POLYGONAL FINITE ELEMENTS FOR FINITE ELASTICITY

BY

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THESIS

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Abstract

Nonlinear elastic materials are of great engineering interest, but challenging to model with standard finite elements. The challenges arise because nonlinear elastic materials undergo large reversible deformations, and often possess complex micro-structures. In this work, we propose and explore an alternative approach to model finite elasticity problems in two dimensions by using polygonal discretizations. To account for incompressible behavior, a general theoretical framework of deriving the two-field variational principle, involving a displacement field and a pressure field, is presented. Within the theoretical framework, by assuming different forms of stored-energy function, two types of variational principles are obtained, each with distinct definitions of the independent pressure field. Based on the theoretical setting, we present both lower order displacement-based and mixed polygonal finite element approximations, the latter of which consist of a piecewise constant pressure field and a linearly-complete displacement field at the element level. Through numerical studies, the mixed polygonal finite elements are shown to be stable and convergent. Finally, in the context of filled elastomers and cavitation instabilities, we present applications of practical interest, which utilize polygonal discretizations, demonstrating the potential of polygonal finite elements in studying and modeling nonlinear elastic materials of complex micro-structures under finite deformations.
To my parents
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## Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Material parameter for incompressible Lopez-Pamies material model</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Cauchy stress tensor</td>
</tr>
<tr>
<td>$\chi_E$</td>
<td>Basis function associated with polygon $E$ for piecewise constant interpolation over the mesh $\mathcal{T}_h$</td>
</tr>
<tr>
<td>$\delta_{kl}$</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>$\epsilon_{0,u}, \epsilon_{1,u}$</td>
<td>Normalized $L^2$-norm and $H^1$-seminorm of the error in finite element solution of displacement field $u$</td>
</tr>
<tr>
<td>$\epsilon_{0,p}, \epsilon_{0,\tilde{p}}$</td>
<td>Normalized $L^2$-norm of the errors in finite element solutions of the hydrostatic pressure field $p$ and pressure field $\tilde{p}$</td>
</tr>
<tr>
<td>$\Gamma_t$</td>
<td>Part of the domain boundary $\partial \Omega$ where traction boundary condition is imposed</td>
</tr>
<tr>
<td>$\Gamma_u$</td>
<td>Part of the domain boundary $\partial \Omega$ where displacement boundary condition is imposed</td>
</tr>
<tr>
<td>$\lambda, \gamma$</td>
<td>Applied macroscopic stretch and shear</td>
</tr>
<tr>
<td>$\langle F \rangle$</td>
<td>Volume average of deformation gradient $F$</td>
</tr>
<tr>
<td>$\langle P \rangle$</td>
<td>Volume average of first Piola-Kirchhoff stress $P$</td>
</tr>
<tr>
<td>$\langle W \rangle$</td>
<td>Volume average of stored-energy function $W$</td>
</tr>
<tr>
<td>$\mathcal{K}$</td>
<td>Set of kinematically admissible displacement fields</td>
</tr>
<tr>
<td>$\mathcal{K}^0$</td>
<td>Set of kinematically admissible displacement fields that vanish on $\Gamma_u$</td>
</tr>
<tr>
<td>$\mathcal{K}_h$</td>
<td>Finite dimensional displacement space defined over the mesh $\mathcal{T}_h$ such that $\mathcal{K}_h \subseteq \mathcal{K}$</td>
</tr>
<tr>
<td>$\mathcal{K}^0_h$</td>
<td>Finite dimensional displacement space defined over the mesh $\mathcal{T}_h$ such that $\mathcal{K}^0_h = \mathcal{K}_h \cap \mathcal{K}^0$</td>
</tr>
<tr>
<td>$\mathcal{Q}$</td>
<td>Space consisting of square integrable functions</td>
</tr>
<tr>
<td>$\mathcal{Q}_h$</td>
<td>Finite dimensional pressure space defined over mesh $\mathcal{T}_h$</td>
</tr>
<tr>
<td>$\mathcal{T}_h$</td>
<td>Partition of the domain into non-overlapping polygons</td>
</tr>
<tr>
<td>$\mathcal{V}(E)$</td>
<td>Space defined by linear combinations of a set of barycentric coordinates over polygon $E$</td>
</tr>
<tr>
<td>$\mu, \kappa$</td>
<td>Shear and bulk moduli of elastic solids</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Gradient operator with respect to the undeformed configuration</td>
</tr>
</tbody>
</table>
Undeformed domain

\(\Pi(v, q)\) Potential energy obtained from the complementary stored-energy function \(\tilde{W}_C(X, \tilde{F}(v), \tilde{q})\)

\(\mathbf{F}\) Modified deformation gradient tensor defined as \(\mathbf{F} = (\det \mathbf{F})^{-\frac{1}{2}} \mathbf{F}\)

\(\mathbf{W}(X, \mathbf{F}, J)\) Modified form of the general stored-energy function by adopting the modified deformation gradient tensor \(\mathbf{F}\)

\(\tilde{W}_C(X, \mathbf{F}, q)\) Complementary stored-energy function obtained from partial Legendre transformations of \(J\) in \(\mathbf{W}(X, \mathbf{F}, J)\)

\(\Pi(v)\) Potential energy obtained from stored-energy function \(W(X, \mathbf{F}(v))\)

\(\mathbf{F}\) Deformation gradient tensor

\(f\) Body force per unit undeformed volume

\(P\) First Piola-Kirchhoff stress

\(t\) Traction vector per unit undeformed area

\(u\) Unknown displacement field

\(u_h\) Finite element solution of displacement field \(u\)

\(v\) Admissible displacement field

\(v_h\) Finite dimensional admissible displacement field

\(w\) Incremental displacement field

\(X\) Initial position vector

\(\varphi_i\) Mean Value coordinates associated with \(i\)th vertex of \(n\)-sided polygon \(E\)

\(\tilde{\Pi}(v, \tilde{q})\) Potential energy obtained from the complementary stored-energy function \(\tilde{W}_C(X, \mathbf{F}(v), \tilde{q})\)

\(\tilde{g}\) Incremental pressure field in the \(\mathbf{F}\)-Formulation

\(\tilde{p}\) Unknown pressure field in the \(\mathbf{F}\)-Formulation

\(\tilde{W}(X, \mathbf{F}, J)\) General form of stored-energy function involving an additional field \(J\)

\(\tilde{W}_C(X, \mathbf{F}, \tilde{q})\) Complementary stored-energy function obtained from partial Legendre transformations of \(J\) in \(\tilde{W}(X, \mathbf{F}, J)\)

\(h, h_{\text{max}}, h_{\text{min}}\) Average, maximum and minimum element diameters of the mesh \(\mathcal{T}_h\)

\(J\) An additional independent field introduced in functions \(\tilde{W}(X, \mathbf{F}, J)\) and \(\mathbf{W}(X, \mathbf{F}, J)\)

\(p\) Unknown hydrostatic pressure field

\(p_h, \tilde{p}_h\) Finite element solutions of hydrostatic pressure field \(p\) and
pressure field $\bar{p}$, respectively

$p_{h|E}, \bar{p}_{h|E}$ Finite element solutions of hydrostatic pressure field $p$ and pressure field $\bar{p}$ over element $E$

$q, \tilde{q}$ Admissible hydrostatic pressure field and pressure field defined in the $F$-Formulation, respectively

$q_{h}, \tilde{q}_{h}$ Finite dimensional admissible hydrostatic pressure field and the pressure field used in the $F$-Formulation, respectively

$W (X, F)$ Stored-energy as a function of deformation gradient $F$

$w_i, \beta_i$ Weight function and angle associated with $i$th vertex of $n$-sided polygon $E$ defined in Mean Value coordinates

$|\Omega|$ Area of the undeformed domain $\Omega$

$|E|$ Area of undeformed polygon $E$
CHAPTER 1

Introduction

1.1 Motivation

Nonlinear elastic materials are distinguished by their ability to undergo large reversible deformations in response to a variety of stimuli, including mechanical forces, electrical and magnetic fields and temperature changes. As an important class of materials, they pervade engineering industry and our daily lives. Polymers and synthetic rubbers are classic examples. More recently, modern advances in material science have demonstrated that soft organic material, such as, electro- and magneto-active elastomers, gels and shape memory polymers, hold tremendous potential for enabling new high-end technologies as a new generation of sensors and actuators. These materials, although complex as they sound, are elastic by nature. Because more often than not, nonlinear elastic materials possess complex micro-structures, the underlying local deformations can be significantly large than the macroscopic deformation. This is indeed the case in filled elastomers, wherein large local deformations can occur due to particle interactions and rotations. Another prominent example is that of large local deformations due to the growth of inherent defects in rubbers, where the stretch of the rubber around the cavities can be tens of orders of magnitude greater than that in the bulk [1].

Computational microscopic studies of nonlinear elastic materials, especially those with complex microstructures, to gain quantitative understanding of their complex behavior are essential in guiding their optimization and actual use in technological applications. The standard finite element approach, however, has been shown to be inadequate in simulating processes involving realistic large deformations. A simple but glaring example can be found in the study of filled elastomers. Experimentally, a synthetic rubber filled with 20% volume fraction of randomly distributed spherical silica particles can be stretched more than four times its original length without any internal damage under uniaxial tension [2]. By contrast, a finite element
model, based on standard 10-node hybrid elements with linear pressure, is only able to deform to a macroscopic stretch of $\lambda = 1.5$ [3]. This is because there are a number of matrix regions squeezed in between particles where the local deformations are very large (involving stretches of up to 5 in this example) and convergence cannot be reached [3]. The use of different elements types, meshes and remeshing has been shown to be inefficient, or of little help, to circumvent this problem [3, 4]. Motivated by the above limitations of the standard finite element method, in this work, we presented a framework using both lower order displacement-based and two-field mixed polygonal finite elements as an alternative approach to study nonlinear elastic materials.

Despite its long history of development, dating back to the work of Wachspress [5], the numerical implementation and application of polygonal finite elements in engineering problems are more recent [6, 7, 8, 9, 10, 11]. Polygonal finite elements have shown to possess advantages over the classical finite elements, i.e. triangular and quadrilateral elements, in many aspects. From a geometric point of view, it offers more flexibility in discretization. Making use of the concept of Voronoi tessellation, a number of meshing algorithms for polygonal meshes have been developed that allow the meshing of arbitrary geometries [12, 13, 14]. In addition, since there is no restriction on the number of sides in polygonal finite element, polygonal elements or $n$-gons ($n = 3, 4, 5, \cdots$) can be useful in mesh transitions and refinement. Representative examples can be found in the fracture literature, where the use of polygonal finite elements makes possible local modifications, such as element splitting and adaptive refinement techniques, to better capture the propagation of cracks and crack branching [15, 16]. In addition to their advantages in mesh generation and refinement, polygonal finite elements can outperform their triangular and quadrilateral counterparts under bending and shear loadings [6]. From an analysis point of view, when incompressible or nearly incompressible materials are considered, mixed finite elements are typically employed, for which numerical stability is a critical issue [17, 18]. Unfortunately, it turns out that many choices of mixed finite elements are numerically unstable [19, 20]. For example, coupled with piece-wise constant pressure approximations, linear interpolations of the displacement field on triangular meshes generally exhibit locking behavior, while bi-linear interpolations of the displacement field on quadrilateral meshes may lead to spurious pressure modes. By contrast, the approximation of the displacement field by
linearly-complete barycentric coordinates with piecewise constant pressure interpolation on Voronoi-type meshes have been shown to be unconditionally stable without the need of any additional treatments [10].

Although shown to be successful in linear analysis, polygonal finite elements have not been extensively studied for nonlinear problems. Biabanaki et al. introduced polygonal finite elements in the context of large deformation elasto-plastic and contact impact problems [21, 22]. They have shown that polygonal discretizations efficiently reduce the computational efforts associated to mesh generation of the arbitrary geometries and boundaries. In this thesis, both displacement-based and mixed polygonal finite elements are extended and formulated for finite elasticity problems. Subsequently, as practical applications, they are utilized in the study of real-life engineering problems, namely filled elastomers and cavitation in rubber. From the numerical examples, the polygonal elements are shown to have the geometrical advantages in discretization when modeling arbitrary inclusions, incorporating periodic boundary conditions, and bridging different length scales. Meanwhile, they also appear to be more tolerant of large local deformations than classic triangular and quadrilateral elements, while being more accurate and numerically stable.

1.2 Thesis organization

The thesis is organized as follows. In Chapter 2, both displacement-based and two-field mixed variational principles are derived and presented in a continuum setting. Their finite element approximations on polygonal meshes and implementation aspects are then discussed in Chapter 3. In Chapter 4, through numerical studies, the convergence and stability of the polygonal finite elements are verified. In Chapter 5, the polygonal finite elements are applied to two practical applications, namely particle reinforced elastomers and a cavitation problem. Finally, we provide some concluding remarks in Chapter 6.
CHAPTER 2

Finite elasticity formulations

In addition to the standard displacement-based formulation [23, 24], we develop a general approach for obtaining two-field variational principles, which involve an independent displacement field and an independent pressure field, to account for the incompressible behavior. Here we adopt hyperelastic constitutive models for finite elasticity [25] and a total Lagrangian description is used based on the first Piola-Kirchhoff stress \( P \).

2.1 Displacement-based formulation

The stress-strain relation of hyperelastic materials is derived from a stored-energy function describing the energy stored in the material, denoted by \( W \). In its most general form, \( W \) is a function of the deformation gradient \( F \), and the initial position vector \( X \). Based on the stored-energy function \( W(X, F) \), the Principle of Minimum Potential Energy can be applied to formulate the variational principle based on the displacement field.

The principle states that the unknown displacement field \( u \) is the one that minimizes the potential energy among the set \( K \) consisting of all kinematically admissible displacement fields:

\[
\Pi(u) = \min_{v \in K} \Pi(v) \tag{2.1}
\]

where \( \Pi(v) \) is the potential energy of the solid:

\[
\Pi(v) = \int_{\Omega} W(X, F(v)) \, dX - \int_{\Omega} f \cdot v \, dX - \int_{\Gamma_t} t \cdot v \, dS \tag{2.2}
\]

In the above expression, \( \Omega \) denotes the undeformed domain, whose boundary \( \partial \Omega \) is partitioned into \( \Gamma_u \) and \( \Gamma_t \), where displacement and traction boundary conditions are imposed, respectively. The tensor \( F \) is the deformation gradient, which is a function of the displacement field \( u \) of the form: \( F(u) = I + \nabla u \), where \( \nabla \) denotes the gradient operator with respect to the
undeformed configuration. $f$ is the body force per unit undeformed volume and $t$ is the traction vector per unit undeformed area.

A necessary condition for Equation (2.1) requires the variation of the potential energy $\Pi(u)$ with respect to all admissible displacement field $v$ in the set $\mathcal{K}^0$, which is known as the Principle of Virtual Work:

$$G(u, v) = D\Pi(u) \cdot v = \int_{\Omega} P(X, F(u)) : \nabla v dX - \int_{\Omega} f \cdot v dX$$
$$- \int_{\Gamma_t} t \cdot v dS = 0 \quad \forall v \in \mathcal{K}^0 \tag{2.3}$$

where $\mathcal{K}^0$ denotes the set of all the kinematically admissible displacement fields that vanish on $\Gamma_u$, and $P(X, F(u))$ is the first Piola-Kirchhoff stress that can be computed from the stored-energy function through:

$$P(X, F(u)) = \frac{\partial W}{\partial F}(X, F(u)). \tag{2.4}$$

Since Equation (2.3) is a nonlinear equation, solutions typically cannot be obtained directly. Therefore, linearizations of Equation (2.3) are needed for the iterative solver in finite element analysis, such as the Newton-Raphson method. Assuming all external loads are deformation independent, the linearization of Equation (2.3) is given by:

$$G(u, v) + DG(u, v) \cdot w = 0 \quad \forall v \in \mathcal{K}^0 \tag{2.5}$$

with:

$$DG(u, v) \cdot w = G(u, v) + \int_{\Omega} \nabla v : \frac{\partial P}{\partial F}(X, F(u)) : \nabla w dX \tag{2.6}$$

where $w$ is the incremental displacement field.

### 2.2 Two-field mixed variational formulations

When the mechanical properties of the material approach the incompressibility limit, the variational principle involving only the displacement field will often perform poorly in standard finite element methods. This phenomenon is usually referred to as volumetric locking [20]. As a standard
remedy, variational principles which involve multiple fields are used [26, 27]. In this section, from the Principle of Minimum Potential Energy, a general derivation of two-field variational principles, valid for elastic materials with any level of compressibility, is presented [28, 29].

Consider a more general stored-energy function of the form \( \tilde{W}(X, F, J) \), involving an additional field \( J \). Through a partial Legendre transformation of \( J \) to a new field \( \tilde{q} \), a complementary stored-energy function \( \tilde{W}_C(X, F, \tilde{q}) \) is defined:

\[
\tilde{W}_C(X, F, \tilde{q}) = \sup_J \left[ \tilde{q}(J - 1) - \tilde{W}(X, F, J) \right].
\]

If \( \tilde{W}(X, F, J) \) is assumed to be a convex function of \( J \), \( \tilde{W}_C(X, F, \tilde{q}) \) will be a convex function of \( \tilde{q} \). Therefore, the following duality relation holds:

\[
\tilde{W}(X, F, J) = \sup_{\tilde{q}} \left[ \tilde{q}(J - 1) - \tilde{W}_C(X, F, \tilde{q}) \right].
\]

If we restrict the field \( J \) to be the determinant of the deformation gradient, the traditional stored-energy function defined in the preceding section is recovered:

\[
W(X, F) = \tilde{W}(X, F, J) \quad \text{with} \quad J = \det F
\]

According to Equations (2.8) and (2.9), the statement of the Principle of Minimum Potential Energy in Equation (2.1) is equivalent to finding \((u, \tilde{p})\) such that:

\[
\tilde{\Pi}(u, \tilde{p}) = \inf_{v \in \mathcal{K}} \sup_{\tilde{q} \in \mathcal{Q}} \tilde{\Pi}(v, \tilde{q})
\]

where

\[
\tilde{\Pi}(v, \tilde{q}) = \int_\Omega \left[ -\tilde{W}_C(X, F(v), \tilde{q}) + \tilde{q}(\det F(v) - 1) \right] dX
- \int_\Omega f \cdot v dX - \int_{\Gamma_t} t \cdot v dS
\]

with the space \( \mathcal{Q} \) consisting of square-integrable functions. The solution \( \tilde{p} \) in the above variational principle represents a pressure field. According to Equations (2.8) and (2.9), it relates the hydrostatic pressure field \( p \) (\( p = \operatorname{tr} \sigma \),
where $\sigma$ is the Cauchy stress) by the following relation:

$$p = \tilde{p} - \frac{1}{3 \det F} \frac{\partial \tilde{W}_C}{\partial F} (X, F, \tilde{p}) : F,$$

(2.12)

In order to obtain a variational principle involving a more physically meaningful pressure field, a deviatoric and dilatational decomposition of the stored-energy function is typically adopted [30, 31, 25, 32]. To accomplish this, we introduce a modified deformation gradient: $\tilde{F} = (\det F)^{-\frac{1}{3}} F$ and a modified stored-energy function: $\tilde{W} (X, \tilde{F}, J)$. By means of the partial Legendre transformation, a similar complementary stored-energy function $\tilde{W}_C (X, \tilde{F}, q)$ is obtained, which also satisfies the duality relation same as Equation (2.8). As a result, the new variational statement becomes finding $(u, p)$ such that:

$$\Pi (u, p) = \inf_{v \in K} \sup_{q \in Q} \Pi (v, q)$$

(2.13)

where $\Pi (v, q)$ is obtained by replacing $\tilde{W}_C (X, F(v), \tilde{q})$ in Equation (2.11) with the new complementary energy $\tilde{W}_C (X, \tilde{F}(v), q)$. In this case, the second field $p$ is identified exactly as the hydrostatic pressure field, which is an attractive feature that makes this method popular in the finite element literature [32, 33, 34, 28, 29].

We note that both variational principles in Equation (2.10) and Equation (2.13) lead to mixed finite element approximations. In the thesis, we will present both. Detailed study and discussion of their performance will be presented in Chapter 4. For convenience, in the remainder of the thesis, we will refer the variational principle in Equation (2.10) as “F-Formulation” and the variational principle in Equation (2.13) as “$\tilde{F}$-Formulation”.

### 2.3 Weak forms of the two-field mixed variational principles

In this section, we present the weak forms and their linearizations of the F-Formulation. In a similar manner, the variations of $\tilde{F}$-Formulation can also be obtained. As a weak statement of Equation (2.10), the variation of $\Pi (u, \tilde{p})$ must vanish with respect to arbitrary admissible displacement field $v$ and pressure field $\tilde{q}$:
\[ D\tilde{\Pi} (u, \tilde{p}) \cdot v = \int_{\Omega} \left[ -\frac{\partial W_C}{\partial F}(X, F(u), \tilde{p}) + \tilde{p} \frac{\partial (\det F)}{\partial F}(u) \right] : \nabla v dX \]

\[ - \int_{\Omega} f \cdot v dX - \int_{\Gamma_t} t \cdot v dS = 0 \quad \forall v \in K^0 \] (2.14)

\[ D\tilde{\Pi} (u, \tilde{p}) \cdot \tilde{q} = \int_{\Omega} \left[ \det F(u) - 1 - \frac{\partial W_C}{\partial \tilde{p}}(X, F(u), \tilde{p}) \right] \tilde{q} dX = 0 \quad \forall \tilde{q} \in Q \] (2.15)

Linearizations of Equations (2.14) and (2.15) are needed for solving the resulting system of equations. The linearized weak statement can be written in the form:

\[ D\tilde{\Pi} (u, \tilde{p}) \cdot v + a_{u,\tilde{p}} (v, w) + b_u (v, \tilde{g}) = 0 \quad \forall v \in K^0 \] (2.16)

\[ D\tilde{\Pi} (u, \tilde{p}) \cdot \tilde{q} + b_u (w, \tilde{q}) + c_{u,\tilde{p}} (\tilde{q}, \tilde{g}) = 0 \quad \forall \tilde{q} \in Q \] (2.17)

where

\[ a_{u,\tilde{p}} (v, w) = \int_{\Omega} \nabla v : \left[ -\frac{\partial^2 W_C}{\partial F \partial F}(X, F(u), \tilde{p}) + \tilde{p} \frac{\partial^2 (\det F)}{\partial F \partial F}(u) \right] : \nabla w dX \] (2.18)

\[ b_u (v, \tilde{g}) = \int_{\Omega} \nabla v : \frac{\partial (\det F)}{\partial F}(u) \tilde{g} dX \] (2.19)

\[ c_{u,\tilde{p}} (\tilde{q}, \tilde{g}) = - \int_{\Omega} \tilde{q} \frac{\partial^2 W_C}{\partial \tilde{p} \partial \tilde{p}}(X, F(u), \tilde{p}) \tilde{g} dX \] (2.20)

Here \( w \) and \( \tilde{g} \) are the incremental displacement and pressure fields, respectively.
CHAPTER 3

Polygonal finite elements

In this chapter, finite element approximations on polygonal meshes are discussed. First, we present the construction of the displacement and pressure spaces for polygonal finite elements. This leads to the subsequent finite element approximations of the weak forms for the displacement-based and mixed variational formulations. Finally, numerical quadrature schemes for polygonal finite elements are compared and discussed.

3.1 Displacement and pressure spaces on polygonal discretizations

While mesh topology has an influence on the performance of the finite element method, the choice of finite element spaces (e.g. interpolants) is also important. Consider $\mathcal{T}_h$ to be a partition of the domain $\Omega$ into non-overlapping polygons. The displacement space is chosen to be a conforming finite dimensional space denoted $\mathcal{K}_h$ with the degree of freedom being the displacements at each vertex of the mesh. At the element level, the displacement field is approximated by a linear combination of a set of barycentric coordinates. If we denote $\mathcal{V}(E)$ as the space spans the basis functions $\varphi_i$ over polygon $E$ with $n$ vertices, i.e. $\mathcal{V}(E) = \text{span}\{\varphi_1, \ldots, \varphi_n\}$, the finite dimensional space $\mathcal{K}_h$ is defined as:

$$\mathcal{K}_h = \{v_h \in [C^0(\Omega)]^2 \cap \mathcal{K} : v_h|_E \in [\mathcal{V}(E)]^2, \forall E \in \mathcal{T}_h\}$$

In the literature, there are quite a few barycentric coordinates available to construct finite dimensional spaces on planar polygons [35, 36, 37, 38, 39, 40, 41, 42]. By definition, they all satisfy the Kronecker-delta property, i.e. $\varphi_i(X_j) = \delta_{ij}$. Moreover, all the barycentric coordinates vary linearly along the edges and, in the interior, they are positive. Finally, all barycentric coordinates interpolates linear fields exactly, which means:
\[ \sum_{i=1}^{n} \varphi_i (X) = 1, \quad \sum_{i=1}^{n} \varphi_i (X) X_i = X \]  
(3.2)

where \( X_i \) is the position vector of vertex \( i \).

Most of the barycentric coordinates require the polygon to be convex, such as Wachspress coordinates, and barycentric coordinates constructed from iso-parametric mapping. To handle discretizations containing initially non-convex polygons, including those with collinear vertices, we adopt the Mean Value coordinates [43], which can be constructed on arbitrary polygons, as shown in Figures 3.1(b) and 3.1(c). The Mean Value coordinates are constructed directly on physical elements. In other words, no iso-parametric mapping is employed.

For a \( n \)-sided polygon \( E \) with \( i \)th vertex located at \( X_i \), its Mean Value coordinates for vertex \( i \) is defined as [43]:

\[ \varphi_i (X) = \frac{w_i (X)}{\sum_{j=1}^{n} w_j (X)} \]  
(3.3)

with \( w_i \) given by:

\[ w_i (X) = \frac{\tan \left[ \frac{\beta_{i-1} (X)}{2} \right] + \tan \left[ \frac{\beta_i (X)}{2} \right]}{{|X - X_i|}} \]  
(3.4)

where the angle \( \beta_i (X) \) is the angle defined in Figure 3.1(a).

In two-field mixed finite element methods, the approximation of the second field is also needed. In the moment, the second field is the pressure field, either \( \tilde{p} \) or \( p \), depending on the two-field variational principle used. For both cases,
as the most simple form of interpolation that leads to a stable approximation on polygonal meshes [10], a piecewise constant interpolation is adopted. It assumes the pressure field to be constant over each element. Accordingly, the basis functions used for this interpolation are:

\[ \chi_E(X) = \begin{cases} 1, & \text{if } X \in E \\ 0, & \text{otherwise} \end{cases} \forall E \in \mathcal{T}_h \]  

(3.5)

Consider the pressure field \( \tilde{p} \) as an example. As a consequence, the finite dimensional space for the pressure field consists of piecewise constant functions over \( \Omega \), denoted by \( Q_h \). It is a subspace of \( Q \) and is defined as:

\[ Q_h = \{ \tilde{q}_h \in Q : \tilde{q}_h|_E = \text{constant}, \forall E \in \mathcal{T}_h \} \]  

(3.6)

### 3.2 Conforming finite element approximations

Considering the finite element space for displacement \( K_h \subseteq K \) for the mesh \( \mathcal{T}_h \), the Galerkin approximation of the displacement-based formulation in Equation (2.3) consists of finding \( \mathbf{u}_h \in K_h \) such that:

\[ G(\mathbf{u}_h, \mathbf{v}_h) = 0 \quad \forall \mathbf{v}_h \in K_h^0 \]  

(3.7)

where \( K_h^0 \) is the defined as: \( K_h^0 = K_h \cap K^0 \).

Additionally, by introducing the finite element space for the pressure field, \( Q_h \subseteq Q \), the Galerkin approximation of the two-field variational principle can also be obtained. Take the \( \mathbf{F} \)-Formulation for example, its Galerkin approximation consists of finding \( (\mathbf{u}_h, \tilde{p}_h) \in K_h \times Q_h \) such that:

\[ D\Pi(\mathbf{u}_h, \tilde{p}_h) \cdot \mathbf{v}_h = 0 \quad \forall \mathbf{v}_h \in K_h^0 \]  

(3.8)

\[ D\Pi(\mathbf{u}_h, \tilde{p}_h) \cdot \tilde{q}_h = 0 \quad \forall \tilde{q}_h \in Q_h \]  

(3.9)

For a given discretization, the quantities in the above nonlinear equations and their linearizations are typically obtained by assembling the contributions from the element levels. In this work, we adopt standard procedures, which can be found in FEM textbooks, e.g., [23, 24].
3.3 Quadrature scheme

Unlike triangles and quads, there is no standard quadrature rule available for general irregular polygons with \( n \) sides \((n \geq 5)\). Alternatively, triangulation or quadrangulation schemes are usually used in the literature, which subdivides each polygon into triangles or quadrilaterals and applies the standard Gauss quadrature rules in each region \([8, 10]\). An illustration of these schemes is shown in Figure 3.2. The triangulation scheme is more flexible, as it can handle certain non-convex polygons where the quadrangulation schemes may lose validity. An example is shown in Figure 3.2(c) and 3.2(d) where the quadrangulation scheme gives one quadrature point outside the polygon while the triangulation scheme does not. Since Mean Value coordinates are adopted with the purpose to handle non-convex elements and elements with collinear vertices, the triangulation scheme is used in this work. For three-sided and four-sided polygons, the standard Gauss quadrature rules are used instead.

![Figure 3.2: Illustration of the “triangulation” and “quadrangulation” schemes for general polygons in physical domain: (a) triangulation scheme for convex polygon; (b) quadrangulation scheme for convex polygon (c) triangulation scheme for non-convex polygon; (d) quadrangulation scheme for convex polygon, a quadrature point is outside of the polygon.](image)

It is worthwhile noting that, because the finite element spaces for polygonal elements include non-polynomial (e.g. rational) functions, the quadrature schemes that discussed above can lead to consistency errors that do not vanish with mesh refinement \([44]\). As a result, the nonlinear version of the patch test, which provides a measure of the polynomial consistency, is not passed, even in the asymptotic sense, on polygonal meshes. This leads to a deterioration of the convergence of the finite element solutions. As will be shown in our numerical studies in Chapter 4, when the mesh size \( h \) become sufficiently small, the consistency errors start to dominate and the convergence rates of the error norms can exhibit noticeable decreases \([44]\). However, we
note that, for the range of the mesh sizes considered in this work, the consistency errors are still dominated by the discretization errors in finite element approximations and therefore the triangular scheme adopted is sufficiently accurate.
CHAPTER 4

Numerical Assessment

In this chapter, two numerical examples are presented to investigate the convergence, accuracy, and stability of the polygonal finite elements. The first example considers the problem of a cylindrical shell expanding under hydrostatic loading, in which we present a thorough verification of the convergence of the mixed polygonal finite element approximations. The second example considers the Cook’s benchmark problem to demonstrate the accuracy and numerical stability of the polygonal elements [45].

Throughout this chapter, plane strain condition is assumed and the material is considered to be Neo-Hookean. Both compressible and incompressible behaviors are investigated. For the compressible Neo-Hookean material, we adopt the commonly used stored energy function:

\[
W(X, F) = \frac{\mu}{2} \left[ (\det F)^{-\frac{2}{3}} F : F - 3 \right] + \frac{\kappa}{2} (\det F - 1)^2 \tag{4.1}
\]

with \(\mu\) and \(\kappa\) being shear and bulk modulus respectively. For the incompressible material, we consider both the complementary stored-energy functions for the so-called \(\bar{F}\)- and \(\tilde{F}\)- Formulations. According to the definitions in Chapter 2, they have the following forms:

\[
\tilde{W}_C (X, \bar{F}, \bar{p}) = -\frac{\mu}{2} (\bar{F} : \bar{F} - 3) \quad \text{and} \quad \tag{4.2}
\]

\[
W_C (X, F, p) = -\frac{\mu}{2} (F : F - 3) \tag{4.3}
\]

respectively. The standard Newton-Raphson algorithm is employed to solve the nonlinear system of equations and each loading step is regarded as convergent once the norm of the residual reduces below \(10^{-10}\) times that of the initial residual.
4.1 Expansion of a cylindrical shell

A cylindrical shell expansion problem is considered in this section to verify the convergence of the mixed polygonal finite element approximations. As illustrated in Figure 4.1(a), the shell is of inner radius $R_{\text{in}}$ and outer radius $R_{\text{out}}$, and is made up of an isotropic solid. The shell undergoes radially symmetric deformations, where the deformed position vector $\mathbf{x}$ has the form: $\mathbf{x} = \frac{r(R)}{R} \mathbf{X}$ with $R = \sqrt{\mathbf{X} \cdot \mathbf{X}}$, and its outer boundary is subjected to hydrostatic displacement loading, namely,

$$r (R_{\text{out}}) = \lambda R_{\text{in}}. \quad (4.4)$$

For incompressible Neo-Hookean solids, the analytical expressions of the displacement field $\mathbf{u} (\mathbf{X})$, the gradient of displacement field $\nabla \mathbf{u} (\mathbf{X})$, the hydrostatic pressure field $p (\mathbf{X})$ and the pressure field $\tilde{p} (\mathbf{X})$ defined in the F-Formulation are derived as:

$$\mathbf{u} (\mathbf{X}) = \left[ \frac{r (R)}{R} - 1 \right] \mathbf{X} \quad (4.5)$$

$$\nabla \mathbf{u} (\mathbf{X}) = \frac{1}{R^2} \left( r' (R) - \frac{r (R)}{R} \right) \mathbf{X} \otimes \mathbf{X} + \left[ \frac{r (R)}{R} - 1 \right] \mathbf{I} \quad (4.6)$$

$$p (\mathbf{X}) = -\frac{2\mu}{3} \left[ r' (R) \right]^2 + \frac{\mu}{3} \left\{ \frac{[r (R)]^2}{R^2} + 1 \right\}$$

$$+ \frac{\lambda^2 - R_{\text{out}}^2}{(\lambda^2 - R_{\text{out}}^2 + R^2) (\lambda^2 - R_{\text{out}}^2 + R_{\text{in}}^2)} + \mu \ln \frac{R r (R_{\text{in}})}{R_{\text{in}} r (R)} \quad (4.7)$$

$$\tilde{p} (\mathbf{X}) = p (\mathbf{X}) - \frac{\mu}{3} \left\{ [r' (R)]^2 + \frac{[r (R)]^2}{R^2} + 1 \right\} \quad (4.8)$$

where the notation $r' = \frac{dr}{dR}$ has been utilized for convenience and $r (R)$ has the following expression:

$$r (R) = \sqrt{R^2 + \lambda^2 - R_{\text{out}}^2} \quad (4.9)$$

We evaluate the convergence of mixed finite element approximations with
both F- and F- Formulations. In the finite element models, making use of symmetry, only a quadrant of the domain is modeled. Two discretizations, centroidal Voronoi tessellation (CVT) mesh and structured hexagonal-dominant mesh, are considered, as illustrated in Figures 4.1(b) and 4.1(c).

Three measures of the error are used to evaluated the convergence of the displacement field \( u \) and hydrostatic pressure field \( p \), including the normalized \( L^2 \)-norms and \( H^1 \)-seminorm, which are defined by the following expressions:

\[
\epsilon_{0,u} = \left[ \frac{\int_{\Omega} (u - u_h) \cdot (u - u_h) \, dX}{\int_{\Omega} u \cdot u \, dX} \right]^{\frac{1}{2}}
\]  
(4.10)

\[
\epsilon_{1,u} = \left[ \frac{\int_{\Omega} \nabla u \cdot \nabla (u - u_h) \, dX}{\int_{\Omega} \nabla u \cdot \nabla u \, dX} \right]^{\frac{1}{2}}
\]  
(4.11)

\[
\epsilon_{0,p} = \left[ \frac{\int_{\Omega} (p - p_h)^2 \, dX}{\int_{\Omega} p^2 \, dX} \right]^{\frac{1}{2}}
\]  
(4.12)

Since the F-Formulation does not directly yield the hydrostatic pressure field, a post processing step is used to obtained the hydrostatic pressure field when its error is to be evaluated. According to Equation (2.12), a piecewise constant hydrostatic pressure field \( p_h \) is recovered and used in the error evaluations in cases of F-Formulation. Within element \( E \), the recovered hydrostatic pressure field \( p_h|_E \) is assumed constant and can be computed by:
\[ p_h|_E = \bar{p}_h|_E - \frac{1}{3 \det \langle \mathbf{F}(\mathbf{u}_h) \rangle_E} \frac{\partial \bar{W}_C}{\partial \mathbf{F}} (\mathbf{X}, \langle \mathbf{F}(\mathbf{u}_h) \rangle_E, \bar{p}_h|_E) : \langle \mathbf{F}(\mathbf{u}_h) \rangle_E, \forall E \in \mathcal{T}_h \]

(4.13)

where \( \langle \cdot \rangle_E \) is the average of operator over element \( E \), defined as:

\[ \langle \cdot \rangle_E = \frac{1}{|E|} \int_E (\cdot) \, d\mathbf{X} \]

(4.14)

in which \( |E| \) denotes the area of element \( E \).

The convergence results are shown in Figures 4.2(a)-4.2(c), where the error measures are plotted against the average element diameter \( (h) \) at the deformation state of \( \lambda = 3 \). For the CVT meshes, each data point is obtained by averaging values from five sets of meshes with the same number of elements. Both numerical results from \( \mathbf{F} \)- and \( \mathbf{F} \)-Formulations indicate optimal convergence rates in the respective error norms. In particular, they display second-order convergence in the \( L^2 \)-norm of the error in displacement field and linear convergences in the \( H^1 \)-seminorm of the error in displacement field and the \( L^2 \)-norm of the error in hydrostatic pressure field. In fact, the \( L^2 \)-norm of the error in hydrostatic pressure field and the \( H^1 \)-seminorm of the error in displacement field for the \( \mathbf{F} \)-Formulation converge at a slightly faster rate than \( O(h) \). In terms of accuracy, numerical results obtained by finite element analysis using the \( \mathbf{F} \)-Formulation are found to be more accurate for this problem, as indicated by comparing the magnitudes of the three error measures in the figures.

Additionally, for the numerical results of the CVT meshes, we observe a noticeable degradation of the convergence rates in the \( H^1 \)-seminorm of the displacement field errors, as the mesh is refined for both formulations. This is similar to the behavior observed in the linear analysis [44] and is due to the persistence of consistency errors in the quadrature scheme used, which is discussed in Chapter 3. Again, we remark that the degradation only begins to show up when the mesh size \( h \) is smaller than 0.01. In the range of practical interest, however, the quadrature scheme used is sufficient and optimal convergence retained.

When undergoing large deformation, local material interpenetration, due to element flipping, tends to occur in finite element analysis when the \( \mathbf{F} \)-
Figure 4.2: Plots of normalized error norms versus average mesh size $h$ at the deformation state of $\lambda = 3$: (a) $\mathcal{L}^2$-norm in the error of displacement field; (b) $\mathcal{H}^1$-seminorm in the error of displacement field; (c) $\mathcal{L}^2$-norm in the error of hydrostatic pressure field.
Formulation is used, an interesting behavior that is not observed with the $\mathbf{F}$-Formulation. Figure 4.3(a) depicts a hexagon element and the corresponding flipped element in the deformed state. Although this appears to be unphysical, the flipping behavior is found to be helpful in some problems, allowing the elements to undergo larger deformation when subjected to constraints. A representative example is the cavitation problem, which will be presented in Chapter 5. Qualitatively speaking, the flipping behavior happens to preserve the area of the element according to the area constraint when a very large deformation field is imposed. As illustrated in Figure 4.3(a), the flipping cause a portion of the deformed element to have negative area, denoted by $A_E^-$, which helps the other portion with positive area $A_E^+$ to deform more while fulfilling the incompressibility constraint, i.e., $A_0^E = A_+^E + A_-^E$, where $A_0^E$ is the undeformed area of the element.

To better understand the flipping behavior and its influence on the convergence of the mixed finite element method, we perform a similar numerical study, which involves much larger local deformations that in turn introduces the flipping behavior. Consider a shell with a much smaller inner radius, $R_{in} = 0.01$, and the same outer radius, $R_{out} = 1$, subjected to a hydrostatic displacement loading on the outer boundary until a global stretch of $\lambda = 2$ is reached. Only CVT meshes are considered in this example. Because the radius of the inner hole is much smaller than the radius of the out boundary, the meshes are graded radially as shown in Figure 4.3(b). In the analysis, as the inner hole expands, the elements around it undergo very large deformations with stretches up to 150. Because of the large local deformations, we
find that finite element approximations using the $\overline{F}$-Formulation have difficulty in numerical convergence and hence are unable to capture the expansion of the inner hole, even with very refined meshes. In contrast, with the flipping behavior, the finite element models using the $F$-Formulation are capable of capturing the hole expansion. Table 4.1 summarizes the convergence of the normalized error norms as the refinement of mesh. In this example, we include all the error measures, i.e., the $L^2$-norm of the errors in the displacement field $u$, the pressure field $\tilde{p}$ and the hydrostatic pressure field $p$ and the $H^1$-seminorm of the error in the displacement field $u$. In the table, as the number of elements increases, all the error norms decrease as expected and their magnitudes stay in reasonable ranges, compared with Figures 4.2(a)-4.2(c). Meanwhile, we also find that the number of flipped elements in the deformed configuration decreases as the number of elements increases. These findings indicate that, even with the flipping behavior, the mixed finite element approximations are convergent. In addition, a distinct difference is observed between the magnitude of the $L^2$-norms of the two pressure fields $p$ and $\tilde{p}$. As a further investigation, in Figures 4.4(a) and 4.4(b), we plot the analytical solution and numerical results of the two pressure fields along the $X$ axis defined in the Figure 4.3(b). In particular, a fine CVT mesh of 25000 elements are used and the numerical results along the $X$ axis are obtained from those elements in the mesh whose edges are on the axis. From the figures, the numerical results of both pressure fields are in good agreements with the analytical solutions. However, as illustrated in the zoomed sections, due to the singular behavior of $p$, the numerical solutions of the pressure field $\tilde{p}$ are more accurate than those of the hydrostatic pressure field $p$. 

### Table 4.1: Summary of the error norms as mesh refinement

<table>
<thead>
<tr>
<th># element</th>
<th>$h_{min}$</th>
<th>$h_{max}$</th>
<th>$\epsilon_{0,u}$</th>
<th>$\epsilon_{1,u}$</th>
<th>$\epsilon_{0,p}$</th>
<th>$\epsilon_{0,\tilde{p}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>6.52E-04</td>
<td>5.99E-02</td>
<td>7.80E-04</td>
<td>2.69E-02</td>
<td>7.21E-01</td>
<td>7.02E-03</td>
</tr>
<tr>
<td>4000</td>
<td>2.10E-04</td>
<td>3.00E-02</td>
<td>2.40E-04</td>
<td>1.67E-02</td>
<td>3.07E-01</td>
<td>4.02E-03</td>
</tr>
<tr>
<td>8000</td>
<td>1.37E-04</td>
<td>2.07E-02</td>
<td>1.37E-04</td>
<td>1.31E-02</td>
<td>1.84E-01</td>
<td>3.54E-03</td>
</tr>
<tr>
<td>16000</td>
<td>9.19E-05</td>
<td>1.45E-02</td>
<td>8.10E-05</td>
<td>1.02E-02</td>
<td>1.03E-01</td>
<td>2.86E-03</td>
</tr>
<tr>
<td>25000</td>
<td>7.11E-05</td>
<td>1.18E-02</td>
<td>5.87E-05</td>
<td>9.02E-03</td>
<td>7.10E-02</td>
<td>2.63E-03</td>
</tr>
</tbody>
</table>
Figure 4.4: (a) Analytical solution and numerical result of the hydrostatic pressure fields $p$ as a function of $R$ along the $X$ axis. (b) Analytical solution and numerical result of the pressure fields $\tilde{p}$ as a function of $R$ along the $X$ axis.

4.2 Cook’s benchmark problem

In order to demonstrate the performance of polygonal finite elements in terms of accuracy and stability, a Cook’s benchmark example is performed with both lower order displacement and mixed finite elements. The problem consists of a tapered swept panel with dimensions depicted in Figure 4.5(a). The left boundary of the panel is fixed and its right boundary is subjected to a uniform shear loading $\mathbf{t} = [0, \tau]^T$ with $\tau = 0.1$. For simplicity, we assume the shear load is independent of deformation and hence it can be converted into nodal forces at the beginning of the finite element analysis. In addition to the CVT meshes, results by triangular and quadrilateral meshes are included as a comparison. An illustration of the three types of meshes is illustrated in Figures 4.5(b)-4.5(d).

Mesh refinements are performed to study the accuracy of the numerical results. In the study, we consider both compressible ($\mu = 1, \kappa = 1$) and incompressible ($\mu = 1$) materials, analyzed by displacement-based finite elements and mixed finite elements, respectively. Figure 4.6(a) shows the convergence of the vertical displacement at point A, obtained by displacement-based finite elements, and Figure 4.6(b) shows the results by mixed finite elements using both $\mathbf{F}$- and $\mathbf{F}'$- Formulations. Again, each data point for the CVT mesh represents an average of the results from five set of meshes. The reference values (11.95 and 8.519, respectively) are obtained by very fine meshes of quadratic
quadrilateral elements using ABAQUS. In both cases, CVT meshes exhibit the fastest convergence and yield the most accurate results with a similar number of elements.

In the refinement study, a non-convergent performance for vertical deflection at point A is observed for the triangular meshes when mixed triangular elements are used, which results from their numerical instability and locking behavior due to the volumetric constraint. In order to qualitatively evaluate the numerical stability of the lower order mixed finite elements, fringe plots of the hydrostatic pressure fields from the $\mathbf{F}$-Formulation in the final deformation state are shown in Figures 4.7(a)-4.7(c), for CVT meshes, quadrilateral meshes and triangular meshes respectively. From the fringe plots, both re-
results in triangular and quadrilateral meshes display numerical instabilities. They show either unphysical pressure field or pressure fields containing spurious checkerboard modes. By contrast, results in CVT meshes exhibit smooth distributions of the pressure field, indicating the stability of the mixed polygonal elements. Identical performances are also observed for the fringe plots from the F-Formulation.

![Fringe plots of hydrostatic pressure fields](image)

**Figure 4.7:** Fringe plots of hydrostatic pressure fields for (a) mixed polygonal elements; (b) mixed quadrilateral elements; (c) mixed triangular elements.
CHAPTER 5

Applications

With the goal of illustrating the applications of polygonal finite elements to study nonlinear elastic materials undergoing finite deformations, this chapter presents three representative examples with in the contexts: i) the finite deformation of an elastomer filled with an isotropic distribution of circular particles, ii) the finite deformation of an elastomer filled with a periodic distribution of anisotropic particles, and iii) cavitation instabilities. As demonstrated in the following sections, polygonal elements provide geometric flexibility to easily model inclusions with arbitrary geometries, incorporating periodic boundary conditions and bridging different length scales. In addition, the polygonal elements appear to be able to accommodate larger local distortions. Again, plane strain condition is assumed throughout this Chapter.

5.1 Elastomers reinforced with circular filler particles

In this example, we study the nonlinear elastic response of a filled elastomer, comprised of a random distribution of monodisperse circular particles firmly bonded to the matrix material, subjected to uniaxial tension. The particles are considered to be rigid, while the matrix is taken to be an incompressible Neo-Hookean rubber ($\mu = 1$). Figure 5.1(a) shows the geometry of a representative volume element (RVE), which is repeated periodically, containing a total of 30 particles at 30% volume fraction. The dimension of the RVE is one by one. To account for periodicity, periodic boundary conditions are applied to the RVE, which are defined as [46]:

\[
\begin{align*}
    u_k(1, X_2) - u_k(0, X_2) &= \langle F \rangle_{k1} - \delta_{k1} \\
    u_k(X_1, 1) - u_k(X_2, 0) &= \langle F \rangle_{k2} - \delta_{k2} \quad \forall k = 1, 2
\end{align*}
\]

(5.1)

where $\delta_{kl}$ is the Kronecker delta and $\langle F \rangle$ denotes the macroscopic deformation gradient with $\langle \cdot \rangle$ being a volume average operator, i.e.,
\[ \langle \cdot \rangle = \frac{1}{|\Omega|} \int_{\Omega} (\cdot) \, d\mathbf{X}. \quad (5.2) \]

Specifically, the macroscopic deformation gradient is \( \langle \mathbf{F} \rangle = \lambda \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda^{-1} \mathbf{e}_2 \otimes \mathbf{e}_2 \) in this case. Moreover, \( u_k \) and \( X_k \) (\( k=1, 2 \)) are the components of the displacement field and the position vector in undeformed configuration respectively, referring to a Cartesian frame of reference with the origin placed at the left lower corner of the RVE, as shown in Figure 5.1(a).

\[ \langle \cdot \rangle = \frac{1}{|\Omega|} \int_{\Omega} (\cdot) \, d\mathbf{X}. \quad (5.2) \]

In order to apply periodic boundary conditions, periodic meshes with matching nodal distribution on the opposing edges of the RVEs are required. For polygonal elements, because of their flexible geometry, the mesh can be

![Image](image_url)

Figure 5.1: (a) Problem set-up and RVE. (b) Domain discretized by a standard triangular mesh composed of 7694 quadratic elements (T6) and 15617 nodes total, with 12112 nodes in the matrix phase. (c) Domain discretized by a polygonal mesh with 6035 n-gons and 12232 nodes. (d) The composition of the polygonal mesh.
locally modified to become periodic by simply inserting nodes at appropriate locations. In addition, the inclusions, no matter their shape, can be modeled as single polygons. These concepts are illustrated in Figure 5.2.

Two discretizations are considered in this example: a polygonal mesh and, for comparison purposes, a triangular mesh. Figure 5.1(c) shows the polygonal mesh utilized to solve the problem where each particle is modeled by a single element, while Figure 5.1(b) depicts the triangular mesh. More specifically, the polygonal mesh consists of mixed linear elements with constant pressure. The triangular mesh, on the other hand, consists of hybrid quadratic elements with linear pressure (CPE6MH in ABAQUS) having a similar total number of degrees of freedom (DOFs), in the matrix phase, as the polygonal one. The polygonal discretizations utilize the $F$-Formulation.

The deformed configurations of the RVE with polygonal elements and triangular elements are shown in Figures 5.3(a) and 5.3(b), at $\lambda = 2.1$ and $\lambda = 1.46$, respectively, which represent the maximum global deformations reached in each case. On the deformed meshes, the maximum stretch of each element is plotted, with those having maximum stretch of 5 or larger shown in red. From the fringe plots of the elemental stretch field, it is clear that a greater number of polygonal elements undergo stretches greater than 5. In addition, the macroscopic quantities including the stored-energy function $\langle W \rangle$ and first Piola-Kirchoff stress $\langle P \rangle_{11}$ are plotted against the macroscopic stretch $\lambda$ for the two meshes in Figures 5.3(c) and 5.3(d). Both meshes agree
reasonably well with the analytical solutions available in the literature, for solids reinforced by a random and isotropic distribution of rigid particles [47]. At large strains, finite element solutions display stiffer responses, possibly due to the effect of particle interactions, which are significant at large deformations. For this problem, the $F$-Formulation and element flipping behavior (see Figure 4.3(a)) are found to be of not much help in making the RVE deform more.

Figure 5.3: (a) Deformed shape using the polygonal mesh, in which the analysis stops at global stretch of $\lambda = 2.1$. (b) Deformed shape using the modified quadratic hybrid elements (CPE6MH) in ABAQUS, in which the analysis stops at $\lambda = 1.46$. (c) Macroscopic stress $\langle P \rangle_{11}$ vs. the applied stretch $\lambda$. (d) Macroscopic stored-energy function $\langle W \rangle$ vs. the applied stretch $\lambda$. 

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5.2 Elastomers reinforced with anisotropic filler particles

At finite deformations, large local deformations within filled elastomers may be generated because of rigid particles coming into close proximity as discussed in the preceding example, but also may be due to the large rigid rotations that anisotropic particles may undergo. In this example, we consider the latter case. To this end, we study the nonlinear elastic response of a filled elastomer, comprised of a periodic square distribution of elliptical particles firmly bonded to the matrix material, that is subjected to simple shear, i.e., \( \langle \mathbf{F} \rangle = \mathbf{I} + \gamma \mathbf{e}_1 \otimes \mathbf{e}_2 \). As in the foregoing example, the particles are considered to be rigid, while the matrix is taken to be a compressible Neo-Hookean rubber with shear and bulk moduli \( \mu = 1 \) and \( \kappa = 100 \), (cf. Equation (4.1)). Figure 5.4(a) shows the geometry of the RVE for the case of a particle of aspect ratio 4 and approximate volume fraction 15%.

For this problem, we make use of a fine polygonal mesh, shown in Figure 5.4(c), with a rigid elliptical particle consisting of a single element (153-gon). Again, nodes are inserted on each boundary to guarantee a periodic mesh. As a comparison, we also solve the problem with a structured mesh comprised of quadrilateral elements. This conventional quadrilateral mesh is also shown in Figure 5.4(b). Both meshes contain a similar number of degrees of freedom in the matrix phase. Due to the applied shear deformation, the elliptical inclusion rotates. The angle of rotation as a function of the applied amount of shear \( \gamma \) is plotted in Figure 5.5(a). For further scrutiny of the result, the final deformed shapes of the RVE and detailed views of the regions around the elliptical particles are displayed in Figures 5.5(a) and 5.5(b). The maximum stretches of each element are plotted on the deformed meshes, with those having maximum stretch of 10 or above shown in red. From the fringe plots, a greater number of polygonal elements undergo stretches greater than 10 when compared to the quadrilateral elements. Together with the preceding example of circular particles, this example demonstrates the ability of polygonal elements to handle large local deformations. The fact that the “particle” consist of just a single element is also of great advantage to model limiting behaviors such as infinitely rigid or vacuous inclusion.
5.3 Cavitation in rubber

In this example, we discuss the cavitation in rubber, that is, the sudden “appearance” of internal cavities in the interior of rubber at critically large loadings. This phenomenon corresponds to the growth of defects inherent in rubber. Such defects can be of various natures (e.g., weak regions of the polymer network, actual holes, particles of dust) and of various geometries ranging from submicron to supramicron in length scale \([48, 49]\). Because of the random distributions of cavities and the huge local deformations in the
regions around cavities, induced by the growth of defects into finite sizes, the modeling of cavitation problems with standard finite elements, especially linear elements, is computationally challenging. A detailed discussion of these issues can be found in the paper by Xu and Henao, in which they propose a non-conforming finite element approach as a solution to the problem [50].

As our first attempt to model such a problem, we study the cavitation problem employing the mixed polygonal finite elements. In particular, the F Formulation is adopted here. We consider a circular disk of radius $R_d = 1$ that contains two circular defects of radius $R_c = 0.001$ in its interior. The disk is centered at $(0, 0)$ and the two defects are placed at $(0, 0)$ and $(0.3, 0)$ respectively. The outer boundary of the disk is subjected to hydrostatic displacement loading until a radial stretch of 2 is reached. The constitutive properties of the disk are characterized by an one-term incompressible Lopez-Pamies material with parameters $\alpha = 0.8$, $\mu = 1$ [51], which ensures growth conditions of the underlying stored-energy function that allow for cavitation [52]:

$$W(X, F, J) = \frac{3^{1-\alpha}\mu}{2\alpha} [(F : F)^{\alpha} - 3^{\alpha}] \quad (5.3)$$

The corresponding complementary stored-energy function $\tilde{W}_C(X, F, \tilde{p})$ has the form:

$$\tilde{W}_C(X, F, \tilde{p}) = -\frac{3^{1-\alpha}\mu}{2\alpha} [(F : F)^{\alpha} - 3^{\alpha}] \quad (5.4)$$
The discretization of such a problem is by no mean an easy task as the mesh has to bridge two very different length scales; the scale of the defects (0.001) and the scale of the disk (1). Making use of the polygonal discretization, and exploiting the flexibility of Voronoi tessellations, we can easily obtain a mesh with two length scales by using specific density functions for mesh gradation [13] tailored to the problem at hand. Figure 5.6(a) illustrates the polygonal mesh of 6000 elements utilized in this example. Figure 5.6(c) shows snapshots of the disk at five different values of the applied hydrostatic stretch.

Qualitatively, the growth of the two cavities is captured very well. From the series of deformed configurations shown in Figure 5.6(c), both defects grow at the beginning of the loading. At around 5% stretch, the defect at the right stops growing and the one in the center starts to dominate and keeps growing till the final stretch 100% is reached. As a result, from the growth of two cavities, very large local deformations are introduced to the elements around the cavities, the maximum of which can be up to 1500 according to the figures. For those elements, flipping behavior is observed, a similar situation to what is discussed in the numerical studies of Chapter 4.

In contrast, finite element models with $F$-Formulation, which are typically employed in the finite element literature, do not contain flipped elements, yet the growth of the defects can not be captured because of difficulties in numerical convergence. Again, we stress that the flipping behavior is helpful to capture the growth of the defects and will not affect the accuracy of the results in this problem.
Figure 5.6: (a) The polygonal discretization of the disk domain of $R_d = 1$ centered at $(0, 0)$. Two circular cavities with initial radius $R_c = 0.001$ are placed at $(0, 0)$ and $(0.3, 0)$. (b) The composition of the polygonal mesh. (c) The growth of the cavities modeled using polygonal mesh under different levels of global stretches and detailed views.
CHAPTER 6

Concluding remarks

The modeling of nonlinear elastic materials by the finite element method at finite deformations is a challenging task because of the large localized deformations. In this work, we present and explore an alternative approach to model nonlinear elastic materials by using polygonal finite elements. In the context of finite elasticity, a general yet simple theoretical framework is proposed that allows the derivation of the two-field variational principle for arbitrary nonlinear elastic materials. Depending on the forms of the stored-energy functions adopted, i.e., with or without the deviatoric and dilatational decompositions, two mixed variational formulations are obtained. Based on the theoretical settings, we present both displacement-based and lower order mixed polygonal finite element approximations for finite elasticity problems. At the element level, the mixed polygonal finite element consists of a linearly complete displacement field approximated by a set of barycentric coordinates and a constant pressure field. With thorough numerical investigations, mixed polygonal elements are shown to be numerically stable on Voronoi-type meshes without any additional stabilization treatment and the convergence of the displacement field and pressure field are verified in the range of mesh size of practical interests for both the $F$- and $F$-Formulations. Furthermore, polygonal finite elements are applied to the study of practical problems within the contexts of filled elastomers and cavitation instabilities. In the applications, the polygonal finite elements are found to be useful in modeling inclusions with arbitrary geometries, incorporating periodic boundary conditions and bridging different length scales. Moreover, polygonal elements appear to be more tolerant of very large local deformations.

The available quadrature schemes on polygonal discretizations will lead to consistency errors that do not vanish under mesh refinement. The persistence of these errors can cause suboptimal convergence or even non-convergence in the finite element solutions. As a remedy, using sufficiently large number of quadrature points can lower the consistency errors such that they are
dominated by the approximations errors. For linear polygonal elements, as shown from the numerical studies in this thesis, the triangulation scheme with three quadrature points in each subdivided triangle appear to be sufficient to ensure accuracy and optimal convergence in practice. However, for higher-order or 3D elements, the number of required integration points can become prohibitively large, which makes such approaches less attractive from a practical point of view. Therefore, for the extension of the current framework to higher-order polygonal or 3D polyhedral elements, better and more efficient quadrature schemes are needed.

As a final remark, when subjected to large local deformation fields, an interesting element flipping behavior in the deformed configuration is observed in the mixed finite element analysis when the F-Formulation is adopted. This effect is localized and such behavior, as demonstrated by the numerical studies and examples in the thesis, is found to be helpful in some problems where elements are allowed to deform more and still yield convergent solutions. However, a rigorous theoretical justification is needed for a better understanding of the flipping behavior and its influence on the quality of finite element solutions.
REFERENCES


