Master’s Dissertation in Mechanical Engineering on

**Ductile Failure Analysis in Metallic Materials through Computational Homogenization**

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Porto, July 2019
To my parents
and Raquel.
Abstract

Ductile Failure Analysis in Metallic Materials through Computational Homogenization

Over the last years, the use of computational tools for the study of the constitutive behavior of materials has received increasing attention, particularly the modeling of heterogeneous materials by an interchange of information between the macro and micro scales. The macroscopic response is obtained by the homogenization of microscopic Representative Volume Elements (RVEs).

The ductile failure of metals at low homologous temperatures is largely determined by the nucleation, growth and coalescence of microstructural voids. These phenomena are strongly dependent on the stress state, specifically on parameters such as triaxiality and Lode angle. High triaxiality stress states tend to increase the void size, whereas lower triaxialities distort them significantly.

In this work, the influence of factors such as porosity, Lode parameter, triaxiality, material properties and void geometry on the overall macroscopic yield response is investigated. Using the Finite Element Method, several RVEs containing voids are analyzed, subject to different boundary conditions, with both isotropic (von Mises) and anisotropic (mono- and polycrystalline FCC slip) matrix material models. A stress-driven homogenization approach is used, allowing for strict control over both triaxiality and Lode angle. Various parametric studies are conducted, and the resulting yield curves are compared with analytical models whenever possible.

For von Mises matrices, the numerical results are compared with the models of Gurson (1977), GTN (Tvergaard and Needleman, 1984), Madou and Leblond (2012a,b) (ML) and Danas and Aravas (2012) (MVAR). The single crystal results are compared with the models of X. Han et al. (2013) and Mbiakop, Constantinescu, et al. (2015b) (MVAR). The numerical solutions capture the same trend as the analytical models. In general, for high triaxialities, void growth up to the yield onset is not negligible. This significantly affects the yield estimates for those loadings. A corrected porosity expression is proposed to predict the porosity at yield as a function of the triaxiality. With isotropic matrices, the effect of the Lode parameter is marginal. For single crystal matrices, its influence is mostly caused by the response of the constitutive model, not by the voids. Even though the Lode parameter also affects the void distortion, the magnitude of this effect is reduced. In the studies conducted, the influence of void geometry and orientation is found to be of the same magnitude as the Lode parameter, for the void volume fractions considered. For
single crystals, lattice orientation plays an important role on the yield onset. The Han et al. model has also been suggested for implementation in the scope of finite element analysis.

**Keywords:** Ductile failure, Homogenization, Yield response, Lode parameter, Triaxiality
Resumo

Análise da Fratura Dúctil em Materiais Metálicos através de Homogeneização Computacional

Nos últimos anos, a utilização de ferramentas computacionais para o estudo do comportamento constitutivo dos materiais tem recebido uma atenção crescente, em particular, a modelação de materiais heterogêneos através de uma troca de informação entre a macro- e micro-escala. A resposta macroscópica é obtida pela homogeneização de Elementos de Volume Representativos (RVEs) microscópicos.

A fratura dúctil dos metais a baixas temperaturas é largamente determinada pela nucleação, crescimento e coalescência de vazios microestruturais. Estes fenômenos são fortemente dependentes do estado de tensão, especialmente de parâmetros como a triaxialidade e o ângulo de Lode. Estados de tensão com elevadas triaxialidades tendem a aumentar o tamanho do vazio, enquanto que triaxialidades mais baixas distorcem-os significativamente.

Neste trabalho, a influência de fatores como a porosidade, o parâmetro de Lode, triaxialidade, propriedades da matriz e geometria dos vazios é analisada. Recorrendo ao Método dos Elementos Finitos, vários RVEs com vazios são analisados, sujeitos a diferentes condições de fronteira, com matrizes isotrópicas (von Mises) e anisotrópicas (mono- e policristais FCC). É utilizada uma abordagem “stress-driven”, na qual é possível ter controlo rigoroso sobre a triaxialidade e ângulo de Lode. Vários estudos paramétricos foram realizados, e as curvas de cedência resultantes são comparadas com modelos analíticos sempre que possível.

estudos efetuados, a influência da geometria e orientação dos vazios é da mesma ordem de grandeza da do parâmetro de Lode. No entanto, para monocristais, a orientação do cristal é importante no início da cedência. É também sugerida a implementação do modelo de Han et al. para análises em elementos finitos.

**Palavras-chave:** Fratura dúctil, Homogeneização, Cedência, Parâmetro de Lode, Triaxialidade
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<td>116</td>
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</tr>
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Chapter 6

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Nomenclature

General notation
\( a \) Scalar
\( \text{\( a \)}} \) Second order tensor
\( \text{\( a \)}} \) Fourth order tensor
\( \mathcal{A} \) Space, set or body
\( \mathcal{A} \) Constitutive functional

Acronyms
2D Bidimensional
3D Tridimensional
BCC Body-centered cubic
CM2S Computational Multi-Scale Modeling of Solids and Structures
FCC Face-centered cubic
FEM Finite Element Method
GTN Gurson-Tvergaard-Needleman
Links Large Strain Implicit Non-linear Finite Element Analysis of Solids Linking Scales
ML Madou-Leblond
MVAR Modified variational
RVE Representative Volume Element

Indices
\( (\bullet)_{\text{iso}} \) Isochoric component
\( (\bullet)_{\text{vol}} \) Volumetric component
\( (\bullet)^{s} \) Matrix subdomain of the RVE
\( (\bullet)^{v} \) Relative to void
\( (\bullet)^{0} \) Reference configuration
\( (\bullet)^{\mu} \) Microscopic domain
\( (\bullet)^{(m)} \) Member \( m \) of a family
\( (\bullet)^{\varphi} \) Field on configuration \( \varphi \)
Field after a transformation

History up to time \( t \)

Field at the instant \( t \)

Field at time \( t_n \)

Interpolated field

Relative to the finite element

Global entity in Finite Element Method

Relative to slip system \( \alpha \)

Incremental constitutive function

Operators

- \( \mathbf{A}(\bullet) \): Finite element assembly
- \( \det(\bullet) \): Determinant
- \( \text{div}_p(\bullet) \): Material divergence
- \( \text{div}_x(\bullet) \): Spatial divergence
- \( \ln(\bullet) \): Natural logarithm
- \( \text{tr}(\bullet) \): Trace
- \( \text{sign}(\bullet) \): Sign function
- \( \max(\bullet) \): Maximum
- \( (\bullet)^\top \): Transposed
- \( (\bullet)^{-1} \): Inverse
- \( (\bullet)^{-\top} \): Inverse of the transposed
- \( \nabla(\bullet) \): Gradient
- \( \nabla_p(\bullet) \): Material gradient
- \( \nabla_x(\bullet) \): Spatial gradient
- \( \partial(\bullet) \): Boundary of domain
- \( (\bullet) \): Material time derivative
- \( (\bullet) \): Material double time derivative
- \( (\bullet) \cdot (\bullet) \): Tensor simple contraction
- \( (\bullet) : (\bullet) \): Tensor double contraction
- \( (\bullet) \times (\bullet) \): Vectorial product
- \( (\bullet) \otimes (\bullet) \): Tensorial product
- \( |(\bullet)| \): Absolute value of scalar
- \( ||(\bullet)|| \): Euclidean norm of vector or tensor

Variables

- \( a \): Area; Generic scalar field; Parameter of corrected porosity
- \( a \): Lattice vector
- \( A \): Generic tensor field
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>Consistent spatial tangent modulus</td>
</tr>
<tr>
<td>A</td>
<td>Consistent material tangent modulus</td>
</tr>
<tr>
<td>b</td>
<td>Parameter of corrected porosity</td>
</tr>
<tr>
<td>b</td>
<td>Body forces per unit deformed volume; Lattice vector</td>
</tr>
<tr>
<td>b₀</td>
<td>Body forces per unit reference volume</td>
</tr>
<tr>
<td>B</td>
<td>Left Cauchy-Green strain tensor; Discrete symmetric gradient operator</td>
</tr>
<tr>
<td>B</td>
<td>Constitutive functional for the specific free energy</td>
</tr>
<tr>
<td>c</td>
<td>Continuum body</td>
</tr>
<tr>
<td>c</td>
<td>Parameter of corrected porosity</td>
</tr>
<tr>
<td>c</td>
<td>Lattice vector</td>
</tr>
<tr>
<td>C</td>
<td>Right Cauchy-Green strain tensor</td>
</tr>
<tr>
<td>C</td>
<td>Fourth-order elasticity tensor</td>
</tr>
<tr>
<td>D</td>
<td>Stretch rate tensor</td>
</tr>
<tr>
<td>e</td>
<td>Specific internal energy</td>
</tr>
<tr>
<td>E</td>
<td>Young’s modulus</td>
</tr>
<tr>
<td>eᵢ</td>
<td>Generic base vector</td>
</tr>
<tr>
<td>Eₑ</td>
<td>Green-Lagrange elastic strain tensor</td>
</tr>
<tr>
<td>Eₑ⁽ᵐ⁾</td>
<td>Lagrangian strain tensor of order m</td>
</tr>
<tr>
<td>f</td>
<td>Void volume fraction</td>
</tr>
<tr>
<td>f*</td>
<td>GTN corrected void volume fraction</td>
</tr>
<tr>
<td>fₖ</td>
<td>GTN critical porosity</td>
</tr>
<tr>
<td>f₀</td>
<td>Initial porosity</td>
</tr>
<tr>
<td>f∞</td>
<td>Corrected porosity for hydrostatic loadings</td>
</tr>
<tr>
<td>fₚ</td>
<td>Porosity at yield</td>
</tr>
<tr>
<td>f</td>
<td>Force vector</td>
</tr>
<tr>
<td>F</td>
<td>Deformation gradient</td>
</tr>
<tr>
<td>Fₑ</td>
<td>Elastic part of the deformation gradient</td>
</tr>
<tr>
<td>Fₚ</td>
<td>Plastic part of the deformation gradient</td>
</tr>
<tr>
<td>G</td>
<td>Constitutive functional for the Cauchy stress tensor</td>
</tr>
<tr>
<td>g</td>
<td>Secondary porosity</td>
</tr>
<tr>
<td>G</td>
<td>Shear modulus</td>
</tr>
<tr>
<td>g</td>
<td>Spatial temperature gradient</td>
</tr>
<tr>
<td>G</td>
<td>Discrete spatial gradient operator</td>
</tr>
<tr>
<td>Iᵢ</td>
<td>i-th invariant of the Cauchy stress tensor</td>
</tr>
<tr>
<td>H</td>
<td>Hardening modulus</td>
</tr>
<tr>
<td>h</td>
<td>ML correction factors</td>
</tr>
<tr>
<td>s₀</td>
<td>Constitutive functional for the specific entropy</td>
</tr>
<tr>
<td>I</td>
<td>Identity tensor</td>
</tr>
<tr>
<td>l</td>
<td>Fourth order identity tensor</td>
</tr>
</tbody>
</table>
\( j \)  
Determinant of the transformation jacobian

\( J \)  
Determinant of the deformation gradient

\( J_i \)  
i-th invariant of the deviatoric stress tensor

\( \mathbf{J} \)  
Hydrostatic projection tensor

\( \mathcal{J} \)  
 Constitutive functional for the heat flux

\( L \)  
Length; Lode parameter

\( l \)  
Ellipsoid axis

\( L_p \)  
Plastic rate of deformation gradient

\( \mathbf{L} \)  
ML localization tensor

\( \mathcal{L} \)  
ML scalar

\( k_i \)  
Lattice integer

\( K \)  
Bulk modulus

\( k \)  
Ellipsoid axis

\( \mathbf{K}_T \)  
Global tangent stiffness matrix

\( \mathcal{K} \)  
Set of kinematically admissible displacements

\( \mathcal{K}^* \)  
Set of minimally constrained kinematically admissible displacements

\( \tilde{\mathcal{K}}^* \)  
Set of minimally constrained kinematically admissible displacement fluctuations

\( m \)  
Mass of a body

\( m \)  
Ellipsoid axis; Normal to the slip plane

\( M^\alpha \)  
Spatial Schmid tensor

\( \mathbf{M}^{\text{var}} \)  
Variational tensor

\( \mathbf{M}^{\text{mvar}} \)  
Modified variational tensor

\( n \)  
Viscoplastic rate-sensitivity parameter

\( n_{\text{slip}} \)  
Number of slip systems

\( N \)  
Shape function

\( n \)  
Normal vector to a surface

\( N \)  
Flow vector

\( N^e \)  
Element interpolation matrix

\( N^g \)  
Global interpolation matrix

\( \Theta^+ \)  
Set of proper orthogonal rotations

\( p \)  
Hydrostatic pressure

\( p \)  
Position of a particle in the reference configuration

\( P \)  
First Piola-Kirchhoff stress tensor

\( \mathcal{P} \)  
ML quadratic form

\( q_i \)  
i-th parameter of GTN model

\( q_j \)  
Correction factor for the hydrostatic point of MVAR

\( q \)  
Position of the center of rotation; heat flux

\( Q \)  
Rotation tensor

\( \mathcal{Q} \)  
ML quadratic form
Density of heat production; Radial coordinate
Residual vector; Point on a lattice
Rotation tensor
Specific entropy
Set of microstructural variables
Deviatoric stress tensor; Slip direction
Unit von Mises stress deviatoric stress tensor
Second Piola-Kirchhoff stress tensor
Variational tensor
Modified variational tensor
Symmetry group
Triaxiality
Surface traction per unit deformed area
Surface traction per unit reference area
Time
Variational effective stress potential
Displacement field
Displacement fluctuation field
Right stretch tensor
Global vector of nodal displacements
Volume
Velocity field
Left stretch tensor
Set of admissible virtual displacements
Position of a particle in the deformed configuration
Translation point
Weight of Gauss points; Ellipsoid semi-axes ratio
Contraction/dilation ratio; Lattice angle
Set of internal variables
Lattice angle
Parameter of the hydrostatic point correction
Elastic domain slope
Convergence tolerance
Virtual displacement vector
Accumulated slip; Lattice angle
Plastic multiplier
Reference slip rate
Slope of homogenized stress-strain curves
Loading factor
\( \nu \) Poisson ratio
\( \Phi \) Yield function
\( \Pi \) Eshelby’s second tensor
\( \psi \) Specific free energy
\( \psi^e \) Elastic strain energy function
\( \Psi \) Flow potential
\( \rho \) Mass density; Magnitude on the deviatoric plane
\( \sigma \) Uniaxial stress
\( \sigma_{eq} \) von Mises equivalent stress
\( \sigma_y \) Uniaxial yield stress
\( \sigma \) Cauchy stress tensor
\( \dot{\sigma} \) Unit von Mises stress Cauchy stress tensor
\( \tau^{\alpha} \) Schmid resolved stress
\( \tau_y^{\alpha} \) Critical resolved shear stress
\( \tau^{\alpha*} \) Effective resolved shear stress
\( \tau \) Kirchhoff stress tensor
\( \theta \) Temperature; Angle on the deviatoric plane
\( \varepsilon \) Uniaxial infinitesimal strain
\( \varepsilon^e \) Uniaxial infinitesimal elastic strain
\( \varepsilon^p \) Uniaxial infinitesimal plastic strain; Accumulated plastic strain
\( \bar{\varepsilon}^p \) Accumulated plastic strain
\( \varepsilon \) Infinitesimal strain tensor
\( \varepsilon^{(m)} \) Eulerian strain tensor of order \( m \)
\( \varphi \) Deformation mapping function
\( \xi \) Projection on the hydrostatic axis
\( \xi \) Coordinates of the Gauss points
\( \Omega \) Domain of a continuum body in the reference configuration
\( \Omega \) Rotation rate tensor
Chapter 1
Introduction

Throughout the last years, computational tools have become fundamental in industrial applications. Using numerical results instead of experimental tests leads to reductions in costs for most engineering applications. Furthermore, the increasing computational power allows for the solution of problems with increasing complexity. Within the scope of structural analysis, where the Finite Element Method is the most widespread technique, accurate representations of the constitutive behavior of the materials is fundamental.

For metals, traditional constitutive models such as the von Mises model have proven to be representative of the response of the material for small strains. Nonetheless, in cases where the plastic strain is close to its rupture value, a group of microscopic phenomena takes place and significantly reduces the strength of the metal, and traditional constitutive models do not capture such damage mechanics. The ductile failure of metallic materials is a consequence of damage by void nucleation, growth and coalescence. These phenomena were first identified in the 1950s, and since then, various authors have conducted micromechanical studies to understand them.

To accurately represent the constitutive behavior of some materials, a recent strategy of interest is Multi-scale modeling. Instead of using a set of constitutive relations for the macroscopic problem, the material behavior is described through a Representative Volume Element (RVE) of its microstructure. Thus, by selecting an appropriate RVE, the complex behavior of an arbitrary microstructure can be modeled. An averaging technique called Homogenization connects both scales.

Even though most materials appear continuous at a macroscopic scale, at smaller scales these are constituted by atoms. In most metallic materials at room temperatures, these atoms are arranged in a crystallographic structure that forms a single crystal (or grain). These structures are known to be highly anisotropic. Nevertheless, as the number of grains increases, the trend is for the response of the material to become isotropic. In most metals, voids are typically found at scales where the single crystal still dominates the behavior of the matrix. For this reason, accurate multi-scale modeling of a void’s influence requires a thorough selection of appropriate constitutive models for the microscopic matrix.

Finally, the ductile failure of metallic materials is dominated by the void nucleation, growth and coalescence. Various models were developed for each of these phenomena. In this work, focus is given to the study of models for void growth, up to the yield onset. These models introduce a dependency of the hydrostatic pressure on the yield function,
and thus the response is now dependent on the stress triaxiality. In contrast, the classical Tresca and von Mises criteria are pressure-insensitive.

At the end of this work, a general review of the yield response of porous media is given, and some improvements to existing analytical models are proposed. It should be mentioned that the yielding response is only the first topic of a constitutive model for porous media. A complete model should incorporate a set of variables that can accurately model the damage induced by the porosity in metals, as well as their appropriate evolution laws.

1.1 Main goals

The main goal of this work is to assess the influence of parameters such as porosity, Lode parameter and triaxiality in the yield response of porous materials using computational homogenization.

Firstly, a set of analytical models for porous media is analyzed and implemented, to serve as a comparison to numerical results obtained. The influence of the parameters mentioned above is studied for these models, as an initial prediction for the yield response.

Then, finite element analyses of RVEs containing voids are carried. By using a stress driven approach, a strict control over the triaxiality and Lode parameter is achieved. In a first study, an isotropic (von Mises) matrix is considered. The numerical results are compared with the analytical models whenever possible. Furthermore, the influence of void geometry and orientation is also assessed. A model accounting for the evolution of the porosity in the elastic region is proposed, and the analytical models are corrected to account for the void growth up to the yield onset.

Finally, a similar study is conducted, but considering a single crystal matrix. A review of the models available in the literature is presented. In addition to the studies mentioned previously, the influence of the lattice orientation and number of grains is assessed. The numerical results are compared with the analytical models. By using these techniques, a model for porous single crystals is studied and its applicability for a constitutive model is assessed.

1.2 Brief literature review

Some of the first evidence of void nucleation, growth and coalescence on ductile failure of metals was identified in Tipper (1949). Over the following years, various micromechanical studies in void growth took place (McClintock, 1968; J. R. Rice and Tracey, 1969). One of the most important works in this subject was the limit analysis of Gurson (1977). After this publication, in Chu and Needleman (1980), Tvergaard (1981), Tvergaard (1982), and Tvergaard and Needleman (1984) further improvements to Gurson’s model were proposed, resulting in the GTN model. Further extensions to the model tried to incorporate void shape effects. For instance, the GLD model proposed in Gologanu et al. (1997) extended Gurson’s model to spheroidal voids. More recently, the ML model in Madou and Leblond (2012a,b, 2013) and Madou, Leblond, and Morin (2013) further extended the model to ellipsoidal shapes. An alternative family of models for porous media resulted from the

Regarding void nucleation, Chu and Needleman (1980) have accounted for two possible contributions: one term controlled by the strain (as described by Goods and Brown (1983)) and other controlled by the stress (Argon et al., 1975; Beremin, 1981). Nevertheless, these two nucleation terms lead to significant differences in ductility prediction (J. Rice, 1976). On the other hand, void coalescence can be interpreted either as a plastic flow localization phenomenon or as a strain concentration within layers of thickness comparable to the void size (Benzerga, Leblond, et al., 2016). The first method predicts that a new plastic deformation mechanism appears abruptly, and results in a sudden decrease in strength (J. R. Rice and Tracey, 1969). Furthermore, the pre-localization constitutive relations no longer provide adequate predictions on the localization. The second method attempts to resolve this issue, using a homogenization approach where the elementary cell is divided into porous and dense regions. Despite these attempts, scale separation is questionable during void coalescence, and should be modeled by elementary cells containing a few voids. At these scales, void coalescence may occur by internal necking of the intervoid ligament, by a micro-shear band or in columns of material leading to necklace coalescence (Benzerga, Leblond, et al., 2016).

Models for porous single crystals have also been also proposed. X. Han et al. (2013) proposed one of the first models, for a rate-independent single crystal containing spherical voids. The yield function is similar to Gurson, using a modified critical resolved shear stress on each slip system. This method is of particular interest because its implementation for a porous single crystal constitutive model is feasible. Another approximate model was given by Paux et al. (2015), where a regularization of the Schmid law was conducted. A variational method was also proposed in Mbiakop, Constantinescu, et al. (2015b) for ellipsoidal voids.

Numerical simulations for RVEs containing voids with von Mises matrices have also been conducted by several authors. In Danas and Ponte Castañeda (2012) the influence of triaxiality and Lode parameter was assessed. For high triaxialities, failure is mostly caused by void growth, leading to a softening effect that eventually overtakes the strain hardening of the solid. In these cases, this limit seems to be independent of the Lode parameter. For low triaxialities, failure happens by void collapse, resulting in an abrupt drop in the load-carrying capacity of the material. Furthermore, while the effect of the triaxiality is preponderant for the yield surface, the Lode parameter does not affect significantly the yielding, but the evolution of the void shape in the plastic domain is strongly dependent on it. Kiran and Khandelwal (2014) also concluded that void collapse is the main cause of ductile failure for deviatoric loadings. Danas, Idiart, et al. (2008) concluded that the influence of the deviatoric stress invariant $J_3$ is non negligible.

Regarding RVEs containing voids with a single crystal matrix, Ha and K. Kim (2010) concluded that the void growth is still strongly dependent of the triaxiality. Furthermore, for lower triaxialities, the crystal orientation is the major factor for the deformation mode of the void. Additionally, void growth is faster for lower initial porosities. However, in a similar analysis, Yerra et al. (2010) concluded that the void growth rate is strongly dependent on crystal orientation. Note that both these conclusions refer to the material behavior after yielding, which is beyond the scope of this work.
1.3 Outline

The general outline of this document and the main aspects of each chapter are described here.

Chapter 2

A brief review of the fundamentals of continuum mechanics is presented. Furthermore, the quasi-static initial boundary value problem is introduced. Finally, the essential aspects of the application of the Finite Element Method within the context of large-strain continuum mechanics are described.

Chapter 3

The fundamentals of multi-scale models based on computational homogenization are presented. Firstly, the concept of Representative Element Volume is introduced. Then, the micro-scale problem is formulated, and the appropriate kinematic restrictions are outlined.

Chapter 4

The principal aspects of ductile failure are introduced, where both micro- and macroscopic phenomenological evidence of damage are presented. A brief review of the theory of plasticity and the concept of limit analysis is also shown. In the context of micromechanical analysis, some theoretical constitutive models for porous media are described and compared.

Chapter 5

The yield response of Representative Volume Elements with voids is analyzed, with an isotropic constitutive model (von Mises) for the matrix. Various parametric studies are conducted, to study the influence of the porosity, Lode parameter, void geometry and void orientation. The numerical results are compared to the analytical models whenever possible. Additionally, a model for the porosity evolution in the elastic region is proposed.

Chapter 6

A brief characterization of crystalline materials is carried, and a large-strain constitutive model for single crystals is presented. Furthermore, a set of models for porous single crystals is also shown. Then, as in Chapter 5, the yield response of RVEs with voids is analyzed, with a single crystal matrix. The influence of the anisotropic matrix on the response is assessed and compared to the analytical models.
Chapter 7

The general conclusions of this work are presented, as well as perspectives for future works regarding the subjects discussed.
Chapter 2
Continuum Mechanics and Finite Element Method

Continuum bodies can be repeatedly subdivided into infinitesimal elements without losing the properties of the bulk material. Even though the matter is discrete (composed of atoms and subatomic particles), if the length of the body is sufficiently larger than its atomic structure, it can be considered as a continuum. In the scope of engineering applications, this assumption is of practical interest and allows the description of the behavior of a solid in terms of a Continuum Mechanics theory. In their most general format, these theories do not restrict the magnitude of the deformation. Furthermore, the resulting equations are generally difficult to solve for complex geometries, and thus, numerical approximation schemes are often employed. The most popular technique used in Continuum Mechanics is the Finite Element Method. By using an appropriate spatial discretization and by interpolation of relevant fields, a solution to the weak form of the problem can be obtained.

In this chapter, a brief review of the basic concepts of Continuum Mechanics is presented. Then, the application of the Finite Element Method for the solution of the quasi-static initial boundary value problem is briefly described. It also serves as a reference for the next sections of this work, that is, the definitions and nomenclature used throughout this thesis are consistent with the ones presented in this chapter. Finally, this chapter is heavily influenced by the work of de Souza Neto, Peric, et al. (2008), which in turn follows many standard textbooks (Billington, 1980; Bonet and Wood, 2008; Gurtin, 1982; Ogden, 1997; Spencer, 2004; Truesdell, 1984).

2.1 Deformation kinematics

Consider a continuum body $\mathcal{B}$, occupying a region $\Omega$ of the three-dimensional Euclidean space, with a boundary $\partial\Omega$ in its reference configuration. The kinematics of deformation allows us to establish a space of possible deformation states of the continuum. Nevertheless, the deformation states are established without a connection to the loading or the stress state the body is subjected to. Firstly, the deformation kinematics of a generic body will be analyzed. Its connection with the stress state will be established in further sections.
2.1.1 Deformation mapping function

Upon deformation, the number of possible configurations of the body is infinite. Therefore, it is useful to take a reference configuration that serves as a basis of comparison for any other possible configuration. It is common to assign the unloaded configuration as the reference, where the region occupied by the body is $\Omega$ and its boundary is $\partial \Omega$. In this reference configuration, let $p$ be the position of a particle in the space, such that $p \in \Omega$.

We can define the position of the particle $p$ upon deformation by the establishment of a deformation function $\varphi(p)$. The smooth and one-to-one deformation function results in

$$x = \varphi(p),$$

where $x$ is the particle’s position in the deformed state. The assumption of a one-to-one function is justified by the requirement that the body cannot penetrate itself upon deformation. Therefore, the region of the space occupied by the body in the deformed configuration will become $\varphi(\Omega)$, implying that $x \in \varphi(\Omega)$.

Generally speaking, the deformation is a time dependent phenomenon. Thus, the deformation function $\varphi$ is better expressed as

$$x = \varphi(p,t),$$

where $x$ becomes the position of the particle $p$ in the deformed state at instant $t$. Such definition allows for both time-dependent deformations, rigid-body movement or, in a more general case, a combination of both. The reference configuration can also be referred now as the configuration at time instant $t_0$ where no loading was applied.

The displacement field $u$ at the instant $t$ of a particle $p$ is the difference of the position of the particle between the deformed and reference configurations. Therefore, recalling Eq. (2.2), it can be written in terms of the deformation mapping function as

$$u(p,t) = \varphi(p,t) - p.$$ \hfill (2.3)

Thus, the position of the particle at the deformed configuration can also be expressed by

$$x = p + u(p,t).$$ \hfill (2.4)
It is worth noting that the motion of a generic particle can be accomplished by deformation of the continuum, a rigid-body motion or a combination of both. Subsequently, a rigid-body displacement can further be a translation, a rotation or a combination of both. Each of these displacements is characterized by:

**Rigid translation:** The displacement $u(t)$ is independent of $p$, resulting in

$$x(p, t) = p + u(t); \quad (2.5)$$

**Rigid rotation:** Generic rotation around a fixed point $q$, given by a rotational tensor $R(t)$, such that

$$x(p, t) = q + R(t)(p - q); \quad (2.6)$$

**Combination of rigid translation and rotation:** A combination of both cases expressed above, with a rotation defined by $R(t)$ around $q$, such that

$$x(p, t) = \varphi(q, t) + R(t)(p - q). \quad (2.7)$$

The velocity of a particle is the derivative of its position $x$ in order to time. According to the definitions in Eqs. (2.2) to (2.4), it can be expressed as

$$\dot{x} = \frac{\partial x}{\partial t} = \frac{\partial \varphi(p, t)}{\partial t}, \quad (2.8)$$

where $\dot{x}$ denotes the velocity of the particle. Furthermore, as the deformation function is a one-to-one function, it admits an inverse function, such that

$$p = \varphi^{-1}(x, t) = x - u(\varphi^{-1}(x, t), t). \quad (2.9)$$

This relation allows us to obtain the position of a particle $p$ in the reference configuration from the deformed position $x$. Similarly, the spatial velocity distribution $v(x, t)$ will be equivalent to

$$v(x, t) \equiv \dot{x}(\varphi^{-1}(x, t), t). \quad (2.10)$$

It is important to notice that both the particle velocity $\dot{x}(p, t)$ and the spatial velocity $v(x, t)$ were defined. These quantities describe the velocity of the body, but they are associated with different coordinate systems. As no restriction is being imposed to the magnitude of the displacements, one must be able to characterize the kinematics of the system whether looking from a particle at the reference configuration or a position on the deformed configuration. Therefore, we define two approaches to describe the quantities under study:

**Lagrangian description (material description):** Expresses the parameters as functions of a material system (i.e. a particle in the reference configuration $p$). It is equivalent to fixing a material particle and following its evolution. Accordingly, any field in terms of a Lagrangian description will be defined over a domain $\Omega$. The particle velocity $\dot{x}(p, t)$ uses a material description.

**Eulerian description (spatial description):** Expresses the parameters as functions of a spatial system (i.e. a spatial position $x$). It is equivalent to fixing a point in the space and following its evolution. Accordingly, any field in terms of a Eulerian description will be defined over a domain $\varphi(\Omega)$. The spatial velocity $v(x, t)$ uses a spatial description.
### 2.1.2 Deformation gradient

Consider a particle \( p \) in the reference configuration and its corresponding point \( x \) in the deformed configuration, such that \( x = \varphi(p, t) \). For each of these points, consider also a neighbour separated by an infinitesimal distance, resulting in points \( p + dp \) and \( x + dx \), respectively. It is shown in Fig. 2.2 a representation of these points in both the reference and deformed configuration. The deformation gradient \( F \) relates both distances in the reference and deformed configuration, this is

\[
dx = Fdp. \tag{2.11}\]

It is a second order tensor, with its components obtained by

\[
F_{ij} = \frac{\partial x_i}{\partial p_j}. \tag{2.12}\]

![Deformation gradient diagram](image)

**Figure 2.2: Deformation gradient: deformation of two neighbouring particles.**

The deformation gradient can also be conveniently expressed in terms of a material gradient of the deformation mapping function, such that

\[
F(p, t) = \nabla_p \varphi(p, t) = \frac{\partial x_t}{\partial p}, \tag{2.13}\]

where \( \nabla_p (\cdot) \) is the material divergence operator\(^1\) and \( x_t \) is the position of a particle in the deformed configuration at the instant \( t \). Recalling Eq. (2.4), the deformation gradient simplifies to

\[
F(p, t) = I + \nabla_p u(p, t), \tag{2.14}\]

where \( I \) is the second order identity tensor.

If a spatial description is adopted, the deformation gradient can be expressed in terms of the spatial coordinate \( x \), such that

\[
F(x, t) = \left[\nabla_x \varphi^{-1}(x, t)\right]^{-1}, \tag{2.15}\]

\(^1\nabla_p (\cdot) = \partial(\cdot) / \partial p\)
where $\nabla_x (\cdot)$ is the spatial gradient operator\(^2\).

When the deformation gradient is uniform (i.e. independent of $p$), the deformation mapping function in a point $p$ can be expressed in terms of the deformation mapping function in a point $q$, such that

$$\varphi (p, t) = \varphi (q, t) + F (p - q),$$

(2.16)

for any $p, q \in \mathcal{B}$. Also, a deformation with $F$ constant is homogeneous. All homogeneous deformations follow Eq. (2.16). Rigid-body motions produce uniform deformation gradients.

### 2.1.3 Isochoric and volumetric decompositions of the deformation gradient

The deformation gradient can be conveniently decomposed and expressed in terms of an isochoric and a volumetric components. These are defined according to:

**Isochoric deformation $F_{\text{iso}}$:** It is a deformation where the volume of the solid is constant before and after deformation. It can be seen as a deformation where the continuum body only changes its shape.

**Volumetric deformation $F_{\text{vol}}$:** It is a deformation where the solid only changes volume. Therefore, the shape is kept constant and the solid expands or contracts equally in all directions. It leads to a spherical tensor such as

$$F_{\text{vol}} = \alpha I.$$

(2.17)

The change in volume of a deformation can be expressed in terms of a quantity $J$ such that

$$J = \frac{dv}{dv_0},$$

(2.18)

where $v_0$ and $v$ are the volumes before and after deformation, respectively. It can be seen that this quantity is the determinant of the deformation gradient ($J = \det(F)$). By this logic, $J$ must be a positive quantity\(^3\). According to the definitions of isochoric and volumetric deformations, we can conclude that

$$\det (F_{\text{iso}}) = 1,$$

(2.19a)

$$\det (F_{\text{vol}}) = \det (\alpha I) = \alpha^3.$$

(2.19b)

The general deformation gradient can be obtained by the product of an isochoric decomposition with a volumetric decomposition, such that

$$F = F_{\text{iso}} F_{\text{vol}}.$$

(2.20)

\(^2\nabla_x (\cdot) = \partial (\cdot) / \partial x\)

\(^3\)Cases where $J = 0$ result in a collapsed volume and destroyed particles, which is impossible. Also, as the deformation is a time-dependent problem, if $J < 0$ it means that at some point $J = 0$ (assuming $\varphi$ is continuous in $t$).
Alternatively, it can also be expressed in terms of the product of a volumetric decomposition with an isochoric decomposition,

$$ F = F_{\text{vol}} F_{\text{iso}}. $$

(2.21)

In order to satisfy Eqs. (2.19) to (2.21), and using $J = \det(F)$, the isochoric component must be

$$ F_{\text{iso}} = (J)^{-1/3} F, $$

(2.22)

and the volumetric component

$$ F_{\text{vol}} = (J)^{1/3} I. $$

(2.23)

### 2.1.4 Polar decomposition of the deformation gradient

In a more general approach, the deformation gradient can contain both changes in shape, rotations and volume changes. It is useful to decompose the deformation gradient in two components, one for the stretch of the solid and another for the rotations. According to the polar decomposition theorem, we can express the deformation gradient in terms of

$$ F = RU = VR, $$

(2.24)

where $R$ is the rotation tensor and $U$ and $V$ are the right and left stretch tensors, respectively. Both $U$ and $V$ are symmetric positive definite tensors, and can also be related by

$$ V = RUR^T. $$

(2.25)

Furthermore, the right and left stretch tensors can also be expressed as follows

$$ U = \sqrt{C}, $$

(2.26a)
2.2 Strain tensor

In the previous section, different measures of the strain state of the solid have been established through decomposition of the deformation gradient. With the decomposition of the deformation gradient in terms of a right or left stretch tensor and a rotation tensor, we can represent the deformation state in terms of a strained component (stretch tensor) and an unstrained component (rotation tensor). Straining happens when the distance between two points in the body changes upon deformation. In an unstrained state, the tensors $U$ and $V$ are identical to $I$. Therefore, any straining will make the stretch tensors deviate from the identity tensor. A strain measure needs to be defined, quantifying this deviation.

If we take a measure of the deformation magnitude, such as

$$||dx||^2 - ||dp||^2 = dx \cdot dx - dp \cdot dp$$

$$= Fdp \cdot Fdp - dp \cdot dp$$

$$= (C - I) dp \cdot dp$$

$$= 2E^{(2)} dp \cdot dp,$$

where $C$ and $B$ denote the right and left Cauchy-Green strain tensors, respectively, given by

$$C = F^T F,$$  \hspace{1cm} (2.27a)

$$B = FF^T.$$  \hspace{1cm} (2.27b)

If we introduce the definition of $F$ in Eq. (2.14), the right and left Cauchy-Green strain tensors can be rewritten as

$$C = I + \nabla_p u + (\nabla_p u)^\top + (\nabla_p u)^\top \cdot \nabla_p u,$$  \hspace{1cm} (2.28a)

$$B = I + \nabla_p u + (\nabla_p u)^\top + \nabla_p u \cdot (\nabla_p u)^\top.$$  \hspace{1cm} (2.28b)
it becomes apparent that a strain measure can be established in terms of the difference between the Cauchy-Green strain tensor and the identity tensor. This is in line with the idea that a strain will deviate a stretch tensor from the identity tensor. Here, \( E^{(2)} \) is the Green-Lagrange strain tensor, explicitly given by

\[
E^{(2)} = \frac{1}{2} (C - I). \tag{2.30}
\]

The Green-Lagrange strain tensor is one of the many possible representations of the strain. In fact, it is a member of the family of Lagrangian strain tensors, whose general definition is given by

\[
E^{(m)} = \begin{cases} 
\frac{1}{m} (U^m - I), & m \neq 0 \\
\ln(U), & m = 0
\end{cases}, \tag{2.31}
\]

where \( m \) is a real number and \( \ln(\cdot) \) is the tensor logarithm operator. These strain tensors are defined in terms of the right stretch tensor. The Green-Lagrange is the case for \( m = 2 \), but other cases are also common, such as the Hencky tensor \( (m = 0) \), the Biot tensor \( (m = 1) \) and the Almansi tensor \( (m = -2) \) (de Souza Neto, Peric, et al., 2008). It is also possible to define a Eulerian strain tensor, function of the left stretch tensor, as

\[
\varepsilon^{(m)} = \begin{cases} 
\frac{1}{m} (V^m - I), & m \neq 0 \\
\ln(V), & m = 0
\end{cases}. \tag{2.32}
\]

Similarly to Eq. (2.25), the Lagrangian and Eulerian strain tensors are related by

\[
\varepsilon^{(m)} = R E^{(m)} R^\top. \tag{2.33}
\]

With these definitions of strain tensor, we can make a short connection between this theory and the infinitesimal strain theory. The assumption of very small strains allows us to simplify the definition of strain tensor. By recalling Eq. (2.28), as long as \( u \) is small, we can ignore the quadratic terms of the right and left Cauchy-Green strain tensors. Moreover, the left and right strain tensors become formally equivalent, such that

\[
C \approx B \approx I + \nabla_p u + (\nabla_p u)^\top. \tag{2.34}
\]

Recalling Eq. (2.26), we now have

\[
U \approx V, \tag{2.35}
\]

which, from Eqs. (2.31) and (2.32) and for any \( m \), ultimately results in

\[
\varepsilon \approx \varepsilon^{(m)} \approx E^{(m)}. \tag{2.36}
\]

The small strain tensor is therefore

\[
\varepsilon = \frac{1}{2} [\nabla_p u + (\nabla_p u)^\top]. \tag{2.37}
\]
2.3 Stress tensor

In previous sections, the kinematic state and strain of a generic continuum were defined. However, up until this point, no reference was made to the concept of forces and their transference within continuum bodies. Mechanical forces can be either

**Surface forces:** Forces per unit of area, typically associated with forces on the boundary of a body. Examples are the contact forces between two bodies and external pressure applied on a surface.

**Body forces:** Forces per unit of volume. Examples are gravitational and magnetic forces.

Generally, the presence of strains will produce a stress state inside the body. In this section, various measures of stress are described, both using a material or a spatial description.

2.3.1 Cauchy stress tensor

Consider a point \( x \) on a surface with a normal \( n \). The traction force \( t \) is given by

\[
  t(x, n, t) = \sigma(x, t) \cdot n,
\]

where the second order tensor \( \sigma(x, t) \) is the Cauchy stress tensor. It is established in the deformed configuration of the solid, such that it is frequently called the real stress tensor. When expressed in terms of an orthonormal basis \( \{e_1, e_2, e_3\} \), each of its components can be expressed by

\[
  \sigma_{ij} = (\sigma e_i) \cdot e_j,
\]

where the term \( \sigma e_i \) is the force per unit of area across a surface with normal \( e_i \). Therefore, the component \( \sigma_{ij} \) is the magnitude of projection of this force along the direction \( e_j \). The terms along the diagonal represent the normal stresses, whilst the others are shear stresses. From the equilibrium of the angular momentum, one can also verify that the Cauchy stress tensor is symmetric. There always exists a orthonormal basis \( \{e'_1, e'_2, e'_3\} \) where the shear stresses are null. In this basis, the stress components \( \sigma \) are known as Cauchy principal stresses and correspond to the eigenvalues of \( \sigma \).

In the same way as the deformation gradient, we can also express the Cauchy stress tensor in terms of deviatoric and volumetric components. It can be stated that

\[
  \sigma = s + pI,
\]

where \( s \) is the deviatoric component and \( pI \) is the volumetric component. Here, \( p \) denotes the hydrostatic pressure, defined as

\[
  p = \frac{1}{3} \text{tr} (\sigma).
\]

Therefore, \( s \) must be a traceless tensor. Just like the Cauchy stress tensor, the deviatoric stress tensor is also symmetric.

The Cauchy stress tensor has three scalar invariants, which are independent of the basis used. The invariants \( I_1, I_2 \) and \( I_3 \) are given by

\[
  I_1 = \sigma_{kk} = \text{tr} (\sigma),
\]

(2.42a)
\[ I_2 = \frac{1}{2} \left( \sigma_{ii} \sigma_{jj} - \sigma_{ij} \sigma_{ji} \right) = \frac{1}{2} \left[ (\text{tr} (\sigma))^2 - \text{tr} \left( \sigma^2 \right) \right], \quad (2.42b) \]

\[ I_3 = \det (\sigma). \quad (2.42c) \]

Similarly, the deviatoric stress tensor also has three invariants, \( J_1, J_2 \) and \( J_3 \), given by

\[ J_1 = s_{kk} = \text{tr} (s) = 0, \quad (2.43a) \]

\[ J_2 = \frac{1}{2} s_{ij} s_{ji} = \frac{1}{2} \text{tr} (s^2), \quad (2.43b) \]

\[ J_3 = \det (s). \quad (2.43c) \]

Note the difference between the invariants of the Cauchy stress tensor and the invariants of the deviatoric stress tensor. For example, the von Mises yield criterion is a function of the second invariant of the deviatoric stress component. The second and third invariants of the deviatoric stress tensor can also be written as a function of the invariants of the Cauchy stress tensor, according to

\[ J_2 = \frac{1}{3} I_1^2 - I_2, \quad (2.44a) \]

\[ J_3 = \frac{2}{27} I_1^3 - \frac{1}{3} I_1 I_2 + I_3. \quad (2.44b) \]

### 2.3.2 First Piola-Kirchhoff stress tensor

The first Piola-Kirchhoff stress tensor is an alternative representation of the stress state. It is a two-point tensor, as the forces are accounted for in the deformed configuration (per unit of reference area), but the normals are in the reference configuration. We can define the first Piola-Kirchhoff stress tensor \( \mathbf{P} \) by

\[ \mathbf{P} = J \sigma \mathbf{F}^{-\top}, \quad (2.45) \]

where \( J = \det (\mathbf{F}) \), \( \sigma \) is the Cauchy stress tensor and \( \mathbf{F} \) is the deformation gradient. It should be noted that, contrary to the Cauchy stress tensor, this tensor is not necessarily symmetric.

The first Piola-Kirchhoff stress tensor can also be written as

\[ \mathbf{P} = \tau \mathbf{F}^{-\top}, \quad (2.46) \]

where \( \tau \) is the Kirchhoff stress tensor, defined by

\[ \tau = J \sigma. \quad (2.47) \]

Note that the Kirchhoff stress tensor is symmetric, and its components are frequently obtained using Cauchy principal stresses.
2.3.3 Second Piola-Kirchhoff stress tensor

The second Piola-Kirchhoff stress tensor is defined as
\[ S = J F^{-1} \sigma F^{-\top}. \]  \hspace{1cm} (2.48)

It is worth noting that similarly to the Cauchy stress tensor, the second Piola-Kirchhoff stress tensor is also symmetric.

2.4 Fundamental laws of Thermodynamics

The foundation for the establishment of the governing equations of the physics of the continuum is the conservation and balance of a set of fields. In essence, in the analysis of a continuum, mass and momentum need to be conserved, and the laws of Thermodynamics must be verified. Throughout this section, these conservation principles will be addressed and summarized.

2.4.1 Mass conservation

Considering a continuous distribution of mass along the body and given a configuration \( \varphi \), its mass \( m(\Omega) \) can be expressed as
\[ m(\Omega) = \int_{\varphi(\Omega)} \rho_{\varphi} dV, \]  \hspace{1cm} (2.49)

where \( \rho_{\varphi} \) is the mass density field on the deformation \( \varphi(\Omega) \). The mass of the body should also be independent of the deformation. Therefore, providing to different configurations \( \varphi_1 \) and \( \varphi_2 \), the mass of the body verifies
\[ m(\Omega) = \int_{\varphi_1(\Omega)} \rho_{\varphi_1} dV = \int_{\varphi_2(\Omega)} \rho_{\varphi_2} dV, \]  \hspace{1cm} (2.50)

for all configurations \( \varphi_1 \) and \( \varphi_2 \), where this expression represents the mass conservation of a deformation.

Note that the mass density field was established in terms of a configuration \( \varphi \). We can define a reference density field \( \rho_0 \) in terms of the reference coordinate \( p \), given by
\[ \rho_0(p) = \lim_{\delta \to 0} \frac{m(\Omega_{\delta})}{\text{vol}(\Omega_{\delta})}, \]  \hspace{1cm} (2.51)

where \( \Omega_{\delta} \) is a sphere of radius \( \delta \). The reference density function in a point \( p \) is related to the density function in the deformed configuration by \( \left( \text{Gurtin, 1982} \right) \)
\[ \rho(x) \det F(p) = \rho_0(p), \]  \hspace{1cm} (2.52)

where \( x \) is the position of \( p \) after the deformation \( \varphi \). Finally, for any point in the deformed configuration \( x \), the principle of local mass conservation in the deformed configuration states that
\[ \dot{\rho} + \rho \text{div}_x \mathbf{u} = 0, \]  \hspace{1cm} (2.53)

where \( \mathbf{u} \) is the velocity field and \( \text{div}_x(\cdot) \) is the spatial divergence operator.
2.4.2 Momentum equilibrium

Considering the deformed configuration, the conservation of linear momentum can be expressed by

\[
\begin{align*}
\text{div}_x \sigma + b &= \rho \ddot{u}, \quad \text{in } \varphi (\Omega) \\
t &= \sigma n, \quad \text{in } \varphi (\partial \Omega),
\end{align*}
\]  

(2.54)

where \( b \) is the body force per unit of volume and \( n \) is the outward normal to the boundary in the deformed configuration. These equations describe the strong or local form of the equilibrium and establish a connection between the forces and stresses with the displacements of the continuum. The first equality of Eq. (2.54) is also known as Cauchy’s equation of motion. We can also express the strong form in terms of a material description, such that

\[
\begin{align*}
\text{div}_p P + b_0 &= \rho_0 \ddot{u}, \quad \text{in } \Omega \\
t_0 &= P n_0, \quad \text{in } \partial \Omega,
\end{align*}
\]  

(2.55)

where \( b_0 \) is the body force per unit of reference volume, \( \rho_0 \) is the mass per unit of reference volume and \( n_0 \) is the outward normal to the boundary in the reference configuration. These quantities can be expressed by

\[
\begin{align*}
b_0 &= J b, \\
\rho_0 &= J \rho.
\end{align*}
\]  

(2.56a, 2.56b)

2.4.3 First Law of Thermodynamics

The first Law of Thermodynamics expresses the conservation of energy in the continuum. The internal energy is a scalar field, which is usually expressed conveniently as an intensive property \( e \), i.e., the specific internal energy. Considering additionally a heat flux \( q \) and a density of heat production \( r \), the first Law of Thermodynamics can be expressed as

\[
\rho \dot{e} = \sigma : D + \rho r - \text{div}_x q,
\]  

(2.57)

where the double contraction \( \sigma : D \) represents the stress power per unit of deformed volume\(^4\). The balance per unit of deformed volume of the stress power, the heat production and the spatial divergence of the heat flux equals the rate of internal energy. For the particular case when no heat production exists and the heat flux is spatially constant, Eq. (2.57) reduces to

\[
\rho \dot{e} = \sigma : D.
\]  

(2.58)

2.4.4 Second Law of Thermodynamics

The second Law of Thermodynamics expresses the irreversibility of entropy production. Expressing the specific entropy by \( s \) and the temperature by \( \theta \), the inequality

\[
\rho \dot{s} + \text{div}_x \frac{q}{\theta} - \frac{\rho r}{\theta} \geq 0
\]  

(2.59)

\(^4D\) is the stretch rate tensor, defined as \( D = \nabla_x v \).
relates the rate of specific entropy production with the heat flux, temperature and heat production.

2.4.5 **Clausius-Duhem inequality**

Combining the first and second Laws of the Thermodynamics, as expressed above, we can write the inequality

\[ \rho \dot{s} + \text{div}_x \frac{q}{\theta} - \frac{1}{\theta} (\rho \dot{e} - \sigma : D + \text{div}_x q) \geq 0. \]  

(2.60)

Developing the spatial divergence

\[ \text{div}_x \frac{q}{\theta} = \frac{1}{\theta} \text{div}_x q - \frac{1}{\theta^2} q \cdot \nabla_x \theta, \]  

(2.61)

Eq. (2.60) simplifies to the Clausius-Duhem inequality

\[ \sigma : D - \rho \left(\dot{\psi} + s \dot{\theta}\right) - \frac{1}{\theta} q \cdot g \geq 0, \]  

where \(\dot{\psi}\) is the specific free energy, given by

\[ \dot{\psi} = e - \theta s, \]  

(2.63)

and \(g = \nabla_x \theta\). We can also express the Clausius-Duhem inequality in terms of the reference configuration by using the Kirchhoff stress tensor, in terms of the dissipation per unit reference volume, as

\[ \tau : D - \bar{\rho} \left(\dot{\psi} + s \bar{\theta}\right) - J\frac{1}{\bar{\theta}} q \cdot g \geq 0. \]  

(2.64)

2.5 **Constitutive theory**

Up until this point, conservation principles, valid for any continuum body, were expressed without a reference to the material of the body. For instance, different materials might have different responses, whilst both verifying the principles expressed in Section 2.4. Constitutive models allow us to distinguish between materials. Along this section, a brief introduction to the constitutive model theory will be exposed.

2.5.1 **Constitutive axioms**

Any constitutive model must verify a set of constitutive axioms. Along this section these axioms will be established. It is important to introduce the difference between a thermokinetic process and a calorodynamic process of \(\mathcal{B}\) (Truesdell, 1984). The former is a pair of functions of fields

\[ \varphi (p, t) \text{ and } \theta (p, t). \]  

\[ \text{ (2.65)} \]

The latter is a set of functions

\[ \sigma (p, t), \ e (p, t), \ s (p, t), \ r (p, t), \ b (p, t) \text{ and } q (p, t), \]  

\[ \text{ (2.66)} \]

whose fields satisfy the balance of momentum, as well as both laws of Thermodynamics. Given these processes, the constitutive axioms of thermodynamic determinism, material objectivity and material symmetry will now be presented.
Thermodynamic determinism

Generally speaking, materials are represented in thermodynamics by constitutive relations, which must hold the principle of thermodynamically compatible determinism (Truesdell, 1984). Specifically, this axiom postulates that for a point \( p \) in a given body \( \mathcal{B} \) at time \( t \), the history of the thermokinetic process to which it has been subject up to and including the time \( t \) determines a calorodynamic process for \( \mathcal{B} \) at \( p \). It is worth noting that, for simple materials, the calorodynamic process of a point \( p \) is only function of the history of the thermokinetic process at the same point, that is, of the local history of the thermokinetic process (de Souza Neto, Peric, et al., 2008). Thus, there must exist constitutive functionals \( \mathcal{F}, \mathcal{B}, \mathcal{S} \) and \( \mathcal{J} \) of the histories of \( F, \theta \) and \( g \) in a point \( p \), such that

\[
\sigma (p, t) = \mathcal{F} \left( F^t(p), \theta^t(p), g^t(p) \right),
\]

\[
\psi (p, t) = \mathcal{B} \left( F^t(p), \theta^t(p), g^t(p) \right),
\]

\[
s (p, t) = \mathcal{S} \left( F^t(p), \theta^t(p), g^t(p) \right),
\]

\[
q (p, t) = \mathcal{J} \left( F^t(p), \theta^t(p), g^t(p) \right),
\]

where \((\bullet)^t\) denotes the history of \((\bullet)\) up to time \( t \). Furthermore, the Clausius-Duhem inequality must be verified for every thermokinetic process of \( \mathcal{B} \).

Material objectivity

The principle of material objectivity or frame invariance states that the material response is independent of the observer. A change of observer of motion \( \varphi \) can be expressed as

\[
\varphi^* (p, t) = y(t) + Q(t) \left[ \varphi (p, t) - x_0 \right],
\]

where \( \varphi^* \) is the motion in the changed observer, \( y(t) \) is a translation and \( Q(t) \) is a rotation around a point \( x_0 \). With this transformation, the deformation gradient as viewed by the second observer becomes

\[
F^* = QF.
\]

Accordingly, the other fields transform according to

\[
\sigma \rightarrow \sigma^* = Q\sigma Q^T,
\]

\[
q \rightarrow q^* = Qq,
\]

\[
g \rightarrow g^* = Qg,
\]

and scalar fields remain constant after transformation.

Therefore, for any transformation similar to Eq. (2.68), the material objectivity principle requires the constitutive relations to verify

\[
\sigma^* (p, t) = \mathcal{F} \left( F^{ts}(p), \theta^{ts}(p), g^{ts}(p) \right),
\]

\[
\psi^* (p, t) = \mathcal{B} \left( F^{ts}(p), \theta^{ts}(p), g^{ts}(p) \right),
\]

\[
s^* (p, t) = \mathcal{S} \left( F^{ts}(p), \theta^{ts}(p), g^{ts}(p) \right),
\]

\[
q^* (p, t) = \mathcal{J} \left( F^{ts}(p), \theta^{ts}(p), g^{ts}(p) \right).
\]
2.5. Constitutive theory

Material symmetry

The symmetry group of a solid material is the set of rotations $Q$ that does not change the response functionals of the constitutive model, i.e.

$$
\mathcal{S} \left( F^t, \theta^t, g^t \right) = \mathcal{S} \left( [FQ]^t, \theta^t, g^t \right), \quad (2.72a)
$$

$$
\mathcal{B} \left( F^t, \theta^t, g^t \right) = \mathcal{B} \left( [FQ]^t, \theta^t, g^t \right), \quad (2.72b)
$$

$$
\mathcal{H} \left( F^t, \theta^t, g^t \right) = \mathcal{H} \left( [FQ]^t, \theta^t, g^t \right), \quad (2.72c)
$$

$$
\mathcal{J} \left( F^t, \theta^t, g^t \right) = \mathcal{J} \left( [FQ]^t, \theta^t, g^t \right). \quad (2.72d)
$$

The symmetry group $\mathcal{S}$ is a set of rotations (such that $Q \in \mathcal{S}$), so it is also a subset of the proper orthogonal group $O^+$. The principle of material symmetry imposes the symmetries of the constitutive model to be consistent with the symmetries of the material. An isotropic solid has its symmetry group coincident with the proper orthogonal group.

2.5.2 Thermodynamics with internal variables

The approach described in Section 2.5.1 for the establishment of the constitutive equations is too general and difficult to use in practice. Thus, to simplify the process, an effective alternative is the use of thermodynamics with internal variables. In essence, this hypothesis states that given a point $p$, a finite set of state variables will completely define the thermodynamic state (defined by $\sigma$, $\psi$, $s$ and $q$) of a thermodynamic process. Additionally, the thermodynamic state is only a function of the instantaneous value of the state variables, not of their history.

For applications in solid mechanics, we can assume that the thermodynamic state of a point can be expressed in terms of a set of state variables,

$$
\{F, \theta, g, \alpha\}, \quad (2.73)
$$

where $F$, $\theta$ and $g$ are the instantaneous values of the deformation gradient, temperature and temperature gradient, and

$$
\alpha = \{\alpha_k\} \quad (2.74)
$$

is a set of internal variables associated with dissipative mechanisms (de Souza Neto, Peric, et al., 2008).

According to this hypothesis, the specific free energy can be expressed in terms of the state variables proposed in Eq. (2.73). However, in order to verify the second law of thermodynamics, it must not be a function of $g$ (Coleman and Gurtin, 1967). Therefore,

$$
\psi = \psi \left( F, \theta, \alpha \right). \quad (2.75)
$$

Its temporal derivative becomes

$$
\dot{\psi} = \frac{\partial \psi}{\partial F} : \dot{F} + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \sum_{k=1}^{n} \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k, \quad (2.76)
$$

$O^+$ is the set of all proper orthogonal rotations $Q$. A proper orthogonal rotation must verify $\det Q = 1$. 

where \( n \) is the number of variables in the set defined in Eq. (2.74). Additionally, expressing the stress power as

\[
\sigma : D = \sigma F^{-T} : \dot{F},
\]

(2.77)

the Clausius-Duhem inequality reduces to

\[
\left( \sigma F^{-T} - \rho \frac{\partial \psi}{\partial F} \right) : \dot{F} - \rho \left( s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} - \rho \sum_{k=1}^{n} \left( \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k \right) - \frac{1}{\theta} q \cdot g \geq 0.
\]

(2.78)

Similarly, in the reference configuration one has

\[
\left( P - \bar{\rho} \frac{\partial \psi}{\partial F} \right) : \dot{F} - \bar{\rho} \left( s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} - \bar{\rho} \sum_{k=1}^{n} \left( \frac{\partial \psi}{\partial \alpha_k} \dot{\alpha}_k \right) - \frac{J}{\theta} q \cdot g \geq 0.
\]

(2.79)

The axiom of thermodynamic determinism imposes that Eq. (2.79) holds for any thermokinetic process, i.e., any pair of functions \( \{ \dot{F}(t), \dot{\theta}(t) \} \). This consequence implies

\[
P = \bar{\rho} \frac{\partial \psi}{\partial F},
\]

(2.80a)

\[
s = -\frac{\partial \psi}{\partial \theta}.
\]

(2.80b)

Equation (2.80a) can also be written in terms of the Cauchy and Kirchhoff stress tensors, that is,

\[
\sigma = \frac{1}{J} \bar{\rho} \frac{\partial \psi}{\partial F} : F^{-T},
\]

(2.81a)

\[
\tau = \bar{\rho} \frac{\partial \psi}{\partial F} : F^{-T}.
\]

(2.81b)

### 2.6 Weak equilibrium equations

In Section 2.4 the strong or local form of the momentum balance was established, where Eqs. (2.54) and (2.55) represent the spatial and material version, respectively. This form imposes several restrictions on continuity and differentiability of the solution. Albeit solutions to the differential problem exist, these are typically obtained for specific geometries, and a general solution for a large set of problems is hard to obtain. For this reason, the weak or global form of the equilibrium equations is used to obtain a solution with less restrictions in terms of continuity and differentiability. In this section, the weak formulation of the momentum balance will be presented, both in a material and spatial version. Furthermore, a quasi-static version will be developed.

#### 2.6.1 Spatial description

The momentum equilibrium equation can be written in a weak form according to an Eulerian description

\[
\int_{\varphi(\Omega)} \left[ \sigma : \nabla \varepsilon(\eta) - (b - \rho \ddot{u}) \cdot \eta \right] \, dv - \int_{\varphi(\partial \Omega)} t \cdot \eta \, d\alpha = 0, \quad \forall \eta \in \mathcal{V},
\]

(2.82)
where $\eta$ is the virtual displacement vector and $\mathcal{V}$ is the set of admissible virtual displacements. The definition of this set will be addressed in Section 3.2.

### 2.6.2 Material description

We can also write a material description based on the weak form of Eq. (2.82). First, recall the relation between the Cauchy stress tensor and the Piola-Kirchhoff stress tensor,

$$\sigma = \frac{1}{J} P F^\top. \tag{2.83}$$

Also, according to the identity

$$\nabla_x a = \nabla_p a F^{-1}, \tag{2.84}$$

valid for any vector field $a$, it is possible to relate the spatial and material gradient of a field. Finally, considering that (Gurtin, 1982)

$$\int_{\varphi(\Omega)} a (x) \, dv = \int_{\Omega} J (p) a (\varphi (p)) \, dv, \tag{2.85}$$

valid for any scalar field $a$, the weak form in a material description follows as

$$\int_{\Omega} \left[ P : \nabla_p (\eta) - (b_0 - \rho_0 \ddot{u}) \cdot \eta \right] \, dv - \int_{\partial \Omega} t_0 \cdot \eta \, da = 0, \quad \forall \eta \in \mathcal{V}. \tag{2.86}$$

### 2.6.3 Quasi-static formulation

The study of the dynamics of a continuum is outside the scope of this work. Therefore, a quasi-static approach was chosen, where the inertia effects are neglected from the weak forms established previously. The spatial quasi-static weak form becomes

$$\int_{\varphi(\Omega)} \left[ \sigma : \nabla_x (\eta) - b \cdot \eta \right] \, dv - \int_{\varphi(\partial \Omega)} t \cdot \eta \, da = 0, \quad \forall \eta \in \mathcal{V}. \tag{2.87}$$

Accordingly, the material quasi-static weak form becomes

$$\int_{\Omega} \left[ P : \nabla_p (\eta) - b_0 \cdot \eta \right] \, dv - \int_{\partial \Omega} t_0 \cdot \eta \, da = 0, \quad \forall \eta \in \mathcal{V}. \tag{2.88}$$

### 2.7 Quasi-static initial boundary value problem

The weak formulation of the momentum balance and its quasi-static version was established in Section 2.6. In this work, the quasi-static version will be used to express the initial boundary value problem, that is, the weak form of the quasi-static fundamental initial boundary value problem.

Recall the body $\mathcal{B}$ from Section 2.1. Consider that the history of prescribed body forces

$$b (x, t), \quad t \in [t_0, T], \tag{2.89}$$

is known. Furthermore, the following boundary conditions are imposed
1. **Natural boundary condition**: history of the prescribed surface traction \( t(x, t) \) over the boundary \( \partial \Omega_t \) of \( \mathcal{B} \) in its reference configuration.

2. **Essential boundary condition**: prescribed boundary displacement field \( \bar{u} \) over the boundary \( \partial \Omega_u \) of \( \mathcal{B} \) in its reference configuration. The boundary displacements become

\[
\varphi(p, t) = p + \bar{u}(p, t), \quad t \in [t_0, T], p \in \partial \Omega_u.
\]  

(2.90)

For simplification, it is assumed that \( \partial \Omega_u \cap \partial \Omega_t = \emptyset \). The set of displacements that satisfies the essential boundary condition allows us to define the set of kinematically admissible displacements of \( \mathcal{B} \), given by

\[
\mathcal{X} = \{ u : \Omega \times \mathcal{B} \to \mathcal{U} | u(p, t) = \bar{u}(p, t), t \in [t_0, T], p \in \partial \Omega_u \}.
\]  

(2.91)

**Figure 2.5**: Illustration of the initial boundary value problem.

Finally, we can define the fundamental quasi-static initial boundary value problem. In its spatial version it reads, as stated by de Souza Neto, Peric, et al. (2008): “Find a kinematically admissible displacement function \( u \in \mathcal{X} \) such that, for all \( t \in [t_0, T] \), the virtual work equation is satisfied

\[
\int_{\varphi(\Omega, t)} \sigma(x, t) : \nabla x \eta - b(x, t) \cdot \eta \, dv - \int_{\varphi(\partial \Omega, t)} t(x, t) \cdot \eta \, da = 0, \quad \forall \eta \in \mathcal{Y}_t,
\]  

(2.92)

where the space of virtual displacements at time \( t \) is defined by

\[
\mathcal{Y}_t = \{ \eta : \varphi(\Omega, t) \in \mathcal{U} | \eta = 0 \text{ on } \varphi(\partial \Omega_u, t) \}''.
\]  

(2.93)

Alternatively, a material version of the problem becomes: “Find a kinematically admissible displacement function \( u \in \mathcal{X} \) such that, for all \( t \in [t_0, T] \), the virtual work equation is satisfied

\[
\int_{\Omega} [P(p, t) : \nabla_p \eta - \bar{b}(p, t) \cdot \eta] \, dv - \int_{\partial \Omega} \bar{t}(p, t) \cdot \eta \, da = 0, \quad \forall \eta \in \mathcal{Y}_t,
\]  

(2.94)

where the space of virtual displacements at time \( t \) is defined by

\[
\mathcal{Y}_t = \{ \eta : \Omega \in \mathcal{U} | \eta = 0 \text{ on } \partial \Omega_u \}''.
\]  

(2.95)
2.8 Finite element method

In previous sections, the weak version of the quasi-static initial boundary value problem was introduced. A universal analytical solution for this problem is generally not available, given the large spectrum of possible geometries and constitutive models one needs to consider. Therefore, an approximate method must be employed to solve the equilibrium problem. In solid mechanics, the finite element method (FEM) is the most popular numerical technique used to solve these problems. The main features of the method are the temporal and spatial discretization. As it will be seen shortly, the temporal discretization allows a numerical integration of the constitutive model, allowing us to solve both path-dependent and path-independent constitutive relations in a straightforward way. Spatial discretization allows us to divide the domain in finite elements and, after appropriate interpolation of field variables, to establish the weak equilibrium equation in terms of a function on the nodal values. Finally, the problem reduces to a root finding process for the discretized weak equilibrium, which is generally non-linear.

2.8.1 Temporal discretization

A generic path-dependent constitutive model is a function of the strain path \( \varepsilon(t) \). The solution of the constitutive initial value problem might be difficult to obtain for complex strain paths. To solve this problem, an appropriate numerical algorithm for the integration of the rate constitutive equations is required. In a rate-independent material behavior, a strategy of pseudo-time discretization is commonly used, where the time domain is divided in increments \( [t_n, t_{n+1}] \), with \( n \) denoting the increment number.

From the axiom of thermodynamic determinism, the stress \( \sigma_{n+1} \) must be uniquely determined from the set of internal variables \( \alpha_n \) at the time \( t_n \) and from the strain tensor \( \varepsilon_{n+1} \) at time \( t_{n+1} \). Thus, one can define the incremental constitutive function \( \hat{\sigma} \) for the stress tensor as

\[
\sigma_{n+1} = \hat{\sigma}(\alpha_n, F_{n+1}),
\]

(2.96)

where \( \sigma_{n+1} \) is expected to converge to the exact solution as increments are reduced. The function is generally nonlinear and path-independent within one increment, i.e., \( \sigma_{n+1} \) is function of the value of \( \varepsilon_{n+1} \) alone and \( \alpha_n \) is assumed constant throughout the increment. Furthermore, an incremental constitutive function for the internal variables is also defined, given by

\[
\alpha_{n+1} = \hat{\alpha}(\alpha_n, F_{n+1}).
\]

(2.97)

It is worth mentioning that the usage of the incremental constitutive functions defined above holds for both path-dependent and path-independent constitutive models. Thus, when the integration scheme is appropriate, it can be seen as a generalization of the constitutive model theory. We can now define the finite strain incremental boundary value problem, as stated by de Souza Neto, Peric, et al.: “Given the field \( \alpha_n \) at time \( t_n \) and given the body forces and surface traction fields at \( t_{n+1} \), find a kinematically admissible configuration \( \varphi_{n+1} (\Omega) \in \mathcal{X}_{n+1} \) such that the virtual work equation

\[
\int_{\varphi_{n+1}(\Omega)} [\sigma(\alpha_n, F_{n+1}) : \nabla^h_u (\eta) - b_{n+1} \cdot \eta] \, dv - \int_{\varphi_{n+1}(\partial \Omega_1)} t_{n+1} \cdot \eta \, da = 0,
\]

(2.98)
is satisfied for any $\eta \in \mathcal{V}$, where $\varphi_{n+1}$ is the deformation map at $t_{n+1}$

$$x_{n+1} = \varphi_{n+1}(p) = p + u_{n+1}(p), \quad (2.99)$$

and

$$F_{n+1} = \nabla_p \varphi_{n+1} = I + \nabla_p u_{n+1}. \quad (2.100)$$

### 2.8.2 Spatial discretization

The finite element method operates on finite elements, which results from the connection of discrete points of interest (nodes) that discretize the domain. Therefore, the domain of the problem $\Omega$ is approximated by the discretized finite element domain $\Omega_d$, given by

$$\Omega \approx \Omega_d = \bigcup_{e=1}^{n_{\text{elems}}} \Omega_e. \quad (2.101)$$

**Interpolation of fields**

Each finite element $e$, occupying a region $\Omega_e$ of the discretized domain $\Omega_d$, has a set of $n_{\text{nodes}}$ nodes. Furthermore, each node $i$ in the element $e$ has a shape function (or interpolation function) $N_i^e(x)$. These shape or interpolation functions must verify the Kroenecker delta property, that is,

$$N_i^e(x_j) = \delta_{ij} = \begin{cases} 1, & \text{if } j = i, \\ 0, & \text{if } j \neq i \end{cases} \quad (2.102)$$

A generic element $e$ also has the interpolation matrix $N_e$, given by

$$N_e = \left[ \text{diag} \left[ N_1^e(x) \right] \, \text{diag} \left[ N_2^e(x) \right] \, \cdots \, \text{diag} \left[ N_{n_{\text{nodes}}}^e(x) \right] \right], \quad (2.103)$$

where the diagonal matrix associated with the node $i$ is square and with the dimensions defined by the number of degrees of freedom of the node $n_{\text{dof}}$,

$$\text{diag} \left[ N_i^e(x) \right] = \begin{bmatrix} N_i^e(x) & 0 & \cdots & 0 \\ 0 & N_i^e(x) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & N_i^e(x) \end{bmatrix}_{n_{\text{dof}} \times n_{\text{dof}}}. \quad (2.104)$$

The interpolation matrices established were defined locally on the element $e$. It is also possible to define a global interpolation matrix $N^g$ in terms of all nodes in the finite element mesh. Before going any further, it is worth remarking that the number of points in the mesh is generally different from the number of nodes per element multiplied by the number of elements, i.e., $n_{\text{points}} \leq n_{\text{elem}} \times n_{\text{nodes}}$. These two numbers are only equal when the finite element mesh is composed of only one element. Finally, the global interpolation matrix becomes

$$N^g = \left[ \text{diag} \left[ N_1^g(x) \right] \, \text{diag} \left[ N_2^g(x) \right] \, \cdots \, \text{diag} \left[ N_{n_{\text{points}}}^g(x) \right] \right], \quad (2.105)$$
where the diagonal matrix $\text{diag} \left[ N_i^g (x) \right]$ is defined similarly to Eq. (2.104), given by

$$
\text{diag} \left[ N_i^g (x) \right] = \begin{bmatrix}
N_1^g (x) & 0 & \cdots & 0 \\
0 & N_2^g (x) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & N_n^g (x)
\end{bmatrix} \in \mathbb{R}^{n_{dof} \times n_{dof}},
$$

with $N_i^g (x)$ being the global shape function associated with node $i$.

Another fundamental aspect of the finite element method is the approximation of the displacement field $u(x)$ by its discretized counterpart $^h u(x)$. The discretized version of the displacement field is given by the interpolation of nodal displacement values, that is,

$$
u(x) \approx ^h u(x) = N^g(x) \nu, \quad \forall ^h \nu \in ^h \mathcal{H},
$$

where $\nu$ is the global vector of nodal displacements, given by

$$
\nu = \left\{ u_1^1, \ldots, u_1^{n_{dof}}, \ldots, u_j^i, \ldots, u_j^{1} \text{points}, \ldots, u_j^{n_{dof}} \text{points} \right\}^T,
$$

and $u_j^i$ is the $i$-th component of the nodal displacement of the global node $j$. The components of $\nu$ on $\partial \Omega_u$ must also satisfy the prescribed kinematic constraints. We can also define a set $^h \mathcal{H}$, result of the spatial discretization, by

$$
^h \mathcal{H} = \left\{ ^h \nu (x) = \sum_{j=1}^{n_{points}} u_j N_j^g (x) \big| u_j = \bar{u}_j (x_j) \text{ if } x_j \in \partial \Omega_u \right\},
$$

where $u_j$ and $\bar{u}_j (x_j)$ are the displacement vector and the prescribed displacement at node $j$. Similarly, the virtual displacements over the domain can be defined as

$$
\eta(x) \approx ^h \eta(x) = N^g(x) \eta, \quad \forall ^h \eta \in ^h \mathcal{V},
$$

with its corresponding set $^h \mathcal{V}$ given by

$$
^h \mathcal{V} = \left\{ ^h \eta (x) = \sum_{j=1}^{n_{points}} \eta_j N_j^g (x) \big| \eta_j = 0 \text{ if } x_j \in \partial \Omega_u \right\}.
$$

Discretization of the equilibrium equations

The incremental boundary value problem requires the usage of gradient operators, in both their material and spatial versions. Therefore, a discretized version of these operators must be introduced. For convenience, let us define the global symmetric discrete gradient operator $^h B^g$. Additionally, we can also define the global discrete spatial gradient operator $^h G^g$. For instance, in two-dimensional problems in a plane strain condition, these operators can be written in a matricial format such as

$$
^h G^g = \begin{bmatrix}
\frac{\partial N_1^g}{\partial x} & 0 & \frac{\partial N_2^g}{\partial x} & 0 & \ldots & \frac{\partial N_{n_{points}}^g}{\partial x} \\
0 & \frac{\partial N_1^g}{\partial x} & 0 & \frac{\partial N_2^g}{\partial x} & \ldots & 0 \\
\frac{\partial N_1^g}{\partial y} & 0 & \frac{\partial N_2^g}{\partial y} & 0 & \ldots & \frac{\partial N_{n_{points}}^g}{\partial y} \\
0 & \frac{\partial N_1^g}{\partial y} & 0 & \frac{\partial N_2^g}{\partial y} & \ldots & 0
\end{bmatrix}.
$$
and

\[
B^g = \begin{bmatrix}
\frac{\partial N_1^g}{\partial x} & 0 & \frac{\partial N_2^g}{\partial x} & \cdots & \frac{\partial N_n^g}{\partial x} & 0 \\
0 & \frac{\partial N_1^g}{\partial y} & 0 & \cdots & 0 & \frac{\partial N_n^g}{\partial y} \\
\frac{\partial N_1^g}{\partial y} & \frac{\partial N_2^g}{\partial y} & \cdots & \frac{\partial N_n^g}{\partial y}
\end{bmatrix}, \quad (2.113)
\]

where \( x \) and \( y \) are the position of a point either in the reference or deformed configuration. Moreover, these matrices can be written locally to a generic element \( e \). We can write the element discrete gradient operators \( G \) and \( B \) as the matrices

\[
G = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial x} & \cdots & \frac{\partial N_n}{\partial x} & 0 \\
0 & \frac{\partial N_1}{\partial y} & 0 & \cdots & 0 & \frac{\partial N_n}{\partial y} \\
\frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \cdots & \frac{\partial N_n}{\partial y}
\end{bmatrix}, \quad (2.114)
\]

and

\[
B = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial x} & \cdots & \frac{\partial N_n}{\partial x} & 0 \\
0 & \frac{\partial N_1}{\partial y} & 0 & \cdots & 0 & \frac{\partial N_n}{\partial y} \\
\frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \cdots & \frac{\partial N_n}{\partial y}
\end{bmatrix}. \quad (2.115)
\]

Having defined the discrete gradient operators, the spatially discretized equilibrium equations can be reduced to a root finding process. In essence, the nodal displacement vector \( u_{n+1} \) at time \( t_{n+1} \) is to be found, such that

\[
\mathbf{r} (u_{n+1}) = \mathbf{f}^{\text{int}} (u_{n+1}) - \mathbf{f}^{\text{ext}}_{n+1} = 0, \quad (2.116)
\]

is satisfied. The vectors \( \mathbf{f}^{\text{int}} (u_{n+1}) \) and \( \mathbf{f}^{\text{ext}}_{n+1} \) are the assembled nodal internal and external forces, respectively, obtained from their element counterparts \( \mathbf{f}^{\text{int}}_e (u_{n+1}) \) and \( \mathbf{f}^{\text{ext}}_e \). In a spatial description, these element forces are given by

\[
\mathbf{f}^{\text{int}}_e = \int_{\varphi_{n+1}} B^T \hat{\mathbf{\sigma}} (\alpha, F (u_{n+1})) \, dv, \quad (2.117)
\]

and

\[
\mathbf{f}^{\text{ext}}_e = \int_{\varphi_{n+1}} N^T \mathbf{b}_{n+1} \, dv + \int_{\partial \varphi_{n+1}} N^T \mathbf{t}_{n+1} \, da. \quad (2.118)
\]

It is worth noting that Eq. (2.116) is in general nonlinear, given the nonlinearity of the incremental constitutive function (de Souza Neto, Peric, et al., 2008). The assembly of nodal force vectors allows building the global nodal force vector from the elementary nodal forces. This operation is commonly expressed in terms of the finite element assembly operator \( \mathbf{A} \) as follows

\[
\mathbf{f}^{\text{int}} = \sum_{e=1}^{n_{\text{ele}}} \mathbf{A} \mathbf{f}^{\text{int}}_e, \quad (2.119a)
\]

and

\[
\mathbf{f}^{\text{ext}} = \sum_{e=1}^{n_{\text{ele}}} \mathbf{A} \mathbf{f}^{\text{ext}}_e. \quad (2.119b)
\]
In essence, each component of the global force on a specific global node is the result of the sum of the corresponding element nodes of all elements that share that global node.

It is worth noting that the assembled nodal internal and external forces have been expressed in a spatial version. Nonetheless, these can also be expressed in terms of a material version, which reads

\[
f^\text{int}_e = \int_{\Omega^e} G^\top \frac{\partial \mathbf{F} (u_{n+1})}{\partial \mathbf{u}} \mathbf{b}_n \, d\mathbf{v}, \tag{2.120}
\]

and

\[
f^\text{ext}_e = \int_{\Omega^e} N^\top b_{0,n+1} \, d\mathbf{v} + \int_{\partial \Omega^e} N^\top t_{0,n+1} \, d\mathbf{a}. \tag{2.121}
\]

**Numerical integration**

The weak formulation established the equilibrium as an integration over the domain of the continuum. Furthermore, the finite element approach allowed the integration over a set of finite elements that approximate the domain \( \Omega \). In practice, this integration is typically performed numerically, using a quadrature rule such as the Gauss-Legendre quadrature. Generally speaking, a Gaussian quadrature approximates an integral of a function \( f \) over a domain \( \Gamma \) by the evaluation of the function on \( n_{\text{gauss}} \) points, such that

\[
\int_{\Gamma} f (\xi) \, d\xi \approx \sum_{i=1}^{n_{\text{gauss}}} w_i f (\xi_i), \tag{2.122}
\]

where \( \xi_i \) \((i = 1, \ldots, n_{\text{gauss}})\) are the coordinates of the Gauss points and \( w_i \) \((i = 1, \ldots, n_{\text{gauss}})\) are the corresponding weights.

Additionally, the integration of a function \( g \) over a domain \( \Omega \), with the function \( x : \Gamma \rightarrow \Omega \) mapping the standard domain \( \Gamma \) onto \( \Omega \) (as shown in Fig. 2.6), can be written in terms of a transformation of variables by

\[
\int_{\Omega} g (x) \, dx = \int_{\Gamma} g (x (\xi)) j (\xi) \, d\xi \approx \sum_{i=1}^{n_{\text{gauss}}} w_i g (x (\xi_i)) j (\xi_i), \tag{2.123}
\]

where

\[
j (\xi) = \det \left[ \frac{\partial x}{\partial \xi} \right], \tag{2.124}
\]

is the determinant of the transformation jacobian. It is also worth noting that the integration can be performed not only over a domain \( \Omega \) but also on the boundary \( \partial \Omega \). Therefore, the integrations in Eqs. (2.117), (2.118), (2.120) and (2.121) are replaced by the Gaussian quadrature with an appropriate number of Gauss points.

**Incremental loading scheme**

The time discretization discussed in Section 2.8.1 introduced the idea of using an incremental constitutive function to evaluate the constitutive properties of the continuum at a
given instant \( t_{n+1} \). The implementation of this methodology constitutes an incremental finite element scheme. In the case of a proportional loading scheme, the body force and surface tractions at any given instant \( t_{n+1} \) are given by

\[
\begin{align*}
  b_{n+1} &= \lambda_{n+1} \tilde{b}, \\
  t_{n+1} &= \lambda_{n+1} \tilde{t},
\end{align*}
\]  

(2.125)

where \( \lambda_{n+1} \) is the prescribed load factor at \( t_{n+1} \) and \( \tilde{b} \) and \( \tilde{t} \) are the prescribed constant body and surface forces.

### 2.8.3 Newton-Raphson method

As stated in previous sections, the resulting equilibrium equations obtained by finite element discretization are nonlinear. Therefore, a robust numerical method must be employed to obtain a valid solution. The Newton-Raphson method is of particular interest, given its quadratic rate of convergence, and suitability for robust nonlinear incremental finite element schemes.

The key aspect of the Newton-Raphson method is the linearization of the nonlinear discretized incremental equilibrium equation, linearized on the current iterative value. Each iteration solves this linearized equation and essentially obtains an estimate of the solution. This estimate is used as the linearization point for the next iteration. The procedure is repeated until the error of the solution is below a given tolerance.

Recall Eq. (2.116) and consider we are solving the iteration \( k \) of the Newton-Raphson method. The global displacement vector at the previous iteration \( u^{(k-1)}_{n+1} \) is known. Upon linearization, the function becomes

\[
\begin{align*}
  r \left( u^{(k)}_{n+1} \right) &\approx r \left( u^{(k-1)}_{n+1} \right) + \left. \frac{\partial r}{\partial u_{n+1}} \right|_{u^{(k-1)}_{n+1}} \left( u^{(k)}_{n+1} - u^{(k-1)}_{n+1} \right) \\
  &= r^{(k-1)} + K_T \left( u^{(k)}_{n+1} - u^{(k-1)}_{n+1} \right) \\
  &= r^{(k-1)} + K_T \delta u^{(k)} \end{align*}
\]  

(2.126)
where $\mathbf{K}_T$ is the global tangent stiffness matrix. Using the linearized version of the function, the value of $\mathbf{u}^{(k)}_{n+1}$ is obtained from the solution of the system of equations

$$\mathbf{K}_T \delta \mathbf{u}^{(k)} = -\mathbf{r}^{(k-1)},$$  \hspace{1cm} (2.127)

by

$$\mathbf{u}^{(k)}_{n+1} = \mathbf{u}^{(k-1)}_{n+1} + \delta \mathbf{u}^{(k)}.$$  \hspace{1cm} (2.128)

This iterative process is repeated until a certain convergence tolerance is satisfied at an iteration $m$, that is, until

$$\frac{|\mathbf{r}^{(m)}|}{|\mathbf{f}_{\text{ext}}^{n+1}|} \leq \epsilon_{\text{tol}},$$  \hspace{1cm} (2.129)

is verified, with $\epsilon_{\text{tol}}$ being the convergence tolerance. The converged value $\mathbf{u}^{(m)}_{n+1}$ then becomes the displacement vector after the increment $n + 1$, that is

$$\mathbf{u}_{n+1} = \mathbf{u}^{(m)}_{n+1}.$$  \hspace{1cm} (2.130)

The global tangent stiffness matrix is given by the assembly of all element tangent stiffness matrices, that is,

$$\mathbf{K}_T = \bigoplus_{e=1}^{n_{\text{elems}}} \mathbf{K}_T^e.$$  \hspace{1cm} (2.131)

Up to this point, no reference was made whether the terms in the Newton-Raphson method are evaluated in a spatial or material version. Either version can be followed, as long as the global nodal forces and the tangent stiffness matrix are evaluated consistently.

In a spatial version, the element tangent stiffness matrix of the element $e$ given by

$$\mathbf{K}_T^e = \int_{\varphi_{n+1}(^e\Omega)} G^T \mathbf{a} G \, dv.$$  \hspace{1cm} (2.132)

The fourth order tensor $\mathbf{a}$ is known as the consistent spatial tangent modulus, and is given by

$$a_{ijkl} = \frac{1}{J} \frac{\partial \tau_{ij}}{\partial F_{km}} F_{lm} - \sigma_{il} \delta_{jk}.$$  \hspace{1cm} (2.133)

Alternatively, in a material version, the element tangent stiffness matrix of the element $e$ becomes

$$\mathbf{K}_T^e = \int_{^e\Omega} G^T \mathbf{A} G \, dv.$$  \hspace{1cm} (2.134)

Similarly, the fourth order tensor $\mathbf{A}$ is known as the consistent material tangent modulus, defined by

$$A_{ijkl} = \frac{\partial P_{ij}}{\partial F_{kl}}.$$  \hspace{1cm} (2.135)

The material and spatial elasticity tensors are related by

$$a_{ijkl} = \frac{1}{J} A_{imkn} F_{jm} F_{ln}.$$  \hspace{1cm} (2.136)
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Chapter 3
Multi-scale Models and Computational Homogenization

The behavior of a solid is strongly dependent of its microstructure. When considering materials whose microstructures are extremely complex, or when a significant amount of defects or damage are present, a macroscopic constitutive model might not be sufficiently accurate to represent the actual behavior of the solid. To introduce the effects of the microstructure on the response of the material, Multi-scale Models are often used, where a microscopic problem is used to derive the constitutive behavior of a macroscopic point. Furthermore, Multi-scale Models based on Computational Homogenization use an averaging technique called Homogenization to derive the material response from a Representative Volume Element (RVE).

In this chapter, the general framework of a Multi-scale Model is presented. The concept of Representative Volume Element (RVE) is introduced. Then, the connection between both scales is established by Homogenization of relevant fields, resulting in a set of microscopic restrictions. Finally, a number of boundary conditions for the RVE is given.

3.1 Representative volume element

The term representative volume element (RVE) was firstly introduced by R. Hill, as an attempt to characterize the microstructure of the material and its influence on the macroscopic response (R. Hill, 1963; Pinto Carvalho, 2015). It can be interpreted as the smallest volume of material where the assumption of material continuity is still valid (de Souza Neto, Peric, et al., 2008). According to R. Hill, the RVE is a sample of material with a structure that is typical, on average, of the entire material, and has enough microscopic defects to make the mechanical properties independent of boundary values. The RVE is defined at a point in the macroscale. On the basis of establishment of an RVE is the principle of scale separation. It states that the characteristic dimension of the RVE should be large enough to be representative of the microstructure of the material (i.e. significantly larger than its heterogeneities), but significantly smaller than the macroscale domain, i.e.

\[ L_\mu \ll L_{\text{RVE}} \ll L_{\text{macro}} \]  

where \( L_\mu \), \( L_{\text{RVE}} \) and \( L_{\text{macro}} \) are the lengths of the microscopic heterogeneities, of the RVE and of the macroscale model, respectively (Hashin, 1983).
An example of a RVE for a macroscopic point $x$ is shown in Fig. 3.1. The domain at the macroscale is $\Omega$, with a boundary $\partial \Omega$. At point $x$, a microscopic domain $\Omega_\mu$ with a boundary $\partial \Omega_\mu$ defines the RVE. A generic point in the microscale is represented as $x_\mu$. Furthermore, the RVE might also contain voids (region $\Omega_v^\mu$ with boundary $\partial \Omega_v^\mu$) and inclusions (region $\Omega_i^\mu$ with boundary $\partial \Omega_i^\mu$). We can additionally define a solid region $\Omega_s^\mu$ that verifies

$$\Omega_\mu = \Omega_v^\mu \cup \Omega_s^\mu. \quad (3.2)$$

The relation between the solid and void part of the RVE can also be expressed as (Nemat-Nasser, 1993)

$$\Omega_s^\mu = \Omega_\mu - \Omega_v^\mu. \quad (3.3)$$

The solid part will be from now referred to as the matrix of the RVE. For the sake of simplicity, in this work we will consider the matrix homogeneous, but not necessarily isotropic (Nemat-Nasser, 1993). Therefore, the presence of inclusions will be neglected ($\Omega_i^\mu = \emptyset$).

Finally, it also needs to be remarked that, in general, the void boundary $\partial \Omega_v^\mu$ can intersect the RVE boundary $\partial \Omega_\mu$. To simplify the problem, and according to the analysis from Nemat-Nasser, this condition will not be considered. Therefore, any void inside the RVE domain is considered to be fully enclosed by the boundary of the RVE, i.e., fully surrounded by the matrix material.

![Figure 3.1: Macro-element and respective RVE at point $x$.](image)

### 3.2 Large strain multi-scale models

In Chapter 2, the formulation of continuum mechanics and thermodynamics was presented considering large strains. Additionally, as covered in Section 3.1, the usage of RVEs allows us to describe a point $x$ in the macro-scale using an appropriate volume element representative of the micro-scale at that point. A model must be developed to connect both scales.

In the employed method, the connection between macro and micro-scale is obtained by an interchange of strain and stress states between them. A schematic representation of the model is shown in Fig. 3.2. The macroscopic problem enforces a deformation measure,
in this case, the deformation gradient $F$ at a given macroscopic point $x$. This field is used to solve the microscopic equilibrium problem, resulting in a stress measure (in this case, the first Piola-Kirchhoff stress tensor $P$). Such stress measure is defined over the microscopic domain $\Omega_\mu$, and is dependent of the microscopic coordinate $x_\mu$. An estimate for its macroscopic counterpart is obtained by an averaging process called homogenization, which will be presented in Section 3.2.1. The homogenized stress measure will then be returned to the macroscopic problem. In essence, the multi-scale model uses a microscopic equilibrium problem over an RVE to establish the macroscopic constitutive model of the macroscopic material. Nevertheless, a constitutive model is still used in the microscopic equilibrium problem.

Throughout this section it will be seen that the imposition of a homogenized deformation gradient at the micro-scale restricts the solution of the microscopic problem. The energy connection between scales also results in additional constraints to the RVE. From these restrictions, a number of boundary conditions for the microscopic problem will be established and discussed. Furthermore, it is worth mentioning that the formulation used is a first order formulation, where only the first term of the Taylor series of the transformation between the reference the deformed configurations is considered, that is (Kouznetsova et al., 2004),

$$dx = F \cdot dp.$$ (3.4)

![Figure 3.2: Schematic representation of a multi-scale model.](image-url)
3.2.1 Homogenization

The transition of properties from the microscale to the macroscale is performed by a process called homogenization. The macroscopic properties at a point $x$ are a volume average of the properties of the RVE. In a general case, a field $A(x, t)$ over a domain in the macroscale can be obtained from the field over the microscopic domain $A_\mu(x_\mu, t)$ by

$$A(x, t) = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} A_\mu(x_\mu, t) \, dv, \quad (3.5)$$

where $x$ is the macroscopic point where the RVE is defined, $x_\mu$ is a point at the microscopic domain and $v_{0,\mu}$ is the volume of the RVE in the reference configuration. Note that the volume integration is performed with the RVE at the reference configuration. Nonetheless, the homogenization could also be performed on the deformed configuration as well.

3.2.2 Homogenization of the deformation gradient

One of the key aspects of a multi-scale model is the connection of properties between the scales. As shown in Section 3.2.1, the homogenization allows to define the properties at the macroscale as a volume average of their counterparts at the microscale. This principle is also on the basis of the imposition of the macroscopic deformation gradient to the microscale. Firstly, accordingly to Eq. (3.5), the macroscopic deformation gradient $F(x, t)$ is related to its microscopic counterpart $F_\mu(x_\mu, t)$ by

$$F(x, t) = \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} F_\mu(x_\mu, t) \, dv. \quad (3.6)$$

Recalling Eq. (2.14), the deformation gradient is the sum of the identity tensor and the material gradient of the displacement field, i.e.

$$F(x, t) = I + \frac{1}{v_{0,\mu}} \int_{\Omega_\mu} \nabla_p u_\mu(x_\mu, t) \, dv. \quad (3.7)$$

We can now transform the integration over the domain $\Omega_\mu$ to an integration over the boundary $\partial \Omega_\mu$ by the application of Gauss’ theorem, such that

$$F(x, t) = I + \frac{1}{v_{0,\mu}} \int_{\partial \Omega_\mu} u_\mu(x_\mu, t) \otimes n_{0,\mu}(p_\mu) \, da, \quad (3.8)$$

where $n_{0,\mu}$ is the normal to the external boundary of the microscopic domain in the reference configuration. This last expression allows us to express the macroscopic deformation gradient as a function of the microscopic displacement field over the boundary of the RVE. As it will be shown soon, the imposition of a macroscopic deformation gradient effectively places a restriction on the set of admissible kinematic microscopic displacements.

3.2.3 RVE kinematics

As shown in Section 3.2.2, the imposition of a macroscopic deformation gradient constrains the displacement field over the boundary of the RVE. We can establish a condition for the
3.2. Large strain multi-scale models

Microscopic displacement field $u_\mu$ to be admissible. A microscopic displacement field $u_\mu$ is kinematically admissible if

$$u_\mu \in \mathcal{K}_\mu^*, \quad (3.9)$$

where $\mathcal{K}_\mu^*$ is the minimally constrained set of kinematically admissible microscopic displacements, as a consequence of Eq. (3.8), given by

$$\mathcal{K}_\mu^* = \{ u_\mu, \text{sufficiently regular} \mid \int_{\partial \Omega_\mu} u_\mu(x_\mu, t) \otimes n_{0,\mu}(p_\mu, t) \, da = \nu_{0,\mu} [F(x, t) - I] \} . \quad (3.10)$$

Moreover, the microscopic displacement field can be decomposed in terms of a linear displacement and a displacement fluctuation,

$$u_\mu(x_\mu, t) = [F(x, t) - I] p_\mu + \tilde{u}_\mu(x_\mu, t) . \quad (3.11)$$

The first component is the linear displacement, which varies linearly with the microscopic position $p_\mu$ (in the reference configuration). The second component is the displacement fluctuation. This decomposition is of interest because the linear displacement is known, making the displacement fluctuations the unknown of the problem. Introducing this decomposition in Eq. (2.14), the deformation gradient at the microscale becomes

$$F_\mu(x_\mu, t) = I + \nabla_p [(F(x, t) - I) p_\mu + \tilde{u}_\mu(x_\mu, t)]$$

$$= I + [F(x, t) - I] I + \nabla_p \tilde{u}_\mu(x_\mu, t)$$

$$= F(x, t) + \nabla_p \tilde{u}_\mu(x_\mu, t) . \quad (3.12)$$

As a result of the microscopic displacement field decomposition, the microscopic deformation gradient is now also decomposed in two terms. The first is the imposed deformation gradient at the macroscale, which represents homogeneous deformation. The second is the material gradient of the fluctuation displacement field. If we introduce the last expression in Eq. (3.6),

$$F(x, t) = \frac{1}{\nu_{0,\mu}} \int_{\Omega_\mu} F_\mu(x_\mu, t) \, dv$$

$$= F(x, t) + \frac{1}{\nu_{0,\mu}} \int_{\Omega_\mu} \nabla_p \tilde{u}_\mu(x_\mu, t) \, dv , \quad (3.13)$$

it becomes apparent that

$$\int_{\Omega_\mu} \nabla_p \tilde{u}_\mu(x_\mu, t) \, dv = 0 . \quad (3.14)$$

Once again, using the Gauss theorem, the volume integral becomes a surface integral over the boundary,

$$\int_{\partial \Omega_\mu} \tilde{u}_\mu(x_\mu, t) \otimes n_{0,\mu}(p_\mu, t) \, da = 0 . \quad (3.15)$$

Finally, this last identity allows us to define the minimally constrained set of displacement fluctuations,

$$\mathcal{\tilde{K}}_\mu^* = \{ \tilde{u}_\mu, \text{sufficiently regular} \mid \int_{\partial \Omega_\mu} \tilde{u}_\mu(x_\mu, t) \otimes n_{0,\mu}(p_\mu, t) \, da = 0 \} . \quad (3.16)$$
We can also define a set of admissible virtual displacements of the RVE, used for the variational formulation proposed. The set can be defined as the difference between two admissible displacements,

\[
\mathcal{Y}_\mu = \{ \eta = u_{\mu,1} - u_{\mu,2} | u_{\mu,1}, u_{\mu,2} \in \mathcal{K}_\mu \}.
\] (3.17)

As can be seen, this set coincides with the set of kinematically admissible displacement fluctuations, this is

\[
\mathcal{Y}_\mu = \tilde{\mathcal{K}}_\mu.
\] (3.18)

Analogously, the set of kinematically admissible velocity fluctuations verifies

\[
\dot{\tilde{u}}_\mu \in \mathcal{V}_\mu.
\] (3.19)

### 3.2.4 RVE equilibrium

The conservation principles expressed in Chapter 2 must be satisfied not only at the macroscopic level but also at the microscopic domain. Given the definition of the representative volume element, and recalling from Section 2.4 the strong form of equilibrium equations with inertial effects neglected, the equilibrium of the RVE is expressed by

\[
\begin{align*}
\text{div}_p P_\mu (x_\mu, t) + b_{0,\mu} (x_\mu, t) &= 0, \forall x_\mu \in \Omega^s_\mu, \\
\text{div}_p P_\mu (x_\mu, t) + b_{0,\mu} (x_\mu, t) &= 0, \forall x_\mu \in \Omega^v_\mu, \\
P_\mu (x_\mu, t) n_{0,\mu} (p_\mu) &= t_{0,\mu} (x_\mu, t), \forall x_\mu \in \partial \Omega_\mu, \\
\| P_\mu (x_\mu, t) n_{0,\mu} (p_\mu) \| &= 0, \forall x_\mu \in \partial \Omega^v_\mu,
\end{align*}
\] (3.20)

where \( P_\mu \) is the first Piola-Kirchhoff stress tensor in the microscopic domain, \( b_{0,\mu} \) is the body force per unit of reference volume and \( t_{0,\mu} \) is the surface traction per unit of reference area on the boundary of the RVE. The first two equations express the conservation of linear momentum in both the matrix and the voids, respectively. The third equation expresses the force equilibrium in the boundary of the RVE. Last equation guarantees continuity of the stress field on the interface between the matrix and the voids. Note that the absence of pressure inside the void automatically satisfies the second and fourth equations.

The weak formulation of the RVE equilibrium can be obtained in a similar fashion, as shown in Section 2.6. Recalling Eq. (2.86) and its quasi-static counterpart Eq. (2.88), the weak formulation of the RVE equilibrium problem becomes

\[
\begin{align*}
\int_{\Omega^s_\mu} P_\mu (x_\mu, t) : \nabla_p (\eta_\mu) \, dv &- \int_{\Omega_\mu} b_{0,\mu} (x_\mu, t) \cdot \eta_\mu \, dv \\
&- \int_{\partial \Omega_\mu} t_{0,\mu} \cdot \eta_\mu \, da = 0, \forall \eta_\mu \in \mathcal{Y}_\mu.
\end{align*}
\] (3.21)

In this version, the weak formulation integrates over the domain of the whole RVE and its boundary. However, one can separate the terms of matrix and void regions on the volumetric integration, resulting in

\[
\begin{align*}
\int_{\Omega^s_\mu} P_\mu (x_\mu, t) : \nabla_p (\eta_\mu) \, dv &- \int_{\Omega^s_\mu} b_{0,\mu} (x_\mu, t) \cdot \eta_\mu \, dv - \int_{\partial \Omega^s_\mu} t_{0,\mu} \cdot \eta_\mu \, da \\
&+ \int_{\Omega^v_\mu} P_\mu (x_\mu, t) : \nabla_p (\eta_\mu) \, dv - \int_{\Omega^v_\mu} b_{0,\mu} (x_\mu, t) \cdot \eta_\mu \, dv = 0, \forall \eta_\mu \in \mathcal{Y}_\mu.
\end{align*}
\] (3.22)
By taking the balance of forces on the voids only, it verifies
\[
\int_{\Omega_{\mu}} P_{\mu} (x_{\mu}, t) : \nabla_p (\eta_{\mu}) \, dv - \int_{\Omega_{\mu}} b_{0, \mu} (x_{\mu}, t) \cdot \eta_{\mu} \, dv \\
+ \int_{\partial \Omega_{\mu}} t_{0, \mu}^i (x_{\mu}, t) \cdot \eta_{\mu} \, da = 0, \quad \forall \eta_{\mu} \in \mathcal{V}_{\mu},
\]
(3.23)
where \( t_{0, \mu} \) is the internal traction force on the boundary of the void, exerted against the matrix. Substituting Eq. (3.23) in Eq. (3.22), the weak equilibrium formulation becomes
\[
\int_{\Omega_{\mu}} P_{\mu} (x_{\mu}, t) : \nabla_p (\eta_{\mu}) \, dv - \int_{\Omega_{\mu}} b_{0, \mu} (x_{\mu}, t) \cdot \eta_{\mu} \, dv - \int_{\partial \Omega_{\mu}} t_{0, \mu} \cdot \eta_{\mu} \, da \\
+ \int_{\partial \Omega_{\mu}} t_{\mu}^i (x_{\mu}, t) \cdot \eta_{\mu} \, da = 0, \quad \forall \eta_{\mu} \in \mathcal{V}_{\mu}.
\]
(3.24)

### 3.2.5 Stress tensor homogenization

In previous sections, the homogenization principle has been introduced. The deformation gradient was then homogenized, which allowed us to establish the minimally constrained set of displacement fluctuations. A similar procedure can be taken for the first Piola-Kirchhoff stress tensor, where its homogenized field becomes
\[
P (x, t) = \frac{1}{v_{0, \mu}} \int_{\Omega_{\mu}} P_{\mu} (x_{\mu}, t) \, dv.
\]
(3.25)
This expression can also be written as
\[
P (x, t) = \frac{1}{v_{0, \mu}} \int_{\Omega_{\mu}} P_{\mu} (x_{\mu}, t) (\nabla_p P_{\mu})^T \, dv.
\]
(3.26)
Integrating by parts the right hand side of the expression,
\[
P (x, t) = \frac{1}{v_{0, \mu}} \left[ \int_{\Omega_{\mu}} P_{\mu} (x_{\mu}, t) n_{0, \mu} (p_{\mu}, t) \otimes p_{\mu} \, da - \int_{\Omega_{\mu}} \text{div} P_{\mu} (x_{\mu}, t) \otimes p_{\mu} \, dv \right].
\]
(3.27)
Recalling the equilibrium equations of the RVE given in Eq. (3.20), the terms involving the first Piola-Kirchhoff stress tensor can thus be written as
\[
P (x, t) = \frac{1}{v_{0, \mu}} \left[ \int_{\Omega_{\mu}} t_{\mu} (x_{\mu}, t) \otimes p_{\mu} \, da - \int_{\Omega_{\mu}} b_{\mu} (x_{\mu}, t) \otimes p_{\mu} \, dv \right].
\]
(3.28)
This last expression makes possible to obtain the macroscopic first Piola-Kirchhoff stress tensor from the volume and surface reactive forces on the RVE.

Regarding the Cauchy stress tensor, it can be expressed in terms of the homogenized first Piola-Kirchhoff stress tensor and the homogenized deformation gradient by
\[
\sigma = \frac{1}{\det F} P F^T.
\]
(3.29)
3.2.6 Hill-Mandel principle

Up until this point, the relationship between field properties in both the macroscale and the microscale has been established by the homogenization of microscale properties. The Hill-Mandel principle (R. Hill, 1963; Hill, 1972; Mandel, 1981) connects both scales by an energy consistency principle. Its general expression states that

\[
P(x, t) : \dot{F}(x, t) = \frac{1}{v_{0, \mu}} \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \dot{F}_{\mu}(x_{\mu}, t) \, dv,
\]  

(3.30)

where \(\dot{F}\) represents the macroscopic rate of deformation gradient and \(\dot{F}_{\mu}\) its microscopic counterpart. In essence, the volume average of the power of an equilibrium stress field over the microscopic domain equals the macroscopic stress power (de Souza Neto, Blanco, et al., 2015). Recalling Eq. (3.12), the microscopic rate of deformation gradient becomes

\[
\dot{F}_{\mu}(x_{\mu}, t) = \dot{F}(x, t) + \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t).
\]  

(3.31)

Moreover, Eq. (3.30) needs to be satisfied for any admissible rate of deformation gradient as well as any microscopic stress field \(P_{\mu}(x_{\mu}, t)\). Therefore, combining last two expressions,

\[
P(x, t) : \dot{F}(x, t) = \frac{1}{v_{0, \mu}} \left[ \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \dot{F}(x, t) \, dv + \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t) \, dv \right]
\]

\[
= \frac{1}{v_{0, \mu}} \left[ \dot{F}(x, t) : \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) \, dv + \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t) \, dv \right]
\]

\[
= P(x, t) : \dot{F}(x, t) + \frac{1}{v_{0, \mu}} \int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t) \, dv.
\]  

(3.32)

From last expression, it follows that

\[
\int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t) \, dv = 0.
\]  

(3.33)

Therefore, the application of the Hill-Mandel principle imposes a restriction on the first Piola-Kirchhoff stress tensor and velocity fluctuations for the domain of the RVE. Separating the domain in terms of the matrix region and the voids region, the integration by parts of Eq. (3.33) results in

\[
\int_{\Omega_{\mu}} P_{\mu}(x_{\mu}, t) : \nabla_{p} \dot{u}_{\mu}(x_{\mu}, t) \, dv = \int_{\partial \Omega_{\mu}} \left[ P_{\mu}(x_{\mu}, t) \cdot n_{0, \mu}(p_{\mu}, t) \right] \cdot \dot{u}_{\mu}(x_{\mu}, t) \, d\alpha
\]

\[
- \int_{\Omega_{\mu}} \text{div} P_{\mu}(x_{\mu}, t) \cdot \dot{u}_{\mu}(x_{\mu}, t) \, dv
\]

\[
- \int_{\Omega_{\mu}} \text{div} P_{\mu}(x_{\mu}, t) \cdot \dot{u}_{\mu}(x_{\mu}, t) \, dv. 
\]  

(3.34)
Recalling Eq. (3.20), the terms involving the first Piola-Kirchhoff stress tensor can be written as functions of the volumetric body or surface traction forces. Considering the body forces null on the voids, Eq. (3.34) reduces to

$$ \int_{\Omega} \mathbf{P}_\mu (\mathbf{x}_\mu, t) \cdot \nabla \hat{\mathbf{u}}_\mu (\mathbf{x}_\mu, t) \, dv = \int_{\partial \Omega} \mathbf{t}_\mu (\mathbf{x}_\mu, t) \cdot \hat{\mathbf{u}}_\mu (\mathbf{x}_\mu, t) \, da + \int_{\Omega} \mathbf{b}_\mu (\mathbf{x}_\mu, t) \cdot \hat{\mathbf{u}}_\mu (\mathbf{x}_\mu, t) \, dv. $$

(3.35)

As both terms are independent, Eq. (3.33) is verified if and only if

$$ \int_{\partial \Omega} \mathbf{t}_\mu (\mathbf{x}_\mu, t) \cdot \eta_\mu \, da = 0, \quad \forall \eta_\mu \in \mathcal{V}_\mu, $$

(3.36a)

$$ \int_{\Omega} \mathbf{b}_\mu (\mathbf{x}_\mu, t) \cdot \eta_\mu \, dv = 0, \quad \forall \eta_\mu \in \mathcal{V}_\mu. $$

(3.36b)

With these conditions and given the definition of the set of the admissible velocity fluctuations field, we can finally conclude that the Hill-Mandel principle indicates that the volume and surface forces correspond to the reactions required by the kinematic constraints,

$$ \int_{\partial \Omega} \mathbf{t}_\mu (\mathbf{x}_\mu, t) \cdot \eta_\mu \, da = 0, \quad \forall \eta_\mu \in \mathcal{V}_\mu, $$

(3.37a)

$$ \int_{\Omega} \mathbf{b}_\mu (\mathbf{x}_\mu, t) \cdot \eta_\mu \, dv = 0, \quad \forall \eta_\mu \in \mathcal{V}_\mu. $$

(3.37b)

### 3.3 Boundary conditions

The microscopic equilibrium problem requires a set of kinematic constraints. Up until this point, a reference was made to the set of minimally constrained kinematic admissible microscopic displacements $\mathcal{K}_\mu^*$, as well as the corresponding set of displacement fluctuations $\mathcal{X}_\mu^*$. However, different restrictions can be imposed in order to correctly model the response of the microstructure, which lead to different sets for the microscopic displacement fluctuations.

As introduced before, the chosen set of kinematic constraints must verify Eq. (3.15), as well as the conclusions from the application of the Hill-Mandel principle, summarized in Eq. (3.37). In what follows, it will be demonstrated that such set can be expressed in terms of the boundary displacement fluctuations and boundary traction forces. These fields effectively pose the boundary conditions of the problem. In this section, four different models will be shown:

1. Taylor model;
2. Linear boundary condition;
3. Periodic boundary condition;
4. Uniform boundary traction model.

It will be shown that these models are sorted in a descending order of level of restriction, that is, the Taylor model enforces the largest constraints (and consequently increases the stiffness of the RVE) and the uniform traction model is the least constraining model (it is, in fact, identical to the minimally constrained set of admissible kinematic displacement fluctuations).

3.3.1 Taylor model

The Taylor hypothesis is the simplest and most restrictive boundary condition of the set considered in this work. In essence, it imposes the displacement on the domain of the RVE to be linear with the reference position, such that

\[ u_\mu(x_\mu, t) = [F(x, t) - I] p_\mu, \quad \forall x_\mu \in \Omega_\mu. \]  

(3.38)

A schematic representation of this condition is shown in Fig. 3.3. From Eq. (3.11), it becomes apparent that

\[ \tilde{u}_\mu(x_\mu, t) = 0, \quad \forall x_\mu \in \Omega_\mu. \]  

(3.39)

Such condition immediately satisfies Eqs. (3.15) and (3.37). Furthermore, the microscopic deformation gradient is constant and coincides with the macroscopic deformation gradient, such that

\[ F(x, t) = F_\mu(x_\mu, t). \]  

(3.40)

This condition imposes a strong restriction on the deformation inside the domain. Therefore, the RVE is not capable of deforming freely enough to characterize geometric or material heterogenities. Ultimately, this results in an overly stiff response of the material (Pinto Carvalho, 2015; Carneiro Molina, 2007; Speirs, 2007).

The set of kinematically admissible displacement fluctuations for the Taylor hypothesis is thus given by

\[ \mathcal{X}_\mu^{Tay} \equiv \{ \tilde{u}_\mu, \text{sufficiently regular} \mid \tilde{u}_\mu(x_\mu, t) = 0, \quad \forall x_\mu \in \Omega_\mu \}. \]  

(3.41)

Figure 3.3: Schematic representation of RVE deformation with a Taylor boundary condition.

3.3.2 Linear boundary condition

The linear boundary condition relaxes Taylor’s hypothesis by enforcing the displacements only on the boundary of the RVE. Therefore, in \( \partial \Omega_\mu \), the displacements are linear with the
coordinate, that is,

\[ u_\mu(x_\mu, t) = [F(x, t) - I] p_\mu, \quad \forall x_\mu \in \partial \Omega_\mu. \]  (3.42)

A schematic representation of this condition is shown in Fig. 3.4. Once again, from Eq. (3.11), it can be easily verified that

\[ \bar{u}_\mu(x_\mu, t) = 0, \quad \forall x_\mu \in \partial \Omega_\mu. \]  (3.43)

As before, this condition immediately satisfies Eqs. (3.15) and (3.37a). However, Eq. (3.37b) is only satisfied in the absence of body forces. In a quasi-static formulation, where inertial effects are neglected, and in the absence of other body forces, this is a reasonable assumption.

It’s also possible to define the set of kinematically admissible displacement fluctuations for the linear boundary condition as

\[ \mathcal{X}_\mu^{\text{Lin}} \equiv \{ u_\mu, \text{sufficiently regular} \mid \bar{u}_\mu(x_\mu, t) = 0, \forall x_\mu \in \partial \Omega_\mu \}. \]  (3.44)

Figure 3.4: Schematic representation of RVE deformation with a linear boundary condition.

### 3.3.3 Periodic boundary condition

Some materials show a repetitive microstructure. The periodic boundary condition attempts to model the response of these materials. Under the assumption that a periodic structure retains its periodicity under deformation, a restriction can be placed in terms of the boundary displacements of the RVE (Speirs, 2007). To do that, the microscopic domain boundary \( \partial \Omega_\mu \) is first split into pairs of boundaries \( (\Gamma_i^-, \Gamma_i^+) \), such that

\[ \partial \Omega_\mu = \bigcup_{i=1}^n (\Gamma_i^-, \Gamma_i^+). \]  (3.45)

Considering two points \( p_{\mu,i}^- \) and \( p_{\mu,i}^+ \) belonging to the boundaries \( \Gamma_i^- \) and \( \Gamma_i^+ \), respectively, their normals must verify

\[ n_{0,\mu}(p_{\mu,i}^+, t) = -n_{0,\mu}(p_{\mu,i}^-, t), \quad \forall p_{\mu,i}^-, \in \Gamma_i^-, \forall p_{\mu,i}^+, \in \Gamma_i^+. \]  (3.46)

In the deformed configuration, consider two points \( x_{\mu,i}^- \) and \( x_{\mu,i}^+ \) belonging to the deformed boundaries of \( \Gamma_i^- \) and \( \Gamma_i^+ \), respectively. Recalling Eq. (3.15), we can now express
the normals and displacement fluctuations in the boundary as

$$
\int_{\partial \Omega} \tilde{u}_\mu (x_\mu, t) \otimes n_{0, \mu} (p_\mu, t) \, da = \sum_{i=1}^{n} \left[ \int_{\Gamma_i^-} \tilde{u}_\mu (x_{\mu,i}^-, t) \otimes n_{0, \mu} (p_{\mu,i}^-, t) \, d\Gamma_i^- \\
+ \int_{\Gamma_i^+} \tilde{u}_\mu (x_{\mu,i}^+, t) \otimes n_{0, \mu} (p_{\mu,i}^+, t) \, d\Gamma_i^+ \right] 
= 0.
$$

(3.47)

Given Eq. (3.46), the condition is automatically satisfied if

$$
\tilde{u}_\mu (x_{\mu,i}^-, t) = \tilde{u}_\mu (x_{\mu,i}^+, t).
$$

(3.48)

As in previous boundary conditions, Eq. (3.37b) is only satisfied in the absence of body forces. Furthermore, Eq. (3.37a) is also satisfied if the traction field on the boundary is anti-periodic, i.e.

$$
t_{0,\mu} (x_{\mu,i}^-, t) = -t_{0,\mu} (x_{\mu,i}^+, t).
$$

(3.49)

A schematic representation of the periodic boundary condition is shown in Fig. 3.5. Equation (3.48) establishes the set of kinematically admissible displacement fluctuations for the periodic boundary condition

$$
\mathcal{K}_\mu^\text{Per} \equiv \left\{ \tilde{u}_\mu, \text{sufficiently regular} \mid \tilde{u}_\mu (x_{\mu,i}^-, t) = \tilde{u}_\mu (x_{\mu,i}^+, t), \right. \\
\forall x_{\mu,i}^- \in \varphi (\Gamma_i^-), \forall x_{\mu,i}^+ \in \varphi (\Gamma_i^+) \right\}.
$$

(3.50)

3.3.4 Uniform traction on the boundary

The uniform traction boundary condition is the less restrictive, when compared with the ones presented here. In fact, it is identical to the set of minimally constrained set of displacement fluctuations, i.e.,

$$
\mathcal{K}_\mu^\text{Uni} = \mathcal{K}_\mu^* \equiv \left\{ \tilde{u}_\mu, \text{sufficiently regular} \mid \int_{\partial \Omega} \tilde{u}_\mu (x_\mu, t) \otimes n_{0, \mu} (p_\mu, t) \, da = 0 \right\}
$$

(3.51)
This condition is shown schematically in Fig. 3.6. As before, Eq. (3.37b) is only satisfied in the absence of body forces. From Eq. (3.37a), the boundary traction is equal to the homogenized traction, that is,

\[ P_\mu (x_\mu, t) n_\mu (x_\mu, t) = P (x, t) n_\mu (x_\mu, t). \]  

(3.52)

Figure 3.6: Schematic representation of RVE deformation with a uniform traction boundary condition.

### 3.3.5 Comparison of models

As was mentioned in Sections 3.3.1 to 3.3.4, the proposed models have different levels of constraints and, therefore, lead to different material responses. The Taylor model is the most constrained model and that the uniform traction is the least constrained. In fact, the sets of kinematically admissible displacement fluctuations of each model can be related as follows:

\[ K_\mu^{\text{Tay}} \subset K_\mu^{\text{Lin}} \subset K_\mu^{\text{Per}} \subset K_\mu^{\text{Uni}}. \]  

(3.53)

Furthermore, the average properties obtained though homogenization are sensitive to the RVE size. A smaller RVE will contain less heterogeneities and, therefore, its response will deviate from the average macroscopic response. As the size of the RVE increases, the homogenized properties converge to their effective value (Terada et al., 2000; de Bortoli, 2017). The choice of boundary condition also influences this convergence. Compared with the effective response, linear and periodic boundary conditions typically give overly-stiff responses, while the uniform traction results in an underestimation of the stiffness. Figure 3.7 shows a schematic example where both the effect of the RVE size and of the boundary conditions are addressed.
Figure 3.7: Convergence of homogenized properties with the RVE size, with different boundary conditions (de Bortoli, 2017).
3.4 Numerical implementation

Combining Chapter 2 with the topics presented in this chapter, a numerical solution to the weak microscopic equilibrium equations can be obtained using the finite element method. The presented multi-scale model allows for the resolution of a macro-scale problem with a constitutive model obtained from microscopic homogenization. In this work, the focus is placed on the study of the macroscopic constitutive models. Although, this is achieved through the analysis of the homogenized response of RVEs. Therefore, only microscopic problems will be solved.

All analyses will use Links (Large Strain Implicit Non-Linear Finite Element Analysis of Solids Linking Scales), a multi-scale finite element analysis program developed and maintained by the research group CM2S (Computational Multi-Scale Modeling of Solids and Structures). The program allows for not only macro-scale and micro-scale analysis, but also coupled analysis (where a microscopic problem is used to derive the macroscopic constitutive model). Within the scope of this work, only the microscopic analysis component of Links will be used. The general inputs and outputs of the program are shown in Fig. 3.8. Furthermore, in the analyses of this work, a stress-driven approach was used. With this method, instead of a macroscopic deformation gradient, it is possible to impose a macroscopic stress tensor to the RVE. The basic algorithm for the stress-driven component is show in Fig. 3.9. In essence, given a prescribed macroscopic stress tensor $\sigma$, an external Newton-Raphson method is applied to the micro-scale equilibrium problem to solve for the macroscopic deformation gradient $F$ imposed to the RVE. As a final note, it must be remarked that this method introduced an increased computational effort, since that for each increment, various micro-scale equilibrium problems may have to be resolved.
Input file:
- Macroscopic deformation gradient or stress tensor;
- Incrementation scheme and convergence tolerance;
- Boundary conditions;
- Constitutive models;
- Mesh properties.

Solve the micro-scale equilibrium problem using

\[ \text{Links} \]

*Large Strain Implicit Non-Linear Analysis of Solids Linking Scales*

Outputs
- Homogenized/Macroscopic quantities;
- Distribution of local variables (stresses, strains, internal variables, etc.) throughout the loading history.

Figure 3.8: Inputs and outputs of Links for the analysis of micro-scale problems.
3.4. Numerical implementation

Begin

Update $\lambda_n$
Update prescribed stress $\sigma_n = \lambda_n \sigma^*$

Set $i = 1$
Initial guess $F_i^n = F_{n-1}$

Evaluate stress residual $R(F_i^n) = \sigma_n - \sigma_i^n(F_i^n)$

$\| R(F_i^n) \| \leq \sigma_{tol}$?

Yes

No

Solve micro-scale equilibrium problem with $F_i^{n+1}$

Newton Raphson method:

$\frac{\partial R}{\partial F} \Delta F_i^{n+1} = -R(F_i^n)$

$F_i^{n+1} = F_i^n + \Delta F_i^{n+1}$

$n = n + 1$

Yes

No

Last increment?

Yes

Stop

Figure 3.9: Stress driven algorithm.
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Chapter 4

Multi-scale Ductile Fracture

In this chapter, the mechanics of ductile damage and failure are presented. Then, a short characterization of the stress state and its connection to the triaxiality and Lode parameter is expressed. A brief review of the theory of plasticity is also given, and the concept of limit analysis is introduced. Furthermore, several models for porous media are presented, in particular, their yield functions and evolution laws. At the end of the chapter, these models are briefly compared.

4.1 Damage phenomena

The effects of void nucleation, growth and coalescence play an important role in the ductile failure of metals. The presence of voids inside a metallic matrix can be seen as damage to the virgin material. At first, damage shows at a microscopic level, with voids nucleating from particle inclusions, growing and finally coalescing with other voids. If sufficient plastic deformation happens, the coalescence of micro-voids generates successively larger voids, eventually reaching the macroscopic level. Once the defects reach a macroscopic level, ductile failure is imminent. In this section, a brief review of the mechanisms of void damage is shown. A bridge between the microscopic and macroscopic experimental evidence is also presented.

4.1.1 Microscopic mechanisms

The ductile failure of metals as a consequence of void nucleation, growth and coalescence was first identified in the 1940s (Tipper, 1949). However, the documentation of these phenomena and their influence on failure was only addressed a few years latter (Rogers, 1960; Beachem, 1963; Puttick, 1959; Gurland and Plateau, 1963). For instance, Rhines (1961) showed the void growth and coalescence in uniaxial stress tests of plasticine containing circular holes (Fig. 4.1), showing similarities with the growth and coalescence of cavities in copper specimens found by Puttick (1959). The first micromechanical studies then appeared in McClintock (1968) and J. R. Rice and Tracey (1969). Over the last decades, various efforts have been made to model these phenomena. In particular, multiple models for void growth have been developed, assuming an initial void volume fraction in the material. Void coalescence has received great attention lately, and various models have been
proposed. Additionally, models for void nucleation typically follow a statistical approach. It is worth mentioning that these mechanisms happen continuously throughout the loading history of the material. In general, while coalescence between voids is occurring, other voids are growing and further voids are being nucleated.

![Figure 4.1: Void growth and coalescence in plasticine specimens under uniaxial tension (Rhines, 1961).](image)

**Void nucleation**

Nucleation of voids is associated with the presence of second-phase particles or inclusions, either inside or at the boundary of grains. It is generally the result of decohesion of the particle-matrix interface (Fig. 4.2a) or of particle cracking (Fig. 4.2b). Generally speaking, the nucleation of voids is influenced by the mechanical properties of the matrix, of the particle and by the loading conditions and strain levels on the inclusion (Benzerga and Leblond, 2010). A summary of the influence of these parameters on each mechanism is shown in Table 4.1, where \( \searrow \) and \( \nearrow \) represent increasing and decreasing tendencies, respectively.

**Void growth**

Following the nucleation stage, the newly created void will grow in size. This phenomenon is referred to as void growth. In general, it is a process mostly controlled by the plastic deformation of the material. Furthermore, the growth of voids induces material softening and aids the appearance of plastic instabilities (Vishwakarma and Keralavarma, 2019). Voids nucleated by particle cracking generally open and grow to rounded shapes, whilst voids resulting from debonding stretch in the direction of the maximum principal stress (Pinto Carvalho, 2015). An example of void growth in copper is shown in Fig. 4.3.
4.1. Damage phenomena

Figure 4.2: Particle debonding and cracking on an 6061 aluminum reinforced with aluminum oxide particles (Kanetake et al., 1995).

Table 4.1: Influence of mechanical properties and loading on the nucleation of voids by particle cracking and decohesion (Benzerga and Leblond, 2010).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Debonding</th>
<th>Cracking</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix yield strength</td>
<td>↘</td>
<td>↗</td>
</tr>
<tr>
<td>Matrix hardening</td>
<td>↘</td>
<td>↗</td>
</tr>
<tr>
<td>Particle stiffness</td>
<td>↗</td>
<td>↗</td>
</tr>
<tr>
<td>Particle elongation</td>
<td>↘</td>
<td>↗</td>
</tr>
<tr>
<td>Axial loading</td>
<td>↘</td>
<td>↗</td>
</tr>
<tr>
<td>Transverse loading</td>
<td>↗</td>
<td>↘</td>
</tr>
<tr>
<td>Triaxiality</td>
<td>↗</td>
<td>↘</td>
</tr>
</tbody>
</table>

It is worth mentioning that the void growth is influenced by the stress state applied to the material. In particular, it is strongly dependent of the stress triaxiality and, to a lesser extent, of the Lode parameter\(^1\) (Benzerga, Leblond, et al., 2016; Bao and Wierzbicki, 2004; Danas and Ponte Castañeda, 2012). Increasing triaxialities tend to induce faster void growths. For low triaxialities, the Lode parameter plays an important role defining the shape of the void.

**Void coalescence**

The coalescence of two voids happens after significant void growth. In this terminal stage, two or more voids are linked, resulting in a microscopic crack that will propagate throughout the microstructure. The most common mode of coalescence is by internal necking between voids (Fig. 4.4a). An alternative mode of failure is by coalescence in a microshear band, or “void-sheet” coalescence (Fig. 4.4b). In this last mode, a sudden decrease in ductility is expected, as stable void growth is abruptly interrupted while the voids are still apart (Benzerga and Leblond, 2010). Nevertheless, this mode is strongly dependent on the relative position of the voids. A less frequent mode results by the formation of voided

\(^1\)These parameters of the stress state are discussed in Section 4.2.
columns, referred to as “necklace coalescence”, as described by Benzerga and Leblond (2010). This last mode is predominant in metals with elongated inclusions in the loading direction.

4.1.2 Macroscopic mechanisms

Among the microscopic mechanisms described, only the coalescence between voids plays a significant effect on the macroscopic response of the material (Benzerga and Leblond, 2010). When the largest voids begin to link, a macroscopic crack initiates. This crack propagates throughout the loaded section and will, eventually, lead to failure. The connection between macroscopic and microscopic mechanisms is shown schematically in Fig. 4.5. Before the point (c), the damage on the material is mostly caused by void nucleation and growth, with occasional coalescence between microscopic voids. At the point (c), the combination of microscopic coalescences results in a macroscopic crack. After (c), the
4.2 Stress state characterization

In the previous section, the basic mechanisms of damage have been addressed. Nonetheless, the stress state strongly influences void growth, especially stress parameters such as triaxiality and Lode parameter. In this section, these parameters are defined and some generalities of the Cauchy stress tensor are presented. To do so, firstly the decomposition into a hydrostatic and deviatoric components, and the importance of the deviatoric component is shown using some yield criteria. Using these yield criteria as example, the concept of yield function is introduced. Afterwards, alternative representations of the stress state are shown, using different coordinate systems. Finally, the Lode parameter and triaxiality are

macroscopic crack propagates, eventually leading to failure in (f). Before fracture, the appearance of shear bands will promote a slight increase in the slope of a stress-strain curve.

Figure 4.5: Macroscopic mechanism of ductile failure and connection with microscopic mechanisms (adapted from Pinto Carvalho (2015)).
introduced, as well as some important properties of the Cauchy stress tensor with respect to them.

Recalling Section 2.3.1, the Cauchy stress tensor $\sigma$ can be decomposed in terms of a hydrostatic and a deviatoric component, such that

$$\sigma = s + pI,$$  \hspace{1cm} (2.40)

where $s$ is the deviatoric component and $p$ the hydrostatic pressure. It will soon be clear that this decomposition plays an important role in the definition of alternative stress state representations.

Some popular yield criteria, such as Tresca and von Mises, are only a function of the deviatoric stress component $s$. For instance, the Tresca yield criterion can be expressed in terms of the principal stresses as

$$\sigma_1 - \sigma_3 \leq \sigma_y,$$ \hspace{1cm} (4.1)

where $\sigma_1$ and $\sigma_3$ are the largest and smallest stress principal stress components and $\sigma_y$ is the uniaxial yield stress of the material. Note that the difference $\sigma_1 - \sigma_3$ is insensitive to hydrostatic components, which goes along with the idea that the Tresca yield criterion is a purely deviatoric criterion. Similarly, the von Mises yield criterion is given by

$$\sqrt{3J_2} = \sqrt{\frac{3}{2}s : s = \sigma_{eq}} \leq \sigma_y,$$ \hspace{1cm} (4.2)

where $\sigma_{eq}$ is the von Mises equivalent stress and $J_2$ is the second invariant of the deviatoric stress tensor. Analogously to the Tresca yield criterion, von Mises yield criterion is only a function of the deviatoric stress component. Both yield criteria are represented in Fig. 4.6, where a plane stress state is considered (i.e. $\sigma_3 = 0$).

![Figure 4.6](image)

Figure 4.6: Graphical representation of the von Mises yield and Tresca yield criteria under plane stress ($\sigma_3 = 0$).

### 4.2.1 Yield functions

Another practical representation of the yield criteria is through yield functions $\Phi$. The onset of yielding is characterized by $\Phi = 0$ (de Souza Neto, Peric, et al., 2008). In this
notation, the Tresca yield criterion can be written as
\[ \Phi(\sigma) = (\sigma_1 - \sigma_3) - \sigma_y. \] (4.3)
Similarly, the von Mises yield function is given by
\[ \Phi(\sigma) = \sqrt{\frac{3}{2} s : s - \sigma_y}. \] (4.4)
The usage of yield functions allows us to establish the condition of pressure insensitivity and isotropy of both Tresca and von Mises yield criteria. A yield function is said to be pressure insensitive if it verifies
\[ \Phi(\sigma) = \Phi(\sigma + p^* I), \] (4.5)
for any hydrostatic pressure \( p^* \). Also, a yield function is said to be isotropic if it verifies
\[ \Phi(\sigma) = \Phi(Q\sigma Q^\top), \] (4.6)
for any rotation tensor \( Q \) (de Souza Neto, Peric, et al., 2008). Both Tresca and von Mises yield criteria are pressure insensitive and isotropic, therefore their yield functions verify the two above conditions.

### 4.2.2 Principal stresses coordinates

It is also possible to represent these yield criteria in a three dimensional space. To do so, we can define a coordinate system with the 3 principal stress components as the unit vectors of the system. In this scenario, the yield function \( \Phi(\sigma) = 0 \) will represent a three dimensional surface, commonly referred to as the yield surface. These representations are shown in Fig. 4.7 for von Mises and Tresca yield criteria.

Using this kind of representation, a few aspects of particular interest emerge. Firstly, according to its definition, a purely hydrostatic stress state has all the principal components of stress equal to \( p \) (i.e. \( \sigma_1 = \sigma_2 = \sigma_3 = p \)). Geometrically, this condition represents a straight line that contains the origin of the coordinate system and has a direction parallel to the vector \((1, 1, 1)\). This geometric entity is typically referred to as the hydrostatic axis. The projection of the stress vector along the hydrostatic axis gives a measure of the hydrostatic stress\(^2\). Secondly, a purely deviatoric stress state will have a null projection on the hydrostatic axis. Such a condition happens on a plane normal to the hydrostatic axis, frequently called the deviatoric plane or the \( \Pi \) plane. Furthermore, the deviatoric plane can be defined anywhere along the hydrostatic axis. Any stress state can then be expressed in terms of the hydrostatic axis projection and the components on the deviatoric plane.

The representation of the Tresca and von Mises yield criteria on this coordinate system results in two surfaces, represented in Fig. 4.7. As both criteria are uniquely function of the deviatoric components, their yield surfaces are independent of the stress state’s projection along the hydrostatic axis. Therefore, the von Mises criterion generates an infinite cylinder along the hydrostatic axis, with a radius equal to the yield stress \( \sigma_y \). Accordingly, the Tresca criterion will be represented by a hexagon extruded along the hydrostatic axis.

\(^2\)Note that the projection on the hydrostatic axis is not the value of the hydrostatic pressure. As it will be shown shortly, if \( \xi \) is the projection on the hydrostatic axis, then \( \xi = \sqrt{3} p \).
4.2.3 Haigh-Westergaard coordinates

Until this point, the stress state has been characterized by the principal stress values $\sigma_1$, $\sigma_2$, and $\sigma_3$, which are the eigenvalues of the Cauchy stress tensor. However, the graphical representation of the stress state and von Mises and Tresca yield surfaces might suggest an alternative set of coordinates to represent the stress state; the coordinate system can be a function of the projection on the hydrostatic axis and its position on the deviatoric plane (Bai and Wierzbicki, 2008; Mirone et al., 2016). Such coordinate system uses Haigh-Westergaard coordinates (Pisano et al., 2013). The representation of the projection of the stress state on the deviatoric plane can be shown in Fig. 4.8. It can been seen that the deviatoric stress $s$ is easily characterized in terms of a polar coordinate system $(\rho, \theta)$. Therefore, the stress state can be defined in terms of the coordinate set $(\xi, \rho, \theta)$, where

**Projection on the hydrostatic axis** $(\xi)$: orthogonal projection of the stress along the hydrostatic axis, also known as the axial coordinate. Defines the position of the deviatoric plane. The coordinate $\xi$ is directly related to the hydrostatic pressure $p$, where

$$\xi = \frac{\sqrt{3}}{3} (\sigma_1 + \sigma_2 + \sigma_3) = \sqrt{3} p. \tag{4.7}$$

**Magnitude on the deviatoric plane** $(\rho)$: magnitude of the projection on the deviatoric plane, also known as the radial coordinate. It can be expressed in terms of the deviatoric stress tensor by

$$\rho = \sqrt{s : s} = \sqrt{2J_2}. \tag{4.8}$$

Recalling the definition of the von Mises yield criterion in Eq. (4.2), the radial coordinate can be related to the von Mises equivalent stress by

$$\sigma_{eq} = \sqrt{\frac{3}{2} \rho}. \tag{4.9}$$

**Angle on the deviatoric plane** $(\theta)$: angle between the projection on the deviatoric plane and the projection of the first principal stress on the deviatoric plane. It is commonly referred as the Lode angle, and is defined over $0 \leq \theta \leq \pi/3$ (Danas and Ponte Castañeda, 2012).
4.2. Stress state characterization

Figure 4.8: Stress state characterization on the deviatoric plane and representation of the von Mises and Tresca criteria.

4.2.4 Lode parameter and triaxiality

As previously stated, both Lode parameter and triaxiality play an important role in the damage and void growth. Firstly, the Lode parameter $L$ is defined in terms of the Lode angle, by

$$L = -\cos(3\theta) = -\frac{27}{2} \frac{J_3}{\sigma_{eq}^2},$$

(4.10)

where $J_3$ is the third invariant of the deviatoric stress tensor and $\sigma_{eq}$ is von Mises equivalent stress (Danas and Ponte Castañeda, 2012). Given the range of the Lode angle ($0 \leq \theta \leq \pi/3$), the Lode parameter varies between $-1 \leq L \leq 1$. It is a more practical measure of the deviatoric stress direction. In Fig. 4.9, the evolution of the principal stress components with the Lode angle and parameter is shown. Some particular values for the Lode parameter are

- $L = -1$ ($\theta = 0$): axisymmetric stress state, with one positive and two negative principal stresses (axisymmetric traction);
- $L = 0$ ($\theta = \pi/6$): one principal component is null, resulting in shear stress in a plane stress condition;
- $L = 1$ ($\theta = \pi/3$): axisymmetric stress state, with two positive and one negative principal stresses (axisymmetric compression).

Secondly, the triaxiality $T$ is the ratio between the hydrostatic pressure and the von Mises equivalent stress, such that

$$T = \frac{p}{\sigma_{eq}}.$$
Given these definitions, we can obtain the principal components of a stress state directly from the Lode parameter, triaxiality and von Mises equivalent stress. The deviatoric stress component can be expressed in terms of the Lode parameter and von Mises equivalent stress by the projection along the principal stress axes, resulting in (Bai and Wierzbicki, 2009)

\[
\mathbf{s} = \mathbf{s}(L, \sigma_{eq}) \equiv \begin{cases} 
\sigma_1 = \frac{2}{3} \sigma_{eq} \cos \theta, \\
\sigma_2 = \frac{2}{3} \sigma_{eq} \cos \left(\frac{2}{3} \pi - \theta\right), \\
\sigma_3 = \frac{2}{3} \sigma_{eq} \cos \left(\frac{4}{3} \pi - \theta\right).
\end{cases}
\]  

(4.12)

These expressions automatically satisfy the condition of a null trace for the deviatoric stress tensor,

\[
\text{tr} (\mathbf{s}) = s_1 + s_2 + s_3 = 0,
\]  

(4.13)

and also ensure that the equivalent von Mises stress of the tensor is the one specified in \(\sigma_{eq}\),

\[
\sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}} = \sqrt{\frac{3}{2} (s_1^2 + s_2^2 + s_3^2)} = \sigma_{eq}.
\]  

(4.14)

This last condition is useful, as it allows us to define a unit deviatoric stress tensor \(\mathbf{\hat{s}}\). Such tensor has a unit von Mises equivalent stress,

\[
\sqrt{\frac{3}{2} \mathbf{\hat{s}} : \mathbf{\hat{s}}} = 1,
\]  

(4.15)
and has its components as a function uniquely of the Lode angle, given by

\[
\hat{s} = \hat{s}(L) \equiv \begin{cases} 
\hat{s}_1 = \frac{2}{3} \cos \theta, \\
\hat{s}_2 = \frac{2}{3} \cos \left( \frac{2}{3} \pi - \theta \right), \\
\hat{s}_3 = \frac{2}{3} \cos \left( \frac{4}{3} \pi - \theta \right).
\end{cases}
\]  

(4.16)

Using these definitions, any deviatoric stress tensor can be written as the product of a unit deviatoric stress tensor and an equivalent von Mises stress, according to

\[
s(L, \sigma_{eq}) = \sigma_{eq} \hat{s}(L).
\]  

(4.17)

The hydrostatic component of the tensor can now be written in terms of the triaxiality \( T \), such that \( p = T \sigma_{eq} \). Therefore, Eq. (2.40) can be rewritten in terms of the principal stresses as

\[
\sigma^* = s + pI = \sigma_{eq} \hat{s}(L) + T \sigma_{eq} I \]  

(4.18)

where \( \sigma^* \) is the Cauchy stress tensor in the principal stress coordinate system, i.e. a diagonal tensor. This last expression allows us to completely define the principal stress components in terms of the Lode parameter, triaxiality and equivalent von Mises stress. The Cauchy stress tensor can then be expressed in terms of any coordinate system by a rotation.

Furthermore, some properties arrive from the expression of the stress state in terms of the Lode parameter and triaxiality. If we consider a scalar \( \lambda \), the Cauchy stress tensor verifies

\[
L(\lambda \sigma) = L(\sigma),
\]  

(4.19a)

\[
T(\lambda \sigma) = T(\sigma),
\]  

(4.19b)

\[
\sigma_{eq}(\lambda \sigma) = \lambda \sigma_{eq}(\sigma).
\]  

(4.19c)

These properties allow us to establish a proportional loading trajectory, whilst keeping the Lode parameter and triaxiality constant throughout the incrementation. In addition, the equivalent von Mises stress is proportional to the increment \( \lambda \). Given these properties, we can also establish a unit Cauchy stress tensor \( \hat{\sigma} \), with a unit equivalent von Mises stress, such that

\[
\hat{\sigma} = \hat{s}(L) + TI.
\]  

(4.20)

Therefore, Eq. (4.19c) reduces to

\[
\sigma_{eq}(\lambda \hat{\sigma}) = \lambda.
\]  

(4.21)

Finally, we can also express the Cauchy and deviatoric stress tensors invariants in terms of the Lode parameter, triaxiality and equivalent von Mises stress. Recalling the definition of the invariants given in Eqs. (2.42) and (2.43), of the von Mises yield criterion.
in Eq. (4.2) and of the Lode parameter in Eq. (4.10), the invariants of the deviatoric stress tensor become

\[ J_2 = \frac{\sigma_{eq}^2}{3}, \]  
\[ J_3 = -\frac{2L\sigma_{eq}^3}{27}, \]  
and of the Cauchy stress tensor

\[ I_1 = 3\sigma_{eq}T, \]  
\[ I_2 = \sigma_{eq}^2 \frac{9T^2 - 1}{3}, \]  
\[ I_3 = \sigma_{eq}^3 \frac{27T^3 - 9T - 2L}{27}. \]

### 4.3 Plasticity theory

In metals, ductile failure happens at stress states where plastic effects are already present. As discussed previously in Section 4.1.1, the microscopic damage mechanisms are strongly dependent on the plastic strain near inclusions and voids. Furthermore, the macroscopic evidence of damage shown in Section 4.1.2 is detected beyond the linear elastic region of the stress-strain curve. For these reasons, it is important to introduce a mathematical formulation for a constitutive model including plasticity effects. In this section, a brief review over the mathematical theory of plasticity will be presented, in the scope of small strains. Furthermore, a rate-independent plasticity model will be considered throughout the section. As an example, a generic one-dimensional constitutive model for a uniaxial stress experiment will be developed, and further relevant generalizations will be discussed. Finally, the concept of limit analysis will be introduced, as a basis for some of the constitutive models presented in the following section. The forthcoming discussion is based on the work by de Souza Neto, Peric, et al. (2008).

#### 4.3.1 Uniaxial constitutive model

In an uniaxial tension model and given a generic elastoplastic material, the total strain \( \varepsilon \) can be decomposed in an elastic \( \varepsilon^e \) and plastic \( \varepsilon^p \) strains, that is,

\[ \varepsilon = \varepsilon^e + \varepsilon^p, \]

or equivalently, the elastic strain can be expressed in terms of the total strain and the plastic (or permanent) strain by

\[ \varepsilon^e = \varepsilon - \varepsilon^p. \]

Given the elastic uniaxial strain defined above, the constitutive law for the uniaxial stress \( \sigma \) becomes

\[ \sigma = E\varepsilon^e, \]
where $E$ is the Young’s modulus of the material. Furthermore, the elastic domain of the material is the set of stresses that verify

$$|\sigma| < \sigma_y,$$

(4.27)

where $\sigma_y$ is the uniaxial yield stress of the model. Consequently, the yield function becomes

$$\Phi (\sigma, \sigma_y) = |\sigma| - \sigma_y.$$  

(4.28)

Using these definitions, the elastic domain can be defined as the set

$$\mathcal{E} = \{\sigma \mid \Phi (\sigma, \sigma_y) < 0\}.$$  

(4.29)

Furthermore, the rate of plastic deformation $\dot{\varepsilon}^p$ can be expressed as

\[
\begin{cases}
\Phi (\sigma, \sigma_y) < 0 \Rightarrow \dot{\varepsilon}^p = 0, \\
\Phi (\sigma, \sigma_y) = 0 \Rightarrow \begin{cases}
\dot{\varepsilon}^p = 0 \text{ for elastic unloading,} \\
\dot{\varepsilon}^p \neq 0 \text{ for plastic loading.}
\end{cases}
\end{cases}
\]

(4.30)

In a general case, the plastic flow rule for the uniaxial model can be expressed as

$$\dot{\varepsilon}^p = \dot{\gamma} \text{sign} (\sigma),$$

(4.31)

where $\dot{\gamma}$ is the plastic multiplier and sign is the sign function. From its definition, the plastic multiplier is non-negative ($\dot{\gamma} \geq 0$) and also satisfies the complementarity condition

$$\Phi \dot{\gamma} = 0.$$  

(4.32)

Finally, a hardening law must be introduced. Generally, it is possible to define the uniaxial yield stress as the function

$$\sigma_y = \sigma_y (\varepsilon^p),$$

(4.33)

where $\varepsilon^p$ is the accumulated axial plastic strain, defined as

$$\varepsilon^p = \int_0^t |\dot{\varepsilon}^p| \, dt.$$  

(4.34)

The constitutive model presented here serves as an example to illustrate the general framework for the development of an elastoplastic constitutive model (de Souza Neto, Peric, et al., 2008). In essence, it is necessary to establish:

- the elastoplastic strain decomposition;
- an elastic law;
- a yield criterion, by the usage of a yield function;
- a plastic flow rule that determines the evolution of plastic strain;
- a hardening law.
4.3.2 General constitutive model

Decomposition of the strain tensor

The generalization of the additive decomposition of the strain tensor $\varepsilon$ reads

$$\varepsilon = \varepsilon^e + \varepsilon^p,$$  \hfill (4.35)

where $\varepsilon^e$ and $\varepsilon^p$ are the elastic and plastic strain tensors, respectively. Furthermore, an equivalent rate form of Eq. (4.35) can be written,

$$\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p,$$  \hfill (4.36)

given the initial condition

$$\varepsilon(t_0) = \varepsilon^e(t_0) + \varepsilon^p(t_0).$$  \hfill (4.37)

Elastic law and free energy potential

In Section 2.4, the free energy function has been introduced. Within the scope of plasticity theories, it is generally assumed that the free energy is a function of the total strain $\varepsilon$, plastic strain $\varepsilon^p$ and of a set of internal variables $\alpha$ associated with the hardening, that is,

$$\psi = \psi(\varepsilon, \varepsilon^p, \alpha).$$  \hfill (4.38)

The free energy can be split in an elastic and plastic part, by

$$\psi(\varepsilon, \varepsilon^p, \alpha) = \psi^e(\varepsilon^e) + \psi^p(\alpha).$$  \hfill (4.39)

With this definition of free energy, upon developing the Clausius-Duhem inequality, the general elastic law follows

$$\sigma = \bar{\rho} \frac{\partial \psi^e}{\partial \varepsilon^e}.$$  \hfill (4.40)

Similarly, the hardening thermodynamical force $A$ can be defined as

$$A = \bar{\rho} \frac{\partial \psi^p}{\partial \alpha}.$$  \hfill (4.41)

In the scope of linear elastic and isotropic materials, the elastic contribution to the free energy becomes

$$\bar{\rho} \psi^e(\varepsilon^e) = \frac{1}{2} \varepsilon^e : D : \varepsilon^e$$

$$= G \varepsilon^e_d : \varepsilon^e_d + \frac{1}{2} K (\varepsilon^e_v)^2,$$  \hfill (4.42)

that, after substitution in Eq. (4.40), results in the constitutive relation

$$\sigma = D^e : \varepsilon^e$$

$$= 2G \varepsilon^e_d + K \varepsilon^e_v I,$$  \hfill (4.43)

where $D^e$ is the standard isotropic elasticity tensor, $\varepsilon^e_d$ and $\varepsilon^e_v$ are the deviatoric and volumetric\(^3\) elastic strain components, respectively, and $G$ and $K$ are shear and bulk moduli.

\(^3\)Note that $\varepsilon^e_v = \text{tr}(\varepsilon^e)$. 

Yield criterion

Just like in the uniaxial case, a yield function for the constitutive model must be defined. By definition, it is negative in the elastic region and zero when plastic flow occurs. In a generic three-dimensional case, it is required that

$$\Phi (\sigma, A) = 0$$

(4.44)

for plastic flow to happen, where the yield function is now dependent on the stress tensor $\sigma$ and the set of hardening variables $A$. The resulting elastic domain is

$$E = \{ \sigma \mid \Phi (\sigma, A) < 0 \}.$$

(4.45)

Plastic flow rule and hardening law

Finally, the constitutive model should provide evolution laws for the internal variables of the model, in this case, the set of hardening variables. Therefore, the plastic flow rule and the hardening law are defined by

$$\dot{\varepsilon}^p = \dot{\gamma} N,$$

(4.46)

$$\dot{\alpha} = \dot{\gamma} H,$$

(4.47)

where the tensors $N$ and $H$ are the flow vector and the generalized hardening modulus, respectively, both function of the stress tensor and the set of hardening variables.

Flow rules and associative flow rule

Up to this point, the general components of an elastoplastic constitutive model have been addressed. In this process, the flow rule can be conveniently stated in terms of a flow (or plastic) potential. Additionally, the hardening law can also be expressed in a similar format. Assuming a flow potential $\Psi$, non-negative convex function of $\sigma$ and $A$, such that

$$\Psi = \Psi (\sigma, A),$$

(4.48)

verifying

$$\Psi (0, 0) = 0,$$

(4.49)

by hypothesis, we can write the flow vector as

$$N = \frac{\partial \Psi}{\partial \sigma}.$$ 

(4.50)

The derivation of the flow rules from potentials is only one modeling possibility among many. Nevertheless, it is an often used method. Optionally, using the same methodology for the hardening law, the hardening modulus can be written as

$$H = -\frac{\partial \Psi}{\partial A}.$$ 

(4.51)
Associative flow rule

It is now appropriate to introduce the concept of an associative plasticity model. Such constitutive models consider the yield function as the flow potential, that is,

\[ \Psi \equiv \Phi. \]  

(4.52)

Using the yield function as potential, one can write

\[ \dot{\varepsilon}^p = \dot{\gamma} \frac{\partial \Phi}{\partial \sigma}, \]  

(4.53)

and

\[ \dot{\alpha} = -\dot{\gamma} \frac{\partial \Phi}{\partial \mathbf{A}}. \]  

(4.54)

Prandtl–Reuss plasticity law

The associative flow rule associated with the von Mises yield criterion is commonly called the Prandtl-Reuss plasticity law. In this case, the flow vector becomes

\[ N \equiv \frac{\partial \Phi}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left( \sqrt{3 J_2(s)} \right) = \sqrt{\frac{3}{2} \frac{s}{\|s\|}}, \]  

(4.55)

resulting in

\[ \dot{\varepsilon}^p = \dot{\gamma} \sqrt{\frac{3}{2} \frac{s}{\|s\|}}. \]  

(4.56)

As the flow vector is the derivative of an isotropic scalar function of a symmetric tensor, \( N \) and \( \sigma \) are coaxial (the principal directions of \( N \) and \( \sigma \) are coincident). Combining the Prandtl-Reuss rule and the von Mises yield criterion, we obtain a model commonly named as the von Mises model.
4.3. Plasticity theory

4.3.3 Limit analysis

In previous sections, an elastoplastic model has been introduced. One can easily conclude that the analysis of such problems is in general complicated. An effective approach to the problem is to use the theorems of limit analysis. Such theories provide estimations to the collapse load of a boundary value problem. As it will be seen shortly, these analysis are of great interest in the development of macroscopic constitutive models for porous media.

The application of limit analysis requires (Chen and X. L. Liu, 1990; Chen and D. J. Han, 2007):

1. A perfect rigid-ideal-plastic material, enforcing the time derivative of the stress tensor $\dot{\sigma}$ to be tangential to the yield surface;
2. A convex yield function;
3. An associated flow rule where the plastic strain rate is obtainable from the yield function;
4. Insignificant changes in geometry at the limit load (infinitesimal strains).

Given these set of restrictions, the usage of limit analysis postulates two theorems: the lower bound for collapse and the upper bound for collapse. Citing Chen and D. J. Han (2007), these theorems state:

**Lower bound theorem:** "If an equilibrium distribution of stress $\sigma^E$ covering the whole body can be found, which balances the body force $b$ in $\Omega$ and the applied loads $t$ on the stress boundary $\partial\Omega$, and is everywhere below yield, $\Phi(\sigma^E) < 0$, then the body at the loads $t, b$ will not collapse."

**Upper bound theorem:** "If a compatible mechanism of plastic deformation $\dot{\epsilon}^p, \dot{u}^p$ is assumed, which satisfies the condition $\dot{u}^p = 0$ on the displacement boundary $\partial\Omega$, then the loads $t$ and $b$ determined by equating the rate at which the external forces do work

$$\int_{\partial\Omega} t \cdot \dot{u}^p \, da + \int_{\Omega} b \cdot \dot{u}^p \, dv,$$

(4.57)

to the rate of internal dissipation

$$\int_{\Omega} D(\dot{\epsilon}^p) \, dv = \int_{\Omega} \sigma^p \dot{\epsilon}^p \, dv,$$

(4.58)

will be either higher than or equal to the actual limit load ($\sigma^p$ is the stress state associated with the strain rate $\dot{\epsilon}^p$)."

These two theorems place two different bounds on the behavior of the problem. A lower bound is obtained when a valid stress state is found that is below yield for the whole domain. As a consequence, it allows the establishment of a lower bound estimate that guarantees that the material does not collapse at the prescribed loads. On the other hand, the upper bound theorem requires the assumption of a compatible velocity field, verifying

---

4A material exhibiting a linear elastic domain followed by a plastic domain with no hardening.
geometric boundary conditions. Afterwards, the rate of work of the external forces and of the internal dissipation must be estimated, according to the velocity field proposed. The upper bound estimate is obtained when the rate of work of external forces is greater than or equal to the rate of internal dissipation. Such estimate guarantees collapse when a set of loads is reached.

4.4 Models for porous media

The mechanics of damage associated with porous media have been introduced in Section 4.1. Various models considering these mechanisms have been published throughout the years, mostly developed in the scope of micromechanical studies of representative volume elements (RVEs) containing voids. These models provide estimates for the macroscopic yielding response of porous media, as well as the evolution laws associated with the set of microstructural variables. Therefore, a constitutive model for porous media can be established when the following expressions are known:

**Yield function:** Also known as the instantaneous effective stress potential. Describes the yielding state of the material, as a function of the stress state, the microstructural variables and the hardening state. It is important to mention that these functions are only dependent of the instantaneous state of the material. For the sake of brevity, the hardening of the yield function is not addressed here, as the focus of this work is on the yield onset (where no significant hardening has occurred).

**Microstructural evolution:** Definition of appropriate laws for the evolution of the microstructural variables after yielding. These laws are typically expressed in terms of differential equations for the microstructural variables. It is common to use the hypothesis of an associative flow rule to establish such laws.

It should be mentioned that these models are defined in terms of stress potentials, and do not depend on the elastic properties of the matrix.

In this section, some models for porous media are presented. Firstly, the Gurson (1977) model is be shown, which was one of the breakthroughs in the scope of micromechanical analysis for RVEs containing spherical voids. In the following years, the model was empirically modified to better fit experimental results and include nucleation effects, rendering the GTN model. Furthermore, some extensions for complex geometries were proposed, namely the GLD model for spheroidal shapes and the ML model for ellipsoidal shapes. In this work, only the ML model is mentioned, as its results for spheroidal shapes are practically coincident with the GLD model. Finally, an alternative approach was taken by Ponte Castañeda and his co-workers, using advanced homogenization techniques. As a result, a family of variational models was developed. From these models, the MVAR model is of particular interest, since it can predict the behavior of RVEs containing ellipsoidal voids. After the presentation of all these models, a short comparison between them is performed.
4.4. Models for porous media

4.4.1 Gurson’s Model

One of the first models for porous media was proposed by Gurson (1977). In his original publication, the model used an upper-bound limit analysis of an RVE containing spherical voids, using approximate homogenization techniques and an homogeneous strain rate at the boundary. As a consequence, the model was derived assuming (Benzerga and Leblond, 2010):

1. A spherical RVE with a single concentric spherical void;
2. A matrix obeying the $J_2$ plastic flow theory (isotropic ideal-plastic von Mises matrix);
3. A trial velocity field decomposed into an incompressible, isotropic expansion field and a linear field (corresponding to a uniform deformation field).

As a consequence of these assumptions, during deformation the voids remain spherical, regardless of the loading conditions. The only microstructural variable of the model is the porosity $f$, defined as the ratio between the volume of the void $V_v$ and the total volume of the domain $V_\mu$, that is,

\[ f = \frac{V_v}{V_\mu}. \]  

(4.59)

Therefore, the set of microstructural variables is

\[ s_\alpha = \{ f \}. \]  

(4.60)

The actual derivation of the Gurson’s yield criterion is beyond the scope of this work. The resulting yield function for a spherical void reads

\[ \Phi_{\text{Gurson}}(\sigma, f) = \left( \frac{\sigma_{\text{eq}}}{\sigma_y} \right)^2 + 2f \cosh\left( \frac{3}{2} \frac{p}{\sigma_y} \right) - (1 + f^2), \]  

(4.61)

where $\sigma_{\text{eq}}$ is the von Mises equivalent stress.

![Figure 4.11: Representative volume element used in the Gurson model (Benzerga and Leblond, 2010).](image)

In essence, this model introduces a dependence on the hydrostatic pressure $p$. A few aspects of particular interest arrive from the analysis of the yield function. Firstly, when the
porosity is zero, Gurson’s criterion reduces to the von Mises criterion and, consequently, becomes independent of the hydrostatic pressure. Furthermore, for high triaxialities, the hypothesis of the voids remaining spherical after deformation is acceptable, as the solicitation approaches the hydrostatic limit. However, for low triaxialities, this assumption is expected to be imprecise, as the deviatoric component of the stress state will most likely distort the void. For low triaxialities it is expected that the Gurson model will fail to capture accurately the response of the material (Danas and Ponte Castañeda, 2012). It is also worth mentioning that the model is not $J_3$-sensitive, i.e. does not depend on the Lode parameter.

**Microstructure evolution**

The model must provide an evolution law for its microstructural variables. In Gurson’s model, the only microstructural variable is the void volume fraction. An evolution law can be deduced by the mass conservation principle. The mass density of Gurson’s RVE is given by

$$\rho = \rho_0 (1 - f), \quad (4.62)$$

where $\rho_0$ is the mass density of the matrix. Under the assumption of an incompressible matrix, i.e., $\dot{\rho}_0 = 0$, the time derivative of $\rho$ becomes

$$\dot{\rho} = -\rho_0 \dot{f}. \quad (4.63)$$

Introducing Eq. (4.62) in last expression, the rate of change of the porosity can be simplified to

$$\dot{f} = -\frac{\dot{\rho}}{\rho} (1 - f). \quad (4.64)$$

Considering the mass conservation principle, it is possible to write

$$\dot{\varepsilon}_v = -\frac{\dot{\rho}}{\rho}, \quad (4.65)$$

where $\dot{\varepsilon}_v$ is the volumetric strain rate. Assuming an additive decomposition of the strain, and assuming that the elastic component of the strain is small when compared to its plastic counterpart, then

$$\dot{f} = (1 - f) \dot{\varepsilon}_v^p, \quad (4.66)$$

where $\dot{\varepsilon}_v^p$ is the plastic component of the volumetric strain rate, obtained from the volumetric strain rate tensor $\dot{\varepsilon}$ by

$$\dot{\varepsilon}_v^p = \text{tr} (\varepsilon_v^p). \quad (4.67)$$

Considering an associative plasticity model, the plastic strain rate can be directly obtained from the yield function by

$$\dot{\varepsilon}_v^p = \dot{\gamma} \frac{\partial \Phi}{\partial \sigma} = \dot{\gamma} \left[ s_0 + f_0 \sigma_y \sinh \left( \frac{3}{2} \frac{p}{\sigma_y} \right) \right] I. \quad (4.68)$$

The volumetric component of the plastic strain rate becomes

$$\dot{\varepsilon}_v^p = \dot{\gamma} f \sigma_y \sinh \left( \frac{3}{2} \frac{p}{\sigma_y} \right). \quad (4.69)$$
Finally, the evolution law for the porosity becomes

$$
\dot{f} = \dot{\gamma} \left( f - f^2 \right) \sigma_y \sinh \left( \frac{3 \, \rho}{2 \, \sigma_y} \right).
$$

(4.70)

It is worth mentioning that this evolution law only considers the growth of existing voids. As a consequence, an initial porosity must be defined for the evolution law.

### 4.4.2 GTN Model

After the original publication by Gurson, some authors proposed an extension of the model to better correlate with experimental data. Two of the most popular proposals were published in Tvergaard (1981) and Tvergaard and Needleman (1984). The resultant model from these works is frequently called the Gurson-Tvergaard-Needleman model (GTN model), and introduced three constants $q_1$, $q_2$ and $q_3$ to the original yield function from Gurson. The resulting yield function becomes

$$
\Phi_{\text{GTN}} (\sigma, f) = \left( \frac{\sigma_{eq}}{\sigma_y} \right)^2 + 2q_1 f^* \cosh \left( q_2 \frac{3 \, \rho}{2 \, \sigma_y} \right) - \left[ 1 + q_3 (f^*)^2 \right],
$$

(4.71)

where $f^*$ is a corrected version of the void volume fraction. In essence, this correction to the porosity attempts to increase the rate of void growth when a critical porosity $f_c$ is reached. It is a function of the porosity $f$ and is defined by

$$
f^* (f) = \begin{cases} 
  f, & f < f_c \\
  f_c + \frac{(f^*_u - f_c) (f - f_c)}{f_f - f_c}, & f \geq f_c,
\end{cases}
$$

(4.72)

where the constant $f^*_u$ is the ultimate value of $f^*$ at fracture, and $f_c$ and $f_f$ are calibrated parameters. The value of $f_c$ corresponds to the porosity at coalescence and $f_f$ is the porosity at fracture. When the volume fraction $f \rightarrow f_f$, then $f^* \rightarrow f_f$. This evolution is shown graphically in Fig. 4.12.

Regarding the parameters $q_1$, $q_2$ and $q_3$, these were firstly estimated as $q_1 = 1.5$, $q_2 = 1.0$ and $q_3 = q_1^2$ (Tvergaard, 1982). However, other values for these parameters have also been adjusted to fit both numerical and experimental results. Various calibrations are shown in Table 4.2, as collected by Bourih et al., 2018. Just like Gurson’s model, the GTN criterion is not $J_3$-sensitive.

### Microstructure evolution

The void growth in the GTN model is assumed similar to the void growth in Gurson’s model. However, as proposed in Chu and Needleman (1980), the porosity evolution can now be split into a void growth evolution and a void nucleation evolution, that is,

$$
\dot{f} = \dot{f}_{\text{growth}} + \dot{f}_{\text{nucleation}}.
$$

(4.73)

In this expression, the void growth term $\dot{f}_{\text{growth}}$ is obtained in a similar fashion to Gurson’s law, by Eq. (4.70). The void nucleation term $\dot{f}_{\text{nucleation}}$ can be controlled by stress or strain.
Chu and Needleman proposed a void nucleation evolution by a statistical modeling of strains, assuming a normal distribution,

\[ \dot{f}_{\text{nucleation}} = \frac{f_n}{s_n \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon^p - \varepsilon_n}{s_n} \right)^2 \right] \dot{\varepsilon}^p, \tag{4.74} \]

where \( f_n \) is the target nucleation porosity and \( \varepsilon_n \) and \( s_n \) are the average and standard deviation of the normal distribution of the plastic strain.

Table 4.2: Values of GTN model parameters, with \( q_3 = q_1^2 \) (adapted from Bourih et al. (2018)).

<table>
<thead>
<tr>
<th>Reference</th>
<th>Calibration</th>
<th>( q_1 )</th>
<th>( q_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gurson (1977)</td>
<td>Analytical</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Tvergaard (1982)</td>
<td>Experimental</td>
<td>1.50</td>
<td>1.00</td>
</tr>
<tr>
<td>Koplik and Needleman (1988)</td>
<td>Numerical</td>
<td>1.25</td>
<td>1.00</td>
</tr>
<tr>
<td>Zuo et al. (1996)</td>
<td>Numerical</td>
<td>1.40</td>
<td>1.00</td>
</tr>
<tr>
<td>Faleskog et al. (1998)</td>
<td>Numerical</td>
<td>1.46</td>
<td>0.93</td>
</tr>
<tr>
<td>Ma and Kishimoto (1998)</td>
<td>Numerical</td>
<td>1.35</td>
<td>0.95</td>
</tr>
<tr>
<td>Corigliano et al. (2000)</td>
<td>Numerical</td>
<td>1.08</td>
<td>0.99</td>
</tr>
<tr>
<td>Zhang et al. (2000)</td>
<td>Numerical</td>
<td>1.25</td>
<td>1.00</td>
</tr>
<tr>
<td>Nègre et al. (2003)</td>
<td>Numerical</td>
<td>1.50</td>
<td>1.20</td>
</tr>
<tr>
<td>J. Kim et al. (2004)</td>
<td>Numerical</td>
<td>1.58</td>
<td>0.91</td>
</tr>
<tr>
<td>McElwain et al. (2006)</td>
<td>Numerical</td>
<td>1.31</td>
<td>1.16</td>
</tr>
<tr>
<td>Nielsen and Tvergaard (2009)</td>
<td>Numerical</td>
<td>2.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Vadillo and Fernández-Sáez (2009)</td>
<td>Numerical</td>
<td>1.46</td>
<td>0.93</td>
</tr>
<tr>
<td>Dunand and Mohr (2011)</td>
<td>Experimental</td>
<td>1.00</td>
<td>0.70</td>
</tr>
<tr>
<td>Fei et al. (2012)</td>
<td>Numerical</td>
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<tr>
<td>Yan et al. (2013)</td>
<td>Numerical</td>
<td>1.55</td>
<td>0.90</td>
</tr>
</tbody>
</table>
4.4.3 Madou-Leblond (ML) Model

Madou and Leblond proposed a Gurson type criterion for voids of ellipsoidal shape (Madou and Leblond, 2012a,b). It is an extension to the GLD model proposed by Gologanu et al. for voids with spheroid shape (Gologanu et al., 1997). The resultant Madou-Leblond (ML) model used an upper bound limit-analysis of an ellipsoid containing a confocal ellipsoidal void. Just like Gurson, the matrix is a rigid-ideal-plastic von Mises material, with a homogeneous boundary strain rate condition. Furthermore, the authors used a set of trial velocity fields developed by Leblond and Gologanu, satisfying conditions of homogeneous strain rate on a family of confocal ellipsoids (Leblond and Gologanu, 2008). The set of microstructural variables for the model is

\[ s_\alpha = \{ f, w_1, w_2, k, l \} , \]  \hspace{1cm} (4.75)

where \( w_1 \) and \( w_2 \) are the ratios between the ellipsoid axes,

\[ w_1 = \frac{a_1}{a_3}, \]
\[ w_2 = \frac{a_2}{a_3}, \]  \hspace{1cm} (4.76)

and \( k \) and \( l \) are the unit vectors of the main axes of the ellipsoid. Furthermore, it was found that the velocity fields proposed by Leblond and Gologanu introduced inaccuracies for very flat oblate spheroid voids. As a result, a hybrid methodology is used, where the coefficients of the model for hydrostatic loadings are determined numerically and the coefficients significant in deviatoric loadings are required to coincide with the bounds of Ponte Castañeda (1991), Willis, 1991 and Michel and Suquet (1992). The resultant yield function of the model becomes

\[ \Phi_{ML}(\sigma, s_\alpha) = \frac{Q(\sigma)}{\sigma_y^2} + 2 (1 + g) (f + g) \cosh \left( \frac{L(\sigma)}{\sigma_y} \right) - (g + 1)^2 - (g + f)^2, \]  \hspace{1cm} (4.77)

where \( g \) is the secondary porosity and \( Q(\sigma) \) and \( L(\sigma) \) are scalar functions of the geometry and stress state. The definition of the terms in the yield function and the details of the implementation are shown in Appendix A.1. In the special case of spherical voids, the ML model reduces to

\[ \Phi_{ML}(\sigma, f) = \left( 1 + \frac{2}{3} f \right) \left( \frac{\sigma_{eq}}{\sigma_y} \right)^2 + 2f \cosh \left( \frac{3p}{2\sigma_y} \right) - (1 + f^2). \]  \hspace{1cm} (4.78)

This last expression is very similar to the Gurson’s yield function. Furthermore, for spheroidal voids, the ML model is practically coincident with the GLD model. For this reason, only the ML model was implemented in this work, as the GLD model can be seen as a particular case of ML model.

**Microstructure evolution**

Madou, Leblond, and Morin (2013) proposed the microstructural evolution for this model, accounting for length and orientation changes of the ellipsoid’s axes. The starting point
for the determination of the evolution laws is the assumption that the strain rate tensor of the void $D^v$ in a plastic material is obtained by

$$D^v = \mathbf{L} : D,$$

(4.79)

where $D$ is the overall strain rate tensor and $\mathbf{L}$ is a new strain localization tensor, obtained from its elastic counterpart

$$\mathbf{L}^{el} \equiv [\mathbf{I} - (1 - f) \mathbf{S}]^{-1},$$

(4.80)

where $\mathbf{I}$ is the unit fourth-rank tensor and $\mathbf{S}$ is Eshelby’s first tensor. The tensor $\mathbf{L}$ is heuristically obtained from its elastic counterpart by

$$\mathbf{L} = \mathbf{h} : \mathbf{L}^{el},$$

(4.81)

where $\mathbf{h}$ are correction factors required to include the plastic effects. Madou, Leblond, and Morin assumed these factors to be interpolated from their solution to particular cases by

$$\mathbf{h} = \lambda \mathbf{h}^{\text{sph}} + \mu \mathbf{h}^{\text{cyl}} + \nu \mathbf{h}^{\text{sand}}$$

(4.82)

where $\mathbf{h}^{\text{sph}}, \mathbf{h}^{\text{cyl}}$ and $\mathbf{h}^{\text{sand}}$ denote the correction factors for a spherical void, a circular cylinder void and an infinite planar empty layer (referred to as the “sandwich” case). The detailed description of these cases is beyond the scope of this work, and the reader is referred to the original publication for the derivation of these terms.

Similarly to the strain rate tensor of the void, the rotation rate tensor of the void $\Omega^v$ is obtained by

$$\Omega^v = \Omega + \mathbf{R} : D,$$

(4.83)

where $\mathbf{R}$ is the rotation localization tensor, obtained from its elastic counterpart by multiplication with a set of correction factors $k_{ij}$. Once again, for brevity, these factors are heuristically obtained from their elastic counterparts by

$$\mathbf{R} = \mathbf{h} : \mathbf{R}^{el},$$

(4.84)

where $\mathbf{h}$ are correction factors required to include the plastic effects. Madou, Leblond, and Morin assumed these factors to be interpolated from their solution to particular cases by

$$\mathbf{h} = \lambda \mathbf{h}^{\text{sph}} + \mu \mathbf{h}^{\text{cyl}} + \nu \mathbf{h}^{\text{sand}}$$

(4.85)

where $\mathbf{h}^{\text{sph}}, \mathbf{h}^{\text{cyl}}$ and $\mathbf{h}^{\text{sand}}$ denote the correction factors for a spherical void, a circular cylinder void and an infinite planar empty layer (referred to as the “sandwich” case). The detailed description of these cases is beyond the scope of this work, and the reader is referred to the original publication for the derivation of these terms.

Figure 4.13: Representative volume element used in the ML model (Pinto Carvalho, 2015).
described in the original publication and will be omitted. The elastic rotation tensor is given by

\[ \mathbf{R}^{el} = \left(1 - f\right) \mathbf{\Pi} : \mathbf{L}^{el}, \]

(4.84)

where \( \mathbf{\Pi} \) is Eshelby’s second tensor.

Given the strain and rotation rate tensors of the void, we can now obtain the evolution of the void’s axes. The method proposed in Madou, Leblond, and Morin (2013) is an alternative to the evolution laws originally proposed by Aravas and Ponte Castañeda (2004), particularly addressing the numerical difficulties arising from divisions by zero. Nevertheless, the original solution is presented in Appendix A.1.3. Considering \( O \) as the center of the void, \( M \) a point on its surface and \( \mathbf{u} \equiv \mathbf{OM} \), the quadratic form \( \mathcal{P} \) for the ellipsoidal void can be written as

\[ \mathcal{P}(\mathbf{u}) = \left(\mathbf{u} \cdot \mathbf{e}_x\right)^2/a^2 + \left(\mathbf{u} \cdot \mathbf{e}_y\right)^2/b^2 + \left(\mathbf{u} \cdot \mathbf{e}_z\right)^2/c^2 = P_{ij}u_iu_j = 1, \]

(4.85)

where \( P_{ij} \) are the coefficients of the quadratic form and with the unit vectors \( \mathbf{e}_x, \mathbf{e}_y \) and \( \mathbf{e}_z \) parallel to the principal directions of the void. After deformation, the point \( M \) must remain on the surface of the void, implying that \( \mathcal{P}(\mathbf{u}) \) must be constant and equal to unity. Therefore, the time derivative of the quadratic form must be zero. This condition finally allows us to establish the evolution law as

\[ \dot{P}_{ij} + P_{kj}(D_{ki}^v + \Omega_{ki}^v) + P_{ik}(D_{kj}^v + \Omega_{kj}^v) = 0. \]

(4.86)

4.4.4 Modified Variational (MVAR) Model

A different approach to void growth was taken by Ponte Castañeda and Zaidman (1994) in the development of their models. These models are originated from extensions to the Hashin-Shtrikman’s homogenization theory of random elastic composites to nonlinear behaviors, as developed by Ponte Castañeda (1991), Willis (1991) and Michel and Suquet (1992). In essence, a comparison between the real nonlinear composite and a reference linear composite is performed, in terms of a number of phases and properties chosen at will (Benzerga, Leblond, et al., 2016). As suggested by Benzerga, Leblond, et al., the major breakthroughs of the model are

- Ponte Castañeda and Zaidman (1994) was the first simple extension to the works of Ponte Castañeda (1991), Willis, 1991 and Michel and Suquet (1992) to nonlinear, plastic or viscoplastic materials, verifying an overall ellipsoidal symmetry. The resulting constitutive model consisted of an instantaneous effective stress potential (yield function) and evolution equations for the state variables, whilst considering finite deformations. This model suffered from an overestimation of the stresses for highly hydrostatic loadings, suggesting that the comparison with a linear material is of less importance for high triaxialities. On the other hand, for low triaxialities, the model provided good predictions.

- Danas and Ponte Castañeda (2009b) and Danas and Ponte Castañeda (2009a) applied the second order method, developed by Ponte Castañeda (2002a,b), in order to improve the linear comparison procedure. In essence, this method dropped some
terms of the linear composite in favor of a Gurson-type analysis, using a set of ad hoc adjustments to the original formulation. As a result, the predictions for high triaxialities improved significantly.

- After the development of the iterative procedure in Ponte Castañeda (2012), a model was proposed in Agoras and Ponte Castañeda (2013, 2014) that does not suffer from the problems at high triaxialities. The notable aspect of this approach is that no ad hoc adjustments are made, while yielding the same results of the exact Hashin solutions.

Given these various versions of models using the variational approach, it is impractical to implement all of them. Therefore, the version proposed by Danas and Aravas, based on the original variational model in Ponte Castañeda and Zaidman (1994) but with a correction on the hydrostatic point (Danas and Aravas, 2012) is chosen for implementation. Furthermore, the model is calibrated to predict the evolution of the microstructural variables according to the second order method of Ponte Castañeda (2002a,b). With that in mind, the model is referred as the modified variational model (MVAR). As before, an ideal-plastic von Mises material is assumed, with the set of microstructural variables

$$s_\alpha = \{\varepsilon^p, f, w_1, w_2, k, l\}, \quad (4.87)$$

where $\varepsilon^p$ is the accumulated plastic strain in the undamaged matrix and the other terms are identical to the ones presented for the ML model in Eq. (4.75). The yield function of the MVAR model is

$$\Phi_{\text{MVAR}}(\sigma, s_\alpha) = \sqrt{\sigma : M^{\text{mvar}} : \sigma} - \sigma_y, \quad (4.88)$$

where $M^{\text{mvar}}$ is a 4th order tensor obtained from the modification of the original variational tensor $M^{\text{var}}$, by

$$M^{\text{mvar}} = M^{\text{var}} + (q_j^2 - 1) J : M^{\text{var}} : J, \quad (4.89)$$

with $J$ representing the hydrostatic projection tensor

$$J_{ijkl} = \frac{1}{3} \delta_{ij} \delta_{kl}, \quad (4.90)$$

and $q_j$ is a correction factor for the hydrostatic point, defined by

$$q_j = \frac{1 - f}{\sqrt{f} \log (1/f)}. \quad (4.91)$$

The usage of this correction factor makes this criterion coincide with the Gurson’s model for hydrostatic loadings (in case of spherical or cylindrical voids). Furthermore, it improves the microstructure evolution with respect to the second order method.

This criterion does not provide any bounds for the material behavior, serving essentially as an estimate of the actual behavior of porous materials. The definition of the tensor $M^{\text{var}}$ and the details of the implementation of the model are described in detail in Appendix A.2.
Microstructure evolution

In Danas and Aravas (2012), the authors propose evolution equations for the accumulated plastic strain by stating that the macroscopic plastic work is equal to the microscopic plastic work, that is

$$\sigma : D^p = (1 - f) \sigma_y \dot{\varepsilon}^p,$$

resulting in the evolution law for the plastic strain

$$\dot{\varepsilon}^p = \frac{\sigma : D^p}{(1 - f) \sigma_y} = \dot{\lambda} \frac{\sigma : N}{(1 - f) \sigma_y}.$$  \hspace{1cm} (4.92)

For the evolution of the volume fraction, the elastic component of strain is assumed to have a negligible effect on $\dot{f}$. Considering the void growth only, the porosity evolution is obtained from the continuity equation, resulting in

$$\dot{f} = (1 - f) \text{tr} (D^p) = \dot{\gamma} (1 - f) \text{tr} (N).$$  \hspace{1cm} (4.93)

The evolution of the aspect ratios are obtained by the average strain rate in the voids, given in terms of a localization tensor $A$ similar to the one presented in Eq. (4.80), by

$$D^v = A : D^p = \dot{\gamma} A : N,$$

with

$$A = \frac{1}{f} \left[ I - \frac{1}{2} K : (M^{\text{mvar}})^{-1} \right].$$ \hspace{1cm} (4.95)

According to these definitions, the aspect ratios $w_s = a_s / a_3$ ($s = 1, 2$) have the evolution law

$$\dot{w}_s = \left[ \frac{\alpha_w}{w_s} \left( n^{(3)} n^{(3)} - n^{(s)} n^{(s)} \right) : A : D^p \right]^{-1}, \quad s = 1, 2,$$ \hspace{1cm} (4.96)

where the factor $\alpha_w$ was heuristically introduced to improve the accuracy of the evolution law. In their publication, Danas and Aravas recommend $\alpha_w = 7 / 4$.

Finally, the evolution of the orientation of the axes of the ellipsoidal void is given by the microstructural spin $\omega$, by

$$n^{(k)} = \omega \cdot n^{(k)}, \quad k = 1, 2, 3.$$ \hspace{1cm} (4.97)

In the last expression, $\omega$ is given by

$$\omega = W^v + \frac{1}{2} \sum_{r,s=1 \atop r \neq s}^3 \frac{w_r^2 + w_s^2}{w_r^2 - w_s^2} \left[ \left( n^{(r)} n^{(s)} + n^{(s)} n^{(r)} \right) : D^v \right] n^{(r)} n^{(s)}, \quad w_3 = 1.$$ \hspace{1cm} (4.98)

The average spin in the void $W^v$ is given by

$$W^v = W - C : A : D^p,$$ \hspace{1cm} (4.99)

with

$$C = -(1 - f) \Pi : A.$$ \hspace{1cm} (4.100)

It should be noted that the evaluation of the microstructural spin tensor is not straightforward when using spherical or spheroidal voids. For additional details, the reader is referred to the original publication.
4.4.5 Comparison between yield criteria

The yielding response of the methods presented so far is now evaluated and compared. Focus is placed on the influence of the void volume fraction, of the void geometry, Lode parameter and configuration. It is also worth mentioning that, even though both the yield function as the microstructural variables evolution are addressed, only the yield function has been implemented and studied. A diagonal stress tensor $\sigma$ defined by its principal components is imposed, as obtained by Eq. (4.18).

Influence of the void volume fraction

At first, the influence of the void volume fraction is studied, using spherical voids. With spherical voids, all the models presented can be compared\(^6\). Three void volume fractions have been chosen; 0.1%, 1% and 10%. The comparison between these models is shown in Fig. 4.14.

As predicted, increasing void volume fraction leads to a decreased material strength, both in purely deviatoric and purely hydrostatic loadings. The von Mises limit, obtained by setting $f = 0$, resulting in a pressure insensitive yielding response, is also represented. Furthermore, for small void volume fractions, the reduction in resistance for purely deviatoric loadings is small. However, for $f = 10\%$ the reduction for these type of loadings is already significant. For hydrostatic loadings, small changes in the void volume fraction lead to a significant reduction in the yield stresses. In essence, the void volume fraction seems to have more influence on the response for high triaxialities than the response for low triaxialities.

Between the models presented, the Gurson model establishes the upper bound of the response for all the volume fractions, as expected. For low values of $f$, the Gurson and ML model are almost coincident, but the ML model predicts smaller stresses at yield when the porosity increases. The GTN model has a similar evolution to the Gurson’s model, but predicts yield at lower stresses. Additionally, with exception of the GTN model, all models have the same value on the intersection with the horizontal axis (hydrostatic loadings). Also, the MVAR and ML model coincide on the vertical axis (deviatoric loadings). Finally, the MVAR model shows a different evolution for intermediate triaxialities, when compared to the other models. Nevertheless, all models exhibit the same trend when varying the void volume fraction.

Influence of the void geometry

In Fig. 4.15, a comparison on the yielding response of different void geometries is shown. Four geometries have been considered: sphere ($1; 1$), prolate spheroid ($5; 1$), oblate spheroid ($0.2; 1$) and ellipsoid ($5; 0.2$). The notation $(w_1; w_2)$ indicates the ratios between the void’s semi-axes, with $w_1 = a_1/a_3$ and $w_2 = a_2/a_3$. Recall that the Gurson and GTN models only account for spherical voids, and, thus, are not able to cover these geometries. For brevity, only a fraction $f = 1\%$ is considered. Furthermore, for anisotropic geometries, the Lode parameter and void orientation are expected to influence the yielding response

\(^6\)If spheroidal or ellipsoidal voids were chosen, only the ML and MVAR models could be compared.
of these models. For this reason, the axes of the voids are considered to be colinear with the axes of imposed stress state. The Lode parameter has been set to $L = -1$.

When considering anisotropic geometries, the yielding response of the material is no longer symmetric with respect to the vertical axes, that is, the material behaves differently in tension and compression. The curves for these models appear to be skewed towards either the left or right. The sensitivity of both models to these distortions seems to be similar. Regarding the void geometry, spherical voids appear to have the highest resistance to yielding, followed by spheroids and finally by the ellipsoid. For this configuration, the prolate void appears to have higher stress at yield than the oblate. However, for deviatoric loadings, the influence of the voids appears to be small. The majority of the differences between the geometries emerge for intermediate to high triaxialities.

**Influence of the Lode parameter**

In Fig. 4.16 a comparison of the yielding response as a function of the Lode parameter is shown. The configuration of the voids is similar to the one shown in the previous study, as well as the void volume fraction considered. Three Lode parameters have been chosen, $L = -1$, $L = 0$ and $L = 1$.

The influence of the Lode parameter seems to be small. Furthermore, for both deviatoric and hydrostatic loadings, the response of the material appears to be independent of the Lode parameter. Additionally, the influence of $L$ appears to be more significant in more anisotropic geometries, that is, it seems to be more significant for ellipsoidal voids than spheroidal voids.

**Influence of the configuration**

Finally, the influence of the configuration is addressed in Fig. 4.17 for spheroidal voids and Fig. 4.18 for ellipsoidal voids. The notation used to define the configuration consists of three numbers in sequence, such as 123. These numbers indicate which axis of the void is parallel to each of the unit vectors of the basis of the stress tensor. The first number dictates which axis of the void is parallel with $e_1$; the second number is relative to $e_2$ and the third to $e_3$. The total set of combinations is shown in Table 4.3 (refer to Fig. 4.13 for the notation of void’s axes). In essence, the principal components of the stress tensor are permuted, whilst the void is kept with the same orientation, leading to different principal stresses on different axes of the void. Such strategy has been proven very useful in Chapter 5, as it is far easier to rotate the prescribed stress tensor than the void’s orientation. As spheroids have two equal axes, only the configurations 123, 213 and 321 produce a different response in the void, i.e., the remaining configurations produce the same response as the first three. For this reason, in Fig. 4.17 only these three configurations are shown. For ellipsoids, all configurations are unique, as shown in Fig. 4.18. Furthermore, $L = 0$ has been chosen, as it guarantees that all principal stress components are different (and thus all permutations of the stress state yield different tensors).

---

7The notation $e_i \parallel (\bullet)$ means “$e_i$ is colinear with (●)”. In the table, (●) must be replaced by the respective unit vector in each row and column. The unit vectors $e_i$, ($i = 1, 2, 3$) are the basis of the stress tensor.
The configuration seems to modify the yielding response at the same regions as the Lode parameter. However, the role played by the configuration appears to be more significant than the one of the Lode parameter. For purely deviatoric and hydrostatic loadings, the response is not altered by the configuration. Furthermore, it seems that for each configuration that exhibits asymmetry relative to the vertical axis, other configuration shows the same asymmetry, but mirrored. Finally, the configuration showing the most resistance in tension is generally the configuration least resistant in compression, and vice-versa.
Figure 4.14: Comparison of yield curves for the models presented for various void volume fractions, considering spherical voids.
Figure 4.15: Comparison of yield curves for the models presented for different geometries, considering the axes of the voids collinear with the axes of the stress tensor, \( f = 1\% \) and \( L = -1 \).
Figure 4.16: Influence of the Lode parameter on spheroidal and ellipsoidal voids, considering the axes of the voids colinear with the axes of the stress tensor and $f = 1\%$. 
Figure 4.17: Influence of the configuration on spheroidal voids, considering $f = 1\%$ and $L = 0$. 
Figure 4.18: Influence of the configuration on ellipsoidal voids, considering $f = 1\%$ and $L = 0$. 

ML (123)  ~  ML (213)  ~  ML (321)  ~  MVAR (123)  ~  MVAR (213)  ~  MVAR (321)  ~  MVAR (312)
Page intentionally left blank.
Chapter 5
Yield response of porous media with isotropic matrices

In this chapter, the yield response of RVEs containing voids is analyzed, considering a von Mises matrix. At first, spherical voids are used. It is studied the influence of the void volume fraction, boundary conditions and Lode parameter on the yield stress of the RVE, for various triaxialities. The respective yield curves are constructed. Furthermore, the GTN model is also calibrated for the numerical results obtained. Additionally, a study of the porosity evolution and the porosity at yield is given, and an appropriate expression for the latter is provided. Then, the influence of the elastic properties of the matrix on the yield response is assessed. Afterward, the study is extended to anisotropic void geometries, i.e., prolate and oblate spheroids and ellipsoid. The influence of the Lode parameter and void orientation is further examined. In the end, the response of all geometries is compared.

5.1 Spherical voids

The analysis of the yielding response of porous media with RVEs containing voids is initiated considering spherical voids. For this geometry, the microstructure of the material can be said to be isotropic. As a von Mises matrix is used, the overall response of the RVE is also expected to be isotropic. Furthermore, all models for porous media implemented are capable of providing results for spherical voids.

With this analysis, the yielding response of the RVE with spherical voids is studied. The dependence of the porosity, boundary conditions and Lode parameter is assessed. Furthermore, estimates of the void growth in the elastic region are provided and introduced in the evaluation of the analytical models implemented. Finally, a preliminary study on the dependence of the elastic properties on the onset of yielding is presented.

5.1.1 Numerical meshes

The finite element meshes used in this work are the same from Pinto Carvalho (2015). The RVE has a cubic shape, with a single spherical void centered in the middle of the domain. Furthermore, the RVE boundary mesh is structured, allowing for periodic boundary conditions to be applied. A total of three void volume fractions are used in the analysis: 0.1 %, 0.5 % and 2 %. A section cut of these meshes is shown is Fig. 5.1, where only 1/8 of the
domain is represented. Additionally, the number of elements in each of these meshes is shown in Table 5.1.

![Meshes with different void volume fractions](image)

Figure 5.1: Section clips of the meshes used in the analysis, containing spherical voids with the specified void volume fraction.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Volume fraction</th>
<th>Number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere (1, 1)</td>
<td>(f = 0.1%)</td>
<td>1654</td>
</tr>
<tr>
<td></td>
<td>(f = 0.5%)</td>
<td>1504</td>
</tr>
<tr>
<td></td>
<td>(f = 2%)</td>
<td>1488</td>
</tr>
</tbody>
</table>

Table 5.1: Number of elements for each of the void volume fractions used, considering spherical voids.

The mesh convergence was also studied by Pinto Carvalho (2015). The refinement level of these meshes has been shown to be sufficient to capture both the elastic and yield response of porous media. For this reason, mesh convergence studies are skipped in this work.

Finally, these meshes use hexahedron elements with 20 nodes, commonly referred to as \(\text{HEXA20}\). In plasticity problems, this type of elements is frequently used with reduced integration schemes. These reduced integration schemes reduce the volumetric locking resultant from the incompressibility of the matrix under plastic deformations (Freischläger et al., 2000). For this reason, the \(\text{HEXA20}\) elements are used with a reduced integration of 8 Gauss points.

### 5.1.2 Matrix properties

The material of the matrix of the RVE is defined accordingly with the assumptions used in the models for porous media, shown in Section 4.4. Therefore, an isotropic elastic ideal-plastic matrix is considered, using the von Mises model. The mechanical properties of the model are chosen to be representative of a structural steel, and are shown in Table 5.2. As previously stated, the models shown in Section 4.4 do not predict a dependency of the elastic properties of the matrix on the macroscopic yielding response of the material.
5.1 Spherical voids

Table 5.2: Mechanical properties of the matrix with von Mises model.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus $E$</td>
<td>200 GPa</td>
</tr>
<tr>
<td>Poisson ratio $\nu$</td>
<td>0.3</td>
</tr>
<tr>
<td>Yield stress $\sigma_y$</td>
<td>240 MPa</td>
</tr>
</tbody>
</table>

5.1.3 Incremental loading scheme

In this work, a stress-driven incremental scheme is used, in order to allow for a strict control over the triaxiality and Lode parameter. This incrementation scheme represents a pseudo-time loading, where the prescribed stress state is increased incrementally. For the study of yielding responses, the incremental procedure must be executed until a certain yield criterion is met.

Recalling Section 4.2.4, in particular Eq. (4.19), the multiplication of a scalar $\lambda$ with a Cauchy stress tensor $\sigma$ does not alter the triaxiality and Lode parameter of the tensor. Additionally, if the equivalent von Mises stress of $\sigma$ is $\sigma_{\text{eq}}$, then the equivalent von Mises stress after the multiplication with $\lambda$ is $\lambda \sigma_{\text{eq}}$. These properties are the foundation for an incremental scheme with controlled triaxiality and Lode parameter. In essence, if a reference stress state $\sigma$ is established, with a triaxiality $T$ and Lode parameter $L$, the usage of a proportional incremental scheme, such that

$$\sigma_n = \lambda_n \sigma,$$  \hspace{1cm} (5.1)

defines a prescribed stress state $\sigma_n$ at the increment $n$, with a load factor $\lambda_n$, having the same triaxiality $T$ and Lode parameter $L$ as the reference $\sigma$. Furthermore, the equivalent von Mises stress of the prescribed stress state is $\lambda_n \sigma_{\text{eq}}$, where $\sigma_{\text{eq}}$ is the equivalent von Mises stress of the reference stress state.

The incremental loading scheme is also shown schematically in Fig. 5.2, using a Gurson-type coordinate system (von Mises equivalent stress on hydrostatic pressure). In summary, after the definition of a triaxiality $T$, the trajectory of the loading becomes a straight line containing the origin, and with angle $\theta$ defined as $\tan \theta = 1/T$. Furthermore, the distance from the origin to a point at the increment $n$ is proportional to $\lambda_n$.

To properly capture the onset of yielding, the increment size should be small. However, using smaller increments leads to an increased computational effort. In an effort to minimize the processor time, the increment size should be small near the yield region, but as large as possible everywhere else. At first glance, the yield region can be estimated with the yield functions given in Section 4.4. To allow for applicability on every void geometry considered in this work, either the ML or MVAR model should be used. As the ML model is closer to the upper bound of Gurson’s model, it is chosen over the MVAR model. The construction of the loading scheme becomes:

1. Define a triaxiality $T$ and Lode parameter $L$ for the stress state;
2. With the parameters defined in the previous step and given the void’s geometry and volume fraction, use the ML model to estimate the stress state at yield;
Chapter 5. Yield response of porous media with isotropic matrices

3. Set the reference stress state to the one obtained in the previous step;

4. Define the increment sizes according to Table 5.3.

A few remarks relatively to the chosen increment sizes must be referred. Firstly, a small size is adopted for the first increment, to allow an accurate estimation of the elastic properties of the RVE. Secondly, a total of four large increments are used to reach the yield region. The yield region is defined from $0.75 \leq \lambda \leq 1.5$, using 0.75 a lower safety margin and 1.5 as an upper margin for the yield.

Table 5.3: Increment sizes prescribed.

<table>
<thead>
<tr>
<th>Number of increments</th>
<th>Increment size</th>
<th>Total load factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.010</td>
<td>0.01</td>
</tr>
<tr>
<td>4</td>
<td>0.185</td>
<td>0.75</td>
</tr>
<tr>
<td>75</td>
<td>0.010</td>
<td>1.50</td>
</tr>
</tbody>
</table>

5.1.4 Macroscopic yield criterion

As previously stated, it is required to define a criterion for the yielding of the incremental loading scheme. In essence, the incrementation scheme should be controlled additionally by this yielding criterion, that is, increment cutting must be triggered to capture the exact onset of yielding, and the analysis should stop when this point is reached. In Pinto Carvalho (2015) it was shown that the usage of the slope of homogenized stress-strain curves is capable of capturing the yielding quite accurately. However, this method was used originally with a strain-driven analysis, and its usage on stress-driven analysis was not developed yet. As a consequence, a preliminary study on the effectiveness of this method was required. It was found that some modifications were required to the criterion. The detailed development of this yielding criterion is shown in Appendix B, where a number of variations of the criterion are discussed.

As it is shown in Appendix B, the chosen criterion uses an hybrid formulation for the increment cutting and yielding evaluation. Increment cutting is triggered by using a
5.1. Spherical voids

A measure of the homogenized plastic strain in the matrix. A set of target values is chosen, and Links tries to find these values one by one. Once a target plastic strain is reached, the stress-strain slope is estimated. If the slope is below a given threshold, it is assumed that this point is beyond the onset of yield and Links will stop. When a sufficiently larger number of target values for the plastic strain are specified, it is expected that this last point is a good estimate of the onset of yielding. Again, for the detailed explanation of the origin of this method, refer to Appendix B. The parameters used in these analysis are shown in Table 5.4.

Table 5.4: Parameters used for the yield criterion.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target slope</td>
<td>0.1(\Gamma_e)</td>
</tr>
<tr>
<td>Slope tolerance</td>
<td>10%</td>
</tr>
<tr>
<td>Slope measure</td>
<td>(\Delta |P|/\Delta |F - I|)</td>
</tr>
<tr>
<td></td>
<td>1 (\times 10^{-5})</td>
</tr>
<tr>
<td></td>
<td>2 (\times 10^{-5})</td>
</tr>
<tr>
<td></td>
<td>5 (\times 10^{-5})</td>
</tr>
<tr>
<td></td>
<td>1 (\times 10^{-4})</td>
</tr>
<tr>
<td></td>
<td>2 (\times 10^{-4})</td>
</tr>
<tr>
<td></td>
<td>5 (\times 10^{-4})</td>
</tr>
<tr>
<td></td>
<td>1 (\times 10^{-3})</td>
</tr>
<tr>
<td></td>
<td>2 (\times 10^{-3})</td>
</tr>
</tbody>
</table>

5.1.5 Cases studied

To study the influence of parameters such as void volume fraction, Lode parameter, boundary conditions and triaxiality, it is required to select and appropriate number of parametric studies. Firstly, the void volume fraction is obtained from the numerical meshes used, as shown in Section 5.1.1. As a consequence, a total of three porosities are considered: 0.1%, 0.5% and 2%. The three boundary conditions of interest are studied: linear boundary condition, periodic boundary condition and uniform traction on the boundary. For brevity, these conditions will from now on be referred to as Linear, Periodic and Uniform, respectively. Furthermore, a set of three equally distant Lode parameters is chosen, \(L = \{-1, 0, 1\}\).

To obtain a yield curve similar to the ones shown in Section 4.4.5, it is required to sweep the whole domain of triaxialities, that is, from negative to positive infinity. Negative triaxialities refer to compressive hydrostatic components, whilst positive triaxialities lead to tension. For brevity, this work is limited only to the study of the yielding response under traction. As a consequence, the domain of triaxialities reduces to \([0, +\infty[\). Furthermore, as shown in Fig. 5.2, it is more appropriate to define a set of triaxialities based on the angle \(\theta\). Therefore, for spherical voids, a set of 10 triaxialities has been chosen, in an attempt to equally divide the domain for a yield curve representation. The various parameters considered in these analysis are shown in Table 5.5. Before going any further, the highest triaxiality chosen is 1000, whereas its theoretical maximum should be \(\infty\). This value is sufficiently close to the case where \(T \to \infty\), and heavily reduces the numerical issues in pre- and post-process of the results.
Table 5.5: Parameters considered in the analysis of the yielding response of spherical voids.

<table>
<thead>
<tr>
<th>Volume fractions $f$</th>
<th>0.1</th>
<th>0.5</th>
<th>2.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lode parameters</td>
<td>-1</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary conditions</th>
<th>Linear</th>
<th>Periodic</th>
<th>Uniform</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>0.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td>Triaxialities</td>
<td>3.5</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>1000</td>
<td></td>
</tr>
</tbody>
</table>

As a final note, the generation of input files for Links for these parametric studies is automated with the help of a set of scripts. These scripts have been developed to speed up and reduce the probability of errors in the combination and generation of cases. In these first studies on spherical voids, 270 cases are analyzed. As the number of cases is very significant, the usage of parallel processing heavily reduced the effective computational time. These simulations were run in the cluster maintained by CM2S, with a total of 40 logical cores. With the incrementation scheme used, the average time for each study is slightly below 1 hour. However, the number of cores effectively used was dependent on the workload of the cluster.

5.1.6 Influence of the void volume fraction and boundary conditions

Yield curves

On a first analysis, the influence of both void volume fraction and boundary conditions is studied. Fig. 5.3 shows the resulting yield curves, with three plots (one for each void volume fraction) and the three boundary conditions per plot, and several solutions from the models shown in Section 4.4. It is worth mentioning that the ML model was omitted for clarity of the results, as it is practically coincident with the Gurson’s model for these cases. Firstly, in agreement with the analytical models, increasing the hydrostatic pressure reduces the von Mises equivalent stress at yield. Therefore, the dependence on the hydrostatic pressure for the yield point is obtained; that is, the material is pressure sensitive according to the simulations.

Regarding the influence of the void volume fraction, an increase in the porosity leads to a reduction in the stress magnitude at yield. However, this effect is significantly more pronounced for high triaxialities; at these porosities, the reduction in strength for deviatoric loadings is minimal. The impact of the boundary conditions on the results also
5.1. Spherical voids

seems to follow the predictions. The linear boundary condition appears to generate an upper bound for the results, in agreement with the premise of it being the most restrictive model. On the other hand, the uniform traction model seems to represent a lower bound. As predicted, the periodic boundary condition returns intermediate results, that in theory are closer to the actual response of the RVE;

When comparing with the implemented models, for low volume fractions, the numerical results show a severe underestimation of the yield point for high triaxialities. As the void volume fraction increases, the numerical results get closer to the theoretical solutions. The increase in void size in the elastic region can explain these last two points, since it could be significant given the large strain formulation used. As will be seen shortly, the evaluation of the yield functions at the initial porosity is the primary source of these discrepancies. Especially for low void volume fractions and hydrostatic loadings, the yield point predicted by these models is very sensitive to the porosity, i.e., a small variation in the porosity results in a significant difference in the yield estimate. Nevertheless, from the results, it can be seen that the Gurson model places an upper bound for the domain of the results, i.e., all numerical results are below the values predicted by this model. These results seem to be closer to the GTN model, that in theory should provide an estimation of the actual response of the material. The MVAR shows a slightly different trend in the yielding response, but the numerical results seem to have an evolution similar to the one predicted by Gurson-type models. The ML model has a response very similar to Gurson’s model, so it shares the same conclusions as the latter.

Section plots

Furthermore, the accumulated plastic strain inside the RVE at yielding is shown in Figs. 5.4 and 5.5, for various void volume fractions, considering the case where \( L = 1, T = 2.5 \) and periodic boundary conditions. The Lode parameter is chosen arbitrarily, the triaxiality is chosen to be an intermediate value, and the periodic boundary condition should provide the most accurate response of the RVE. Most of the plastic deformation happens near the void. Furthermore, the maximum plastic strain increases as the void volume fraction decreases. The higher stresses at yield shown by lower void volume fractions can justify such condition, which in turn leads to higher strains. For this triaxiality level, the response of the RVE already seems to be dominated by the hydrostatic term, as the void shows roughly the same level of plastic strain on all of its surface.

Finally, the accumulated plastic strain inside the RVE at yielding is shown in Figs. 5.6 and 5.7, for the different boundary conditions, considering \( L = 1, T = 0 \) and \( f = 2\% \). Firstly, with a purely deviatoric loading \((T = 0)\), the strain on the void’s surface is now localized in a plane, in contrast with the results for \( T = 2.5 \). Then, as the boundary condition becomes less restrictive, the maximum plastic strain increases. Furthermore, the plastic strain seems to be less localized for the lesser restrictive boundary conditions. If the RVE can deform more freely, the strains should increase. Lastly, it is possible to observe some shear bands at roughly \(45^\circ\) on the section plane, specially in the periodic boundary condition.
Figure 5.3: Influence of the volume fraction and boundary conditions on a von Mises matrix with spherical voids and $L = -1$. 
5.1. Spherical voids

Figure 5.4: Accumulated plastic strain on 1/8th of the RVE with spherical voids at yielding, for varying void volume fractions, considering $L = 1$, $T = 2.5$ and periodic boundary conditions.

Figure 5.5: Accumulated plastic strain on a section cut of the RVE with spherical voids at yielding, for varying void volume fractions, considering $L = 1$, $T = 2.5$ and periodic boundary conditions.
Figure 5.6: Accumulated plastic strain on 1/8th of the RVE with spherical voids at yielding, for varying boundary conditions, considering $L = 1$, $T = 0$ and $f = 2\%$.

Figure 5.7: Accumulated plastic strain on a section cut of the RVE with spherical voids at yielding, for varying boundary conditions, considering $L = 1$, $T = 0$ and $f = 2\%$. 
5.1.7 Influence of the Lode parameter

Yield curves

The next study analyzes the influence of the Lode parameter on the yielding response of the RVEs. In Fig. 5.8 the yield curves for different void volume fractions and Lode parameters are shown, considering periodic boundary conditions. The Lode parameter influences the yielding response, specially in the region of intermediate triaxialities ($1.5 \leq T \leq 7$). As the void volume fraction increases, the influence of the Lode parameter increases. Furthermore, the domain of triaxialities where the Lode parameter seems to play a significant role increases as the void volume fraction also increases.

For low triaxialities, the effect of the Lode angle is minimal for low void volume fractions, but increases as the void volume fraction increases too. This effect was expected because as the voids increase in size, their distortion should affect the yielding response in a more noticeable manner. For high triaxialities, the effect of the Lode parameter also increases with the increase in void size, but in a reduced magnitude. In this type of loadings, the deviatoric component is small, and therefore the effect of the Lode parameter will not be as noticeable.

From this analysis, the yield response for $L = 1$ appears to place an upper-bound for the results. On the other hand, $L = 0$ and $L = -1$ seem to have similar responses. Additionally, $L = -1$ predicts a slightly higher yield point in lower triaxialities, while $L = 0$ indicates a marginal increase in resistance for high triaxialities. It is worth mentioning that the theoretical solutions do not predict the influence of the Lode parameter in the yielding response of spherical voids, but numerical solutions show otherwise.

To better characterize the influence of the Lode parameter, further analyses are carried to cover the remaining domain of $L$. To do so, a triaxiality level $T = 2.5$ is fixed and more Lode parameters are considered. Such triaxiality value apparently shows the largest dependence on the Lode angle of all other cases considered. Eight more Lode parameters are added to the three originally studied, resulting in a total of eleven equally spaced Lode parameters. To reduce computational cost, only the periodic boundary condition and a void volume fraction of 2% are considered. These results are shown in Fig. 5.9, for various void volume fractions and boundary conditions, considering $T = 2.5$. It should be mentioned that the stress measure used here is $\| r \|$, representing the distance to the origin of the yield point in a $p - \sigma_{eq}$ system, i.e., $\| r \| = \sqrt{\sigma_{eq}^2 + p^2}$. This type of measure is more practical than $\sigma_{eq}$ or $p$, as it does not tend to zero when either $\sigma_{eq} \to 0$ or $p \to 0$.

Firstly, from the scale of the plots, it can be seen that the influence of the Lode parameter on the yielding response is small. However, its influence seems to be more noticeable for larger void volume fractions, corroborating the idea that the distortion of larger voids impacts the yielding response. The boundary conditions follow a similar pattern to the one discussed in Section 5.1.6. There seems to exist a trend for an increase in the stress at yield as the Lode parameter increases. Even though such trend is visible, some of the cases show a non-smooth evolution of the yielding response. It remains unclear whether such fluctuations are the actual response of the RVE or imprecisions in evaluating the yielding criterion used.
Void distortion

Figure 5.10 shows the distortion of the voids at yield with a 200x magnification of the displacement fluctuations, considering periodic boundary conditions, $T = 0$ and $f = 2\%$. These three pictures are shown considering section cuts containing the center of the void and normal to $x$, $y$ and $z$, respectively. Firstly, considering the $xz$ plane, as the $\sigma_1$ component is always positive and $\sigma_3$ is always negative for all Lode parameters, the void will always follow an elliptical shape. In the $yz$ plane, in the case where $L = -1$, the components $\sigma_2$ and $\sigma_3$ are equal, and the resulting void remains spherical. For every other case in that plane, $\sigma_2 > \sigma_3$, and the void will become an ellipse with the largest semi-axis aligned with $y$. Finally, in the $xy$ plane, for $L = 1$ it is known that $\sigma_1 = \sigma_2$, yielding a spherical void. As before, for the remaining cases of that plane, the void is an ellipse resulting from stretching along the $x$ axis.

Section plots

Finally, in Figs. 5.11 and 5.12 the accumulated plastic strain for varying Lode parameters is shown, considering periodic boundary conditions, $T = 0$ and $f = 2\%$. The maximum values of the plastic strain seem to be weakly affected by the Lode parameter. Furthermore, as the loading is purely deviatoric, the regions of maximum strain are localized on the void’s surface. Depending on the Lode parameter, these localizations take place in different regions of the void. For the cases where $L = 0$ and $L = 1$, it is possible to see some shear bands on the results. For the case with $L = -1$, these shear bands are found in planes perpendicular to the one shown in Fig. 5.12a.
5.1. Spherical voids

Figure 5.8: Influence of the Lode parameter on a von Mises matrix with spherical voids and a periodic boundary condition.
Figure 5.9: Yield radius as a function of the Lode parameter on a von Mises matrix with spherical voids and $T = 2.5$. 

\[ ||r|| = \sqrt{\sigma^2_{eq} + p^2} \]
5.1. Spherical voids

$\bar{L} = -1 \quad \bar{L} = 0 \quad \bar{L} = 1$

--- Unloaded void

Figure 5.10: Distortion of the voids for various Lode parameters and planes, with displacement fluctuations magnified by 200x and considering periodic boundary conditions, $T = 0$ and $f = 2\%$.

Figure 5.11: Accumulated plastic strain on 1/8th of the RVE with spherical voids, for varying Lode parameters, considering periodic boundary conditions, $T = 0$ and $f = 2\%$. 
Figure 5.12: Accumulated plastic strain on a section cut of the RVE with spherical voids, for varying Lode parameters, considering periodic boundary conditions, $T = 0$ and $f = 2\%$. 
5.1.8 Calibration of GTN model

As suggested in Section 4.4.2, it is common to use numerical or experimental results to calibrate the $q_1$ and $q_2$ parameters of the GTN model. To compare with the values in the literature, these parameters are calibrated considering the numerical results obtained, using a non-linear least-squares method. The resulting parameters are shown in Table 5.6, for various Lode parameters and void volume fractions, and considering periodic boundary conditions. It can be seen that the dispersion of these parameters is quite large, and that there are significant differences from the originally proposed values of $q_1$ and $q_2$. However, it can be seen in Fig. 5.13 that the fitting is capable of capturing the yield curve obtained numerically. This discrepancy in the fitted parameters can be justified by the void growth in the elastic region that, as will be seen shortly, induces a significant error in the yield evaluation. It should be remarked that, in particular for $q_1$, a strong dependency was found between the fitted and Lode parameters. In general, $q_1$ was maximum for $L = 0$ and minimum for $L = 1$, whilst $q_2$ showed exactly the opposite trend. In practice, these differences in the fitted parameters modify the shape of the yield curve for intermediate triaxialities, and hardly change the response for deviatoric and hydrostatic loadings.

Table 5.6: Calibration of GTN parameters for varying Lode parameters and volume fractions, given a periodic boundary condition on RVEs with spherical voids.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$f = 0.1%$</th>
<th>$f = 0.5%$</th>
<th>$f = 2%$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$q_1$</td>
<td>$q_2$</td>
<td>$q_1$</td>
</tr>
<tr>
<td>$-1$</td>
<td>1.2099</td>
<td>1.1487</td>
<td>2.3603</td>
</tr>
<tr>
<td>$0$</td>
<td>2.1421</td>
<td>1.0460</td>
<td>3.5363</td>
</tr>
<tr>
<td>$1$</td>
<td>0.1713</td>
<td>1.4833</td>
<td>0.8975</td>
</tr>
</tbody>
</table>

Figure 5.13: Yield curves with the GTN criterion fitted, considering periodic boundary conditions, $f = 0.1\%$ and $L = -1$. 
5.1.9 Porosity evolution

In Pinto Carvalho (2015), it was suggested that the void volume fraction at the onset of yielding is larger than the initial volume fraction. In particular, for high triaxialities, the voids appear to grow significantly in the elastic region of the loading. As the models presented in Section 4.4 depend on the instantaneous value of the porosity, the usage of the initial porosity for the assessment of the yield point should over-estimate the strength of the material. This tendency is identified in Section 5.1.6, specially for low initial void volume fractions.

To assess the void growth up to the onset of yielding, the porosity increase throughout the loading is first studied. In Fig. 5.14 the percentual increase of the void volume fraction with the loading factor $\lambda$ is shown, with $L = 0$ and periodic boundary conditions. For simplicity, only 5 triaxialities are shown. From these results, it is possible to conclude that the voids indeed grow significantly in the elastic region. Furthermore, the growth is mostly noticeable after $2/3$ of the load factor, and most of it happens near the yield point. Such a trend was expected, as the region near the voids begins to exhibit plasticity at these stress levels. The triaxiality also plays an important role in the rate of growth. For low triaxialities, the void is mostly distorted, and thus does not increase significantly in size. At high triaxialities, the void growth is notable, specially for initially small void volume fractions. Note that for an initial porosity $f = 0.1\%$, the final porosity was roughly double at yield, whilst for an initial porosity $f = 2\%$, the final porosity increased less than 10\%.

Finally, it appears that the rate of growth saturates at some triaxiality, that is, after a certain level of triaxiality is reached, further increases in $T$ do not increase the rate of growth of the void. Such phenomenon also appears to exist for the porosity at yield, but it was not possible from these figures to conclude it with the same level of certainty.

As the dependence of the triaxiality on the yield porosity is not clear in Fig. 5.14, a different representation is shown in Fig. 5.16, where the yield porosity is represented as a function of the triaxiality (on a logarithmic scale), considering $f = 0.1\%$ and $L = 0$. The influence of the boundary conditions is also shown, exhibiting the same trend shown for the yield curves, where the linear boundary condition leads to the largest estimation and the uniform traction to the lowest. However, in this type of plot it is evident that the yield criterion used does not capture exactly the yield onset. As it can also be seen in Fig. 5.14, the rate of growth of the voids near yielding is very large. As a consequence, a small error in the yield point results in a large error on the porosity value at yield. Any porosity study will therefore be very sensitive to the accuracy of the yield criterion used.

In the representation of Fig. 5.16, the hypothesis of a saturation of the yield porosity becomes more evident. Furthermore, for low triaxialities, the void only appears to grow after a certain value of the triaxiality is reached. This suggests that, in tension, the porosity at yield is bounded below and above by the values at $T = 0$ and $T = \infty$, respectively, and that a smooth and monotonic transition happens around a certain triaxiality. The lower bound for the porosity corresponds to the initial void volume fraction, and the upper bound would be the yield porosity for a purely hydrostatic loading. This behavior can be modeled by a function of the triaxiality, such as

$$f_y(T, f_0) = \frac{c}{1 + e^{-a(\log T - b)}} + f_0,$$  \hspace{1cm} (5.2)

where $f_y$ is the porosity at yield, $f_0$ is the initial porosity and the parameters $a$, $b$ and $c$
must be calibrated. This function provides an estimate of the void volume fraction at yield as a function of the triaxiality and the initial porosity. By using this expression, it is assumed that the porosity for \( T = 0 \) is equal to the initial porosity. From the numerical results, this assumption is reasonable, as the porosity at yield diverges marginally from the initial porosity for \( T = 0 \), as shown in Fig. 5.15. The parameter \( a \) defines how steep is the transition between both bounds, \( b \) defines where the transition occurs and \( c \) is the difference between the upper and lower bounds. Additionally, if we consider \( f_\infty \) as the porosity at yield with \( T = \infty \), the parameter \( c \) can be written as

\[
c = f_\infty - f_0.
\]  
(5.3)

This relation allows the calculation of the upper bound of the yield porosity directly. The parameters \( a \), \( b \) and \( c \) can now be fitted from the numerical results, using a non-linear least squares method. It is shown in Fig. 5.17 the porosity at yield for \( f_0 = 0.1\% \) and \( L = 0 \), plus the fitted curves obtained from Eq. (5.2). The numerical values of the constants are shown in Table 5.7 for the same case. It appears that the proposed expression follows the trend of the numerical results. However, due to the inaccuracies of the yield criterion, it remains a doubt whether the fitted upper bound is accurate. Nevertheless, the transition appears to be correctly captured by the proposed function, as well as the lower bound value.

Table 5.7: Fitted parameters for the void volume fraction at yield, considering \( f_0 = 0.1\% \) and \( L = 0 \).

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>( a )</th>
<th>( b )</th>
<th>( c )</th>
<th>( f_\infty /% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>2.6055</td>
<td>1.9220</td>
<td>0.001238</td>
<td>0.2238</td>
</tr>
<tr>
<td>Periodic</td>
<td>4.4856</td>
<td>1.5849</td>
<td>0.000854</td>
<td>0.1854</td>
</tr>
<tr>
<td>Uniform</td>
<td>3.1528</td>
<td>1.6792</td>
<td>0.000829</td>
<td>0.1829</td>
</tr>
</tbody>
</table>

In order to assess the influence of the corrected porosity on the yield functions of the analytical models, the function in Eq. (5.2) is introduced in the evaluation of the yield estimates for all the models implemented. As a consequence, the model uses a porosity that depends on the value of the triaxiality and on the initial porosity. The resulting yield functions are compared with the numerical results in Fig. 5.18\(^1\), for \( L = -1 \). It must be noted that the corrected porosity used for the yield functions was obtained considering the case of periodic boundary condition of each plot. It can be seen that the usage of the corrected porosity greatly improves the yield estimate for all the cases, specially for low porosities.

Finally, to provide improved fittings of the proposed corrected porosity, further triaxialities are tested. A total of 25 triaxialities are considered, logarithmically spaced from 0.1 to 1000. Furthermore, the accuracy of the yield criterion is improved for these analyses, by using a set of 21 target plastic strains, logarithmically scaled from \( 1 \times 10^{-6} \) to \( 1 \times 10^{-2} \). The numerical results and respective fits are shown in Fig. 5.19. It can be seen that the porosity at yield appears to follow the trend of the proposed corrected porosity. That said, some fluctuations in the results are found for high triaxialities. This emphasizes the difficulty of capturing the yielding point accurately for high triaxialities. Even with a refined

\(^1\)In this plot, the original GTN parameters were used.
yield criterion, some estimates were poor for the porosity values at yield. As a conclusion, for the accurate evaluation of the proposed corrected porosity, further improvements on the yield criterion evaluation must be considered. Nevertheless, the strategy of using a corrected porosity for the yield estimate seems to be very promising in the prediction of the yield response of porous media.
Figure 5.14: Evolution of the porosity with the load factor $\lambda$, considering periodic boundary conditions and $L = 0$. 
Chapter 5. Yield response of porous media with isotropic matrices

Figure 5.15: Evolution of the porosity for a purely deviatoric loading ($T = 0$), considering a spherical void, $f = 0.1 \%$ and periodic boundary conditions.

Figure 5.16: Porosity at yield as a function of the triaxiality, considering a spherical void, $f = 0.1 \%$ and $L = 0$. 
5.1. Spherical voids

Figure 5.17: Porosity at yield as a function of the triaxiality and its corresponding curve fitting with Eq. (5.2), considering a spherical void, $f = 0.1\%$ and $L = 0$. 
Figure 5.18: Yield curves and analytical models with corrected porosity (based on the periodic boundary condition), considering spherical voids and $L = -1$. 

- Linear
- Periodic
- Uniform
- Gurson $f = f_y(T)$
- GTN $f = f_y(T)$
- MVAR $f = f_y(T)$
Figure 5.19: Porosity at yield as a function of the triaxiality and curve fitting, with refined yielding criterion, considering a spherical void, $f = 0.5\%$ and $L = -1$. 
5.1.10 Influence of the matrix stiffness

In previous sections, the void growth up to the onset of yielding is found to be significant. By using a large strain formulation, the effects of such growth are reflected on the yielding response of the RVE. The region near the void enters the plastic domain far earlier than the remaining of the domain, and the plastic deformation near that region is responsible for most of the void growth. In theory, a more substantial deformation up to yield will induce a higher void growth in the elastic region. Therefore, the void growth in the elastic region should be dependent on the elastic deformation at yield, that is, $\sigma_y/E$. Under this assumption, in this section, a study is presented on the relation between $\sigma_y/E$ and the yielding response of the material. For brevity, only the void volume fraction $f = 2\%$ is considered, with periodic boundary conditions and $L = -1$. A total of four values of $\sigma_y/E$ were considered, as shown in Table 5.8. It is worth noting that the second case is already studied in previous sections, and this simulation is not repeated.

Table 5.8: Values of $\sigma_y/E$ considered in the analysis of the yielding response of RVEs with spherical voids.

<table>
<thead>
<tr>
<th>$\sigma_y/E$</th>
<th>$\sigma_y$ / MPa</th>
<th>$E$ / MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.2 \times 10^{-4}$</td>
<td>24</td>
<td>200000</td>
</tr>
<tr>
<td>$1.2 \times 10^{-3}$</td>
<td>240</td>
<td>200000</td>
</tr>
<tr>
<td>$1.2 \times 10^{-2}$</td>
<td>2400</td>
<td>200000</td>
</tr>
<tr>
<td>$1.2 \times 10^{-1}$</td>
<td>24000</td>
<td>200000</td>
</tr>
</tbody>
</table>

The resulting yield curves are shown in Fig. 5.20. It can be seen that an increase in $\sigma_y/E$ leads to a significant reduction in the non-dimensional stresses at yield. This condition was predicted, as larger elastic strains would lead to increased void growths, and consequently to reduced strengths. The porosity at yield is also shown in Fig. 5.21, with the respective porosity fit. The porosity for low values of $\sigma_y/E$ barely increases, whilst for high values of $\sigma_y/E$ the porosity might increase over 300%. Table 5.9 shows the fitted parameters of the porosity correction and void volume fractions at infinite triaxialities. Here it becomes evident that the void growth is strongly influenced by the ratio $\sigma_y/E$. Finally, in Fig. 5.22, the porosity corrections are introduced in the analytical solutions and compared to the numerical results. For clarity, only the GTN model was displayed. For low values of $\sigma_y/E$, the GTN model with corrected porosity is practically coincident with the model with the initial porosity, as there’s only a slight increase in $f$ at yield. However, for the remaining cases, the differences in porosity modify significantly the yield curve, as the porosity at yield for high triaxialities increases dramatically. The resulting yield curves for these cases appear to have a strong reduction in strength for nearly hydrostatic loadings. It is worth mentioning however that the numerical results do not show the same trend. As most of the porosity correction happens at high triaxialities, the response for low triaxialities is not corrected in such a significant manner. For this reason, even with porosity corrections, the yield curves shown largely overestimate the resistance of the material for intermediate triaxialities. For nearly deviatoric loadings, the material does not have a reduction in strength as significant.

As a final note, the validity of the models presented in Section 4.4 is brought into question for high values of $\sigma_y/E$. Firstly, the hypothesis of smalls strains seems to be
invalid, as the uniaxial elastic strains at yield are already significant, and the void volume fraction shows a measurable increase. Furthermore, in these models, the elastic strain component is typically ignored, and the void growth only takes into consideration the volumetric plastic strains. For these elastic strain levels, such assumption results in an underestimation of the void growth. Finally, the models do not predict a dependency of the yielding response on the elastic properties of the matrix. As seen in this section, under large strains, the onset of yielding is influenced by the relation between the yield stress and Young’s modulus. When the matrix is overly stiff when compared to the yield stress, the voids do not grow significantly in size and the yielding response is more closely captured by the models. When the stiffness is reduced, the void growth in the elastic region is significant, and the onset of yielding happens at lower stress levels. Nevertheless, it must be emphasized that the range of $\sigma_y/E$ considered is well beyond the typical range for most materials, and this example was mostly to show that the response should be dependent of the elastic properties of the material.

![Graph showing yield curves for varying $\sigma_y/E$](image)

**Figure 5.20:** Yield curves for varying $\sigma_y/E$, considering spherical voids with $f = 2\%$, periodic boundary conditions and $L = -1$.

**Table 5.9:** Fitted yield porosity parameters (Eq. (5.2)) and $f_\infty$ for various values of $\sigma_y/E$, with $f_0 = 2\%$.

<table>
<thead>
<tr>
<th>$\sigma_y/E$</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$f_\infty$ /%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.2 \times 10^{-4}$</td>
<td>1.2127</td>
<td>1.8408</td>
<td>0.00021</td>
<td>2.021</td>
</tr>
<tr>
<td>$1.2 \times 10^{-3}$</td>
<td>1.7428</td>
<td>1.1104</td>
<td>0.00142</td>
<td>2.142</td>
</tr>
<tr>
<td>$1.2 \times 10^{-2}$</td>
<td>1.7959</td>
<td>1.3804</td>
<td>0.01001</td>
<td>3.001</td>
</tr>
<tr>
<td>$1.2 \times 10^{-1}$</td>
<td>1.2640</td>
<td>2.0082</td>
<td>0.04527</td>
<td>6.527</td>
</tr>
</tbody>
</table>
Figure 5.21: Porosity at yield in function of the triaxiality, for varying $\frac{\sigma_y}{E}$, considering spherical voids with $f_0 = 2\%$, periodic boundary conditions and $L = -1$. 

$\sigma_y/E = 1.2 \times 10^{-4}$

$\sigma_y/E = 1.2 \times 10^{-3}$

$\sigma_y/E = 1.2 \times 10^{-2}$

$\sigma_y/E = 1.2 \times 10^{-1}$
Figure 5.22: Yield curves for varying $\sigma_y/E$ with corrected porosity for the analytical solutions, considering spherical voids with $f_0 = 2\%$, periodic boundary conditions and $L = -1$. 
5.2 Spheroidal voids

Following the work in the previous section, an anisotropic void geometry are introduced. With this in mind, the response of the RVE should now be dependent on the direction of loading. The analysis firstly focus spheroidal voids, which exhibit axisymmetry. A prolate spheroid with $w_1 = 2$ and $w_2 = 1$ and an oblate spheroid with $w_1 = 0.5$ and $w_2 = 1$ is used. At the outset, the conclusions from Section 5.1 relative to spherical voids is checked for spheroidal voids. Then, the focus will be on studying the influence of the loading direction and on the comparison between the prolate and oblate geometries.

5.2.1 Cases studied

A similar analysis to the one in Section 5.1 is taken for voids with spheroidal geometries. Figure 5.23 shows 1/8th of the meshes used in the finite element analyses. Once again, these meshes are also used in Pinto Carvalho (2015), and are sufficiently refined for the analysis of their yielding response. As before, a total of three void volume fractions are used. The number of elements for each porosity and geometry is shown in Table 5.10. The mechanical properties of the matrix are the same as the ones used in the analysis of spheres. The incremental loading scheme and the macroscopic yield criterion are also exactly the same as before.

Table 5.10: Number of elements for each of the void volume fractions used, considering spheroidal voids.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Volume fraction</th>
<th>Number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prolate (2, 1)</td>
<td>$f = 0.1%$</td>
<td>2046</td>
</tr>
<tr>
<td></td>
<td>$f = 0.5%$</td>
<td>1856</td>
</tr>
<tr>
<td></td>
<td>$f = 2%$</td>
<td>1666</td>
</tr>
<tr>
<td>Oblate (0.5, 1)</td>
<td>$f = 0.1%$</td>
<td>2046</td>
</tr>
<tr>
<td></td>
<td>$f = 0.5%$</td>
<td>1872</td>
</tr>
<tr>
<td></td>
<td>$f = 2%$</td>
<td>1488</td>
</tr>
</tbody>
</table>

Regarding the cases studied, it should be mentioned that the study of spheroidal voids introduces a dependency on the orientation of the void. In practice, this new dependency introduces one more parameter to the parametric study conducted for the spheres, which leads to a considerable increase in the total number of cases that need to be accounted for. For this reason, in a first stage, the Lode parameter was fixed to $L = 0$ and the configuration 123 was chosen\(^2\). In this study, the influence of the boundary conditions and void volume fraction is assessed. Then, an additional study on the influence of the configuration and Lode parameter is performed, by considering periodic boundary conditions and $f = 2\%$. The Lode parameter is either $-1, 0 \text{ or } 1$, and the configurations considered are 123, 213 and 321. As the spheroidal voids have only one different semi-axis, only rotations that lead to different stress states along that axis should produce different responses. For this reason,

\(^2\)For reference on the notation for the configurations, please refer to Section 4.4.5. In this case, a configuration of 123 indicates that the void’s axes are colinear with the basis of the prescribed macroscopic stress tensor.
configurations 132, 231 and 312 should produce the same response as the ones considered in this analysis. To analyze these configurations, the void orientation is kept constant and the prescribed stress tensor is transformed accordingly. Furthermore, it should be mentioned that some combinations of Lode parameter and configuration lead to equal stress states applied to the RVE. These duplicate cases resulted in two exactly equivalent input files for Links, so these are removed by the generator script. Considering the same 10 triaxialities in Table 5.5 for each study above, a total of 342 cases are covered. These cases are shown in Table 5.11.

5.2.2 Analysis of the results

In Figs. 5.24 and 5.25 the yield curves obtained for the void volume fractions and boundary conditions considered are shown. The ML and MVAR models are also displayed and compared to the numerical results. Firstly, the influence of the boundary conditions follows the same trend as before, with the response above and below bounded by the linear and uniform traction boundary conditions, respectively. Furthermore, as the void volume fraction increases, the strength of the material reduces. These results also show the same trend as the ones obtained by the spheres, where the numerical results show lower stresses at yield than the ones predicted by the analytical models, specially for lower void volume fractions.
Table 5.11: Parameters considered in the analysis of the yielding response of spheroidal voids.

<table>
<thead>
<tr>
<th>Study</th>
<th>Porosities /%</th>
<th>Boundary Conditions</th>
<th>Lode parameters</th>
<th>Configurations</th>
<th>Number of cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>First</td>
<td>0.1</td>
<td>Linear</td>
<td>0</td>
<td>123</td>
<td>180</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>Periodic</td>
<td>-1</td>
<td>123</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>Uniform</td>
<td>0</td>
<td>213</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>321</td>
<td></td>
</tr>
<tr>
<td>Second</td>
<td>2.0</td>
<td>Periodic</td>
<td>0</td>
<td>213</td>
<td>180</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>360</td>
</tr>
<tr>
<td>Unique cases</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>342</td>
</tr>
</tbody>
</table>

Comparing the prolate and oblate voids, both geometries appear to show roughly the same results. However, the analytical models predict a dependency on the geometry. When compared to the results for the spherical void, these spheroidal voids appear to show only a slight reduction in resistance.

Figures 5.26 and 5.27 show the influence of the Lode parameter on the yield curves for each configuration. In general, the influence of the Lode parameter on these geometries is similar to that of the spheres. Purely hydrostatic loadings seem to be unaffected by the Lode parameter. The influence of the Lode parameter seems to be maximum for triaxialities around $\frac{2}{5}$. Additionally, the response for $L = 1$ seems to be an upper bound for the results, just like it happened with the spheres.

The dependence of the configuration is shown in Figs. 5.28 and 5.29. The effects of the configuration are very similar to the ones observed for the Lode parameter. For purely hydrostatic loadings, the influence of the configuration vanishes. Furthermore, this independence of the configuration happens earlier for oblate voids, i.e., for triaxialities above 7, the response seems to be independent of the configuration.

In Figs. 5.30 and 5.31 the void geometry at yield for prolate and oblate voids is shown, respectively, considering periodic boundary conditions, $T = 0$, $f = 2\%$ and configuration 123. As previously, the voids remain either circular or elliptical, depending on the orientation of the stress state. Nevertheless, up to the yield point, no significant change in the void geometry is found, even for spheroidal voids, that is, prolate voids remain prolate and oblate voids remain oblate.

Furthermore, in Figs. 5.32 and 5.33 the accumulated plastic strain in a section of the RVE for two triaxialities is shown. For deviatoric loadings, the distribution of strain is similar to the one found in spheres, where it is mostly localized in the intersection of the void with a plane. However, for high triaxialities, the distribution of the strain is not as uniform as it was on the spheres; the strains are localized in the region of highest curvature in the void surface. Even though these differences were found relatively to spherical voids, the yielding response was very similar. Additionally, for this loading, the maximum plastic strain seems to be higher in the prolate void for deviatoric loadings, and higher in the oblate void for hydrostatic loadings.
Finally, Fig. 5.34 shows the porosity at yield in function of the triaxiality for prolate and oblate spheroidal voids, with periodic boundary conditions, $f = 0.1\%$, $L = 0$ and configuration 123. It can be seen that the void volume fraction at yield is very similar for both geometries, with the fitting of the corrected porosity showing two practically coincident curves. Those results have been omitted for brevity, but it was also found that the Lode parameter and configuration do not play a significant role in the porosity evolution. This was expected, as most of the void growth is caused by the hydrostatic part of the stress state. Despite the similarities between both geometries, $f_\infty$ seems to be slightly higher for spheroids than spheres. However, the differences are still small, and if more accurate conclusions are demanded on this subject, the yielding criterion used must be once again revised.
Figure 5.24: Influence of the boundary conditions on a von Mises matrix with prolate voids and $L = 0$. 
5.2. Spheroidal voids

Figure 5.25: Influence of the boundary conditions on a von Mises matrix with oblate voids and $L = 0$. 

- Red: Linear
- Blue: Periodic
- Green: Uniform
- Orange: ML ($L = 0$)
- Gray: MVAR ($L = 0$)
Chapter 5. Yield response of porous media with isotropic matrices

Figure 5.26: Influence of the Lode parameter on a von Mises matrix with prolate voids for different void orientations, periodic boundary conditions and $f = 2\%$. 
Figure 5.27: Influence of the Lode parameter on a von Mises matrix with oblate voids for different void orientations, periodic boundary conditions and $f = 2\%$. 

\[ L = -1 \quad \text{ML (} L = -1 \text{)} \quad \text{MVAR (} L = -1 \text{)} \]
Figure 5.28: Influence of the configuration on a von Mises matrix with prolate voids for different Lode parameters, periodic boundary conditions and $f = 2\%$. 

\[
L = -1
\]

\[
L = 0
\]

\[
L = 1
\]
5.2. Spheroidal voids

Figure 5.29: Influence of the configuration on a von Mises matrix with oblate voids for different Lode parameters, periodic boundary conditions and $f = 2\%$. 

Oblate (0.5, 1)
Figure 5.30: Distortion of prolate voids for multiple Lode parameters and planes, with displacement fluctuations magnified by 200x and considering periodic boundary conditions, $T = 0$, $f = 2\%$ and configuration 123.

Figure 5.31: Distortion of oblate voids for multiple Lode parameters and planes, with displacement fluctuations magnified by 200x and considering periodic boundary conditions, $T = 0$, $f = 2\%$ and configuration 123.
5.2. Spheroidal voids

Figure 5.32: Accumulated plastic strain on 1/8th of the RVE with prolate voids at yielding, for varying triaxialities, considering $L = 1$, $f = 2\%$, periodic boundary conditions and configuration 123.

Figure 5.33: Accumulated plastic strain on 1/8th of the RVE with oblate voids at yielding, for varying triaxialities, considering $L = 1$, $f = 2\%$, periodic boundary conditions and configuration 123.
Figure 5.34: Porosity at yield as a function of the triaxiality and corresponding curve fitting using Eq. (5.2), considering spheroidal voids, periodic boundary conditions, $f = 0.1\%$, $L = 0$ and configuration 123.
5.3 Ellipsoidal voids

Finally, the ellipsoidal voids with $w_1 = 2$ and $w_2 = 1.5$ are analysed. The numerical meshes used are, once again, the same used in Pinto Carvalho (2015), and are shown in Fig. 5.35. The number of elements for each porosity is shown in Table 5.12. The approach for this analysis is equal to the one used to study the yield response of spheroidal voids. The only difference that has to be accounted for is the removal of radial symmetry in the geometry. For this reason, configurations that could be removed in previous analysis have to be included for ellipsoidal voids, resulting in a total of 6 distinct cases. That said, the collection of duplicate cases increases, and the total number of cases to analyze was reduced to 209 from the total number of 270.

![Section clips of the meshes used in the analysis, containing ellipsoidal voids (2, 1.5, 1) with the specified void volume fraction.](image)

(a) $f = 0.1\%$
(b) $f = 0.5\%$
(c) $f = 2\%$

Table 5.12: Number of elements for each of the void volume fractions used, considering spherical voids.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Volume fraction</th>
<th>Number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ellipsoid (2, 1.5)</td>
<td>$f = 0.1%$</td>
<td>1504</td>
</tr>
<tr>
<td></td>
<td>$f = 0.5%$</td>
<td>1504</td>
</tr>
<tr>
<td></td>
<td>$f = 2%$</td>
<td>1504</td>
</tr>
</tbody>
</table>

In Fig. 5.36 the yield curves for the ellipsoidal voids in function of the boundary conditions and void volume fraction are shown, with $L = 0$ and configuration 123. Comparing to the void geometries shown before, the ellipsoidal shape results in a very similar yielding response. Furthermore, in Figs. 5.37 and 5.38 the yielding response as a function of the Lode parameter for various configurations are shown, for periodic boundary conditions and $f = 2\%$. Once again, the majority of the influence of the Lode parameter happens at low and medium triaxialities, but the differences between the extremes is relatively small. Even for the new configurations added in the analysis, the influence of the Lode parameter was similar. As before, the response seems to be above bounded by the case of $L = 1$. Finally, Fig. 5.39 shows the influence of the configuration on the yield curve for multiple Lode parameters, periodic boundary conditions and $f = 2\%$. The influence of the configuration seems to be of the same magnitude as the Lode parameter. In contrast
with $L$, specific bounds for the response were not evident; each Lode parameter led to different bounds for the yielding response of the RVE.
Figure 5.36: Influence of the boundary conditions on a von Mises matrix with ellipsoidal voids, $L = 0$ and configuration 123.
Figure 5.37: Influence of the Lode parameter on a von Mises matrix with ellipsoidal voids, periodic boundary conditions and $f = 2\%$ for configurations 123, 213 and 321.
Figure 5.38: Influence of the Lode parameter on a von Mises matrix with ellipsoidal voids, periodic boundary conditions and $f = 2\%$ for configurations 132, 231 and 312.
Figure 5.39: Influence of the configuration on a von Mises matrix with ellipsoidal voids for different Lode parameters, periodic boundary conditions and $f = 2\%$. 
5.4 Conclusions

In this chapter, the yielding response of RVEs containing voids and with a von Mises matrix is studied. Both isotropic (spherical) and anisotropic (prolate, oblate and ellipsoidal) geometries are considered. For prolate voids, \( w_1 = 2 \); for oblate voids, \( w_1 = 0.5 \) and for elliptical voids, \( w_1 = 2 \) and \( w_2 = 1.5 \). Even though the von Mises model is pressure insensitive, when voids are present in the micro structure, the actual response of the material becomes pressure sensitive. This behavior is captured by the numerical analyses performed. Generally, the initial porosity is the predominant factor on the onset of yielding of porous media. Increasing the porosity will reduce the yield stress. Furthermore, the response at high triaxialities is far more sensitive to the porosity than the response at lower triaxialities. The yield curves obtained numerically are also compared to the analytical models shown in Section 4.4. In general, the numerical results agree with these models. However, for low void volume fractions, the models overestimate the yield stress compared to the numerical results.

These numerical analyses are run with different boundary conditions. As already predicted in Section 3.3.5, the linear boundary condition appears to be an upper bound for the numerical results, while the uniform traction model showed the lower response, and the periodic boundary condition captured an intermediate response of the RVE. This trend is verified for all the cases considered, regardless of the void volume fraction, Lode parameter, void geometry and triaxiality. The Lode parameter shows a small influence on the response of the RVE, and the response is apparently independent of this parameter for high triaxialities. Nevertheless, the yield response is apparently above bounded for \( L = 1 \), but once again, the actual differences in the response are reduced. For low triaxialities, the Lode parameter influences the geometry of the deformed void at yield, but the void geometry remains either spheroidal or ellipsoidal. For anisotropic geometries, the influence of the configuration, i.e., of the orientation of the void relative to the stress state, seems to be of the same magnitude as that of the Lode parameter.

The void growth up to yielding is analyzed. With the large strain formulation used, it is found that the voids grow significantly in size for \( T > 0 \). As a consequence, for these cases, the porosity at yield is higher than the initial porosity. For lower initial porosities, the percentual void growth is larger. For these reasons, a study has been conducted to estimate the porosity at yield. The porosity at yield in function of the triaxiality has an asymptotic trend to certain values when \( T \to 0 \) and \( T \to \infty \). By convenience, these extremes are called \( f_0 \) and \( f_\infty \). Furthermore, as the void growth is insignificant for deviatoric loadings \((T = 0)\), \( f_0 \) is assumed equal to the original void volume fraction of the RVE prior to loading. The porosity at yield was then fitted to a function of the triaxiality and initial void volume fraction. As a result, it is possible to predict a corrected porosity that is closer to the porosity at yield. Introducing this corrected porosity at the yield models, their prediction of the numerical results improves significantly.

Finally, the influence of the void geometry and orientation is assessed. These two parameters play a relatively small influence on the yielding response, both in terms of stresses at yield and void growth in the elastic region, as shown in Figs. 5.40 and 5.41 and Table 5.13. Nevertheless, the anisotropic geometries used are not very skewed, since the ratios \( w_1 \) and \( w_2 \) are not significantly different from 1. If highly anisotropic geometries are used, their influence on the response would probably be greater.
On a final note, by far the most important parameter in the yielding response of porous media is the initial void volume fraction. Other parameters such as void geometry, void orientation and Lode parameter play a secondary role on the response of the RVE. Furthermore, the analytical models do not predict void growth up to the onset of yielding. As a consequence, they overestimate the yielding response of the RVE when compared to the yielding criteria used for the numerical analyses here. By correcting the porosity at yield, much better estimates of the behavior for the RVE were found.

Table 5.13: Fitted parameters for the porosity correction for various geometries and void volume fractions, considering periodic boundary conditions, $L = 0$ and configuration 123.

<table>
<thead>
<tr>
<th>Porosity /%</th>
<th>Geometry</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$f_\infty$ /%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>Sphere</td>
<td>4.485</td>
<td>1.584</td>
<td>0.000854</td>
<td>0.185</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>3.634</td>
<td>1.616</td>
<td>0.000918</td>
<td>0.192</td>
</tr>
<tr>
<td></td>
<td>Oblate</td>
<td>4.242</td>
<td>1.609</td>
<td>0.000907</td>
<td>0.191</td>
</tr>
<tr>
<td></td>
<td>Ellipsoid</td>
<td>4.341</td>
<td>1.577</td>
<td>0.000865</td>
<td>0.187</td>
</tr>
<tr>
<td>0.5</td>
<td>Sphere</td>
<td>2.437</td>
<td>1.624</td>
<td>0.001418</td>
<td>0.642</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>1.797</td>
<td>1.715</td>
<td>0.001438</td>
<td>0.644</td>
</tr>
<tr>
<td></td>
<td>Oblate</td>
<td>2.863</td>
<td>1.505</td>
<td>0.001324</td>
<td>0.632</td>
</tr>
<tr>
<td></td>
<td>Ellipsoid</td>
<td>2.703</td>
<td>1.353</td>
<td>0.001273</td>
<td>0.627</td>
</tr>
<tr>
<td>2.0</td>
<td>Sphere</td>
<td>2.288</td>
<td>1.158</td>
<td>0.001470</td>
<td>2.147</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>2.130</td>
<td>1.232</td>
<td>0.001680</td>
<td>2.168</td>
</tr>
<tr>
<td></td>
<td>Oblate</td>
<td>1.514</td>
<td>1.500</td>
<td>0.001887</td>
<td>2.189</td>
</tr>
<tr>
<td></td>
<td>Ellipsoid</td>
<td>2.268</td>
<td>1.105</td>
<td>0.001583</td>
<td>2.158</td>
</tr>
</tbody>
</table>
Figure 5.40: Comparison of the yielding response of the RVE as a function of the void geometry, for various porosities, periodic boundary conditions, $L = 0$ and configuration 123.
Figure 5.41: Comparison of the porosity at yield as a function of the void geometry, for various porosities, periodic boundary conditions, $L = 0$ and configuration 123.
Chapter 6
Yield response of porous media with single crystal matrices

In this chapter, an analysis of the yield response of RVEs with voids is conducted, considering a single crystal matrix. At first, a brief review of crystalline materials and large-strain formulation for single crystals are shown. Then, some models for porous single crystals are presented, showing their yield functions and performing a brief comparison between them. After this short review, the numerical results are shown, considering at first spherical voids. In a first analysis, the influence of the viscoplastic parameters is investigated. Afterward, in the rate-independent case, the influence of void volume fraction, boundary conditions, Lode parameter and crystal orientation is assessed. A porosity evolution study is also conducted. Additionally, an initial study on the yield response of polycrystals is performed, considering spherical voids and varying the number of grains. Then, the analysis is extended to anisotropic geometries (prolate and oblate spheroids and ellipsoids), and the results are compared with the ones for spherical voids.

6.1 Crystalline materials

Solid materials are constituted by atoms, arranged in a specific manner. A crystalline material exhibits periodicity in its atomic structure, that is, the atoms are placed in a repetitive pattern relative to each other. At room temperatures and under normal solidification conditions, all metals and certain ceramics and polymers possess crystalline structures. Depending on the material, these crystalline structures can vary significantly; metals form relatively simple structures, whilst some polymers and ceramics show large and complex ones (Callister, 2007).

In the scope of crystalline materials, it is frequent to use the term lattice as an array of points corresponding to the centers of the atoms in a three-dimensional space. A generic lattice is shown in Fig. 6.1. Given the periodicity of the lattice, these are commonly divided in unit cells. Such unit cell is the basic structural unit of the crystalline structure, characterized by a set of three noncoplanar vectors \( \mathbf{a}, \mathbf{b} \) and \( \mathbf{c} \) and the angles \( \alpha, \beta \) and \( \gamma \). Any point \( \mathbf{r} \) in the lattice can be obtained relative to the origin \( \mathbf{o} \) by

\[
\mathbf{r} = k_a \mathbf{a} + k_b \mathbf{b} + k_c \mathbf{c},
\]  

(6.1)
where \( k_i \) \( (i = a, b, c) \) are a set of integers. A schematic representation of a unit cell is shown in Fig. 6.2.

![Figure 6.1: Lattice for a generic crystalline system.](image1)

Figure 6.1: Lattice for a generic crystalline system.

![Figure 6.2: Unit cell for a generic crystalline system.](image2)

Figure 6.2: Unit cell for a generic crystalline system.

The symmetries of the lattice imply that certain geometric transformations result in identical atomic configurations. When a rotation by 90° around an axis preserves atomic structure, the crystal is said to have a four-fold rotational symmetry about that axis. If instead of 90°, a 180° rotation exhibits symmetry, then it is called a two-fold rotational symmetry. Additionally, symmetries may arise from mirror planes and translational symmetries. Finally, compound symmetries are the result of a combination of translations and rotational/mirror symmetries. The assessment of all these symmetries is required for a complete characterization of the crystal (Engler and Randle, 2009). Furthermore, it is important to introduce the lattice centerings, which define the position of the lattice points with respect to the unit cell. The four possible lattice centerings are:

**Primitive (P):** Lattice points on the corners of the unit cell;

**Body-centered (B):** Lattice points on the corners of the unit cell and at its center;

**Face-centered (F):** Lattice points on the corners and centers of the faces of the unit cell;
6.1. Crystalline materials

**Base-centered** (C): Lattice points on the corners and on the center of the bases of the cell.

Finally, the combination of a crystal system and a lattice centering results in a Bravais lattice. Only 14 unique Bravais lattices exist, as certain combinations of crystal systems and lattice centerings result in the same lattice (Engler and Randle, 2009). These Bravais lattices are shown in Table 6.1. In this work, only cubic crystal systems are be considered, in particular, face-centered cubic (FCC) lattices.

Table 6.1: Characterization of the 7 crystal systems and corresponding 14 Bravais lattices.

<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Unit cell parameters</th>
<th>Lattice centering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>(a \neq b \neq c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha \neq \beta \neq \gamma)</td>
<td>Primitive</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>(a \neq b \neq c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = 90^\circ \neq \gamma)</td>
<td>Primitive Base-centered</td>
</tr>
<tr>
<td>Orthorombic</td>
<td>(a \neq b \neq c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = \gamma = 90^\circ)</td>
<td>Primitive Body-centered Face-centered Base-centered</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>(a = b \neq c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = \gamma = 90^\circ)</td>
<td>Primitive Body-centered</td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>(a = b = c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = \gamma \neq 90^\circ)</td>
<td>Primitive</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>(a = b = c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = 90^\circ , \gamma = 120^\circ)</td>
<td>Primitive</td>
</tr>
<tr>
<td>Cubic</td>
<td>(a = b = c)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\alpha = \beta = \gamma = 90^\circ)</td>
<td>Primitive Body-centered Face-centered</td>
</tr>
</tbody>
</table>

6.1.1 Elastic properties of single crystals

Single crystals exhibit an elastic response. Under small strains, the constitutive relation between stress and strain in the elastic regime is given by Hooke’s law

\[ \sigma = C : \varepsilon, \]

(6.2)

where \(C\) is the fourth order elasticity tensor. Furthermore, given the symmetries of the Cauchy stress tensor and of the infinitesimal strain tensor, and energy considerations, \(C\) possesses major and minor symmetries, that is (Tenreiro Vieira, 2018),

\[ C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klcj}. \]

(6.3)

This condition is of particular interest, as it reduces dramatically the number of independent terms in the elasticity tensor from 81 to 21. If material symmetries are present, the number of independent parameters is further reduced. For instance, an isotropic material
(that is, with an infinite number of symmetry planes) only has 2 unique parameters. For cubic single crystals, with 9 planes of symmetry, 3 independent constants are required. The constitutive relation using Voigt notation\(^1\)\(^2\)\(^3\) for a cubic single crystal becomes

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\sigma_4 \\
\sigma_5 \\
\sigma_6
\end{bmatrix}
= 
\begin{bmatrix}
C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & C_{44} & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\varepsilon_1 \\
\varepsilon_2 \\
\varepsilon_3 \\
\varepsilon_4 \\
\varepsilon_5 \\
\varepsilon_6
\end{bmatrix},
\]

(6.4)

where \(C_{11}, C_{12}\) and \(C_{44}\) are the elastic parameters to be determined. For additional reference on the elastic properties of single crystals under small strains, please refer to Tenreiro Vieira (2018).

### 6.1.2 Crystal plasticity

One of the most important factors in the anisotropic behavior of single crystals is their plastic deformation mechanism. Plastic deformation happens mostly by the slip of blocks of atoms in certain planes. As a consequence, the crystal is highly anisotropy under plasticity. Throughout this section, the constitutive model used for single crystals will be presented, formulated under finite strains. Furthermore, a rate-dependent law for plastic slip will be introduced, resulting in a viscoplastic constitutive model.

#### Plastic deformation by slip

The most relevant plastic deformation mechanism in single crystals is by crystallographic slip, where blocks of the crystal slide over one another along certain crystallographic planes (or slip planes) (Dieter, 1986). As a shorter atomic bond is stronger, slip typically happens between planes with higher atomic density. The slip mechanism involves cyclic temporary breakage, moving of the block of atoms and subsequent reestablishment of these bounds (de Bortoli, 2017). In a similar fashion, slip also happens in directions where the atomic bonds are stronger (directions with the highest linear atomic density), commonly referred as slip directions. A slip system is a combination of a slip plane with a slip direction. Figure 6.3a shows a schematic representation of slip planes and slip directions and their connection to the atomic structure.

FCC crystals have a total of 12 slip systems. These systems are shown in Table 6.2, where \(m\) is the normal to the slip plane and \(s\) is the slip direction. In this crystal, there are only 4 slip planes, with 3 directions each. Figure 6.3b shows a unit cell of a FCC crystal with one slip plane represented, as well as the respective slip directions.

\(^1\)\(\{\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{21}, \sigma_{13}, \sigma_{12}\} \equiv \{\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6\}\)

\(^2\)\(\{\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12}\} \equiv \{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6\}\)

\(^3\)\(C_{1111} = C_{11}, C_{1212} = C_{12}, C_{2323} = C_{44}\)
The general finite strain elastoplasticity formulation used in this work is supported by the hypothesis of a multiplicative decomposition of the deformation gradient in an elastic and plastic part

\[ F = F^e F^p, \]

where \( F^e \) and \( F^p \) are the elastic and plastic parts of the deformation gradient, respectively. This is also known as the Lee-Kröner decomposition and was firstly introduced by Lee and D. T. Liu (1967) and Lee (1969). It is shown schematically in Fig. 6.4. This split assumes the existence of a local unstressed intermediate configuration defined by the plastic deformation gradient \( F^p \). Such configuration can be obtained by elastic unloading from the final configuration (de Bortoli, 2017). The slip system remains unaltered in the unstressed slip lattice configuration. The lattice distortions and rotations are only a result of elastic deformations (de Souza Neto, Peric, et al., 2008). Furthermore, the unit vectors
in the deformed configuration remain orthogonal, and are given by

\[ s^\alpha = F^e s^\alpha_0, \quad (6.6a) \]
\[ m^\alpha = (F^e)^{-\top} m^\alpha_0, \quad (6.6b) \]

where \( m^\alpha \) and \( s^\alpha \) are the unit vectors of the slip system \( \alpha \) in the deformed configuration and \( m^\alpha_0 \) and \( s^\alpha_0 \) are their counterparts in the original configuration.

**Hyperelastic law**

The elastic behavior of the crystal is strongly dependent on its crystallographic structure and orientation. Therefore, an anisotropic elasticity model must be employed. Furthermore, during elastic loading, the distortion of the lattice can be considered infinitesimal, but its rotations cannot, as they have a large impact on the texture development of the grain. For these reasons, a hyperelastic law of Saint-Venant Kirchhoff is used, whose strain energy function is

\[ \psi^e = \frac{1}{2} E^e : C : E^e, \quad (6.7) \]

where \( C \) is the stiffness tensor (as defined in Eq. (6.2)) and \( E^e \) is the Green-Lagrange elastic strain tensor, expressed as

\[ E^e = \frac{1}{2} ((F^e)^{-\top} F^e - I). \quad (6.8) \]

The conjugate quantity of the Green-Lagrange elastic strain tensor is the second Piola-Kirchhoff stress tensor, defined in the intermediate unstressed configuration. The second Piola-Kirchhoff stress tensor becomes

\[ S = \frac{\partial \psi^e}{\partial E^e}, \quad (6.9) \]
where $\bar{\rho}$ is the mass density in the intermediate configuration. The linear elastic constitutive relation can be written as

$$ S = C : E^e. \quad (6.10) $$

**Schmid law and resolved Schmid shear stress**

According to the Schmid law, in FCC crystals, slip on a system takes place when a resolved shear stress on that system reaches a critical value, that is,

$$ \tau^\alpha_y = \tau^\alpha, \quad (6.11) $$

where $\tau^\alpha_y$ and $\tau^\alpha$ are the critical resolved shear stress and the Schmid resolved stress, respectively, on a slip system $\alpha$. The Schmid resolved shear stress is the shear stress acting on the slip plane along the slip direction, and can be expressed in the current configuration by

$$ \tau^\alpha = \sigma : (s^\alpha \otimes m^\alpha). \quad (6.12) $$

The dyadic product is also called the spatial Schmid tensor $M^\alpha$, that is,

$$ M^\alpha = s^\alpha \otimes m^\alpha. \quad (6.13) $$

Recalling the hyperelastic law, the resolved Schmid stress can also be written in the intermediate configuration as

$$ \tau^\alpha = (F^e)^T F^e S : M^\alpha_0, \quad (6.14) $$

where $M^\alpha_0$ is the Schmid tensor expressed in the reference configuration ($s^\alpha$ and $m^\alpha$ are replaced by their counterparts in the reference configuration).

Before going any further, it should be mentioned that BCC crystals violate Schmid’s law, resulting in further anisotropic effects not observed in FCC crystals (Yalcinkaya et al., 2008). As a consequence, non-Schmid laws must be employed when dealing with such crystals. These effects are beyond the scope of this work, as only FCC crystals are used in the analyses conducted.

Finally, the Schmid law can be represented as a set of yield surfaces, associated with each slip system. The yield function associated with each yield surface can be written as

$$ \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) = |\tau^\alpha| - \tau^\alpha_y, \quad \alpha = 1, \ldots, n_{\text{slip}}, \quad (6.15) $$

where $n_{\text{slip}}$ is the number of slip systems of the crystal.

**Plastic flow rule**

When the stress state in the yield surface, the slip may occur. Considering a plastic slip $\gamma^\alpha$ on the system $\alpha$, the plastic deformation gradient can be expressed as

$$ F^p = I + \gamma^\alpha s^\alpha_0 \otimes m^\alpha_0. \quad (6.16) $$

The plastic rate of deformation gradient $L^p$ is given by

$$ L^p = \dot{\gamma}^\alpha s^\alpha_0 \otimes m^\alpha_0. \quad (6.17) $$
In the case of a crystal with \( n_{\text{slip}} \) systems, Eq. (6.17) becomes

\[
L^p = \sum_{\alpha=1}^{n_{\text{slip}}} \dot{\gamma}^\alpha s_0^\alpha \otimes m_0^\alpha, \tag{6.18}
\]

where \( \dot{\gamma}^\alpha \) is the rate of plastic slip in the system \( \alpha \). Finally, the following criteria must be verified

\[
\Phi^\alpha \leq 0, \tag{6.19a}
\]
\[
\dot{\gamma}^\alpha \geq 0, \tag{6.19b}
\]
\[
\Phi^\alpha \dot{\gamma}^\alpha = 0. \tag{6.19c}
\]

In this work, no hardening has been considered on the matrix. Nevertheless, it is important to notice that the accumulated slip \( \gamma \) is an internal variable, more specifically, a hardening variable, given by

\[
\gamma = \int_0^t \sum_{\alpha=1}^{n_{\text{slip}}} |\dot{\gamma}^\alpha| \, dt, \tag{6.20}
\]

and its respective evolution law

\[
\dot{\gamma} = \sum_{\alpha=1}^{n_{\text{slip}}} |\dot{\gamma}^\alpha|. \tag{6.21}
\]

**Rate-dependent formulation**

Single crystals are often employed in high temperature applications. Under these conditions, creep and other rate-dependent phenomena cannot be neglected. Therefore, a viscoplastic law is of interest in the formulation of the plastic slip rate of a single crystal’s constitutive model. Such a law introduces a dependence on the rate of deformation, reason for which this formulation is commonly referred to as a rate-dependent formulation. Nevertheless, these viscoplastic models are also capable of recovering the rate-independent case, which is still the case of most interest in practical applications. It should also be mentioned that the rate-independent case typically exhibits numerical issues. Some often-used laws for viscoplastic slip are

- Perić’s law (Perić, 1993): Uses yield surfaces to define the onset of plastic slip. Furthermore, depends on two parameters, \( n \) and \( \dot{\gamma}_0 \). The former is a rate-sensitivity parameter, and the latter is a viscosity-like parameter. A rate-independent behavior is obtained for \( \dot{\gamma}_0 \to \infty \) and \( n \to \infty \).

\[
\dot{\gamma}^\alpha = \begin{cases} 
\dot{\gamma}_0 \left( \frac{|\tau^\alpha|}{\tau^\alpha_y} \right)^n \text{sign}(\tau^\alpha), & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) \geq 0, \\
0, & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) < 0.
\end{cases} \tag{6.22}
\]

- Perzyna’s law (Perzyna, 1963): Similar to the Perić’s law, with yield surfaces for the plastic slip. The limit \( \dot{\gamma}_0 \to \infty \) results in the rate-independent case. However, \( n \to \infty \)
leads to a rate-independent case, but it converges to a state where the critical resolved shear stress is the double of $\tau^\alpha_y$.

$$\dot{\gamma}^\alpha = \begin{cases} 
\dot{\gamma}_0 \left( \frac{|\tau^\alpha|}{\tau^\alpha_y} - 1 \right)^n \text{sign} (\tau^\alpha), & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) \geq 0, \\
0, & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) < 0.
\end{cases} \quad (6.23)$$

- Norton’s law: Does not use yield surfaces, i.e., plastic slip occurs whenever $\tau^\alpha > 0$. It is a function of two parameters, $n$ and $\dot{\gamma}_0$, representing the rate-sensitivity and reference shear rate parameters, respectively. As before, $\dot{\gamma}_0 \to \infty$ and $n \to \infty$ recover the rate-independent case.

$$\dot{\gamma}^\alpha = \begin{cases} 
\dot{\gamma}_0 \left( \frac{|\tau^\alpha|}{\tau^\alpha_y} \right)^n \text{sign} (\tau^\alpha), & \tau^\alpha > 0, \\
0, & \text{otherwise}.
\end{cases} \quad (6.24)$$

- Rate-insensitive Perić: A rate-insensitive version of Perić's law can be obtained if the flow rules are modified to be homogeneous functions of degree one with respect to the total strain rate, that is

$$\dot{\gamma}^\alpha = \begin{cases} 
\|\dot{\varepsilon}\| \left[ \left( \frac{|\tau^\alpha|}{\tau^\alpha_y} \right)^n - 1 \right] \text{sign} (\tau^\alpha), & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) \geq 0, \\
0, & \Phi^\alpha (\tau^\alpha, \tau^\alpha_y) < 0.
\end{cases} \quad (6.25)$$

The above modification makes the formulation rate-independent when discrete plastic multipliers are used, as $\Delta \gamma^\alpha = \Delta t \dot{\gamma}^\alpha$. When the strain rate is approximated between increments by

$$\dot{\varepsilon} \approx \frac{\varepsilon_{n+1} - \varepsilon_n}{\Delta t},$$

Eq. (6.25) becomes only a function of the magnitude of strain increments.

## 6.2 Models for porous single crystals

Following the analysis of porous von Mises models, a similar review is conducted for models of porous single crystals. One model of interest was proposed by X. Han et al. (2013), where rate-independent single crystals containing spherical voids have been considered. An approximate yield criterion was proposed in Paux et al. (2015), by using a regularized form of the Schmid law, in a single crystal matrix containing spherical voids. Furthermore, Mbiakop, Constantinescu, et al. (2015b) also proposed a model derived from the variational method, resulting in a MVAR model for porous single crystals, with ellipsoidal voids.

In this work, the models proposed by X. Han et al. (2013) and Mbiakop, Constantinescu, et al. (2015b) are implemented. Their relevant expressions are presented in this section and, at the end, their results are compared.
6.2.1 Han et al. model

One of the first models for porous single was proposed by X. Han et al. (2013). It was derived considering the variational formulation of Ponte Castañeda and Suquet (1997), using spherical voids. The yield function for a slip plane becomes

$$\Phi^{\alpha} = \tau^{\alpha*} - \tau_0,$$  \hspace{1cm} (6.27)

where $\tau^{\alpha*}$ is the effective resolved stress on the slip plane $\alpha$. Considering a rate-independent formulation, the overall yielding of the material happens when slip initiates on any slip plane. From the variational formulation, $\tau^{\alpha*}$ is obtained by

$$\tau^{\alpha*} - \frac{1}{1-f} \sqrt{\left(\tau^\alpha\right)^2 + \frac{2}{45} f \sigma_{eq} + \frac{3}{20} fp^2} = 0,$$  \hspace{1cm} (6.28)

where $\tau^\alpha$ is the resolved stress on the slip system $\alpha$, $f$ is the void volume fraction, $\sigma_{eq}$ is the von Mises equivalent stress and $p$ the hydrostatic pressure. However, motivated by the idea that a Gurson-like model is a better representation of the actual yielding of porous materials, the authors proposed the following alternative expression:

$$\left[\frac{\left(\frac{\tau^\alpha}{\tau^{\alpha*}}\right)^2}{\tau^{\alpha*}} + \frac{\alpha}{45} f \left(\frac{\sigma_{eq}}{\tau^{\alpha*}}\right)^2\right] + 2q_1 f \cosh \left(q_2 \sqrt{\frac{3}{20} \frac{\sigma_m}{\tau^{\alpha*}}}\right) - 1 - q_1^2 f^2 = 0.$$  \hspace{1cm} (6.29)

This last definition also introduces three parameters for calibration, $q_1$, $q_2$ and $\alpha$. In the original publication, these parameters were calibrated numerically, resulting in $\alpha = 6.456$, $q_1 = 1.471$ and $q_2 = 1.325$. It is important to mention that this model was calibrated for the rate-independent case, and no expressions for yield or gauge surfaces were provided for any rate-dependent case. The main interest of this model was its simplicity and resemblance with the Gurson and GTN models for isotropic materials. Its implementation for finite element analysis would therefore be feasible.

The use of an associative plastic flow rule implies that

$$\dot{\varepsilon}^p = (1-f) \sum_{\alpha=1}^{n_{slip}} \dot{\gamma}^{\alpha} \frac{\partial \Phi^{\alpha}}{\partial \sigma},$$  \hspace{1cm} (6.30)

where $\dot{\gamma}^{\alpha}$ is the slip rate of the slip system $\alpha$, with the assumption of small strains.

6.2.2 Variational method of Mbiakop et al.

Mbiakop, Constantinescu, et al. (2015b) developed a fully analytical model for porous single crystals with the variational linear comparison composite approach of Ponte Castañeda (1991). Subsequently, a modification similar to the one in Danas and Aravas (2012) was introduced, resulting in a modified variational model (MVAR). Furthermore, this model for porous single crystals considered ellipsoidal voids. The analysis begins with the definition of a representative ellipsoidal void, with its semi-axes colinear with $k$, $l$ and $m$ and with the ratios $w_1$ and $w_2$. Therefore, the set of microstructural variables is

$$s_\alpha = \{f, w_1, w_2, k, l, m\}.$$  \hspace{1cm} (6.31)
The model was developed under the assumption of a viscoplastic single crystal, with the slip rate defined as

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{\tau_0} \right)^n, \]  

(6.32)

where \( \tau^\alpha \) is the resolved stress on the system \( \alpha \). Here, the reference slip stress \( \tau_0 \) and slip rate \( \dot{\gamma}_0 \) are assumed to be equal for all slip systems\(^4\). Employing the variational formulation, the effective stress potential becomes

\[ \tilde{U}_{\text{mvar}} = (1 - f)^{-n} \sum_{\alpha=1}^{n_{\text{slip}}} \dot{\gamma}_0 (\tau_0)^{-n} \left( \sigma : \hat{S}^{\alpha,\text{mvar}} : \sigma \right)^{(n+1)/2}. \]  

(6.33)

The modified fourth-order microstructural tensor \( \hat{S}^{\alpha,\text{mvar}} \) results from the modification of the \( \hat{S}^{\alpha,\text{var}} \) tensor from the variational formulation, in order to correct the hydrostatic point. It is given by

\[ \hat{S}^{\alpha,\text{mvar}} = \hat{S}^{\alpha,\text{var}} + (q_j^2 - 1) J : \hat{S}^{\alpha,\text{var}} : J, \]  

(6.34)

where \( J \) is the hydrostatic projection tensor (see Section 4.4.4, page 75) and \( q_j \) is a scalar for the correction of the hydrostatic point, given by

\[ q_j = \sqrt{\frac{15}{f}} \left[ \frac{(1 - f) (\beta_n)^{1/n}}{n (f^{-1/n} - 1)} \right]^{n/(n+1)}, \quad \beta_n \approx \frac{4}{25} 6^{-n/2}. \]  

(6.35)

In a rate independent formulation, the yield surface defines the onset of yielding. However, in rate dependent formulations, gauge surfaces must be used instead. These gauge surfaces characterize the domain of statically admissible stresses. Furthermore, in the limit of a rate-independent material, these are analogous to the yield surfaces. Therefore, Mbiakop, Constantinescu, et al. defined a gauge surface in terms of the gauge function \( \tilde{\Phi} \) as

\[ \tilde{\Phi} (\sigma, s_\alpha) = (n + 1) \tilde{U}_{\text{mvar}} (\sigma, s_\alpha) - \dot{\gamma}_0 \tau_0^{-n} = 0. \]  

(6.36)

By introducing Eq. (6.33) in the gauge function, a gauge surface is obtained for a rate dependent formulation. In the limit case of \( n \to \infty \) (rate independent), the respective yield function simplifies to

\[ \Phi (\sigma, s_\alpha) = \max_{\alpha=1, n_{\text{slip}}} \left\{ \sqrt{\sigma : \hat{S}^{\alpha,\text{mvar}} : \sigma} - \dot{\gamma}_0 \tau_0^{-n} \right\} = 0. \]  

(6.37)

Furthermore, \( q_j \) simplifies to

\[ q_j = \frac{5}{2} \frac{1 - f}{\sqrt{f \log(1/f)}}. \]  

(6.38)

The definition of \( \hat{S}^{\alpha,\text{mvar}} \) and the details of the implementation of the method are shown in Appendix A.4. The authors did not develop evolution laws for the microstructural variables.

\(^4\)It should be mentioned that, in the original formulation, this assumption was not considered. Nevertheless, in the cases when this model was applied, these terms were effectively equal for all slip systems. For this reason and notational convenience, this will be assumed from this point on.
Even though the model was derived under the hypothesis of rate-dependent materials, its applicability for such cases is object of discussion. Firstly, the slip rate depends on both the creep exponent $n$ and the reference slip rate $\dot{\gamma}_0$. These terms are accounted in the variational estimate of the effective stress potential, but the reference slip rate dependency disappears once it is introduced in the gauge function. Furthermore, the results shown in the article do not mention any value used for $\dot{\gamma}_0$, but are shown in terms of a normalized stress measure accounting for the reference slip rate. For these reasons, the influence of $\dot{\gamma}_0$ on the response predicted by the model is not clear. Additionally, various numerical difficulties have arrived in the evaluation of the microstructural tensor, as discussed in Appendix A.4. The current implementation of the model is a result of various attempts to obtain similar results to the ones shown in the publication, but it remains unclear whether it is sufficiently accurate or not. For this reason, comments of the numerical results against the MVAR model will be made with caution.

### 6.2.3 Analysis of the models

Figure 6.5 compares the yield curves obtained by these models for different porosities. For low void volume fractions, Han’s model predicts higher strengths than the MVAR model. However, for $f = 10\%$, this trend is reversed. The models predict different values for purely deviatoric loadings, and these differences increase with increasing porosities. For purely hydrostatic loadings, some differences also appear, and the magnitude of these differences also depends on the porosity.

In Fig. 6.6 the influence of the Lode parameter on the response predicted by the models is shown. It can be seen that the Lode parameter strongly affects the yielding stresses for purely deviatoric loadings. Both models predict significantly less strength in those cases for $L = 0$. As the triaxiality increases, the influence of the Lode parameter vanishes. These conclusions already show possible differences in the behavior of the single crystal matrix, when compared to the von Mises one. The influence of the Lode parameter seems to be of far greater magnitude for low triaxialities than the influence of the void volume fraction. Such result was not verified for von Mises matrices.
Figure 6.5: Analysis of the yield curves predicted by the models for porous single crystals presented, considering spherical voids and $L = -1$. 
Figure 6.6: Analysis of the yield curves predicted by the models for porous single crystals presented for varying Lode parameters, considering spherical voids and an FCC crystal.
6.3 Yield response with spherical voids

In this section, a similar approach to the one in Section 5.1 is taken to study the yielding response of single crystals with spherical voids. Unlike the previous case, now the single crystal is anisotropic, and thus the response of the RVE should no longer be isotropic. The yielding response is analyzed in detail for the rate-independent case. Nevertheless, a brief study of the rate-dependent case is also presented.

The numerical meshes used are the same in Section 5.1. Therefore, void volume fractions of 0.1%, 0.5% and 2% are studied. The material of the matrix has been replaced by the single crystal model implemented in Links, for an FCC single crystal. As stated before, for cubic crystals, three independent elastic parameters are required. For consistency, the elastic properties of the single crystal are chosen to be equivalent to the ones in Section 5.1.2. Therefore, for the isotropic case, the terms $C_{11}, C_{12}$ and $C_{44}$ can be directly obtained from the elastic parameters $E$ and $\nu$ by

\[
C_{11} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)},
\]
\[
C_{12} = \frac{E\nu}{(1+\nu)(1-2\nu)},
\]
\[
C_{44} = \frac{E}{2(1+\nu)}.
\] (6.39)

Furthermore, the slip rate in each system requires a slip rate law and a set of viscoplastic parameters. Firstly, the critical resolved shear stress is defined so that the homogenized stress levels are similar to the ones obtained for the von Mises model. As the yield stress of the von Mises matrix used in Section 5.1 was 240 MPa, and the analytical models predicted that $\sigma_{eq}/\tau_0 \approx 2.4$ at yield for deviatoric loadings, $\tau_0$ is set at 100 MPa. To capture the rate-independent limit, $n = 100$ and $\dot{\gamma}_0 = 0.01 \text{ s}^{-1}$ are used. In addition, Links provides a modified rate-insensitive option for viscoplastic laws, that dynamically adjusts $\dot{\gamma}_0$ to ensure both rate-insensitivity at any $n$ (Vieira de Carvalho et al., 2019). As a result, $\dot{\gamma}_0$ ends up not being used in the analysis. These parameters are also assumed constant in all slip systems. As most of the routines for viscoplastic models in Links were developed and tested for a Perić law, this has been chosen as the viscoplastic law for these analysis. It should be mentioned that in the limiting case of rate-independent behavior, both Norton and Perić’s laws should converge for the same solution. All these parameters are shown in Table 6.3.

Finally, both the incremental loading scheme and the macroscopic yielding criterion are similar as the ones in the von Mises cases. The same increment numbers and sizes are chosen. However, the evaluation of the yielding estimate was now obtained using the model of Han et al. Even though this model was only defined for spherical voids, the incrementation used proved to be capable of capturing the onset of yielding even in the cases of non-spherical voids. Nevertheless, as concluded in Chapter 5, the influence of the void geometry should be relatively reduced when compared to the porosity. The yielding criterion was also revised, as it was found that the homogenized plastic strain could evolve non-monotonically. For this reason, the homogenized hardening variable was used instead, as it is guaranteed to be monotonically non-decreasing. As a consequence, the target values for the sub-incrementation have been updated. These new values are
Table 6.3: Mechanical properties of the matrix with the single crystal model.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>269.23 GPa</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>115.38 GPa</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>76.92 GPa</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>100 MPa</td>
</tr>
<tr>
<td>$n$</td>
<td>100</td>
</tr>
<tr>
<td>$\dot{\gamma}_0$</td>
<td>0.01 s$^{-1}$</td>
</tr>
<tr>
<td>Slip rate law</td>
<td>Perić (Rate-insensitive)</td>
</tr>
</tbody>
</table>

shown in Table 6.4. Note that the number of target values for the homogenized hardening variable increased significantly, as it was found that this new variable had much larger variations from case to case.

Table 6.4: Parameters used for the yield criterion with the homogenized hardening variable.

<table>
<thead>
<tr>
<th>Target slope</th>
<th>$0.1 \Gamma_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slope tolerance</td>
<td>10%</td>
</tr>
<tr>
<td>Slope measure</td>
<td>$\Delta |P|/\Delta |F - I|$</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$5 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$2 \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-2}$</td>
</tr>
<tr>
<td>Target homogenized $\gamma$</td>
<td>$5 \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>$2 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>$1$</td>
</tr>
<tr>
<td></td>
<td>$5$</td>
</tr>
<tr>
<td></td>
<td>$2 \times 10^1$</td>
</tr>
</tbody>
</table>

6.3.1 Influence of the rate dependent parameters

Before an analysis similar to the one in Chapter 5 is performed, the influence of the rate-dependent formulation is assessed. To do so, four values of $n$ and three values of $\dot{\gamma}_0$ are combined, resulting in a total of 12 cases for analysis. Furthermore, for each of these cases, 5 triaxialities have been used to build the yield curve, considering $f = 2\%$ and $L = -1$. The maximum number of increments had to be adjusted, as some cases had the yielding point beyond the previously established safety margin. Additionally, a fixed homogenized strain rate of $0.01\,s^{-1}$ has been imposed. Finally, no rotations were applied to the either the crystal or the stress tensor.

The results are shown in Fig. 6.7. Firstly, for $\dot{\gamma}_0 = 100\,s^{-1}$, the yielding response of the RVE appears to be independent of $n$. This result may indicate that this magnitude of $\dot{\gamma}_0$ induces a near rate-independent behavior of material, for this homogenized strain rate. As
the value of the reference slip rate decreases, the influence of \( n \) increases. For \( \dot{\gamma}_0 = 1 \text{s}^{-1} \), an increasing \( n \) leads to a decreasing stress value at yield. This effect is more pronounced in hydrostatic loadings. Finally, for \( \dot{\gamma}_0 = 0.01 \text{s}^{-1} \), the influence of \( n \) becomes very significant.

These results illustrate that there is a dependency on both viscoplastic parameters on the yielding response of the RVE. As stated before, the model proposed by Mbiakop, Constantinescu, et al. (2015b) included an explicit dependence on \( n \), but the dependency of \( \dot{\gamma}_0 \) is not clear. Nevertheless, their results did not mention any value for the reference slip rate. Given this inconsistency, a direct comparison between the numerical results and the MVAR model could lead to wrong conclusions, and thus is skipped. These analyses are made with a different slip rate law than the one used in the model.

As a conclusion, since the results raised a significant number of questions relating to the influence of these parameters on the yielding response, and since the rate-independent case is of far more interest in general applications of ductile media, all the studies from now on will focus only on the rate-independent case.
Figure 6.7: Influence of the viscoplastic parameters on yielding of a single crystal matrix with spherical voids, $f = 2\%$ and $L = -1$. 
6.3. Yield response with spherical voids

6.3.2 Influence of the boundary conditions and void volume fraction

As in Chapter 5, the first study is focused on the influence of the boundary conditions and void volume fraction on the yielding response of the material. In this case, a single crystal matrix is considered, with a rate-independent formulation. Furthermore, neither the crystal or the stress state are rotated. In Fig. 6.8 the yield curves obtained numerically for all the boundary conditions and porosities considered are shown, considering $L = -1$. These results show a very similar trend to those with the von Mises matrix. The linear and uniform boundary conditions represent the upper and lower bound for the results, respectively. Furthermore, an increase in the void volume fraction leads to a decrease in the stress levels at yield, mostly noticeable for hydrostatic loadings. The yield curve obtained numerically seems to be in agreement with the curves predicted by the models. The Han et al model shows a trend very similar to the one shown by Gurson’s model for a von Mises matrix, apparently providing an upper bound for the results. Similarly, the MVAR model for single crystals behaves like its von Mises counterpart, showing a slight underestimation of the stresses at yield for medium triaxialities. Finally, for low porosities, the models show a slight overestimation of the stresses at yield for hydrostatic loadings. Such trend is similar to the one in the results for a von Mises matrix. As before, it may be justified by the void growth in the linear elastic region, which is not accounted in the models.
Figure 6.8: Influence of the void volume fraction and boundary conditions on yielding of a single crystal matrix with spherical voids and $L = -1$. 
6.3. Yield response with spherical voids

6.3.3 Influence of the Lode parameter

The influence of the Lode parameter on the yielding response of the RVEs is also studied. As in Section 5.1, three values of the Lode parameter have been chosen (−1, 0 and 1). For each Lode parameter, the three boundary conditions and porosities are analyzed. Once again, no rotations to the crystal or stress tensor are considered.

Yield curves

The yield curves for various Lode parameters are shown in Fig. 6.9, for the three void volume fractions and periodic boundary conditions. As predicted by the models, the yield response for low triaxialities is now significantly dependent of the Lode parameter. For these cases, the stresses at yield are lower for \( L = 0 \) than the two other values. Nevertheless, for very high triaxialities, the response seems to be independent of the Lode parameter.

Comparing with the results for a von Mises matrix, now the influence of the Lode is significant for low triaxialities. In the von Mises case, the effects of the Lode are mostly felt at triaxialities from 1.5 to 7. With a single crystal matrix, the influence of the Lode parameter appears in the whole region of triaxialities below 7. This difference has a strong impact on practical applications in engineering, as the maximum values of triaxiality are typically below 3 (Ferreira, 2017). Finally, both materials are independent of the Lode parameter for nearly hydrostatic loadings.

To better characterize the influence of the Lode parameter for deviatoric loadings, a parametric study is conducted where more values of \( L \) are accounted. Thus, considering \( T = 0 \), Fig. 6.10 shows the yielding point for various triaxialities. Firstly, \( L = 0 \) seems to be the case of minimum strength of the material. On the other hand, \( L = −1 \) and \( L = 1 \) are the cases with the maximum yield stresses. Furthermore, these results are apparently symmetric relative to \( L = 0 \). All the results for the various boundary conditions and porosities show the same trend.

In Fig. 6.10 is also shown the response for a nonporous single crystal\(^5\). It can be seen that the dependence of the Lode parameter is mostly caused by the response of the single crystal constitutive model. By using a porous material, the yield stresses are inferior, but the overall dependency of the Lode parameter is very similar to the nonporous material. Nevertheless, this does not invalidate the conclusion that the yielding response of porous single crystals is dependent of the Lode parameter, but the dependency is mostly caused by the matrix constitutive model used and not the porosity.

Section plots

Figures 6.11 and 6.12 show plots of the hardening variable in sections of the RVE for 3 triaxialities, considering \( L = 0 \) and \( f = 2\% \). For a purely deviatoric loading, the slip localizes in certain regions of the void, just like it happened with the von Mises model. As the triaxiality increases, the localization starts to appear on the remaining regions of the void surface. However, unlike the von Mises material, in single crystals, slip only occurs in certain planes and directions. As a consequence, the value of the hardening

\(^5\)Obtained by the analysis of one element with a single crystal model.
variable is not evenly distributed in the void’s surface. When the triaxiality increases, a checkerboard pattern appears on the void. Each region of high hardening variable values is associated with a slip system. For instance, in Fig. 6.12c, 4 bright points can be seen on the section plane and 4 more points are visible in the void’s surface. As the section plane is also a symmetry plane for an FCC system, 4 more points should exist on the other side of the section plot, yielding a total of 12 points on the void’s surface, the same number of slip systems in an FCC crystal.

**Void distortion**

Figure 6.13 shows the distortion of the voids at yield for periodic boundary conditions, considering $T = 0$ and $f = 2\%$. It can be seen that the section cuts of the voids no longer remain perfectly circular or elliptical. In a few of these cases, the voids show some vertices that are not present in the response of the von Mises material. The Lode parameter plays the same role as before, stretching or compressing the void along an axis depending on the stress along that direction. Furthermore, in Fig. 6.14 the influence of the triaxiality in the shape of the voids is shown, considering $L = 0$, $f = 2\%$ and periodic boundary conditions. It can be seen how strongly dependent the void growth is on the triaxiality. For $T = 0$, the void is mostly distorted and does not expand, since the volumetric stresses are null. For $T = 2.5$, the resulting void shape is a combination of the volumetric and deviatoric components of stress. Finally, for $T = 1000$, the void is mostly expanded equally in all directions, as the deviatoric components are very small. Nevertheless, in this final case, the void is severely distorted from its original shape, thanks to the single crystal anisotropic behavior. As a result, the void expands significantly more in certain directions and less in others (in this case, maximum expansion appears to happen for a set of directions with an angle of $45^\circ$ between them). In a final note, Fig. 6.15 shows the evolution of the void shape throughout the incrementation, colored by the hardening variable and considering $L = 0$, $f = 2\%$, $T = 2.5$ and periodic boundary conditions. It must be remarked that the displacement fluctuations in these plots are significantly magnified, to better demonstrate the effects of the material anisotropy. The actual shape of the void at yield still resembles a sphere, as these displacement fluctuations are in fact small.
6.3. Yield response with spherical voids

Figure 6.9: Influence of the Lode parameter on yielding of a single crystal matrix with spherical voids and periodic boundary conditions.
Figure 6.10: Yield point as a function of the Lode parameter on a single crystal matrix with spherical voids and $T = 0$. 

\[ ||r|| = \sqrt{\sigma_{eq}^2 + p^2} \]
6.3. Yield response with spherical voids

Figure 6.11: Accumulated plastic strain on 1/8th of the RVE with spherical voids, for varying triaxialities, considering periodic boundary conditions, $L = 0$ and $f = 2\%$.

Figure 6.12: Accumulated plastic strain on a section cut of the RVE with spherical voids, for varying triaxialities, considering periodic boundary conditions, $L = 0$ and $f = 2\%$. 
Figure 6.13: Distortion of the voids for various Lode parameters and planes, with displacement fluctuations magnified by 200x and considering periodic boundary conditions, $T = 0$ and $f = 2\%$. 
Figure 6.14: Distortion of the voids for various triaxialities and planes, with displacement fluctuations magnified by 200x and considering periodic boundary conditions, $L = 0$ and $f = 2\%$. 
Figure 6.15: Evolution of the void geometry through the incrementation, with displacement fluctuations magnified by 200x, considering $L = 0$, $f = 2\%$, $T = 2.5$ and periodic boundary conditions.
6.3. Yield response with spherical voids

6.3.4 Influence of the crystal orientation

The influence of the orientation of the crystal relative to the stress state is also studied. As the material is highly anisotropic, its response is expected to also be strongly dependent on the direction of loading. Therefore, two extreme cases are considered:

- A set of rotations that results in the largest maximum Schmid stress on all slip systems;
- A set of rotations that results in the smallest maximum Schmid stress on all slip systems.

These cases should be the limiting cases of the RVE’s response; the first case should represent a lower bound for the yielding response, and the second should be its corresponding upper bound. As the intent is only to obtain the directions where these conditions are verified, a simple direct search method is used. The space of Euler angles is discretized and all its points are evaluated. As in Houtte (1987), the cubic symmetry of FCC crystals reduces the space of unique Euler angles. Therefore, the space of Euler angles has been reduced from $0 \leq \phi_1 < 360^\circ$, $0 \leq \Phi < 180^\circ$ and $0 \leq \phi_2 < 360^\circ$ to $0 \leq \phi_1 < 90^\circ$, $0 \leq \Phi < 90^\circ$ and $0 \leq \phi_2 < 90^\circ$. The greatest and smallest maximum Schmid stress are obtained by sweeping all these points, with a domain discretization of $1^\circ$, and the angles obtained are shown in Table 6.5.

Table 6.5: Euler angles used for the analysis of the orientation of the crystal.

<table>
<thead>
<tr>
<th>Lode parameter</th>
<th>Case</th>
<th>$\phi_1 /^\circ$</th>
<th>$\Phi /^\circ$</th>
<th>$\phi_2 /^\circ$</th>
<th>Maximum $\tau^\alpha / \tau_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>Maximum</td>
<td>64</td>
<td>27</td>
<td>23</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>Minimum</td>
<td>64</td>
<td>84</td>
<td>78</td>
<td>0.2459</td>
</tr>
<tr>
<td>0</td>
<td>Maximum</td>
<td>12</td>
<td>25</td>
<td>13</td>
<td>0.5773</td>
</tr>
<tr>
<td></td>
<td>Minimum</td>
<td>84</td>
<td>81</td>
<td>55</td>
<td>0.2056</td>
</tr>
<tr>
<td>1</td>
<td>Maximum</td>
<td>13</td>
<td>25</td>
<td>13</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>Minimum</td>
<td>78</td>
<td>48</td>
<td>45</td>
<td>0.2753</td>
</tr>
</tbody>
</table>

The results are shown in Fig. 6.16, for three Lode parameters, periodic boundary conditions and $f = 2\%$. As can be seen, the cases with the minimum Schmid resolved stress result in the higher stresses at yield, as predicted. Conversely, the cases with the maximum Schmid stress result in the lower stresses at yield. The case with no rotations ($\phi_1 = \Phi = \phi_2 = 0^\circ$) is an intermediate between these two extremes. The extreme cases should represent upper and lower bounds of the yielding response. The influence of the crystal orientation appears to be of great significance for deviatoric loadings.

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Using the Bunge convention.
Figure 6.16: Influence of the orientation of the crystal on yielding of a single crystal matrix with spherical voids, periodic boundary conditions and $f = 2\%$. 

No rotations

Maximum $\tau_s$

Minimum $\tau_s$
6.3.5 Porosity evolution

As in Chapter 5, the porosity evolution before yield onset is also studied. The single crystal model can also exhibit a significant void growth up to the yielding. The porosity at yield in function of the triaxiality is shown in Fig. 6.17. Furthermore, the same function given in Eq. (5.2) is fitted to the results, and the resulting parameters are shown in Table 6.6. These results show the same trend seen in the von Mises matrices, with two asymptotes when \( T \to 0 \) and \( T \to \infty \). Additionally, the range of values of the porosity at yield seems to be similar for both cases. However, unlike previous results, for \( T = 1000 \), the periodic boundary condition shows a smaller value for \( f_\infty \) than the uniform traction boundary condition. Nevertheless, the fits show otherwise. Such condition might be justified by the errors of the yielding criterion used. Finally, Fig. 6.18 shows the numerical results compared with the analytical models with corrected porosity. It can be seen that the prediction of these models greatly improves with a corrected porosity.

It is possible to conclude that even though the matrix is highly anisotropic, the void growth still resembles the isotropic case. As such, the proposed expressions for the porosity at yield still apply.

![Porosity at yield as a function of triaxiality and curve fitting](image-url)

Figure 6.17: Porosity at yield as a function of the triaxiality and curve fitting, considering a spherical void, \( f = 0.1 \% \) and \( L = 0 \).
Table 6.6: Fitted parameters for the void volume fraction at yield, considering $f_0 = 0.1\%$ and $L = 0$. 

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$f_\infty$</th>
<th>$f%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>3.1954</td>
<td>1.8451</td>
<td>0.001177</td>
<td>0.2177</td>
<td></td>
</tr>
<tr>
<td>Periodic</td>
<td>3.8850</td>
<td>1.7168</td>
<td>0.000884</td>
<td>0.1884</td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>2.0520</td>
<td>2.0704</td>
<td>0.001000</td>
<td>0.2000</td>
<td></td>
</tr>
</tbody>
</table>
6.3. Yield response with spherical voids

Figure 6.18: Yield curves and analytical models with corrected porosity (based on the periodic boundary condition), considering spherical voids and \( L = -1 \).
6.4 Influence of the number of grains considered

A preliminary study on the yielding response of polycrystals containing spherical voids is conducted. With an increasing number of grains in a RVE, it is expected that the response tends to the isotropic case (Tenreiro Vieira, 2018). To assess this idea, a set of polycrystals with different numbers of grains have been created and analyzed. A total of three intermediate cases for the number of grains is considered, resulting in polycrystals with 3, 7 and 24 grains. These polycrystals have been generated manually by assigning each mesh region to a single crystal. The orientations of the crystals are generated using the open-source software Neper, with the orientations uniformly distributed and taking into account crystal symmetry (Quey et al., 2011). These meshes are shown in Fig. 6.19. Finally, an additional case is considered, where each element of the mesh is a single crystal (the same methodology used in Savage et al. (2018)). For a void volume fraction of 2%, this results in a total of 1488 grains, whose orientations were also obtained with Neper.

![Figure 6.19: Polycrystal meshes used, with a void volume fraction of 2%.

These results are shown in Fig. 6.20, for a void volume fraction of 2% and periodic boundary conditions. It can be seen that the response seems to be bounded above and below by the 1488 grain case and the single crystal case, respectively. All the remaining cases are between these bounds, but their responses are very similar. Furthermore, as the number of grains increases, the response seems to become less dependent of the Lode parameter. These conclusions can be further seen in Fig. 6.21. The polycrystals also appear to display minimal strength for \( L = 0 \). Nevertheless, such difference in strength reduces as the number of grains increases. By using uniformly distributed crystal orientations, the response is expected to recover the isotropic case with less grains than if random orientations were used instead.

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\[7\] For additional reference on the generation of these meshes, please refer to Pinto Carvalho (2015).
6.4. Influence of the number of grains considered

Figure 6.20: Influence of the number of grains on yielding of a polycrystalline matrix with spherical voids and $L = -1$. 

- Single crystal
- 3 grains
- 7 grains
- 24 grains
- 1488 grains
- Han
- MVAR
Figure 6.21: Influence of the number of grains on yielding of a polycrystalline matrix with spherical voids and $L = -1$. 

\[ \| \mathbf{r} \| = \sqrt{\sigma_{eq}^2 + p^2} \]
6.5 Yield response with anisotropic voids

Finally, the influence of the void geometry with single crystal matrices is assessed. As concluded in Sections 5.2 and 5.3, the influence of an anisotropic geometry should be of small magnitude when compared to the influence of, for example, the void volume fraction. For this reason, this brief study is focused on a direct comparison of the yielding response between isotropic (spherical) voids and anisotropic (prolate, oblate and ellipsoidal) voids. For the anisotropic voids, the meshes are the same as used in Chapter 5, and the remaining properties are identical to the ones used for spherical voids. Additionally, for brevity, only the cases with periodic boundary conditions, $L = 0$ and configuration 123 are considered.

The resulting yield curves are shown in Fig. 6.22. As concluded previously, the influence of the void’s anisotropy is relatively small and roughly of the same magnitude as for von Mises matrices. Most differences occur for higher void volume fractions. Nevertheless, as in previous cases, the oblate spheroid apparently shows the most reduced strength. For the remaining voids, the highest stresses at yield are shown either by prolate or spherical voids, depending on the triaxiality.

Figure 6.23 shows the results for the porosity at yield and the fitted curves. Here the influence of the void geometry seems to play a more significant role, specially for low initial porosities. The prolate and oblate void seem to show less void growth for these lower values of $f_0$. Nevertheless, the differences between geometries is reduced as $f_0$ increases, and no particular conclusion to whether geometry promotes greater void growth can be extracted.
Figure 6.22: Comparison of the yielding response of the RVE in function of the void geometry, for various porosities, periodic boundary conditions, \( L = 0 \) and configuration 123.
6.5. Yield response with anisotropic voids

Figure 6.23: Comparison of the porosity at yield as a function of the void geometry, for various porosities, periodic boundary conditions, $L = 0$ and configuration 123.
6.6 Conclusions

The yielding response of RVEs with single crystal matrices containing void is analyzed. A similar approach to Chapter 5 is taken, and the influence of the porosity, boundary conditions and Lode parameter is assessed. Furthermore, a preliminary study on the yielding of viscoplastic porous single crystals is conducted, to evaluate the influence of the rate-dependent formulation and its parameters. A brief analysis to the influence of the crystal’s orientation is also performed. As in the von Mises case, the porosity at yield is studied and fitted, resulting in a corrected porosity function that is latter introduced in the analytical models, thereby improving their estimations. Still within the scope of spherical voids, an initial study on the yielding response of polycrystals with voids is presented. Finally, the results for spherical voids are compared against other anisotropic void shapes.

From the results, it is verified that the parameters of the viscoplastic laws strongly influence the yielding response of the RVE. For low values of $\dot{\gamma}_0$, the value of $n$ plays a critical role in the yielding, whereas for high $\dot{\gamma}_0$ the response is practically independent of $n$. In the MVAR model, this dependency is not clear, as the term referring to the reference shear rate disappears in the gauge function. As a suggestion for future works, a deeper study should be carried for the influence of these viscoplastic parameters on the yielding response of porous single crystal matrices.

For the rate-independent case, the boundary conditions and void volume fraction play a similar role to the one shown in Chapter 5 for von Mises matrices. The response predicted by the models is an overestimation of the response obtained numerically, in particular for low initial porosities. These differences are justified by the void growth up to the onset of yielding that is not accounted in the models. Regarding the Lode parameter, a significant difference from the von Mises case is found. For deviatoric loadings, this parameter strongly influences the yielding response of the single crystal. The strength is minimum for $L = 0$ and maximum for $L = 1$ or $L = -1$. However, these influences are mostly caused by the response of the constitutive model, as nonporous media show the same trend in respect with the Lode parameter. The orientation of the crystal also plays a significant role in the response. In general, the orientation that results in the greatest maximum Schmid resolved stress leads to a smaller resistance, whereas the smallest maximum resolved shear stress leads to a greater resistance. The case without lattice rotations is an intermediate of these two extremes.

The porosity evolution before yield onset also followed the same trend as in a von Mises matrix. As a result, the same function is fitted, and similar values are found for the maximum porosity at yield. Introducing the corrected porosity in the analytical models improved greatly their predictions.

The yielding response of the polycrystals showed a dependence on the number of grains. As the number of grains increases, the response of the aggregate tends to the isotropic case. Such trend is also found for the yielding response. As the number of grains increases, the response becomes more independent of the Lode parameter and the strength of material increases.

In a final study, the influence of the void anisotropy is reduced, as in the von Mises case. However, the porosities at yield showed some differences in some cases, but it is unclear if this is due to the actual behavior of the RVE or to errors in the yielding criterion.
Conclusions and perspectives for future works

The main goal of this work is the study of the yield response of porous media, through computational homogenization, using a finite strain formulation. Furthermore, the influence of parameters such as triaxiality and Lode angle on different porosities and void shapes is assessed using a stress-driven analysis. The porous microstructure is modeled with Representative Volume Elements containing voids, where both isotropic (von Mises) and anisotropic (FCC single crystal) matrices are considered.

Ductile failure in metals is caused by void nucleation, growth and coalescence. Even though the von Mises and single crystal models are pressure insensitive, the presence of voids in the microstructure induces pressure-sensitivity in the macroscopic response of the material. Thus, with increasing triaxialities, the equivalent von Mises stress at yield reduces, i.e., the loading capacity for deviatoric stress states is decreased. Furthermore, a brief review of models currently available in the literature is conducted. These models provide estimates for the yield onset of porous media, as well as appropriate evolution laws for the internal damage of the material (void volume fraction, shape and orientation).

From the numerical results, it is possible to conclude that the predominant factor in the yield response of porous media is the initial porosity. Using a stress-driven approach allows for a strict control over the Lode parameter and triaxiality. Higher porosities induce lower yield stresses, and the response at high triaxialities is far more sensitive to the porosity than the response at lower triaxialities. In general, the yield curves predicted by the models are similar to the ones obtained numerically. However, the models appear to overestimate the yield stress when compared to numerical results, especially for lower void volume fractions.

In general, the linear boundary condition appears to be an upper bound for the numerical results. On the other hand, the uniform traction model shows the lower bound of the response. The periodic boundary condition captures an intermediate response of the RVE. Both von Mises and single crystal matrices verify this trend. This last boundary condition is expected to be the closest to the actual response of the material.

For von Mises matrices, the influence of the Lode parameter on the yield response was marginal. Purely hydrostatic loadings show no influence of the Lode parameter. The overall influence of this parameter increased with higher porosities. Apparently, $L = 1$ is an upper bound for the response, but the differences are not significant. Furthermore, the Lode parameter affects the geometry of the void at yield. Nevertheless, with von Mises
matrices, the voids remain either spherical or elliptical. The influence of the void geometry and orientation seems to be of the same magnitude as that of the Lode parameter, for the void volume fractions considered.

However, for single crystal matrices, the homogenized response is significantly dependent of the Lode parameter for deviatoric loadings. Without lattice rotations, \( L = 0 \) shows the smallest values of yield stress, whereas \( L = 1 \) and \( L = -1 \) are both maxima of the strength of the material. However, this trend is mostly caused by the constitutive model, as nonporous monocrystalline media show the same results. Furthermore, the orientation of the crystal is a crucial factor in its yield stress. The geometry of the voids at yield is also affected by the Lode parameter in a similar fashion as in von Mises matrices. However, the voids no longer remain spherical or ellipsoidal, and their shape is strongly affected by the anisotropic behavior of the matrix. Nevertheless, the displacements near the void have to be significantly magnified for these distortions to be visible. Finally, a brief study on the response of polycrystalline matrices is conducted. In general, as the number of grains increases, the response became similar to the isotropic case.

The porosity up to the yield onset is also analyzed. For high triaxialities, the void growth is not negligible, specially for lower initial porosities. As the analytical models do not predict void growth in the elastic region, the yield estimate for high triaxialities overestimates the actual response. To improve their estimate, an expression for a corrected porosity is proposed, as a function of the initial porosity and triaxiality. Thus, instead of using the initial porosity, this corrected porosity accounting for void growth in the linear elastic region is used. Consequently, the estimates of the models for nearly hydrostatic loadings improve significantly. Furthermore, these conclusions display a dependency of the relative values of the elastic properties on the yield stress, and such evidence is found in additional numerical studies on the subject.

As a final note, the Han et al. model for single crystals proposes a simple modification to the critical resolved shear stress. As such, its implementation in finite element constitutive models is feasible and attractive. This work is an effort to validate the model and assess whether its predictions are close to the numerical results of RVEs. It becomes clear that the model captures the overall yielding trend of the single crystal. Furthermore, calibration of its parameters would possibly lead to an improvement of its response.

7.1 Future works

In this work, the spheroideal and ellipsoidal voids considered are relatively close to spheres, as the values of the ratios \( w_1 \) and \( w_2 \) used are close to 1. To better characterize the influence of void shape, more extreme ratios should be studied.

Only three void volume fractions are used in this work. Explicit expressions for the parameters \( a, b \) and \( c \) of the corrected porosity in Eq. (5.2) could be fitted if more porosities were considered.

Further studies with single and polycrystals on porous media can also be conducted. The generation of polycrystalline RVEs could be improved by experimental data of interaction between voids and grains in metals.
In this work, focus is given to the yielding response of porous media. Nonetheless, the ductile failure of metals happens at large values of plastic strain. The influence of parameters such as Lode parameter and triaxiality in the material response beyond yield was not addressed here and could be subject of further study.

Finally, the implementation of Han et al. model is suggested. Preliminary studies on the model have already been conducted, and promising results were obtained. These are shown in Figs. 7.1 and 7.2, where the response of the RVE with a void is compared to the response of the non-porous single crystal model and Han et. al model. Three cases are shown, where the prescribed deformation gradient is determined from the parameter $\alpha$ by

$$F = I + \begin{bmatrix} \sqrt{\frac{\alpha^2}{3}} & \sqrt{1 - \alpha^2} & 0 \\ 0 & \sqrt{\frac{\alpha^2}{3}} & 0 \\ 0 & 0 & \sqrt{\frac{\alpha^2}{3}} \end{bmatrix}. \quad (7.1)$$

It can be seen that the Han et. al model captures the same trend of the porous RVE, that is significantly different from the non-porous model. For the triaxial expansion case, the non-porous model does not predict yielding. As a further example, a polycrystalline tensile specimen was obtained using Neper, as shown in Fig. 7.3. Figure 7.4 shows the force-displacement curve for the specimen, using both non-porous and porous (Han et. al) models. The difference between these cases is significant beyond the yield onset. Nevertheless, a fully analytical implementation is not complete, and is left as a future work. Additionally, optimal values for its parameters could be calibrated, in order to reproduce in an accurate way the microscopic response.
Figure 7.1: Comparison between the stress responses of the non-porous single crystal model, of the porous single crystal RVE and of the Han et. al model.
7.1. Future works

Figure 7.2: Comparison between the porosity evolution of the non-porous single crystal model, of the porous single crystal RVE and of the Han et. al model.
Figure 7.3: Polycrystal tensile specimen used: tessellation and numerical mesh.

Figure 7.4: Comparison between the force-displacement curves for porous and non-porous single crystals in the tensile specimen.
Appendix A
Details on the implementation of yielding criteria for porous media

A.1 Parameters of the ML Model

In this section, the implementation of the yield criterion proposed by Madou and Leblond is summarized. Mostly, this is a transcription of the summary of Madou and Leblond, 2012b, for usage as a reference in future works. However, the expressions are presented here in the same order they should be evaluated. Furthermore, any relevant detail in the implementation is addressed.

Considering a rigid-ideal-plastic von Mises matrix with an uniaxial yield stress $\sigma_y$, containing an ellipsoidal void with semi-axes $a_1, a_2, a_3$ (such that $a_1 \geq a_2 \geq a_3$), with a porosity $f$, the ML model requires the evaluation of both $L(\sigma)$ and $Q(\sigma)$.

A.1.1 Evaluation of $L(\sigma)$

- Semi-axes of the outer ellipsoidal representative cell
  \[ A_1 = \sqrt{a_1^2 + \Lambda}, \quad A_2 = \sqrt{a_2^2 + \Lambda}, \quad A_3 = \sqrt{a_3^2 + \Lambda}, \quad \text{(A.1)} \]
  where $\Lambda$ is the unique positive solution of
  \[ (a_1^2 + \Lambda) (a_2^2 + \Lambda) (a_3^2 + \Lambda) - \frac{a_1^2 a_2^2 a_3^2}{f^2} = 0. \quad \text{(A.2)} \]

- Semi-axes of the completely flat confocal ellipsoid
  \[ \bar{a}_1 = \sqrt{a_1^2 - a_3^2}, \quad \bar{a}_2 = \sqrt{a_2^2 - a_3^2}, \quad \bar{a}_3 = 0 \quad \text{(A.3)} \]
  and shape parameter
  \[ k = \frac{\bar{a}_2}{\bar{a}_1}. \quad \text{(A.4)} \]

- Second porosity
  \[ g = \frac{\bar{a}_1 \bar{a}_2^2}{A_1 A_2 A_3}, \quad g_1 = \frac{g}{g + 1}, \quad g_f = \frac{g}{g + f}. \quad \text{(A.5)} \]
• Eccentricities of the inner and outer ellipsoids

\[ e_{xz} = \frac{a_1}{a_1} \times \frac{a_1}{A_1} \]  

(A.6)

• \( F \) factor for a general case (non prolate)

\[ F = 1 + \frac{1}{\log \left( \frac{g_f}{g_1} \right)} \left[ (k - 1) \left( 1 - \frac{\sqrt{3}}{2} \right) \log \frac{11k^2 + 5g_f}{11k^2 + 5g_1} \right. \\
\left. + \frac{3}{5} (1 - k)^2 \log \frac{8 - 5g_1}{8 - 5g_f} + \frac{13}{10} k (g_f - g_1) - \frac{3}{10} k \left( g_f^5 - g_1^5 \right) \right], \]  

(A.7)

and for a prolate spheroid

\[ F = 1 + \frac{1 - \sqrt{3}/2}{\log f} \log \left( \frac{11 + 5e_{xz}^3 / (1 - e_{xz}^2)}{11 + f e_{xz}^3 / (1 - e_{xz}^2)} \right) \]  

(A.8)

• \( H \) shape factors

\[ H^\text{prol}_y = \frac{1}{3} \left( 1 + E_{xz}^2 - \frac{E_{xz}^4}{2} \right), \quad H^\text{obl}_y = \frac{1}{32} - 7E_{xz}^2 + 5E_{xz}^4, \]  

(A.9)

\[ H^\text{prol}_y = 1 - 2H^\text{prol}_y, \quad H^\text{obl}_y = H^\text{obl}_y. \]  

(A.10)

• \( \alpha \) and \( \beta \)

\[ \alpha = \frac{4k}{1 + 9k^2}, \quad \beta = \frac{3k^2}{1 + 30k^2}. \]  

(A.11)

• \( H \) factors

\[ H_x = \left( 1 - k^2 \right) H^\text{prol}_x + k^2 H^\text{obl}_x. \]  

(A.12)

If using a prolate spheroid

\[ H_y = H^\text{prol}_y, \]  

(A.13)

else

\[ H_y = (1 - k) H^\text{prol}_y + k H^\text{obl}_y + \frac{1}{2} \left( 1 - k \right) \frac{\alpha^2 + \beta^2}{\alpha} \frac{E_{xz}^2 (1 - \alpha - E_{xz})}{\alpha \left( 1 - \alpha - E_{xz}^2 \right) + \beta^2}. \]  

(A.14)

Finally

\[ H_z = 1 - H_x - H_y. \]  

(A.15)

• \( \kappa \) factor

\[ \kappa = \frac{3}{2F}. \]  

(A.16)

• \( \sigma_h \)

\[ \sigma_h = H_x \sigma_{xx} + H_y \sigma_{yy} + H_z \sigma_{zz}. \]  

(A.17)

• \( \mathcal{L} (\sigma) \)

\[ \mathcal{L} (\sigma) = \kappa \sigma_h. \]  

(A.18)
A.1.2 Evaluation of $Q(\sigma)$

- Evaluation of tensor $T$

$$T = \lim_{\nu \rightarrow 1/2} \frac{1}{2G} C(G, \nu) : [I - S(\nu)], \quad (A.19)$$

where $S$ is the Eshelby tensor. Alternatively, it can be evaluated by the usage of Eshelby integrals $I_i$ and $I_{ij}$, defined in Appendix A.3, resulting in

$$
\begin{align*}
T_{iii} &= 2 - \frac{I_i + 3a_i^2 I_{ii}}{4\pi}, \\
T_{iij} &= 1 - \frac{I_i + I_j + (a_i^2 + a_j^2) I_{ij}}{8\pi}, \\
T_{ijj} &= \frac{1}{2} - \frac{(a_i^2 + a_j^2) I_{ij}}{8\pi},
\end{align*}
$$

where $i$ and $j$ ($i, j = 1, 2, 3$) must be cyclically permuted to obtain all components of the tensor$^1$.

- Tensors $M^{dg}$ and $M^{offdg}$

$$M^{dg} = (1 - f) \left[ \begin{array}{ccc} 1 & -1/2 & -1/2 \\
-1/2 & 1 & -1/2 \\
-1/2 & -1/2 & 1 \end{array} \right] + \frac{3f}{2} \left[ \begin{array}{ccc} T_{1111} & T_{1122} & T_{1133} \\
T_{2211} & T_{2222} & T_{2233} \\
T_{3311} & T_{3322} & T_{3333} \end{array} \right]^{-1}, \quad (A.21)$$

$$M^{offdg} = 3 (1 - f) \left[ \begin{array}{ccc} 1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \end{array} \right] + \frac{3f}{2} \left[ \begin{array}{ccc} T_{1212} & 0 & 0 \\
0 & T_{2323} & 0 \\
0 & 0 & T_{1313} \end{array} \right]^{-1}. \quad (A.22)$$

- Definition of $\sigma^{dg}$ and $\sigma^{offdg}$

$$\sigma^{dg} = \left[ \begin{array}{ccc} \sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \end{array} \right], \quad (A.23)$$

$$\sigma^{offdg} = \left[ \begin{array}{ccc} \sigma_{xy} \\
\sigma_{yz} \\
\sigma_{zx} \end{array} \right]. \quad (A.24)$$

- Quadratic Willis form $Q^W(\sigma)$

$$Q^W(\sigma) = \sigma^{dg} \cdot M^{dg} \cdot \sigma^{dg} + \sigma^{offdg} \cdot M^{offdg} \cdot \sigma^{offdg}. \quad (A.25)$$

- $Q(\sigma)$

$$Q(\sigma) = Q^W(\sigma) \left( (1 + g) (f + g) \kappa^2 \sigma_h^2 \right). \quad (A.26)$$

$^1$Note that $T$ has major and minor symmetries, that is, $T_{ijk} = T_{kij} = T_{jik} = T_{ijk}$. 
A.1.3 Alternate evolution law

As stated in Section 4.4.3, Madou, Leblond, and Morin originally used an alternate method for the evaluation of the evolution law for the axes of the void, in order to solve some numerical issues with the solution proposed by Aravas and Ponte Castañeda, 2004. For completeness of the definition of the model, this last solution of Aravas and Ponte Castañeda is now presented.

Considering an ellipsoidal void with semi-axes \( a \), \( b \), and \( c \) aligned with the unit vectors \( e_x \), \( e_y \), and \( e_z \), their evolution is given by

\[
\frac{\dot{a}}{a} = D_{xx}^v, \quad \frac{\dot{b}}{b} = D_{yy}^v, \quad \frac{\dot{c}}{c} = D_{zz}^v \tag{A.27}
\]

and

\[
\dot{e}_x = \left( \frac{a^2 + b^2}{a^2 - b^2} D_{yx}^v + \Omega_{yx}^v \right) e_y + \left( \frac{a^2 + c^2}{a^2 - c^2} D_{zx}^v + \Omega_{zx}^v \right) e_z, \tag{A.28a}
\]

\[
\dot{e}_y = \left( \frac{b^2 + c^2}{b^2 - c^2} D_{zy}^v + \Omega_{zy}^v \right) e_z + \left( \frac{b^2 + a^2}{b^2 - a^2} D_{xy}^v + \Omega_{xy}^v \right) e_x, \tag{A.28b}
\]

\[
\dot{e}_z = \left( \frac{c^2 + a^2}{c^2 - a^2} D_{xz}^v + \Omega_{xz}^v \right) e_x + \left( \frac{c^2 + b^2}{c^2 - b^2} D_{yz}^v + \Omega_{yz}^v \right) e_y. \tag{A.28c}
\]

As pointed by Madou, Leblond, and Morin, numerical difficulties arrive from the usage of these expressions when the sizes of the axes are equal, as the terms in the denominators of Eq. (A.28) become zero. For this reason, it is recommended to use the method proposed in Section 4.4.3.

A.1.4 Implementation

Regarding the implementation of the method, the evaluation of \( \kappa \) and the terms \( H_i \) is required, with \( i = x, y, z \). The term \( \mathcal{L}(\sigma) \) is a function of the stress state, so it will be evaluated later. Afterwards, the tensors \( M_{\text{dev}} \) and \( M_{\text{dev}}^{\text{dev}} \) must be evaluated. The strategy used for the evaluation of the yield curve consisted in sweeping the range of triaxialities, whilst keeping the Lode parameter and stress basis constant. Recalling the definition of the unit deviatoric stress and the properties discussed in Section 4.2.4, the stress tensor is written as

\[
\sigma = Q \left( pI + \sigma_{\text{eq}} \hat{s} \right) Q^\top. \tag{A.29}
\]

If a polar coordinate system \((r, \theta)\) is used in the \( p - \sigma_{\text{eq}} \) plane, one can write

\[
p = r \cos \theta, \tag{A.30}
\]

\[
\sigma_{\text{eq}} = r \sin \theta.
\]

The triaxiality can be written as

\[
T = \frac{1}{\tan \theta}, \tag{A.31}
\]

and allows for the direct calculation of \( \theta \) from \( T \). Introducing these last two expressions in Eq. (A.29),

\[
\sigma = Q \left( r \cos \theta I + r \sin \theta \hat{s} \right) Q^\top. \tag{A.32}
\]
If \( Q, \hat{s} \) and \( \theta \) are known, \( \sigma \) becomes a function of only \( r \). Introducing this stress tensor in \( L(\sigma) \) and \( Q(\sigma) \), for a certain triaxiality, the yield function becomes a function of only \( r \). Such equation is solved conveniently using the bisection method, to guarantee convergence of the method. With the value of \( r \) obtained, \( p \) and \( \sigma_{eq} \) are calculated from Eq. (A.30). After the range of triaxialities is swept, a set of points is obtained, representing the yield curve.

A.2 Parameters of MVAR Model

The MVAR model was introduced in Section 4.4.4, but the definition of some of its terms was skipped. These terms will now be presented, and further details on the implementation will be shown.

The proposed yield function for the MVAR model depends on the fourth order tensor \( M^{\text{mvar}} \), which in turn is a modification of the original variational tensor \( M^{\text{var}} \). This last term is defined as
\[
M^{\text{var}} = \frac{3}{2} K + \frac{3f}{1-f} \lim_{K \rightarrow \infty} G Q^{-1},
\]
where the fourth order shear projection tensor \( K \) is defined as
\[
K = I - J,
\]
and \( I \) and \( J \) are the identity and hydrostatic projection tensors, respectively, defined as
\[
I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (A.35a)
\]
\[
J_{ijkl} = \frac{1}{3} \delta_{ij} \delta_{kl}. \quad (A.35b)
\]
The microstructural tensor \( Q \) is defined as
\[
Q = C : (I - S(\nu)), \quad (A.36)
\]
where \( C \) is the stiffness tensor and \( S \) is the Eshelby tensor. The stiffness tensor can be conveniently expressed from the shear and bulk moduli as
\[
C = 2G K + 3K J. \quad (A.37)
\]
However, as shown in Pinto Carvalho (2015), the evaluation of \( Q \) can be conveniently replaced by the solution to the Eshelby problem, in the coordinate system defined by the principal axes of the void. As a result, the components of \( Q \) become
\[
\begin{align*}
Q_{1111} &= \frac{G}{4\pi (1-\nu)} \left(8\pi - I_1 - 3a_1^2 I_{11}\right), \\
Q_{1122} &= \frac{G}{8\pi (1-\nu)} \left[16\pi \nu (1-4\nu) (I_1 + I_2) - (a_1^2 + a_2^2) I_{12}\right], \\
Q_{1122} &= \frac{G}{8\pi (1-\nu)} \left[8\pi (1-\nu) - (1-2\nu) (I_1 + I_2) - (a_1^2 + a_2^2) I_{12}\right],
\end{align*}
\]
where \( I_i \) and \( I_{ij} \) are the Eshelby integrals, given in Appendix A.3. The remaining components of the tensor are obtained by cyclic permutation of \((1, 2, 3)\) and \((a_1, a_2, a_3)\), as well as the symmetry properties
\[
Q_{ijkl} = Q_{jikl} = Q_{ijlk} = Q_{klij}. \quad (A.39)
\]
In the incompressibility limit, Eq. (A.38) must be evaluated with \( \nu = 0.5 \).
A.2.1 Implementation

The critical aspect of the implementation is the evaluation of the $M^{\text{var}}$ tensor. From the analysis of the expressions, Eq. (A.33) can be written as

$$M^{\text{var}} = \frac{3}{2} K + \frac{3f}{1 - f} \left( \frac{Q|_{\nu=0.5}}{G} \right)^{-1}, \quad (A.40)$$

where $Q/G$ is directly obtained by dividing Eq. (A.38) by $G$. This result is then used to evaluate $M^{\text{invvar}}$, which is then introduced in the yield function. If a polar coordinate system equivalent to Eq. (A.30) is used, the radial coordinate can be explicitly obtained by

$$r = \sqrt{\frac{1 - f}{a \sin^2 \theta + b \sin \theta \cos \theta + c \cos^2 \theta}}, \quad (A.41)$$

where $a$, $b$ and $c$ are

$$a = \hat{s} : M^{\text{invvar}} : \hat{s},$$
$$b = I : M^{\text{invvar}} : \hat{s} + \hat{s} : M^{\text{invvar}} : I,$$
$$c = I : M^{\text{invvar}} : I. \quad (A.42)$$

A.3 Eshelby integrals

The Eshelby inclusion problem describes the elastic behavior of a continuum in the neighborhood of an inclusion (Eshelby John Douglas and Peierls Rudolf Ernst, 1957; Pinto Carvalho, 2015). The actual derivation of the Eshelby tensor is beyond the scope of this work (for additional reference, see Mura (1987) and Eshelby John Douglas and Peierls Rudolf Ernst (1957)). The focus is on the Eshelby integrals $I_i$ and $I_{ij}$, which are required in the evaluation of microstructural tensors for the ML and MVAR model. These integrals, obtained by respective cyclic permutations, are shown below for different geometries:

- **Ellipsoidal inclusion**
  
  $$3I_{11} + I_{12} + I_{13} = \frac{4}{a_1^2}, \quad (A.43a)$$
  $$3a_1^2I_{11} + a_2^2I_{12} + a_3^2I_{13} = 3I_1, \quad (A.43b)$$
  $$I_{12} = \frac{I_2 - I_1}{a_1^2 - a_2^2}. \quad (A.43c)$$

- **Spheroidal inclusion** $w = a_3/a_1$
  
  - **Oblate**: $w < 1$
    
    $$g = \frac{w}{(1 - w^2)^{3/2}} \left( \arccos w - w\sqrt{1 - w^2} \right), \quad (A.44)$$
  
  - **Prolate**: $w > 1$
    
    $$g = \frac{w}{(1 - w^2)^{3/2}} \left( w\sqrt{w^2 - 1} - \arccosh w \right), \quad (A.45)$$
\[ I_1 = I_2 = 2\pi g, \quad (A.46a) \]
\[ I_3 = 4\pi - 2I_1, \quad (A.46b) \]
\[ I_{11} = I_{22} = I_{12} = \frac{\pi}{a_1^2} - \frac{I_1 - I_3}{4(a_3^2 - a_1^2)}, \quad (A.46c) \]
\[ I_{13} = I_{23} = \frac{I_1 - I_3}{a_3^2 - a_1^2}, \quad (A.46d) \]
\[ 3I_{33} = \frac{4\pi}{a_3^2} - 2I_{13}. \quad (A.46e) \]

- **Sphere**

\[ I_1 = I_2 = I_3 = \frac{4\pi}{3}, \quad (A.47a) \]
\[ I_{11} = I_{22} = I_{33} = I_{12} = I_{13} = I_{23} = \frac{4\pi}{5a^2}. \quad (A.47b) \]

## A.4 Parameters of MVAR Model for porous single crystals

Just like the MVAR model for von Mises matrix, it is required to obtain the microstructural tensor \( \hat{S}_{\alpha,\text{var}} \), for each slip system. In Mbiakop, Constantinescu, et al. (2015b) it is proposed

\[ \hat{S}_{\alpha,\text{var}} = \frac{1}{2} E^\alpha + \frac{f}{K} \hat{S}^*, \quad (A.48) \]

where \( E^\alpha \) is the fourth order Schmid projection tensor on the slip system \( \alpha \) and \( \hat{S}^* \) is a fourth order microstructural tensor. The former is given by

\[ E^\alpha = 2\mu^\alpha \otimes \mu^\alpha, \quad (A.49) \]

where \( \mu^\alpha \) is the second order symmetric Schmid tensor on the slip system \( \alpha \),

\[ \mu^\alpha = \frac{1}{2} (m^\alpha \otimes s^\alpha + s^\alpha \otimes m^\alpha). \quad (A.50) \]

Then, \( \hat{S}^* \) is given by

\[ \hat{S}^* = \hat{Q}^{-1} - \sum_{\alpha=1}^{n_{\text{slip}}} \frac{1}{2} E^\alpha, \quad (A.51) \]

where \( \hat{Q} \) is given by the limits

\[ \hat{Q} = \lim_{\hat{\rho} \to \infty} \lim_{\hat{\kappa} \to \infty} \left[ S^{-1} - S^{-1} \hat{P} S^{-1} \right]. \quad (A.52) \]

The limit \( \hat{\rho} \to \infty \) represents the absence of slip in the perpendicular directions to the slip direction, and \( \hat{\kappa} \to \infty \) is the incompressibility limit. Furthermore, \( S \) is a reduced fourth order tensor, given by

\[ S = \sum_{\alpha=1}^{n_{\text{slip}}} \frac{1}{2} E^\alpha + \frac{1}{2\hat{\rho}} \sum_{\alpha=1}^{n_{\text{slip}}} F^\alpha + \frac{1}{3\hat{\kappa}} J, \quad (A.53) \]
where $F^\alpha = K - E^\alpha$ (with $K$ and $J$ obtained by Eqs. (A.34) and (A.35)). Finally, the microstructural tensor $\mathbf{P}$ is related to the Eshelby tensor and is given by

$$
\hat{P}_{ijkl} = \frac{1}{4\pi \det Z} \int_{\|\xi\|=1} \frac{\left(S^{-1}_{ab} \xi_a \xi_b\right)^{-1} \xi_j \xi_l (ij)(kl)}{Z^{-1} \cdot \|\xi\|^3} \, da,
$$

(A.54)

where $\xi$ is a unit three-dimensional unit vector, $(ij)(kl)$ denote symmetrization with respect to the corresponding indices\(^2\) and $Z$ is a second order tensor related to the shape and orientation of the voids,

$$
Z = w_1 k \otimes k + w_2 l \otimes l + m \otimes m.
$$

(A.55)

In the original publication, the authors evaluate the integral in Eq. (A.54) and the limits in Eq. (A.52) numerically. However, for two-dimensional cases, a fully analytical solution was presented in Mbiakop, Constantinescu, et al. (2015a).

### A.4.1 Implementation

As in the MVAR model for von Mises matrices, the key aspect is the evaluation of the microstructural tensor $\hat{S}_{\alpha,\text{var}}$, as given by Eq. (A.48). In particular, the evaluation of $\hat{Q}$ is not straightforward. The main problem arises in the inversion of the $S$ tensor. In the limits $\hat{\rho} \to \infty$ and $\hat{k} \to \infty$, $S$ is singular. For this reason, the authors introduce the limit only in the definition of $\hat{Q}$, not before. Numerically, this singularity is very difficult to overcome.

In a first attempt, these tensors were evaluated numerically using very high values of $\hat{\rho}$ and $\hat{k}$ (around $1 \times 10^{100}$), in order to numerically solve the limits. The integrals were evaluated numerically, using a Gauss-Legendre quadrature. The integration domain is a surface whose points are at a unit distance from the origin, i.e., a sphere with unit radius. As such, a spherical coordinate system was firstly used, resulting in

$$
\int_{\|\xi\|=1} A(\xi) \, da(\xi) = \int_0^\pi \int_0^{2\pi} A(\xi(\phi, \theta)) \sin \theta \, d\theta \, d\phi,
$$

(A.56)

with $\xi = (\sin \phi \cos \theta, \sin \phi \sin \theta, \cos \phi)$. In his thesis, Mbiakop (2015) suggests the usage of a cylindrical coordinate system instead, by

$$
\int_{\|\xi\|=1} A(\xi) \, da(\xi) = \int_{z=-1}^1 \int_0^{2\pi} A(\xi(z, \theta)) \, d\theta \, dz,
$$

(A.57)

where $\xi = (\sqrt{1-z^2} \cos \theta, \sqrt{1-z^2} \sin \theta, z)$.\(^3\) By using this integration scheme, the kernel of the integral becomes less oscillatory for highly anisotropic voids.

However, for such values of $\hat{\rho}$ and $\hat{k}$, the singularity was still present. These values were lowered until these numerical issues disappeared. Such condition only happened for values around $1 \times 10^5$, where the representability of the limit becomes very questionable.

\(^2\)As in Aravas and Ponte Castañeda (2004), $A_{(ij)(kl)} = \frac{1}{4} (A_{ijkl} + A_{ijlk} + A_{jikl} + A_{jkli})$.

\(^3\)In Mbiakop (2015), this expression is missing the exponent in the $z$ terms inside the square root.
A second iteration consisted in the evaluation of these tensors using a computer algebra system (CAS). As such, in theory, both the limits and the integration could be carried out algebraically. In practice, the numerical integration was significantly faster, yet yielding the same results, so it was preferred over the analytical one. The inversions were carried algebraically, and thus the singularity could be resolved. However, the computational effort was very substantial, both in terms of CPU time and memory, which made this calculation impractical for relatively anisotropic geometries (where a high number of Gauss points is required). Furthermore, even in the case of spheres (where only one Gauss point should be sufficient), the results obtained were questionable. The hydrostatic projection of the $\hat{S}^*$ tensor was always zero, which led to a yield function that was pressure insensitive. Nevertheless, for deviatoric loadings, the predicted values appeared correct.

In an attempt to make this calculation faster, an arbitrary numerical precision library was used. With this tool, the singularity that appeared for values of $\hat{\rho}$ and $\hat{\kappa}$ of $1 \times 10^{100}$ disappeared. Furthermore, the results were equal to the ones obtained by the CAS solver, yet took only a small fraction of the time. For this reason, this method was preferred over the CAS solver. However, the same anomalies were found for the hydrostatic component of the tensor.

In a final attempt, the values of $\hat{\rho}$ and $\hat{\kappa}$ were varied, to see if the results improved. Counterintuitively, the hydrostatic terms began to appear when these values were lowered. At regions with $\hat{\rho} \approx \hat{\kappa} \approx 1$, the results returned by the implementation of the model were very close to the ones in Mbiakop, Constantinescu, et al. (2015b) for the rate-independent case. After some calibration, the optimal values were found to be $\hat{\rho} = 1$ and $\hat{\kappa} = 0.89$. As no better estimate for the response of the criterion was found, this last iteration was the one used in this work. Nevertheless, the results provided by this implementation should be interpreted with caution.

As a final note, once the relevant microstructural tensors are evaluated, a similar procedure to the one in the MVAR model for von Mises matrices is used to obtain the yield curve. An explicit expression for $r$ can be written from both the yield function for the rate-independent case, and from the gauge function in the rate-dependent case.
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Appendix B

Numerical yield criterion development

For the analyses performed in this work, it is fundamental to establish a macroscopic yielding criterion. In the previous work of Pinto Carvalho (2015), the usage of slope based criteria was found to be very adequate to accurately capture the yielding point. In Fig. B.1 an example of a homogenized stress-strain curve is shown for a perfectly plastic material. The yield onset would be defined as the point where the slope of the curve was below a certain threshold. Nevertheless, in a stress-driven approach, some issues were found in determination of the yielding point. In this appendix, all the iterations of the development of this criterion are presented, as well as the major advantages and drawbacks of using each one. It must be remarked that a universal criterion was searched, such that it was capable of finding the yielding point sufficiently well for the vast majority of the cases considered.

![Figure B.1: Example of a homogenized stress-strain plot of an RVE with voids for various triaxialities.](image)
B.1 Derivative of the tangent modulus

At the beginning, an analytical approach was attempted to establish the point where the yielding begins. By using a closed form expression, analytically obtained from the principles in Chapter 2, its application would be independent of the incrementation scheme used. The slope of curve $\Gamma$ we are trying to capture is defined as

$$\Gamma = \frac{\Delta ||P||}{\Delta ||F - I||}, \quad (B.1)$$

where $||P||$ and $||F - I||$ are the norm of the first Piola-Kirchhoff and deformation gradient minus identity, respectively. In essence, the slope should be a measure of the rate of change in the magnitude of the stress in respect to the magnitude of the deformation. As an alternative, we could also use the Cauchy stress tensor and the Hencky strain tensor, such as

$$\Gamma = \frac{\Delta ||\sigma||}{\Delta ||\varepsilon||}, \quad (B.2)$$

or even the second Piola-Kirchhoff stress tensor in respect to the Green-Lagrange strain tensor,

$$\Gamma = \frac{\Delta ||S||}{\Delta ||E||}. \quad (B.3)$$

All these definitions represent different quantities. Nevertheless, the magnitude of the deformations at the yielding point in most metals is low, so we expect that all stress and strain tensors mentioned to be similar at the region of interest. Indeed, it will be shown in Appendix B.2 that all three definitions proposed are nearly identical for the domain of deformations used.

However, a closed expression for these definitions could not be found, and an alternative definition of the slope needs to be defined. A strong candidate for a slope definition is the homogenized material tangent modulus $A$, given by

$$A = \frac{\partial P}{\partial F}. \quad (B.4)$$

Note, however, that we are looking for a scalar measure of the slope, whereas the tangent modulus is a fourth order tensor. Thus, the first idea for the slope was to simply use the norm of the tensor, by

$$\Gamma = ||A|| = \left\| \frac{\partial P}{\partial F} \right\|. \quad (B.5)$$

Yielding is considered to occur when the slope reaches a critical value. Such value can be conveniently expressed in terms of the slope value on the linear elastic domain. Therefore, the yield region was defined as

$$\Gamma \leq \delta \Gamma_e, \quad (B.6)$$

where $\Gamma_e$ is the value of $||A||$ in the linear elastic region and $\delta$ is a tolerance parameter. In essence, in the transition between the linear elastic and plastic region, we expect a decrease in the slope $\Gamma$. In the linear elastic region, $\Gamma$ should be approximately constant and equal to $\Gamma_e$; in the plastic region, assuming a perfectly plastic material, $\Gamma$ should tend to
B.1. Derivative of the tangent modulus

zero. The value of the parameter $\delta$ establishes where the yielding occurs in this transition. Values close to 1 will be near the linear elastic region, where values close to 0 will be near the plastic region. A calibration of $\delta$ is required to ensure that the criterion captures the yielding point correctly. Thus, upon calibration of $\delta$, the macroscopic yielding function becomes

$$\Phi(\sigma) = \delta \Gamma_e - \Gamma.$$  \hfill (B.7)

In order to capture accurately the yielding point, the criterion was implemented in Links. The program proceeded as normal until it found that the current increment was already inside the yield region. The program would then discard the recently calculated increment and cut the incrementation scheme, i.e. resolve from the last valid increment with half step size. This procedure is executed until the yielding point is captured accurately. Figure B.2 shows the algorithm implemented. It it worth noting that this is equivalent to the root finding process of Eq. (B.7) with the bisection method. As long as the yield function is monotonic and continuous, the bisection method guarantees convergence to a solution, given an interval whose extremes lead to function values of opposite sign. The yield function is negative before reaching the yield region and positive afterwards. We also expect the function to be monotonic, as shown in Fig. B.1, as the evolution of stress magnitude with strain magnitude appears to lack inflection points. These conditions should satisfy the requirements for the bisection method to converge.

However, $||A||$ is not representative of the slope we were trying to capture. Figure B.3 shows the evolution of the stress magnitude and slope (normalized by the linear elastic slope) with the deformation magnitude. It can be seen that, for low triaxialities, the slope should be very close to zero for deformations above $1.5 \times 10^{-3}$, however the slope measure is far from that range. For high triaxialities there seems to exist a better agreement between $||A||$ and the slope of the curve, but there still appears to exist an error. From these results, it becomes clear that an alternative measure of the slope needs to be defined, as the norm of the tangent modulus is not representative of the actual slope.
Figure B.2: Algorithm for the yielding criterion implemented.
Figure B.3: Evolution of the stress magnitude and norm of the tangent modulus with the deformation magnitude, for various triaxialities, uniform traction boundary conditions, $L = -1$ and $f = 0.5 \%$. 
B.2 Finite difference approximation

As shown in previous section, the norm of the tangent modulus is not a representative measure of the slope we are trying to capture. Furthermore, an analytical expression representative of the slope could not be found. Therefore, in the next iteration a finite difference approximation of Eq. (B.1) was used, defined as

\[
\Gamma \approx \Gamma_n = \frac{||P||_n - ||P||_{n-1}}{||F - I||_n - ||F - I||_{n-1}},
\]  
(B.8)

where \( ||P||_n \) and \( ||F - I||_n \) are the norm of the first Piola-Kirchhoff stress tensor and of the deformation gradient minus identity at the increment \( n \), respectively, and \( \Gamma_n \) is the backward finite difference approximation of \( \Gamma \). Similarly to Eq. (B.2) and Eq. (B.3), the slope \( \Gamma \) can alternatively be expressed in terms of other stress and strain measures, such as

\[
\Gamma \approx \Gamma_n = \frac{||\sigma||_n - ||\sigma||_{n-1}}{||\varepsilon||_n - ||\varepsilon||_{n-1}},
\]  
(B.9)

or

\[
\Gamma \approx \Gamma_n = \frac{||S||_n - ||S||_{n-1}}{||E||_n - ||E||_{n-1}},
\]  
(B.10)

where the subscript denotes the increment number where the term was evaluated. The finite difference evaluated with one of these definitions would then be compared with the slope in the elastic domain, also obtained as a finite difference of the first increment. It is then required that the first increment lies within the elastic region, i.e. the first increment should be relatively small.

Another aspect that should be mentioned is the relation of the terms in Eqs. (B.8) to (B.10) to the incrementation scheme. As the loading used in Links is stress driven, we are controlling the stress state prescribed, or the numerator in these expressions. In a proportional loading scheme, the step size of the incrementation explicitly gives the difference of stress magnitude between two increments. Additionally, the terms in the denominator are functions of the terms in the numerator. It becomes clear that the variation of the terms in the numerator and denominator between increments should be proportional to the increment size. For instance, in the elastic region, the variation of the terms in the numerator should be similar to the variation of terms in the denominator, yielding a constant slope. When reaching the plastic region, the rate of variation of the denominator (strain) should be significantly larger than the rate of variation of the numerator (stress), yielding a decreasing slope. The quality of the approximation by finite differences will be dependent on the increment size, where a smaller increment will provide a more accurate result.

It is also important to select one of the measures described in Eqs. (B.8) to (B.10). An example of simulations performed with the three definitions is shown in Fig. B.4, with the slope relative to the elastic domain in terms of the increment number. It can be seen that all three measures are very similar, with differences hardly measurable. This goes into agreement with the premise of small strains up to the yielding point; the different stress and strain measures should be very similar. From this idea, we can conclude that the choice of the stress and strain measures does not play an important part on the calibration of the yielding criterion. Therefore, for convenience, we will use the magnitude of the
first Piola-Kirchhoff stress tensor and the magnitude of the deformation gradient minus identity as the measures for finite difference evaluation.

![Graph showing comparison between various measures](image)

**Figure B.4: Comparison between the three proposed stress and strain measures.**

The yielding criterion used is identical to the one used in Eq. (B.6), with the evaluation of the slope \( \Gamma \) by finite differences. Both the yield function and the root finding process were equal to the ones explained in Appendix B.1. An example of the evolution of the stress magnitude and the finite difference with the deformation magnitude is shown in Fig. B.5. It was found that this approximation of the slope was representative of the phenomena we are trying to capture. For low triaxialities it can be seen that the slope estimation does tend to zero, where the transition between both regions is quite sharp\(^1\). For high triaxialities the transition is softer, and zero slope was not reached up to the increment the simulation ended.

However, the usage of finite differences led to problems in the evaluation of the slope. As the function’s slope is monotonically decreasing, we expect the finite difference approximation to overestimate the true slope of the function. Therefore, at an increment \( n \), the true slope \( \Gamma(\lambda_n) \) should be smaller than the finite difference estimation \( \Gamma_n \). This is shown in Fig. B.6, in an extreme case where the step is very large. Note that the error will increase if the rate of variation of the slope is large, as a small increment will induce a large variation in the slope. This fast variation happens typically in the transition between the elastic to plastic region. The root finding process will fail because of this numeric error. When searching a target slope \( \delta \Gamma_e \), the error in the finite difference calculation might be sufficient to miss the target slope. This scenario is also shown in Fig. B.6. At increment \( n \), the finite difference predicted a slope \( \Gamma_n \) larger than the actual slope \( \Gamma(\lambda_n) \) and the target slope \( \delta \Gamma_e \), while the actual slope is already smaller than the target slope. Consequently, at the increment \( n + 1 \) the algorithm will believe that the target slope is ahead, when it actually already missed it. In terms of the root finding process, the bisection method will be used with an interval that does not contain a root of the yield function. This is not easily detected, because the function value of the first extreme is not accurate, and the method will essentially try to converge to the beginning of the increment.

In essence, this criterion and its implementation in theory works, but the convergence of the root finding process is very sensible to the incrementation size in the transition between

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\(^1\)It’s worth remarking that in the case where \( T = 0 \), the end of the incrementation is different in Fig. B.3 and Fig. B.5. Upon implementation of the finite difference criterion, some issues were fixed with the stress driven component of Links, which improved the stability of the incrementation scheme.
Figure B.5: Evolution of the stress magnitude and finite difference with the deformation magnitude, for various triaxialities, uniform traction boundary conditions, $L = -1$ and $f = 0.5\%$.

Figure B.6: Graphical representation of the finite difference error. The finite difference overestimates the actual slope of the curve. If the target slope is $\delta \Gamma_e$, at increment $n$ we would have already passed the target, and the finite difference scheme would fail.

When the transition is very sharp (typically at low triaxialities), the increments need to be very small, increasing significantly the computational effort. An
hybrid incrementation scheme was required, with large increments in the linear elastic region and small increments in the transition. Such scheme was difficult to design, as the transition is not known \textit{a priori}.

B.3 Finite difference with dynamic step size

From previous section, it was concluded that the slope based criterion with finite differences was capable of capturing the yield point, but was too sensitive to the increment size in the transition between elastic and plastic region. A hybrid incrementation scheme was proposed to reduce computational cost, where a large increment size is used in the linear elastic region and a smaller step is used in the transition. In this section, a method is proposed to adjust increment size when the transition is detected.

When we approach the yield point, it's expected for the deformation magnitude to increase faster than the stress magnitude. As discussed before, this results in a decreasing slope $\Gamma$. Such decrease in slope should only start to be measurable in the neighborhood of the yielding point. Therefore, the proposed criterion adds one more condition to trigger the increment cutting: at increment $n$, the absolute value of the difference between the slope $\Gamma_n$ and $\Gamma_{n-1}$ should be less or equal to a specific tolerance $\gamma$, such that

$$\left| \frac{\Gamma_n - \Gamma_{n-1}}{\Gamma_e} \right| \leq \gamma.$$  

(B.11)

The slope magnitude is normalized relatively to the slope in the linear elastic region $\Gamma_e$, for convenience on the calibration of $\gamma$. In essence, this condition imposes a maximum variation of the slope between increments, in an attempt to solve the problems described in Appendix B.2. We expect this condition to trigger when approaching the yield point, leading to a fine incrementation scheme near the zone where the finite differences produce the greatest error. Such condition also allows for the increment size to be controlled dynamically by Links, allowing a large step in the linear region and a smaller one near the yield point, and effectively reducing computational cost. Figure B.7 shows the algorithm used.

This condition effectively allowed some control of the incrementation on the yield transition. Increment cutting would start when approaching the critical region, and the increment size was kept at a reasonable level. However, the problems described in Appendix B.2 were still happening. One of the causes was that this new increment cutting condition was also suffering from the error in the evaluation of the finite difference slope. In some cases, the value that satisfied the tolerance $\gamma$ was missed, just like it happened when looking for the target $\delta \Gamma_e$. Reducing the tolerance was not enough to solve this problem, as more increment cuts were activated and more errors in the finite differences were propagated. In some other cases, the tolerance required for some target slopes was so low that the computational cost increased significantly, which ultimately resulted in non converging root finding for the yield function.
B.4 Strain offset method

From Appendices B.2 to B.3, it becomes clear that a yield criterion defined from the slope of the homogenized stress-strain curve is not practical. The main problem arrives with the dependence of the yield function with the increment size. Controlling effectively the increment size is also difficult, as computational time quickly increases when using smaller increments. Therefore, in the next iteration, we tried to establish the yield criterion in terms of a function of only point values, i.e. independent of the incrementation scheme used.
In uniaxial stress experiments, it is common to define the yielding point by the usage of a straight line parallel to the elastic portion, with a strain offset of 0.002. The yield point is the intersection between that straight line and the stress-strain curve (Callister, 2007). As this method is only dependent of the stress and strain measures at a given point, the incrementation scheme used will not have an influence on the yield point. For calibration purposes, the offset \( \delta \) should be adjustable, and a graphical representation of the condition is shown in Fig. B.8. According to the geometric representation shown, the yield function becomes

\[
\Phi (\sigma) = (\varepsilon_m - \delta) \Gamma_e - \sigma_m,
\]

where \( \sigma_m \) and \( \varepsilon_m \) are stress and strain measures, respectively, and \( \Gamma_e \) is the slope on the linear elastic region. These stress and strain measures need to be chosen. Candidates are the measures expressed in Eqs. (B.8) to (B.10).

\[
\sigma_m
\]

\[
\varepsilon_m
\]

**Figure B.8: Graphical representation of the strain offset method.**

However, it was soon realized that this criterion should be similar to a measure of the accumulated plastic strain. Furthermore, the choice of stress and strain measures is not straightforward. Even though the stress and strain measures used by previous criteria were similar (the strain magnitude is small at yielding), this criterion is normally used in uniaxial stress experiments, where the stress and strain measures are their uniaxial counterparts. It remains unclear whether a scalar representation of the three-dimensional stress and strain states is as meaningful as the uniaxial measures for the yielding criterion proposed. For these reasons, this criterion was dropped in favor of the plastic strain measure.
B.5 Homogenized plastic strain

In this next iteration, a plastic strain measure as the target variable was chosen. The yield function becomes

\[ \Phi(\sigma) = \varepsilon_{i}^{p} - \varepsilon^{p}, \]  

(B.13)

where \( \varepsilon_{i}^{p} \) is a target value of homogenized plastic strain and \( \varepsilon^{p} \) is the current value of the homogenized plastic strain. The latter is a scalar measure of the homogenized tensor \( \varepsilon^{p} \), evaluated at each Gauss point. Even though the physical meaning of this measure is questionable, it was only used to control the sub-incrementation and estimate the yielding point.

The algorithm used is the same as Fig. B.2. The convergence of this variable was very good, as it evolved monotonically for the vast majority of the cases and was not dependent on the increment size. However, two main issues were found with this measure. Firstly, it was not as representative of the yielding as the slope, as shown in Fig. B.9. If this method was to be used for the estimation of the yielding point, the optimal values of the target plastic strain would be dependent of the triaxiality. This would invalidate the intent of developing a universal yielding criterion that works for most cases. Secondly, for some triaxialities on certain geometries, the plastic strain measure did not evolve past a certain level, and for very small increment sizes in those regions, its evolution was non-monotonic. The origin of such behavior is unclear. Mostly because of the first issue, this iteration of the criterion was discarded.

Figure B.9: Stress-strain curves and points with equal Homogenized plastic strain.
B.6 Homogenized plastic strain with slope evaluation

The final iteration of the yielding criterion attempted to combine the best aspects of both measures used up to this point: the good convergence of the plastic strain with the good estimate of the yield of the slope measure. As a result, sub-incrementation was controled by a plastic strain measure and the yielding was evaluated considering the slope. Whenever a target plastic strain is reached, the slope is evaluated. If it is below a certain threshold, Links will stop, and the yielding point will be the last converged increment. This algorithm is show in Fig. B.10. As the estimation of the slope is always in excess, it is guaranteed that the actual slope is lower than the one evaluated. Thus, when the criterion is verified, it is guaranteed that the true slope is below the given threshold, i.e., the exact yielding point is behind the last converged increment, not ahead of it. By defining an appropriate set of target plastic strains, the incrementation near the yielding region will be relatively refined and the slope evaluation will be moderately accurate. Furthermore, in cases where the criterion cannot find the yielding point (for example, if a set of unreachable target plastic strains is given), it was found that Links will typically stop not far from the yielding point. As a result, the last converged increment is always the best estimate of the yielding point, as it the one used in all the studies shown in this work.
Appendix B. Numerical yield criterion development

End of converged increment

Evaluate plastic strain $\varepsilon_p$ and slope $\Gamma_n$

$\varepsilon_p$ within tolerance?
$|\varepsilon_p - \varepsilon_p^i| \leq \text{tol}$

Yes

Acceptable slope?
$\Gamma_n \leq \delta \Gamma_e$

Yes

Increment cut

No

Missed target?
$|\varepsilon_p - \varepsilon_p^i| > \text{tol}$

Yes

Increment target $i = i + 1$

No

Go to next increment

Stop Links

Figure B.10: Algorithm for the hybrid plastic strain-slope criterion.
Bibliography


