^T a_3(x_0) = \nabla a_3(y)^T a_3(x_0) - \nabla a_3(y)^T a_3(y),
\]
so that
\[
\| \nabla a_3(y)^T a_3(x_0) \| \leq \| \nabla a_3(y)^T \| \| a_3(x_0) - a_3(y) \|
\leq C_\omega \| \nabla a_3 \|_{L^{\infty}(\omega; \mathbb{M}_{32})}^2 \|y - x_0\|
\]
almost everywhere. Therefore,
\[
\| \nabla a_3^T a_3(x_0) \|_{L^{\infty}(\overline{B}(x_0, \|x-x_0\|)) \cap \omega; \mathbb{R}^2} \leq C_\omega \| \nabla a_3 \|_{L^{\infty}(\omega; \mathbb{M}_{32})}^2 \|x - x_0\|,
\]
hence the result with \( C = C_\omega^2 \| \nabla a_3 \|_{L^{\infty}(\omega; \mathbb{M}_{32})}^2 \cdot \). \( \square \)

Remark. Note that the above geometrical result holds true under the weaker, “minimal” regularity hypotheses advocated in [1] for a shell midsurface, namely \( \varphi \) bilipschitz and such that \( a_3 \) is Lipschitz. \( \square \)

Lemma 5.5 Under the same hypotheses, there exists a constant \( C > 0 \) such that for all \( x \) and almost all \( y \) in \( \omega \),
\[
|a_3(x) \cdot \partial_\alpha a_3(y)| \leq C \|x - y\|. \tag{29}
\]

Proof. Let \( y \) be a point of differentiability of \( a_3 \). We have
\[
a_3(x) \cdot \partial_\alpha a_3(y) = (a_3(x) - a_3(y)) \cdot \partial_\alpha a_3(y),
\]
so that
\[
|a_3(x) \cdot \partial_\alpha a_3(y)| \leq C_\omega \| \nabla a_3 \|_{L^{\infty}(\omega; \mathbb{M}_{32})}^2 \|x - y\|,
\]
for all \( x \in \omega \). \( \square \)
We now turn to the inf-sup condition per se. Let \( \Pi_h \) denote either the vector-valued Lagrange interpolation operator from \( C^0([\Omega; \mathbb{R}^3]) \) into \( X_h \) or the scalar-valued Lagrange interpolation operator from \( C^0([\tilde{\Omega}]) \) into \( M_h \), depending on the context, and \( \psi_j^h \) the shape function associated with vertex \( S_j \) of the triangulation.

**Lemma 5.6** For all \( \mu_h \in M_h \), we let \( R_h(\mu_h) = \Pi_h(\mu_h a_3) \). There exists a constant \( C > 0 \) independent of \( h \) such that

\[
b(R_h(\mu_h) \cdot a_3; \mu_h) \geq C\|\mu_h\|_{M}^2.
\]

**Proof.** Note that while \( \mu_h \) is scalar piecewise \( P_1 \), \( \mu_h a_3 \) is vector-valued and \( R_h(\mu_h) \) is vector-valued piecewise \( P_1 \). Let us set

\[
\delta_h = R_h(\mu_h) \cdot a_3 - \mu_h,
\]

so that

\[
b(R_h(\mu_h) \cdot a_3; \mu_h) = \|\mu_h\|_{M}^2 + b(\delta_h; \mu_h),
\]

with

\[
|b(\delta_h; \mu_h)| \leq \|\mu_h\|_M \|\delta_h\|_M.
\]

We thus just need to estimate \( \delta_h \) in the norm of \( M \). By Lagrange interpolation, we have

\[
\mu_h(x) = \sum_{S_j} \mu_h(S_j) \psi_j^h(x)
\]

and

\[
R_h(\mu_h)(x) = \sum_{S_j} \mu_h(S_j) \psi_j^h(x) a_3(S_j).
\]

Therefore

\[
R_h(\mu_h) \cdot a_3(x) = \sum_{S_j} \mu_h(S_j) [a_3(S_j) \cdot a_3(x)] \psi_j^h(x),
\]

and

\[
\delta_h(x) = \sum_{S_j} \mu_h(S_j) [(a_3(S_j) - a_3(x)) \cdot a_3(x)] \psi_j^h(x),
\]

since \( a_3(x) \) is a unit vector. Consequently, we arrive at the formula

\[
\partial_\alpha \delta_h(x) = \sum_{S_j} \mu_h(S_j) [a_3(S_j) \cdot \partial_\alpha a_3(x)] \psi_j^h(x)
\]

\[
+ \sum_{S_j} \mu_h(S_j) [(a_3(S_j) - a_3(x)) \cdot a_3(x)] \partial_\alpha \psi_j^h(x)
\]

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almost everywhere (namely inside the triangles). At every point of differentiability in \( \omega \), at most three terms in the sums are non zero, therefore we can estimate

\[
\| \partial_\alpha \delta h \|_{L^\infty(\omega)} \leq 3 \| \mu h \|_{L^\infty(\omega)} \max_{j} \left[ |a_3(S_j) \cdot \partial_\alpha a_3(x)| + \frac{C}{h} \left| (a_3(S_j) - a_3(x)) \cdot a_3(x) \right| \right],
\]

where \( K_{k,j} \) stand for all the triangles having \( S_j \) as vertex. Since all triangles have diameter bounded by a constant times \( h \), we deduce with the help of Lemmas 5.4 and 5.5 that

\[
\| \partial_\alpha \delta h \|_{L^\infty(\omega)} \leq C h \| \mu h \|_{L^\infty(\omega)},
\]

where \( C \) does not depend on \( h \) nor on \( \mu h \).

We now appeal to the classical discrete Sobolev estimate, see [9], and deduce that

\[
\| \nabla \delta h \|_{L^2(\omega; \mathbb{R}^2)} \leq C \| \nabla \delta h \|_{L^\infty(\omega; \mathbb{R}^2)} \leq C h \| \mu h \|_{L^\infty(\omega)} \leq C h (\ln h)^{1/2} \| \nabla \mu h \|_{L^2(\omega; \mathbb{R}^2)}.
\]

Taking \( h \) small enough so that \( C h (\ln h)^{1/2} \leq \frac{1}{2} \), we obtain estimate (30). \( \square \)

We now are in a position to prove the crucial uniform discrete inf-sup condition which guarantees the convergence of the finite element scheme applied to the mixed formulation.

**Theorem 5.7** There exists \( \beta^* > 0 \) independent of \( h \) such that

\[
\inf_{\mu h \in M_h} \sup_{V h \in X_h} \frac{b((s h \cdot a_3); \mu h)}{\| V h \|_X \| \mu h \|_M} \geq \beta^*.
\]

(31)

**Proof.** Let thus

\[
\beta_h = \inf_{\mu h \in M_h} \sup_{V h \in X_h} \frac{b((s h \cdot a_3); \mu h)}{\| V h \|_X \| \mu h \|_M}.
\]

By construction, since \( \mu h \) vanishes on \( \partial \omega \), we see that \( V h = (0, R h(\mu h)) \in X_h \) and that \( \| V h \|_X = \| \nabla R h(\mu h) \|_{L^2(\omega; \mathbb{R}^2)} \). Therefore

\[
\beta_h \geq C \inf_{\mu h \in M_h} \frac{\| \mu h \|_M}{\| \nabla R h(\mu h) \|_{L^2(\omega; \mathbb{R}^2)}},
\]

and it suffices to estimate the denominator from above independently of \( h \).

Since we have

\[
\partial_\alpha R h(\mu h)(x) = \sum_{S_j} \mu h(S_j) \partial_\alpha \psi_j^h(x) a_3(S_j),
\]

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it follows that
\[ \| \nabla R_h(\mu_h) \|_{L^2(\omega; \mathbb{M}_{32})}^2 = \sum_{S_j, S_k} \mu_h(S_j) \mu_h(S_k) [a_3(S_j) \cdot a_3(S_k)] (\partial_\alpha \psi^k_j) (\partial_\alpha \psi^k_k) L^2(\omega). \] (32)

Now we notice that
\[ a_3(S_j) \cdot a_3(S_k) = 1 + a_3(S_j) \cdot (a_3(S_k) - a_3(S_j)) = 1 + \varepsilon_{jk}(h), \]
where
\[ |\varepsilon_{jk}(h)| \leq C h^2, \]
for all nonzero terms in the right-hand side of equation (32), due to Lemma 5.4 again. Moreover, all shape functions are positive, which implies that
\[ |(\partial_\alpha \psi^k_j) (\partial_\alpha \psi^k_k) L^2(\omega)| \leq \frac{C}{h^2} (\psi^j_j) (\psi^k_k) L^2(\omega), \]
an inverse inequality easily established by going back to the reference triangle. Therefore, we see that
\[ \| \nabla R_h(\mu_h) \|_{L^2(\omega; \mathbb{M}_{32})}^2 = \| \nabla \mu_h \|_{L^2(\omega; \mathbb{R}^{32})}^2 + \sum_{S_j, S_k} \mu_h(S_j) \mu_h(S_k) \varepsilon_{jk}(h) (\partial_\alpha \psi^k_j) (\partial_\alpha \psi^k_k) L^2(\omega) \]
\[ \leq \| \nabla \mu_h \|_{L^2(\omega; \mathbb{R}^{32})}^2 + C \sum_{S_j, S_k} |\mu_h(S_j)| |\mu_h(S_k)| (\psi^j_j) (\psi^k_k) L^2(\omega) \]
\[ = \| \nabla \mu_h \|_{L^2(\omega; \mathbb{R}^{32})}^2 + C \| \Pi_h(\mu_h) \|_{L^2(\omega)}^2. \] (33)

To conclude, we now proceed to show that
\[ \| \Pi_h(\mu_h) \|_{L^2(\omega)} \leq C \| \mu_h \|_{L^2(\omega)} \] (34)
for some constant \( C \) that does not depend on \( h \). To do this, we compare the squared \( L^2 \) norms on each triangle, and then by way of the standard affine change of variable, on the reference triangle \( \hat{K} \). We are thus reduced to comparing two functions defined on \( \mathbb{R}^3 \)
\[ f(a) = \int_{\hat{K}} \sum_{i,j=1}^3 |a_i| a_j \hat{\lambda}_i \hat{\lambda}_j d\hat{x} \text{ and } g(a) = \int_{\hat{K}} \sum_{i,j=1}^3 a_i a_j \hat{\lambda}_i \hat{\lambda}_j d\hat{x}, \]
where \( \hat{\lambda}_i \) are the barycentric coordinates in \( \hat{K} \). Both functions are homogeneous of degree two, hence
\[ \sup_{a \in \mathbb{R}^3 \setminus \{0\}} f(a) = \sup_{\|a\|_{\mathbb{R}^3} = 1} f(a). \]
Now the function \( f(a)g(a) \) is continuous on the unit sphere of \( \mathbb{R}^3 \) since its denominator is a positive definite quadratic form. Therefore, there exists \( C > 0 \) such that \( \frac{f(a)}{g(a)} \leq C \) for all \( a \neq 0 \), which immediately implies estimate (34).

Replacing now the latter estimate in estimate (33), we see that

\[
\| \nabla R_h(\mu_h) \|_{L^2(\omega;\mathbb{R}^3)} \leq C \| \mu_h \|_{\mathcal{M}},
\]

so that

\[
\inf_{\mu_h \in \mathcal{M}_h} \frac{\| \mu_h \|_{\mathcal{M}}}{\| \nabla R_h(\mu_h) \|_{L^2(\omega;\mathbb{R}^3)}} \geq \frac{1}{C} > 0,
\]

which completes the proof of the Theorem. \( \square \)

**Remark.** It is fairly clear that the proof works the same if we replace \( P_1 \) interpolation by another Lagrange interpolation, for example \( P_2 \), which is also available in FreeFem++.

The proof of Theorem 5.3 follows as in [15].

Naturally, if we assume some regularity of the solution, we obtain error estimates.

**Proposition 5.8** Assume that the solution \( ((u, r), \lambda) \) of problem (4.1) belongs to \( H^2(\omega;\mathbb{R}^3)^3 \), then there exists a constant \( C \) independent of \( h \), such that

\[
\| (u_h, r_h) - (u, r) \|_X + \| \lambda_h - \lambda \|_{\mathcal{M}} \leq Ch \| ((u, r), \lambda) \|_{H^2},
\]

(35)

**Proof.** See [15] for example. \( \square \)

### 6 Numerical tests

In this section, we implement the discretization of both penalized and mixed approaches using FreeFem++, compare them on a literature benchmark and apply them to genuinely \( W^{2,\infty} \) shells.

#### 6.1 Implementation details

Both model formulations only require the knowledge of \( a_\alpha, a_3 \) and \( \partial_\alpha a_3 \). All other quantities, either geometrical like the elasticity tensor, or kinematical like the strain tensors, can be expressed by means of dot products of these quantities. Since FreeFem++ includes a language with C++-like syntax, it is convenient to define these vectors as FreeFem++ functions. The dot products are expressed as
FreeFem++ macros, which are then combined into other macros that eventually expand to all the other quantities of interest. The net result is that our code automatically constructs the bilinear forms, with minimal user input, typically between ten and twenty lines of code. This works well if an analytic description of the mid-surface is available. In the case of midsurfaces implicitly defined via interpolation of nodal values, as in [12], the same approach should be possible, provided the interpolated surface chart retains $W^{2,\infty}$ regularity. We plan to address this issue in a further iteration of the code.

The user must also input the chart domain, boundary conditions and linear form for the loading terms, which is again minimal work. FreeFem++ automatically meshes the domain, constructs the stiffness matrix based on the bilinear and linear forms, and solves the linear system using a direct solver (UMFPACK by default). If asked to, it can automatically refine the mesh during successive iterations, based on an estimate of the second derivatives of given solution components, in order to minimize the local interpolation error. The mesh adaption is quite efficient in general.

Let us note that, with respect to user input, our approach compares favorably with classical formulations which require the computation of the covariant and mixed components of the second fundamental form and of the Christoffel symbols of the chart, see for example [3].

Concerning the expressivity of FreeFem++, it should be noted that all the shell-specific work in our code, essentially the various macros, is contained in about a hundred lines of code.

We also compute the chart $\varphi$ itself as a FreeFem++ function for purposes of 3D visualization of the undeformed and deformed shells. Visualization uses Medit\(^1\), a free mesh visualization software available at http://www.ann.jussieu.fr/~frey/logiciels/medit.html.

All the tests were run on 1.5GHz Apple PowerBook G4 laptops and 2GHz, single processor, Apple Xserve G5.

### 6.2 The hyperbolic paraboloid shell

This test is a literature benchmark for shell elements. We use this example, in which the midsurface of the shell is represented by a chart of class $C^\infty$, mainly to validate our FreeFem++ code. It does not constitute a relevant test for the $W^{2,\infty}$ case.

The reference domain of the midsurface is given by

$$\omega = \{|x| + |y| < \sqrt{2}b\},$$

\(^1\)Legal mention: This software was designed and developed at the Laboratoire Jacques-Louis Lions of the University Pierre et Marie Curie.
and the chart is defined by
\[ \varphi(x, y) = (x, y, \frac{c}{2b^2}(x^2 - y^2))^T, \]
where \( b = 50 \) cm and \( c = 10 \) cm.

The shell is clamped on \( \partial \omega \) and subjected to a uniform pressure \( q = 0.01 \) kp/cm\(^2\). The mechanical data are
\[ E = 2.85 \times 10^4 \text{ kp/cm}^2, v = 0.4, \]
The thickness of the shell is \( e = 0.8 \) cm.

The reference value for this test is the normal displacement at the center \( A \) of the shell. Its value computed by various methods is of \(-0.024 \) cm, see [3].

Due to the symmetries of the problem, we use the computational domain
\[ \omega' = \{ 0 < x, 0 < y, x + y < \sqrt{2}b \}, \]
and enforce the symmetry conditions
\[ u_2 = 0, r_2 = 0 \text{ on } y = 0 \]
and
\[ u_1 = 0, r_1 = 0 \text{ on } x = 0. \]
These conditions are obtained by expressing the continuity of the three-dimensional Kirchhoff-Love displacement \( U = u + x_3r \) along these edges.

We give below results for both methods using mesh adaption and \( P_2 \) elements.

<table>
<thead>
<tr>
<th>Degrees of freedom</th>
<th>((u \cdot a_3)(A))</th>
<th>Range of values for ((r \cdot a_3)(B))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Penalized</td>
<td>7005</td>
<td>(-0.0241419, -3.46456e^{-8}, 3.52366e^{-8})</td>
</tr>
<tr>
<td>Mixed</td>
<td>7279</td>
<td>(-0.0241416, -3.52081e-08, 3.51064e-08)</td>
</tr>
</tbody>
</table>

In the penalized test, the penalization parameter was \( 10^3 \frac{E}{2(1+v)} \). Both methods achieve excellent tangency for the rotation vector and similar performance in terms of the reference value.

![Figure 1: The initial and final meshes](image_url)
Remark. We also performed tests on another benchmark, the Scordelis-Lo roof. Unfortunately, in this case, $P_1$ and $P_2$ elements present significant locking (we obtain a maximum normal displacement that is only 65% of the reference value). Until more sophisticated elements become integrated into FreeFem++, such tests cannot yield satisfactory results. We were however able to confirm that both Cartesian formulations provide the same (locked) result as the classical covariant formulation using $P_1$ and $P_2$ elements.

6.3 A plane-cylinder $W^{2,\infty}$-shell

Our next test is a genuine $W^{2,\infty}$ test with curvature discontinuities. The shell consists of a plane part and a cylindrical part with a $C^1$-join, see Figure 2. The reference domain of the midsurface is given by

$$\omega = ]-R,R[ \times ]-L/2,L/2[,$$

and the chart is defined by

$$\varphi(x,y) = \begin{cases} (x,y,0)^T & \text{if } x < 0, \\ (R\sin(x/R),y,R(1-\cos(x/R)))^T & \text{if } x \geq 0, \end{cases}$$

with $R = 300$ in and $L = 600$ in (these values come from the Scordelis-Lo test). The thickness of the shell is $e = 3$ in.
The mechanical data are

\[ E = 3.0 \times 10^6 \text{ psi}, \nu = 0.0. \]

The shell is submitted to a uniform downward pressure of 0.625 lb/sq in.

Concerning boundary conditions, we consider the case of hard clamping on lines \( AB \) and \( DC \)

\[ u_1 = u_2 = u_3 = 0 \quad \text{and} \quad r_1 = r_2 = r_3 = 0, \]

and the shell is free on its remaining edges. Thanks to the symmetry, we only consider half of the midsurface, \( y > 0 \). The corresponding symmetry conditions on \( AD \) are

\[ u_2 = r_2 = 0. \]

Note that the initial mesh ignores the curvature discontinuity at \( x = 0 \).
Note that in Medit, the coordinate axes are attached to the bounding box: although it seems that the clamped left side of the shell has moved up in Figure 5 compared to Figure 4, this is not actually the case.

It is interesting to note that mesh adaption concentrates around the curvature discontinuity, thus indicating the lack of regularity of the solution across this line. In the following isovalues, the leftmost half of the domain corresponds to the planar part of the shell for \( x_1 < 0 \), and the other half to the cylindrical part of the shell. The line \( AD \) is represented by the bottom side of the domain.

![Figure 6: Isovalues of \( u_1 \). The range of values is \([-0.967042, 0.0130627]\).](image)

![Figure 7: Isovalues of \( u_2 \). The range of values is \([-0.00181261, 0.00234357]\).](image)

![Figure 8: Isovalues of \( u_3 \). The range of values is \([-6.31062, 0.949939]\) (isovalues for \( u \cdot a_3 \) are practically identical and those for \( r_1 \) and \( \lambda \) show similar features).](image)

Note that even though the pressure acts downward, the cylindrical part of the shell lifts a little bit to compensate for the large deflection of its planar part.

Concerning the rotation vector, we have the following isovalues (\( r_1 \) is not represented, see Figure 8).

![Figure 9: Isovalues of \( r_2 \). The range of values is \([-0.0011471, 0.000972632]\).](image)
Figure 10: Isovalues of $r_3$. The range of values is $[-0.00547512, 0.0128569]$.

To see how the mixed formulation manages to enforce the tangency constraint, we also plot the isovalues of the normal rotation $r \cdot a_3$. We see that the curvature discontinuity makes it harder to capture this constraint than in the $C^\infty$ case of the hyperbolic paraboloid.

Figure 11: Isovalues of $r \cdot a_3$. The range of values is $[-9.18161 \times 10^{-6}, 0.00474402]$.

Finally, we compare our results with those of [16] for the same geometry, but for the Koiter model, using the Argyris element on a structured mesh that respects the curvature discontinuity. The vertical displacement of point $O$ is found to be approximately $-4.0$ in (value based on a graph in [16]). We find $u_3(0) = -3.83631$ in, which is in good agreement.

6.4 A basket-handle tunnel

A basket-handle is a classical approximation of an arc of ellipse, and a very good one, constructed with three circles. It has long been used in architecture as a replacement for an ellipse. Clearly this arc presents two curvature discontinuities and the same will be true for arches based on it.

Figure 9: AMNB is basket handle or three-centered arch
We present numerical results for a long, tunnel-like shell based on a slightly extended basket-handle arc. Similar structures have recently been used in architecture, with mixed results.

We use the same mechanical data as for the plate-cylinder shell. Clamping is assumed on both rectilinear sides of the shell. These sides are of length 3000 in. The large circle radius is 400 in and the small circle radius 200 in.

The natural chart for this shell is of class $W^{2,\infty}$. It is obtained by parametrizing the basket-handle by arclength. The computational domain is a rectangle $[-628.32, 628.32] \times [-1800, 1800]$ (we compute the whole shell without using the symmetries for better visualization).

The vertical displacement of the center of the shell is $u_3(0, 0) = -27.3815$ in.

Figure 10: The initial mesh on the midsurface

Figure 11: The deformed shell (displacement magnified by a factor of 3)
Figure 12: Isovalues of \( u \cdot a_3 \) (left), \( r \cdot a_3 \) (middle), and \( u_2 \) (right)

**Remark.** Naturally, the isovalues for \( u_2 \) should respect the shell symmetries. However, since the range of values for \( u_2 \) is of the order of \([-2e^{-5}, 2e^{-5}]\), the shape of the isovalue lines is very sensitive to errors. It nonetheless becomes more symmetrical when the mesh is further refined.

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**References**


[18] B. Maury, personal communication.