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DOCTORAL THESIS

Phenomenological data-driven procedures for the characterization of soft materials

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“Over very large timescales, and thinking of materials rather than the structures referred to just now, we are discovering that nature has evolved a number of biomaterials with the auxetic effect. We are trying to understand now why nature has done this, but it is likely to be relevant to the application for which the material has been developed”

Andrew Alderson

Abstract

From the very early days, materials have become scope of interest. Stone age, iron age, and so on, first epoches were coined by the dominance of materials. Young civilizations already realized the importance of the study of the materials and their properties. It was not until recent centuries that it became a discipline of science. Modelization thrived as an important branch of characterization and prediction of their mechanical behaviour, and mathematics the cornerstone. Already in the XIX century, analytical modelization covered entirely this activity. However, nature does not respond generally to an exact mathematical formula, mainly because of the complexity that implies the reality. In the past century computers emerged, and with them new possibilities to cover the study of all sciences. In particular in the prediction of the mechanical behaviour of complex structures. The Finite Element Method (FEM) boosted engineering to a new era. Nevertheless in some branches of rheology, analytical studies still effectuate an important role.

Depending on the circumstances, today there are two mayor ways of characterizing the mechanical behaviour of a material. The first one is with a phenomenological approach, in which an analytical formulation of stored strain energy functions with flexible parameters is fitted to get the closest response to certain referential experimental data. Thus it consists in a minimization problem of a certain error function that quantifies the differences between the reproduction of the experimental data and the data itself. The second way is directly with a Finite Element Analysis (FEA from now on) that comprises both scales the micro and the macro in the same model. The nature of the microscale will be reflected by a basic cell unit called Representative Volume Element or RVE, and the macrostructure of the specimen is covered by repetition of the RVE along of the macroscale, so that the model results in a very fine, heavy numerical mesh. The drawback of this method are the very high computational costs that, in some cases, makes the study unrealizable in practice. We will refer from now on to this approach as a *complete FEA*.

In the case of the phenomenological evaluation of stored strain energy functions the procedure is computationally very cheap, but the error functions associated with the guess of the stored energy functions itself have a minimum bigger than zero (considering a numerical zero of computational round-off error). This zero is unreachable because the analytical formulation is a guess, but also a constraint. This implies that the analytical approach cannot numerically solve the system of functional equations that arise from stress-strain equilibrium, but only get an approximate solution of the system (the functional unknowns are the stored strain energy functions, and the functional data are the curves defined by the experimental data).

The main line of the contribution of this Doctoral Thesis is the development of data-driven techniques that allow to solve numerically the system of functional equations that govern the behaviour of the solid. The found stored energy functions are expressed spline-wise (i.e. spline functions), with a similar approach as FEM does: the discretization of the domain, in this case applied to the stored energy functions.

This approach is a trade-off between the analytical method and the complete FEA. It has the benefits of showing better accuracy than the former, and better computational costs than the latter. As a matter of fact, computational times are of the same order of magnitude than the conventional analytic phenomenological approach. There are also, more qualitative than quantitative positive aspects of this methodology. One is the quantification of the differences between the assumptions that yields the stress-strain system of functional equations, and the complexity of

real nature of the mechanical behaviour of the material (fully anisotropic, non-linear, non-affine deformations, etcetera). We will call this difference "*assumption error*" from now on. Usually, in the analytical approach there is another source of error. This error quantifies the differences between the approximate and the exact mathematical solutions of the system of functional equations generated by the accepted assumptions (leaving experimental noise from the functional data, and machine round-off errors aside). This error exists because the minimization of the analytical formulation leads to a non-zero residual error (i.e. functional equations are not completely satisfied). Let this source of error be called simply *mathematical error*. Since our data-driven approach aims to erase the mathematical error, this phenomenological procedure offers for the first time (up to the author's knowledge) the possibility of quantifying the assumption error. Another positive qualitative aspect of this procedure, is that it specifies how many independent experimental data curves are required to determine the energies. The reason behind is that this approach considers the problem as a system of functional equations. Therefore, in order to be a compatible, determinate system, it is required that the number of functional unknowns be the same than the number of independent functional data, as simple as an algebraic system of equations. Finally, also as a consequence, because the number of independent functional data is definite, these are the referential experimental curves that guarantee that the found energy functions will reproduce these referential tests. Usually, energy functions obtained from conventional analytical approach shows unrealistic and unpredictable results out of the referential frame (i.e. stress-strain conditions different from referential experimental data). In opposition to that, energy functions from the procedure developed in this Doctoral Thesis, will reproduce with predictable and reasonable good results the mechanical behaviour out of the referential scenario.

In this Thesis further advances of the data-driven methods are made.

- Extension to the compressible regime for different hyperelastic possibilities.
- Extension to invariants beyond the logarithmic strains in the methodology.
- Extension of the procedures beyond the use of the inversion formula.
- Development of algorithms to cover general loading circumstances.
- Extension of the method beyond the Valanis - Landel decomposition.
- Extension to auxeticity for both isotropic and orthotropic materials.

Resumen

Desde siempre los materiales han sido foco de interés. La edad de piedra, la edad de hierro, etc, las primeras épocas se acuñan con el nombre del uso de los materiales que la caracterizan. Las primeras civilizaciones ya se dieron cuenta de la importancia de los materiales y sus propiedades. Ya en los últimos siglos se ha convertido en una disciplina de la ciencia. La modelización prosperó como una rama importante de caracterización y predicción del comportamiento elástico de los materiales, y en el que las matemáticas son la piedra angular. Ya en el s.XIX, la modelización analítica cubrió completamente esta actividad. Sin embargo, la naturaleza no responde generalmente a una fórmula matemática exacta, principalmente debido a la complejidad que implica la realidad. En el siglo pasado surgieron las computadoras, y con ellas nuevas posibilidades para cubrir el estudio de todas las ciencias en general, y en la predicción del comportamiento mecánico de estructuras complejas en particular. El método de elementos finitos (FEM) impulsó la ingeniería a una nueva era. Sin embargo, en algunas ramas como la reología los estudios analíticos siguen desempeñando un papel importante.

Dependiendo de las circunstancias, hoy existen dos formas principales de caracterizar el comportamiento mecánico de un material. El primero es con un enfoque fenomenológico, en el que una formulación analítica describe las energías de deformación, que se ajustan con unos parámetros flexibles para obtener la respuesta más cercana a ciertos datos experimentales que se usan de referencia. Por lo tanto, se trata de un problema de minimización de una función de error que cuantifica las diferencias entre la reproducción de los datos experimentales a partir del modelo y los datos en sí. La segunda forma es directamente con un análisis de elementos finitos (FEA de ahora en adelante) completo, que comprende las escalas micro y macro en el mismo modelo. La naturaleza de la microescala se refleja en una unidad básica llamada Elemento de Volumen Representativo (acrónimo inglés RVE), mientras que la macroestructura de la muestra está cubierta por repetición de la RVE a lo largo de todo el volumen del modelo, que da como resultado una malla numérica muy fina y pesada. El inconveniente de este método es el elevado coste computacional. Son costes que, en algunos casos, hacen que el estudio sea irrealizable en la práctica. En adelante nos referiremos a este enfoque como un FEA completo.

En el caso del enfoque fenomenológico, la evaluación de las funciones de energía sale muy barata, pero las funciones de error minimizadas que dieron lugar a la expresión analítica de dichas funciones de energía tienen un mínimo mayor de cero (considerando el cero como un cero numérico, con la correspondiente tolerancia numérica). Esto es en parte porque la prescripción analítica supone una restricción para alcanzar el cero numérico en las funciones de error. Esto implica que el enfoque analítico no puede resolver numéricamente el sistema de ecuaciones funcionales que surgen del equilibrio tensión-deformación, sino que solo obtiene una solución aproximada del sistema (las incógnitas funcionales son las funciones de energía de deformación almacenadas, y los datos funcionales son las curvas definidas por los datos experimentales).

La contribución principal de esta Tesis Doctoral es el desarrollo de técnicas basadas en datos experimentales que permitan resolver numéricamente el sistema de ecuaciones funcionales que rigen el comportamiento del sólido. Las funciones de energía despejadas del sistema de ecuaciones se expresan en forma de spline (es decir, funciones de spline), con un enfoque similar al de FEM: la discretización del dominio, en este caso aplicada a las funciones de energía almacenada.

Este enfoque de esta Tesis es una relación de compromiso entre el método analítico y el FEA detallado. Tiene los beneficios de mostrar una mejor precisión que la primera, y mejores costes computacionales que la segunda. De hecho, los tiempos computacionales son del mismo orden de magnitud que con el enfoque fenomenológico analítico convencional. También hay aspectos positivos más cualitativos que cuantitativos de esta metodología. Una es la cuantificación de las diferencias causadas por la aceptación de determinadas hipótesis simplificativas en comparación con la complejidad de lo real (deformaciones completamente anisotrópicas, no lineales, no afines, etc.). Llamaremos a esta diferencia "*error por hipótesis*". Por lo general, en el enfoque analítico hay otra fuente de error. Este error cuantifica las diferencias entre las soluciones matemáticas aproximadas y exactas del sistema de ecuaciones funcionales generadas a partir de dichas hipótesis simplificativas (dejando de lado el ruido experimental de los datos funcionales y los errores de redondeo de la máquina). Este error existe porque la minimización de la formulación analítica conduce a un error residual distinto de cero (es decir, las ecuaciones funcionales no están exactamente resueltas). Para diferenciarlo del anterior error, llamaremos a éste *error matemático*. Dado que nuestro enfoque *data-driven* tiene como objetivo anular el error matemático, este procedimiento fenomenológico ofrece por primera vez (según nuestro conocimiento) la posibilidad de cuantificar el error de hipótesis. Otro aspecto cualitativo positivo de este procedimiento es que especifica cuántas curvas de datos experimentales independientes se requieren para determinar las energías. La razón subyacente es que este enfoque considera el problema como un sistema de ecuaciones funcionales. Por lo tanto, para ser un sistema compatible y determinado, se requiere que el número de incógnitas funcionales sea el mismo que el número de datos funcionales independientes, algo tan simple como un sistema algebraico de ecuaciones. Finalmente, también como consecuencia, debido a que el número de datos funcionales independientes es definido, se sabe que las curvas experimentales empleadas son la referencia que garantiza que las funciones de energía encontradas reproducirán precisamente esas referencias. Las funciones de energía obtenidas a partir del enfoque analítico convencional pueden mostrar resultados poco realistas e impredecibles fuera del marco referencial (es decir, condiciones de tensión-deformación diferentes de los datos experimentales referenciales). En oposición a eso, las funciones de energía del procedimiento desarrollado en esta Tesis Doctoral, reproducirán con buenos resultados predecibles y razonables el comportamiento mecánico fuera del escenario referencial si las hipótesis de partida son adecuadas.

En esta Tesis se han desarrollado los siguientes avances de los procedimientos data-driven.

- Extensión al régimen compresible para distintas posibilidades hiperelásticas.
- Extensión de uso de invariantes más allá de los logarítmicos.
- Extensión de los procedimientos más allá de la fórmula de inversión.
- Desarrollo de los algoritmos para cubrir condiciones de ensayo generales.
- Extensión del método más allá de la descomposición Valanis-Landel.
- Extensión al régimen auxético de materiales isótropos y ortótropos.

Agradecimientos

Hace ya unos años, yo tenía cierta curiosidad matemática por las hiperoperaciones aritméticas, que a primera vista parecían tan atractivas como improductivas. La curiosidad era mayor que el sentido de la rentabilidad. Cierta día entré en el despacho del profesor Francisco Javier Montáns, (o Paco, que además de más cómodo de decir, con una mínima confianza le gusta más) y le comenté mi quijotesca inquietud. Lejos de sacarme a librazos del despacho, le pareció curioso y no sólo me animó a seguir, sino que además me compró un libro dedicado a lo que se sabía sobre las hiperoperaciones. Un tiempo después y gracias a su apoyo no solo se encontraron posibles utilidades, sino que además hicimos una publicación con la primera hiperoperación aritmética fraccional. Esa experiencia hizo que yo quisiera seguir trabajando con él, y ya antes de terminar el trabajo de dicha publicación empecé a adentrarme en la mecánica de sólidos computacional. Con Paco, más que un jefe que te exige resultados, tienes a un compañero de trabajo que te acompaña a lo largo de la Tesis y que te contagia ilusión por cada avance investigado. Al mismo tiempo no había tenido hasta ahora a un superior con unos conocimientos tan inmensos que, sencillamente no ves dónde acaban. Gracias por todo lo que me has enseñado, y más aún por hacerme ver la inmensidad de lo que aún me queda por conocer. Supongo que es así como se siente un explorador que ama lo que hace.

Por el camino de la Tesis he encontrado durante mi estancia en Sheffield gente de una calidad personal y profesional asombrosa, como es el caso del profesor Andrew Alderson o Andy como a él le gusta. Siempre que veo a alguien por primera vez me imagino cómo será, incluso antes de que hable, como una especie de primera impresión. Esto ocurrió en un congreso de materiales auxéticos que organizó, y me imaginé que era una persona muy relevante y distante. En lo segundo me equivoqué completamente. Es una persona cercana, muy humana y de la que he recibido muchísimo más de lo que yo haya podido darle. Es una persona que deja el listón altísimo, que equilibra a la par la calidad humana, el orden metódico, la profesionalidad y los conocimientos. Si yo consiguiera ser la mitad de quién es Andy hoy me sentiría muy satisfecho. Si esta Tesis tiene finalmente la mención internacional se lo debo a él, así como a otras personas maravillosas que conocí en Sheffield como Shruti Mandhani, Olly Duncan (al principio de conocerle como Mr.Olly, y después como Dr.Olly), Mirjam Skof, Ronak Janani, Amy McNally, y más. Todos allí de una calidad humana encomiable. Doy las gracias así mismo a Tom Allen por la ayuda prestada y por haber accedido a ser miembro del tribunal de mi Tesis, así como también a Victoria Lapuerta, Pablo Fajardo y Mario Merino por el mismo motivo.

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FIGURE 1: Despedida de mi estancia en Sheffield con mis compañeros
(publicación con permiso)

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Chapter 1

Introduction

The study of materials has always been a key role in engineering. In the first stages, only natural materials were available. With the surge of new techniques, the first modified materials appeared and with them the alloys. Such progress was a leap in the technical capabilities available, to such an extent that new materials could only have been produced thanks to the technological level of that moment. New materials implied new properties. Since then, human beings have tried to study how to improve materials, study their properties and their mechanical behavior. To reach the current state several milestones have had to be met. The concepts of center of gravity, static and balance date back to Archimedes. Aristotle, considered the inventor of the scientific method, contributed significantly to the methodology that science requires. The Arabic notation of numbers significantly enhanced mathematics. Indian mathematics was the first to register this notation. In the period of 400 - 1200, they developed contributions such as the concept of zero, negative numbers, arithmetic, algebra, and even the functions of sine and cosine. Francis Bacon introduced the experimental method within the current of empiricism, which says that knowledge must come from experience. Galileo Galilei (1564-1642) established the first stones of theory of structures, and Robert Hooke (1635-1703) developed the law of linear relations between force and deformation of materials. Issac Newton formulated the laws of movement and developed the calculus. John Bernoulli (1667-1748) formulated the principle of virtual work. Louis Navier (1785 - 1836) wrote the first treatise on the elastic behavior of structures. Already in the 19th century, an important leap was when Willard Gibbs [1] proved the relationship between the properties of a material and its microstructure. One of the most relevant properties of a material is its mechanical behavior. The study of the mechanical behavior is necessary for countless fields such as structural analysis, employed for most of the structures, such as bridges, ships, highways, buildings or the space station, or disciplines such as mechanical engineering, architecture, or aerospace engineering. But it is also essential for other branches such as deformation mechanics, fracture mechanics, fracture, mechanical testing, biomechanics and much more. In the last century, the possibilities of mechanical properties experienced a boom with polymeric materials and later with composites, in which the properties of materials, including mechanical ones, were directly the subject of work. Initially, these advances took place by altering the chemistry of materials, but currently these changes also occur in a mesoscopic and even macroscopic scale, with the use of 3D printers, for example. The change of the structure can be so decisive in the mechanical properties that they are able to reach achievements such as the anti-intuitive behavior of the auxetic materials. These materials have a great implication in the latest advances in the mechanical properties of the materials, with multiple fields of application such as sports, military, aerospace, medical or biomechanics. Nowadays, biomechanics and the study of biological materials are undergoing a breakthrough. One of the characteristics of these materials,

in addition to their complexity, is their specificity. Each tissue specimen is unique on each individual. For example, the stiffness of an aortic artery varies according to genetics, but even for the same individual it may vary according to the health, habits (food, sport), or youth. If we think about the importance of knowing the mechanical behavior of a tissue, the success or disaster of an operation of a surgeon robot, it depends, among other things, on the ability to predict the mechanical behavior of the tissues of a specific patient.

1.1 The importance of a model

1.1.1 The assumption

In order to make a prediction of the mechanical behavior of a material, it is a priority to model it first. The mechanical behaviour of a material may be extraordinarily complex, so this implies applying different experimentally verifiable assumptions that simplify the real problem. In general, deformations are neither linear nor conservative; the effects of the different deformations and their history are not governed by the principle of superposition. From the mechanical point of view, materials are neither ideally orthotropic, nor perfectly viscous, or plastic, or hyperelastic. Therefore, it is necessary to undertake a set of simplifying but reasonable assumptions that make the calculation of the mechanical behavior somewhat approachable. Depending on the type of material, some assumptions will be more accurate than others. In the case of materials whose relationship between deformation and stress does not depend on the history or on the load path, hyperelasticity is a successful assumption that can considerably simplify the problem. The great advantage of hyperelasticity from the analytical approach is that it greatly simplifies the modeling of the problem. It implies that there is a potential energy that yields a system of equations that describe the stress-strain equilibrium of the material. Therefore an analytical form of the problem is a quick way from the computational point of view to model the mechanical behavior of the material. Another strong point of the analytical approach is that the proposal of an analytical stored energy guarantees *per se* the conditions of a potential function (by definition), as well as the necessary stability criteria. This can be an advantage when addressing for example issues such as errors due to the influence of experimental noise, and therefore the quality of the employed data. Usually, the arguments of the energy functions are the strains, and from these functions the corresponding stresses can be determined with their derivatives. Theoretically, the dual problem can also be expressed, that is, using the stresses as arguments to determine the corresponding strains. These functions need certain objectivity requirements, such as the invariance of energy (the energy is the same independently of the reference system). Other assumptions that affect the computation of some energy functions are hypoelastic materials, in which the mechanical response depends on the history of the loads, but not on the speed at which they have are applied; viscoelasticity, in which it does not depend on the past but on the speed of application of the loads; or plasticity, in which the information from the past defines the mechanical behavior of the material.

Because the mechanical energy of the material is objective, it is smart to consider some invariants from the strain tensors as arguments of the strain energy functions. The most immediate are the principal stretches, where the stretch is defined as the ratio final/initial length of certain geometry of the material. Mathematically the principal stretches are the eigenvalues of the stretch tensor, $\mathbf{U}$. Other options, grounded mainly on experimental evidences, are the Rivlin-Spencer invariants [2]

especially for incompressible materials, and the J invariants adopted by Blatz and Ko [3] and Horgan and Saccomandi for compressible foams [4]. Another assumption is required based on the compressibility of the material, such as the case of incompressible, quasi-incompressible or simply compressible materials. The topology of the response is also quite relevant when characterizing a material, and there is a similar relationship with a Taylor polynomial. We have the isotropic case that would be a case of order 0, in which the response of the material does not vary with the direction of the applied load, if reference is aligned with the principal stress directions. In other words, the principal directions of the stress and strain tensors are the same. In the next order of complexity we would find the materials that are transversally isotropic and orthotropic. Generally, this is the modeling of composites or materials that covers effects caused by aligned fibers along special directions of the material, known as preferred directions. In that preferred direction the mechanical behavior will be different from the rest. If each one of the symmetries of the material is characterized by a strain energy function, then the assumption of orthotropy is applied. In that case, each of the three-dimensional symmetries is a preferred direction of the material. Following the analogy with Taylor, grade 2 would imply coupling of the described effects and could be simply considered as anisotropy. Other hypotheses to consider are related with deformations, such as the *affine deformation*, which is applicable to materials characterized by an isotropic matrix and fibers nested in it. The simplification assumes that the deformation experienced by the fibers and the matrix is the same. According to experimental evidences it is quite a rough approximation, although in many cases is an admissible assumption that simplifies dramatically the model. In general, it is critical to know the degree of satisfaction of certain assumption in the application of a model, and more importantly the quantification of the error derived from such assumption. Experimental evidence is therefore another factor to consider in the construction of a model and the methodology required to the correct reproduction of the mechanical behavior of the material. The characterization and quantification of the sources of error (that is, the classification and the corresponding weight that affects the quality of a model) is paramount to control the limitations of the model and the procedure, and gives the understanding to answer questions such as to what extent does the experimental noise affect the quality of the experimental data? Do the model lead to a mechanical instability if it is not based on an analytical formulation? If not, what guarantees the stability? What is the weight of numerical rounding errors in the obtained energy functions? What is the mathematical error of a model due to minimizing a residual function that quantifies the satisfaction of the equilibrium equations? What is the error inherent to a specific assumption that contributes to define the mechanical behavior of the material? Are the different sources of error classifiable and quantifiable? (e.g. Valanis – Landel assumption, hyperelasticity, the choice of a certain family of strain invariants, or the affine strains assumption? These issues have both quantitative and qualitative importance since they determine the degree of control that the modeler possesses about the weakness and strengths of the model. Therefore these questions have to be considered in the genesis of a model when applying certain simplifying assumptions (in which the rheological experience of the modeler and the experimentalist is of importance), as well as in the theoretical verification phase, if applicable (e.g. the use of some pseudo-experimental data to recover the theoretical reference energy functions and resolve the inverse problem). These questions are also relevant during the experimental validation, since the observation is required to compare the reproduced results by the model and the experimental results, especially for load cases different from the ones employed for the determination of the energy. This is

because the goal of a model is to cover all possible cases and to contribute to the understanding of the mechanical behavior of the material.

1.1.2 The approach

In general, the assumption of affine deformations is employed by the phenomenological approach that considers energy functions as a manifestation of the mechanical behavior of a solid, defined as a continuous and homogeneous medium. The great advantage of this method is that it simplifies the complexity that entails the microscale aspects, and it allows to address the problem in a mathematical frame that is generally analytical. This approach is called phenomenological because it does not explicitly consider the microstructure, and it was adopted with complete acceptance in the twentieth century. Numerous important advances were developed applying this approach. Examples are the simple Neo-Hookean model [5], the Rivlin's energy functions and the Mooney - Rivlin model [2], Ogden [6], Gent [7], Arruda - Boyce [8] models, among others. Some models are combinable, such as the one that contemplates the compressibility effects of Hartmann-Neff [9]. One of the most important and accepted models by the community is the small strains model, which keeps a linear relationship between the stress response and the undergone deformation. This model is interesting and important for several reasons. First, it is an extremely simple formulation that facilitates the understanding and the control of the experimentalist over the model. Second, since the dependencies are all linear, its implementation on FEA generates fast simulations computationally speaking because the first iteration on each time step of the finite elements is directly the solution of equilibrium. It would be interesting and intuitive that the casuistry of small strains model were recovered by the aforementioned models at small deformations, especially because the importance of the understanding that the experimentalist requires about the model. Otherwise, the model behaves as a black box, and it reduces the possibility of anticipating results and avoiding unwanted effects. Unfortunately, this recovery of the small strains is not accomplished for the majority of the analytical formulations employing the phenomenological approach. This point is discussed in detail later on. There are more approaches available to model a mechanical response. Attending to the microstructure, it is possible to define a model with numerical parameters related with geometric elements of the microscale that trigger the macromechanical response [10]. With the arrival of computers, new methods thrived with the aim of improving the efficiency of previous models, or even covering new scenarios. One of the new possibilities that computers offers is to perform a complete micro-macro finite element analysis (FEA, from now on) of the entire structure, so that both the microstructure and the macrostructure are covered in the FEA, and the model collects all the scales. This has the advantage of being able to model in a more realistic way the mechanical behavior of the material directly with its microstructure. The drawback is that computational costs are very high, usually unapproachable. In these cases, the microstructure can be modified and covered by a repetitive pattern that expands to the entire macroscopic domain. This pattern is the minimum volume with unrepeatable topology and is called the RVE or representative volume element. RVE is therefore the basic unit that defines by extension all the entire macroscopic domain of the specimen. These models assume what is known as *separation of scales*, which means that deformations at the microscale are characterized by a deformation gradient and periodic boundary conditions in the RVE. In this multi-scale models, FEA is applied to the different discretized levels. One of them, FE^2 , considers each point of integration of the macroscopic domain as

a RVE domain that must be resolved using FEA on each step, so that the response is averaged and assigned to the macroscopic integration point [11]. It is therefore an attempt to reduce the very high computational FEA costs of making a single very fine and large mesh for the entire geometry.

Another approach that is gaining prominence is the so-called data-driven, which is characterized by a correct management of the experimental data to model the problem and not necessarily using an analytical framework. The alternatives for this approach yield an extensive bibliography. An example of this approach is a method that involves the characterization of the mechanical behavior of a nanocomposite material by applying the concept of surface energy of bodies. The surface energy of particles encapsulated in a matrix material is calculated according to chemical, topological reasons, and thus the dispersion of the particles within the material. Subsequently, a FEA is performed using the concept of RVE for the particles, and the results are compared with the experimental evidence. Finally, applying Machine Learning concepts, the RVEs are updated with iterations until the error between the model and the experimental evidence is minimized [12]. Other data-driven options generally employ the combination of a conveniently managed database, which requires the use of FEA to estimate the deviations between the result obtained and reality as a control element. Finally a corrective algorithm, applies the necessary corrections for the next iteration. After several iterations the differences between the results produced by the model and the reality are minimal [13]. Usually these methods aim to minimize the number of possible restrictions, at expenses of requiring a great amount of data. An example of this type applies the data to compare the results and updates some penalty functions that act directly on the algorithm inside the finite elements. These penalty functions are related with the quantification of the differences between the estimation of the model and the reality. This quantification is performed with a correct management of the data. In these circumstances it is observed that the smaller the differences between the model and the reality, the greater the amount of data required for the procedure [14, 15]. Generally, another cost that must be considered in these cases is the curse of dimensionality because of the exponential effect of the increment of the degrees of freedom that the data-driven approach frequently involves [16]. It does not necessarily imply that this curse needs to happen, though. In any case, especially for implementation, this paradigm has the necessity of a global database capable of covering the increasing demand of the computational challenges of the data-driven procedures [17].

1.2 The phenomenological approach

The only considered behavior is the macroscopic one, and it is usually determined by the computation of energies that are collected in the form of functions. In the case of hyperelastic materials, the energy functions respond to the mathematical requirements of a potential function, such as the condition of Schwartz's theorem applied to the tensorial derivatives of the strain energies, which is the reason for the major symmetry of the constitutive tensor. Conventionally, phenomenological approach provides an analytical frame to the strain energy functions that define the mechanical behaviour of the material. The derivatives of the strain energy functions relate the stresses with the strains in the equilibrium equations. These analytical functions have a set of parameters that are determined by fitting the model to the experimental evidences. For that purpose, the method employ residual functions to be minimized

that quantify the differences between the reference experimental data and the prediction of the model. In this way, it is found an approximative solution of the strain energy functions that satisfy to certain extent the system of equilibrium equations.

1.2.1 Invariants and tensors

This approach generated a big number of analytical models that pursue the same goal. The differences between them are mainly analytical, but also they differ on the physical meaning behind the formulation. These analytical functions have specific arguments that are related with the strains in a special way so that they satisfy the principles of invariance and objectivity. This is important, because although the stress components vary with the system of reference, they must represent the same tensorial object. Since the energy cannot change with the system of reference, the corresponding strain energy functions must be evaluated by these invariants, so that the corresponding stress tensors satisfy objectivity. There are many functional arguments eligible as invariants, and in fact there are many proposals in literature. The best known are the stretches, which are the eigenvalues of the stretch tensor $\mathbf{U}$. Rivlin-Spencer invariants I_i are also used, especially for incompressible formulations. J invariants are a variant sometimes used for compressible formulations, although nothing prevents them from being used instead of the Rivlin-Spencer ones. Regarding stresses, they are also abundant in literature. They are subjected to a certain relation with a specific kind of strain, known as work-conjugacy. This relation is grounded in the invariance of the energy. For example, the space stress tensor of Kirchhoff can be related to the 2nd of Piola – Kirchhoff,

$$\int_{\Omega} \mathbf{S} : \dot{\mathbf{A}} d\Omega = \int_{\Omega} \boldsymbol{\tau} : \mathbf{d} d\Omega \quad (1.1)$$

Where $\dot{\mathbf{A}}$ is the derivative of the Green-Lagrange strain tensor, $\mathbf{d}$ is known as the strain rate tensor, and they are another example of work-conjugacy. One tensor is the conjugate of the other, because the scalar product between them yields the energy rate. It is one of the mathematical conditions of the phenomenological formulation. Another work-conjugacy pair widely used throughout the Thesis are the tensor of logarithmic deformations (material description) and the corresponding generalized Kirchhoff stress tensor. The main reason of this pair is the advantage offered by the logarithmic strain tensor. The benefits are that the corresponding material and spatial descriptions are reduced to a mere rotation, and that the small strain formulation is recovered at moderate deformation. All of this makes the procedure intuitive, clean and simple. Other known stress tensors are the 1st Piola – Kirchhoff and the Biot. 1st Piola – Kirchhoff stress tensor is of interest because is the real stress magnitude obtained from experiments, so that the load force of the mechanical test is divided by the initial section of the specimen (undeformed area). Using the Nanson's formula,

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^T \quad (1.2)$$

Regarding strains, other strain tensors of interest in literature are the right – Cauchy $\mathbf{C}$ (material description) and left – Cauchy $\mathbf{b}$ (spatial description) that are expressed in terms of the quadratic stretches, the Euler – Almansi $\mathbf{a}$ which is the push – forward of the Green – Lagrange $\mathbf{A}$, and of course the stretch tensor $\mathbf{U}$. The right-Cauchy tensor is related with some of the commented strain tensors,

$$\mathbf{C} = \mathbf{U}^2 \quad (1.3)$$

Using spectral decomposition can be re-expressed as

$$\mathbf{C} = \sum_{i=1}^3 \lambda_i^2 N_i \otimes N_i \quad (1.4)$$

Left-Cauchy strain tensor is also very frequent in literature, and it is obtained simply by the rotation of the right-Cauchy stress tensor. Left-Cauchy is in spatial description due to the rotation transformation,

$$\mathbf{b} = \mathbf{R} \mathbf{C} \mathbf{R}^T \quad (1.5)$$

Finally, the small strains work conjugacy pair is defined by the Cauchy stress σ and the true strain ε .

1.2.2 Proposal of hyperelastic formulations

There are many analytical proposals to cover similar problems, although the motivation of each of them focused on particular conditions. This does not prevent applying several proposals to cover the same problem of mechanical characterization. The most emblematic formulations are here described. The model of small strains is the first of them, and is applicable at moderate deformations or materials characterized by a linear response. In other words, there is a linear relationship between the stress σ and the strain ε , so they respond to the Hooke's law. The stored strain energy function is the potential function that defines the hyperelasticity in this model.

$$w(\varepsilon) = \frac{1}{2} \varepsilon : \mathbf{C} : \varepsilon \quad (1.6)$$

where ε is the small strain tensor and $\mathbf{C}$ represents the tangent modulus, which is a fourth-order tensor. Inside $\mathbf{C}$ there are material parameters such as the young modulus E and the Poisson's ratio ν in the case of isotropy. The strain tensor can be devised as the volumetric strain tensor $\varepsilon^v = \text{tr}(\varepsilon) \mathbf{I}$ and the isochoric (deviatoric) strain tensor $\varepsilon^d = \varepsilon - \varepsilon^v$, which is the complementary contribution. Following with isotropy, the corresponding stresses are expressed in terms of the shear modulus μ for deviatoric effects and the bulk modulus κ for volumetric contributions that accompany the respective strain tensors. For instance, the stress in the uniaxial test is,

$$\sigma_u = \frac{2}{3} \mu \varepsilon_u^d - \frac{2}{3} \mu \varepsilon_t^d + \kappa \varepsilon^v \quad (1.7)$$

where ε_u^d is the deviatoric strain in the load direction and ε_t^d is the one in the transverse direction.

Other models are applicable to large deformations, where the response between stress and strain is no longer linear. Unlike small strains, some of the existing formulations fulfill a more adaptive than intuitive function. One of the first proposals for large strains was developed by Mooney in 1940 [18]. The model emerged as an adaptive response to the experiments of isotropic materials, and resulted to be useful even for large strains in materials that kept a linear relationship between the applied shear force and the amount of cumulative shear strain. Rivlin-Spencer invariants [2] are employed in this model, motivated by experimental evidences, forming the so-called Mooney – Rivlin model [2],

$$W = C_1 (\bar{I}_1 - 3) + C_2 (\bar{I}_2 - 3) \quad (1.8)$$

which is applicable to incompressible materials and therefore uses isochoric invariants. The model is an extension of the Neo-Hookean model $W = C_1(I_1 - 3)$. Other known models that use Rivlin invariants are the Arruda - Boyce, Gent, or the models of Holzapfel - Gasser - Ogden and Gasser - Ogden - Holzapfel, known as HGO and GOH respectively [8, 19, 20]. The Arruda - Boyce model has a statistical mechanics approach and it is also applied to biological tissues. We dedicate here a space for its explanation. It takes into account the microstructure of the material and the physics of the problem, but from a statistical and entropic approach. It is based on an entropic decomposition of the possible configurations adopted by the angles of the carbon bonds of the molecule, so that each link of the chain can rotate freely. This allows having a macroscopic description of the physical phenomenon behind the mechanical behavior. The model states that on a microscopic scale, the mechanical behavior is complex and anisotropic; however a macroscopic, homogeneous isotropic behavior can be modeled on average. For this purpose, a unitary cube-shaped microstructure is modeled, in which molecular chains born in the 8 vertices of the cube, and all die in the center of the cube. There are also geometrical characterizations in the literature for three [35] and four chains [36-39], but the most prominent configuration is for the eight chains. Each of these chains represents a complex structure such as a polymeric molecule. Whenever the material is subjected to a field of strains and stresses, the microstructure is always working on the preferred directions, such that λ_1 works along the local, "i", λ_2 along "j" and λ_3 along "k", causing the macroscopic behaviour to work on principal strains despite microscopic anisotropy. The model assembles several pieces from statistical and entropic approaches, as is the case with the application of the random walk criterion to determine the average radius of the r_0 chain. One of the eight chains is considered to be subdivided into N sections of equal length l . So applying random walk it yields,

$$r_0 = \sqrt{N}\ell \quad (1.9)$$

And taking into account the load configuration, the averaged distance is,

$$r_{ch} = \sqrt{\frac{N}{3}} I_1^{1/2} \quad (1.10)$$

Applying both expressions it is possible to determine the invariant that really defines the approach of this model, which is the chain stretch (it is an invariant as long as it does not depend on the reference system)

$$\lambda_{ch} = \frac{r_{ch}}{r_0} \quad (1.11)$$

The configuration of the subdivision of the chain length into N equidistant sections of length " ℓ " allows addressing the entropic configuration of the chain. There is a probability distribution of the angular configuration of the chain. In fact, for each length r_{ch} the most probable state of this distribution can be determined. In particular, the entropy of the chain is,

$$s_{ch} = k \left[c - N \left(\frac{r_{ch}}{N\ell} \right) \beta + \ln \left(\frac{\beta}{\sinh \beta} \right) \right] \quad (1.12)$$

$$\beta = \mathcal{L}^{-1}(r_{ch}/N\ell) \quad (1.13)$$

Where $\mathcal{L}$ represents the Langevin function, whose inverse describes efficiently the

limiting chain extensibility, k is the Boltzmann's constant and n is the chain density. One of the basis of the model is that the work of deformation is proportional to the entropy change of the chains during the stretching. Thanks to Eq. 1.12, it is possible to formulate the sought stress-strain relation,

$$\sigma_1 - \sigma_2 = \frac{nk\Theta}{3} N \mathcal{L}^{-1} \left[\frac{\lambda_{ch}}{\sqrt{N}} \right] \frac{\lambda_1^2 - \lambda_2^2}{\lambda_{ch}} \quad (1.14)$$

where Θ is the absolute temperature. Using series expansion and knowing that $\lambda_{ch} = I_1^{1/2}/\sqrt{3}$ it is possible to express finally the stored strain energy formulation,

$$W = nk\Theta \left[\frac{1}{2}(I_1 - 3) + \frac{1}{20N}(I_1^2 - 3^2) + \frac{11}{1050N^2}(I_1^3 - 3^3) + \frac{19}{7000N^3}(I_1^4 - 3^4) + \dots \right] \quad (1.15)$$

The strength of the method is that it permits simulate efficiently the network response of the coordinated stretched chains effect and at the same time keep a relative simple mathematical formulation. To this regard, it is important to mention that using the advances of WYPiWYG procedure for quadratic invariants developed in this Thesis, an application was done to get the exact solution of the functional equations from the Arruda-Boyce formulation [21]. In relation to the Gent model, as in the case of Arruda - Boyce, it takes into account a certain view of the physics of the micromechanics and its influence on the macroscopic behavior of the material. It includes the effect of the extensibility of the chains of the material. This effect of the extensibility of the chains is constrained to a maximum, reaching a limiting state I_m as the state of maximum extensibility. This model is grounded on the hypothesis of a Gaussian effect

$$W = \frac{E}{6} I_1 \quad (1.16)$$

where E represents the macroscopic Young modulus of the material. The model includes the effect of maximum extensibility of the chains, whose limit is for $I_1 = I_m$.

$$W = -\frac{E}{6} J_m \ln \left(1 - \frac{I_1}{I_m} \right) \quad (1.17)$$

Therefore, mathematically it is a simpler model than Arruda - Boyce, which does take into account certain common aspects such as the characterization of a microscopic physical phenomenon and give it a meaning of macroscopic contribution, as well as the concepts of cooperative chain network. In fact in this work there is a comparison of the results produced by the proposal of Arruda - Boyce and the own results. One of the strengths of this formulation is the simplicity, since it only requires the characterization of Young's modulus of the material and the maximum extensibility of the chain, which in turn is indirectly obtained from the maximum extensibility of the material to be characterized from the macroscopic point of view.

Another type of relevant phenomenological approach applied to soft tissues are the Generalized Structure Tensor models (GST). This type of approach is mainly applied to constitutive models that reflects anisotropic, fiber reinforced materials whose fibers are dispersed. It is applicable to soft materials such as biological tissues. Generally, a superposition of the matrix effects together with the influence of the fibers is applied. As observed in Figure 1.1, the skin is a good example of application, in which there are some dispersed elastic fibres (elastin fibres) nested in the matrix (collagen).

FIGURE 1.1: Skin illustration based on the image from Benítez and Montáns [22]. A fibre dispersion (elastine) is immersed into the matrix (collagen)

Often, the detail of the model is focused on the interpretation of the micromechanics and its influence on the macromechanical response. In the fiber directions, a modification of the strain tensor is usually included as an argument, which is projected on the structural tensor that provides information on the deformation along the fiber direction, also known as pseudo-invariant. The application of this argument to the energy function related to the fiber or family of fibers implies the imposition of the assumption of affine strains, which is an idealization of reality, more or less accurate depending on each case. It is common in this type of models to employ modifiers such as the switch [20], which disconnects the influence of the energy of the fiber when the fiber works under compression; or the distribution function of the fiber orientation [23], which gives an impression of the pre-integrated influence of the orientation of the fiber distribution. This type of formulations has been successfully implemented in the study of the mechanical behavior of angiological structures. A simple and representative model of the phenomenological GST approach is the HGO model [19]. It is a model adapted to the phenomenon of the mechanical behavior of the arteries. The formulation is the same for all the structure, and it only modifies the coefficients of each layer (media and adventitia). As observed in Figure 1.2, in this model there are two fiber families, which are distributed symmetrically, distancing a β angle from a plane of symmetry.

FIGURE 1.2: Image extracted from reference [19]. In the model two layers are devised, namely media and adventitia (reserved subindices M and A respectively for the notation). In each layer, two families of fibres are distributed symmetrically with an angle β with the plane of symmetry. The thickness of each layer is denoted with the letter H

The corresponding energy functions are evaluated by the pseudo-invariants I_4 , I_6 , which are the projection of the quadratic stretches in the direction of the fibers, $\mathbf{C} : \mathbf{a}_0 \otimes \mathbf{a}_0$, where $\mathbf{a}_0$ is the verifier in the direction of fiber 0. The energy of each of the two fiber families, expressed as a function of the pseudo-invariant I_i ($i = 4, 6$) is,

$$\Psi_f(I_i) = \frac{k_1}{2k_2} \exp(k_1 I_i) \quad (1.18)$$

where k_1 and k_2 are material constants. General expression of the total energy is the sum of the matrix influence (isotropic, Neo-Hookean) and the contribution of the fibbers.

$$\Psi(I_1, I_4, I_6) = \Psi(I_1) + \sum_{i=4,6} \Psi_f(I_i) \mathbf{a}_i \otimes \mathbf{a}_i \quad (1.19)$$

Some of the formulations for compressible models employ the J invariants. This is the case of the Blatz and Ko model for compressible foams, and the Ciambella – Saccomandi model for auxetic foams. The J invariants are defined as follows,

$$\begin{aligned} J_1 &= \text{tr}(\mathbf{b}) \\ J_2 &= \text{tr}(\mathbf{b}^{-1}) \\ J_3 &= J \end{aligned}$$

Where $\mathbf{b}$ is the left Cauchy strain tensor and J is the Jacobian. The description of the model of Blatz and Ko is the following one,

$$W(J_1, J_2, J_3) = W_1(J_1) + W_2(J_2) + W_3(J_3) \quad (1.20)$$

$$W_1(J_1) = f \mu / 2 (J_1 - 3) \quad (1.21)$$

$$W_2(J_2) = (1 - f) \mu / 2 (J_2 - 3) \quad (1.22)$$

$$W_3(J_3) = \mu / 2 [2/\alpha] [f(J_3^{-\alpha} - 1) + (1 - f)(J_3^\alpha - 1)] \quad (1.23)$$

$$\alpha = \frac{2\nu}{1 - 2\nu} \quad (1.24)$$

The work of Blatz and Ko is worth of mention. First, they develop a set of systematic experiments on the mechanical behavior of compressible foam. They perform, in addition to the uniaxial test, pure shear experiments and equibiaxial tests for the same material. This allows a detailed study not only on that specific foam, but on the mechanical behavior of foams in general. The experiments shed new light on the actual macroscopic behavior of a material with a complex microstructure and a compressible macroscopic behavior. They provide the opportunity to study real behaviors such as the influence of coupled strains in terms of contribution of the strain energy. Second, they propose a compressible model based on a modification of the Rivlin - Spencer invariants. For the formulation, an assumption of the decomposition of the strain energy is done in terms of the J invariants. In other words, the effects of the invariants J_1 , J_2 and J_3 over the strain energies are decoupled. The form of the assumption is analytically similar to the one of the Valanis-Landel decomposition, but in J invariants instead of stretches. In addition, this assumption is also considered for the phenomenological proposal of Ciambella and Saccomandi to model the hyperelastic, isotropic behavior of the auxetic foam developed experimentally by Lakes [24]. The fact of being isotropic and auxetic implies the compressibility of the material. The formulation of Ciambella-Saccomandi [4] is more complex. Although at a last extent it only depends on three physical parameters: the shear modulus μ_0 , the infinitesimal Poisson's ratio ν_0 , and the lateral stretch at inversion λ_I , which is the last value of lateral stretch before adopting auxeticity. The advantage of this model is that these three parameters are easily measurable quantities and with clear physical meaning. One of the strengths of the phenomenological approach is that it offers the possibility of a physical understanding of the mechanical behavior behind the experimental evidences. This makes this model to be a reference in the literature review for this Doctoral Thesis. A comparative study is performed in this work between the proposal of Ciambella – Saccomandi and the extension of the WYPiWYG methodology for auxetic, isotropic hyperelastic materials. However, a phenomenological approach not necessarily requires to be based on a physical interpretation of the mechanical behavior. The model of Ogden [6] is widely accepted by the scientific community.

$$W = \sum_{p=1}^N \frac{\mu_p}{\alpha_p} (\lambda_1^{\alpha_p} + \lambda_2^{\alpha_p} + \lambda_3^{\alpha_p} - 3) \quad (1.25)$$

where μ_p are shear-like parameters and α_p are also fitting parameters. The strength of this model lies on its adaptive capacity. It offer great results during the minimization process of the residual error functions that quantify the accuracy of the required fitting of the model. It uses the main stretches as invariants of the evaluation of the strain energy functions. The model requires the assumption of the Valanis – Landel decomposition, which is in great accordance with the experimental evidence [25]. The model is successfully implemented for rubber-like materias with hyperelastic, isotropic mechanical behaviour [26, 27]. Additionally it shows some coherence with the statistical theory of the micromechanical network of fibers [28]. This proposal is also employed in biomechanics, such as for skeletal muscle tissues [29] and the skin [30].

1.3 Data-driven WYPiWYG hyperelasticity

WYPiWYG (What You Prescribe is What You Get) hyperelasticity, was so-named because of the similarities with the WYSIWYG display method. It argues that the

energy functions obtained depend on the experimental prescriptions that are introduced and the assumptions to be considered. More specifically, it consists in directly solving the stress-strain equilibrium equations that emanate from the energy functions of the material. The system of equations relates the curves from the experimental tests with the strain energies. One might think that this is the conventional method already mentioned, which consists in fitting analytical energy formulations to minimize an error function that quantifies the differences between the prediction and the experimental evidence. However, WYPiWYG differs in several aspects. The first of these is that it does not seek to minimize any error function, but to make it zero, and therefore to solve the problem numerically, determining the energy functions that satisfy, from the numerical point of view, the equilibrium equations. As a matter of fact, there is no need of any error function in the process. The first work in this line is proposed by Sussmann and Bathe. They use the Kearsley-Zapas solution for the case of a hyperelastic isotropic, incompressible material. It solves directly a functional equation. The unknown to be found is the strain energy, and the corresponding functional datum is the experimental curve. This paper confirms that it is not necessary to analytically force the form of the energy function, but more on the contrary, it is directly attainable. An explicit formula is obtained in its reduced form that expresses the exact mathematical solution of the problem. The second advance in this line is the work done by M. Latorre and F.J. Montáns, in which the method is extended with the same vision to hyperelastic, incompressible transversely isotropic [31] and incompressible orthotropic materials [32]. Additionally, the method is also extended to the viscoelastic case [33], and to the damage [34]. The basic assumptions of this work are common to those made by the Sussmann and Bathe. That is, the employed invariants are logarithmic strains, and the requirement of the Valanis – Landel decomposition is a constant throughout all the work. This work also emphasizes the importance of the application of logarithmic strains, as they are the natural extension of the problem of small deformations, and therefore, when applying WYPiWYG to the case of moderate deformations, it recovers naturally and progressively the behavior of the small strains formulation.

The inclusion of compressibility signifies an enhancement, regardless of the material to be considered. It entails not only a quantitative contribution in terms of the number of materials that can be modeled with this extension, but also a qualitative aspect. In reality, all materials are compressible to a greater or lesser extent. Incompressibility is then a limit that can be naturally recovered with this extension. One of the immediate advances of this improvement is that FEA procedures for quasi-incompressible materials no longer require the implementation of a pressure-like penalty function. Regarding the extension to different types of invariants, the method is adapted for J invariants, which is capable of recovering, among others, the model of Blatz and Ko for compressible foams [3], as well as the model of Ciambella and Saccomandi for auxetic foams [4]. Additionally a formulation to an anisotropic case using Rivlin-Spencer invariants is extended using the reduced form of the HGO formulation on fiber distribution [19]. All these advances open the door to new possibilities and show the power of this procedure. The choice for invariants different from the logarithmic strains allows solving the problem for situations in which Valanis - Landel is not fulfilled, and therefore it is capable of covering a mechanical behavior in which there is a coupling of main stretches. In addition, for the first time (up to the author's knowledge) the same case can be resolved with one type of invariants and then with another, so that the differences between them can

be analyzed. Discrepancies in results are caused by the application of a certain assumptions instead of others. This opens the possibility of quantifying the error inherent to a certain assumption. This error is called from now on assumption error, and it is different for the error caused by the approximation of the strain energy functions that comply with the equilibrium equations. This source of error is called from now on mathematical error. Regarding the different methods to be applicable, both functional refresh and matrix methods are developed for different kind of invariants. The matrix method is capable of solving the energy functions for linear functional equations (it does not mean the functions are linear), as such is the case of the stress-strain equilibrium equations. The functional refresh method is a qualitative advance in solving problems of energy functions, because it finally focuses on the problem as a system of functional equations to solve. This allows knowing exactly how many independent experimental data set inputs are needed to uniquely solve the problem, since the energy functions are considered functional unknowns, and the experimental curves as functional data. The relationship between them is the system of functional equations that allows solving the problem in a unique way. The functional refresh method also represents a breakthrough for its simplicity of implementation, its ability to solve functional equations that, unlike previous methods, may be nonlinear. Note that linearity is specified in terms of functions, not the arguments (e.g. linear: $f(x) = g(x) + h(x)$; non-linear: $f(x) = g(x)h(x)$). The method is applied along the Thesis to different materials, progressively from easy to complex problems. Within this facet of compressibility, the problem is determined for the conventional compressible isotropic case, the auxetic compressible isotropic case, the orthotropic case for moderate compressibility, for any generic condition of experimental data (off-axis experimental data), and finally the auxetic, compressible orthotropic case, which is of greater complexity when dealing with non-injective strain relation functions, as the inverse functions of strain relation are not uniquely defined in that case. The improvements of the methodology allows recovering not only specific assumptions such as incompressibility, small strains, Valanis – Landel or a particular combination of invariants in a model, but in practice any model based on analytical, phenomenological approach. This fact is put into practice when recovering several models available in literature, such the Neo-Hookean, Mooney, Ogden, Gent, Blatz - Ko, Horgan - Saccomandi, HGO, Hartmann – Neff, etc [5, 18, 6, 3, 35, 19, 9]. Regarding the auxetic isotropic case, in this work hyperelastic isotropic auxeticity implies compressibility. Auxeticity exhibits a particular response due to its microstructure. The material shows a negative Poisson coefficient, which means that when a specimen of these characteristics is stretched out, the cross-section does not narrow, but widens. This property is so unusual that in the recent past it was only considered on the theoretical plane or as a rare and isolated circumstance [36], but this fact changed when Lakes synthesized the first man-made auxetic material [37]. The importance of these materials is fundamental in countless fields, such as medicine, biomechanics, sports or the military, among others. Far from being a stress concentrator, it is a natural stress dissipator, which makes it ideal for applications such as a biomechanical implant or a bulletproof vest. However, the available models in literature cannot cover all the requirements. Some of them are very expensive because they require fine meshes that are capable of capturing the micro and macro mechanical behavior of the material. There are analytical models from the phenomenological approach with fast but with insufficient precision, but this is mandatory especially in fields as delicate as medicine (for example, surgical implant). Therefore, the extension of the method to auxetic materials is of great importance. Additionally, this work covers the resolution of the problem with the use

of different invariants (logarithmic invariants, J invariants) and different methods (inversion formula, functional refresh method). The advances not only focus on the efficiency, but on the understanding. This is the case of the study done in the Thesis that considers all the possibilities from the theoretical point of view for a bimodular, auxetic orthotropic material. Likewise, a resolution in J invariants is performed for compressible materials with coupled stretches. The matricial method for this type of materials is extended, and the convergence procedure of the functional refresh method is improved. Regarding orthotropic materials, the extension of the method is relevant for several reasons. As in the case of compressible isotropy, it is able to recover the incompressibility, so it is really means an extension. Additionally, significant improvements are made for this case. In particular, different algorithms are developed for a specific loading configuration, including a generic case whose test directions do not require to be aligned with the preferred directions of orthotropy of the material. Finally, the case of orthotropic auxetic materials is interesting. To date, the author does not know any method that can solve a general case of auxetic orthotropy. Although the existence of isotropic auxetic foams (isotropy is just an idealization) was already mentioned, usually the microstructure of auxetic materials causes an observable anisotropic response. Precisely because of that, another strength of the method is that it provides a solution when the modeling of a RVE it is a difficult issue (e.g. the microstructure apparently does not follow a specific pattern but there is no isotropy since there is a clear evidence of anisotropy in the macroscopic response). Given the importance of this type of material, either found in nature in biological materials or fabricated, the development of this model is considered a relevant issue. It offers a trade-off between precision and speed for both the strain energy computation and the corresponding computational simulations. Additionally, a theoretical study of auxetic orthotropy is performed. This contributes to a greater understanding of the phenomenon, so the inherent advances and its importance is not merely quantitative.

1.4 Mathematical background

1.4.1 Tensorial algebra

In solid mechanics, as in the case of Fluid Mechanics, there is a tensorial background. Hereby some of the operations necessary for the development of the Doctoral Thesis are summarized. One of the common operations is the dyadic product. It appears for example in some tensorial derivative operations. One of the most important utilities of this operation is the basis for specifying the dimension of a tensor (e.g. the dyadic product of 4 vectors generates a fourth order tensor). In general, a tensor of order N requires the dyadic product of N vectors. For example, if a tensor $\mathbf{T}$ is defined component-wise by the dyadic product of two vectors $\mathbf{a}$ and $\mathbf{b}$. The operation is defined as follows:

$$\mathbf{T} = \mathbf{a} \otimes \mathbf{b}$$

$$T_{ij} = a_i b_j$$

Tensorial scalar product of order 2. It appears for example in the chain rule in tensorial derivation, but the main application in this Thesis is the projective property that this operator possesses, such as the projection of a 4th order tensor onto a tensor of order 2, or the projection of a tensor of order 2 on another one of order 2. The name

of the scalar product comes from the analogies with the conventional scalar product between two vectors. In the next example, first for vectors and then for tensors, the scalar product of vectors $\mathbf{a}$, $\mathbf{b}$ yields the scalar c , and then the same operation is done for second order tensors $\mathbf{A}$, $\mathbf{B}$ that yields the scalar C . The component-wise description (i.e. Einstein notation) is also provided.

$$\begin{aligned}\mathbf{a} \cdot \mathbf{b} &= c \\ a_i b_i &= c \quad (\text{sum on } i) \\ \mathbf{A} : \mathbf{B} &= C \\ A_{ij} B_{ij} &= C \quad (\text{sum on } i \text{ and } j)\end{aligned}$$

With the combination of the aforementioned operations, it is possible for example to compute a vector $\mathbf{c}$ that is the projection of the vector $\mathbf{a}$ onto another $\mathbf{b}$, so that the module c corresponds to the projected vector $\mathbf{a}$ in the direction of the projecting one $\mathbf{b}$. Mathematically,

$$\mathbf{c} = \mathbf{a} \cdot (\mathbf{b} \otimes \mathbf{b}) = (\mathbf{a} \cdot \mathbf{b})\mathbf{b} = c\mathbf{b} \quad (1.26)$$

If the dimension of the previous example is doubled, then we have the projection of a 2nd order tensor $\mathbf{A}$ onto another one, so that the norm C corresponds to the projected tensor $\mathbf{A}$ over $\mathbf{B}$ with the tensorial direction of $\mathbf{B}$. Mathematically,

$$\mathbf{C} = \mathbf{A} : (\mathbf{B} \otimes \mathbf{B}) = (\mathbf{A} : \mathbf{B})\mathbf{B} = C\mathbf{B}$$

If the fourth order tensor $\mathbf{B} \otimes \mathbf{B}$ satisfies unitary norm for $\mathbf{B}$ (i.e. $\mathbf{B} : \mathbf{B} = 1$) then it is usually called *projector*, because that is the function that complies. Another interesting operation is the spectral decomposition. It consists in decomposing the components of a tensor in the eigenvalues multiplied by their corresponding eigentensors. The eigentensors are expressed in terms of the dyadic product of the corresponding eigenvectors, so that the dimension of the eigentensors is the same than the original tensor. Mathematically if the spectral decomposition is applied to a 3×3 tensor $\mathbf{U}$, and the pair λ_i , $\mathbf{N}_i$ are the corresponding eigenvalues and eigenvectors respectively, then

$$\mathbf{U} = \sum_{i=1}^3 \lambda_i \mathbf{N}_i \otimes \mathbf{N}_i \quad (1.27)$$

As observed spectral decomposition is applied to symmetric tensors, since $\mathbf{N}_i \otimes \mathbf{N}_i$ yields symmetric tensors and therefore the sum of all of them is also symmetric. In solid mechanics, the notation for $\mathbf{U}$ is usually reserved for the stretch tensor, whose eigenvalues are the stretches in the principal directions of the deformed solid, and $\mathbf{N}_i$ are the corresponding eigenvectors (direction of stretches) in the material description.

Mapping operations are important because they allow one tensor to be converted into another according to a compendium of rules. For example, due to the variety of stresses and strains, it is common for experimental data to be in different measures than the ones required by a given method or formulation, so that the experimental stresses/strains cannot be directly introduced as inputs. An example of mapping operation is the one that maps the second Piola Kirchhoff stress tensor $\mathbf{S}$ into the generalized Kirchhoff stress tensor $\mathbf{T}$ using the corresponding fourth order mapping

tensor $\mathbb{M}$,

$$\begin{aligned}\mathbf{T} &= \mathbf{S} : \mathbb{M} \\ \mathbb{M} &= \sum_{i=1}^3 \lambda_i^2 \mathbf{M}_i \otimes \mathbf{M}_i + \sum_{i=1}^3 \sum_{j \neq i} \frac{\lambda_j^2 - \lambda_i^2}{2(\ln \lambda_j - \ln \lambda_i)} \mathbf{M}_{ij}^S \otimes \mathbf{M}_{ij}^S \\ \mathbf{M}_i &= \mathbf{N}_i \otimes \mathbf{N}_i \\ \mathbf{M}_{ij}^S &= 1/2 \mathbf{N}_i \otimes \mathbf{N}_j + 1/2 \mathbf{N}_j \otimes \mathbf{N}_i\end{aligned}$$

where λ_i , $\mathbf{N}_i$ are respectively the eigenvalues and eigentensors of the aforementioned stretch tensor $\mathbf{U}$. Generally, in order to accomplish the required mapping operations it is necessary to apply successive intermediate transformations that are common in solid mechanics. Some of these operations are the polar decomposition, and the transformations of push forward and pull back, which change the representation of tensors in materials or space configuration. Polar decomposition consists in the separation of the effects of the strain gradient tensor $\mathbf{F}$ into a change of the size of the eigenvectors (covered by the stretch tensor $\mathbf{U}$) on one side and the rotation of the eigenvectors (covered the rotation matrix $\mathbf{R}$) on the other one. This operation intervenes in many of the mapping operations, and is essential in operations such as the Lie derivative. The polar decomposition is a multiplicative decomposition.

$$\mathbf{F} = \mathbf{R}\mathbf{U} \quad (1.28)$$

The push forward and pull back transformations allow working with tensors from the reference of the deformed (spatial) configuration or prior to the deformation (material). The operations vary depending on whether it is treated with covariant or contravariant tensor objects (vectors, tensors). The push forward operation changes the representation from material to space description, while the pull back does the contrary. Next, given a strain gradient tensor $\mathbf{F}$, the push forward operation for the covariant and contravariant cases is defined for a vector in materials $\mathbf{V}$ that becomes $\mathbf{v}$ in the spatial description.

$$\begin{aligned}X(\mathbf{V}) &= \mathbf{F}^{-\top} \mathbf{V} = \mathbf{v} && \text{(covariant)} \\ X(\mathbf{V}) &= \mathbf{F} \mathbf{V} = \mathbf{v} && \text{(contravariant)}\end{aligned}$$

Pull back transformation is the inverse operation.

1.4.2 Numerical treatment for manipulation with functions

Mathematical procedures generally need function evaluations, as well as transformations of functions, whether scalar, tensorial, etc. However, there are some difficulties to overcome. The set of experimental data is discrete instead of continuous (e.g. a set of points are retrieved from a load curve of an uniaxial test), but the phenomenological approach is based on energy functions that by definition are continuous. Therefore is necessary to convert the discrete experimental points of the experimental curves into a functional representation for its evaluation (i.e. functional data). The simplest idea is to perform a linear interpolation between the given experimental points, but there are some other options (splines, Fourier, Chebyshev, or even the hyperoperational techniques developed in the first article of the Thesis). However, it is not just a matter of choices, but restrictions (experimental noise, stability, mathematical conditions for hyperelasticity). In addition to the problem

of functional evaluation aforementioned, there is the difficulty of functional manipulation. Both problems are present during the construction and evaluation of the inverse of a given function that lacks an analytical expression and in the functional composition, also without an analytical form.

Regarding the inverse evaluation, the number of functions without an explicit analytical inverse is infinitely greater than the opposite case. To this fact it should be added that, functional data from experiments does not usually follow any analytical pattern, what makes it even harder (if not impossible) to find an exact analytical form for the inverse function. Regarding the composition of functions, except in simple cases, it is an impediment to obtain the analytical expression resulting from a composition of functions. The situation is critical if all these situations take place at once, namely the composition of several functions with some of them being the inverse of a known function without an analytical form. Some of the procedures of this Thesis face this situation, and therefore they cannot be fulfilled without the proper numerical treatment. Throughout the development of the thesis, splines (cubic, not-a-knot, B-splines, linear for some academic examples) are applied for the functional representation of the set of curves initially defined by discrete points. For example, consider the case of an experimental load curve from a uniaxial test. The curve is defined by experimental points that relate a load y_i to a stretch x_i so that together they constitute an experimental set $\{x_i, y_i\}$, and they are transformed into a functional representation.

$$\{x_i, y_i\} \rightsquigarrow y(x) \quad (1.29)$$

The straightforward benefits of this treatment make the compositional or inverse evaluations a trivial issue.

$$\begin{aligned} \{y_i, x_i\} &\rightsquigarrow x(y) \\ x_j &= x(y_j) \end{aligned}$$

We are aware that the obtained function $x(y)$ is not exactly the inverse of the function $y(x)$, but there are three reasons to operate in this way. Firstly, an analytical formulation of $x(y)$ is generally not available, and the construction of an approximate analytical function for each specific evaluation becomes less efficient when not unapproachable. Secondly, in case that an analytical form of $x(y)$ is reachable by means of mathematical techniques such as infinite terms or the application of an algorithm, there are three errors to take into account: i) the truncation error, ii) the error of converting the discrete data into a functional representation and iii) the inherent round-off errors during the functional conversion and the successive evaluations. Thirdly, the error of the numerical treatment dwindles with the size of the available data. Last but not least, conventionally the experimental noise error is bigger than the rest of aforementioned errors, what makes negligible the derived errors from the numerical treatment. This is also applicable to the evaluation of functional compositions.

$$\begin{aligned} \{x_i, y_i\} &\rightsquigarrow y(x) \\ \{y_j, z_j\} &\rightsquigarrow z(y) \\ \{x_i, z(y_i)\} &\rightsquigarrow \hat{z}(x) \end{aligned}$$

This numerical treatment allows the fulfillment of the goals of this Thesis.

1.5 Tools and equipment

In order to undertake the developments in this thesis, an infrastructure is required to cover the activities of experimentation, computing and visualization of results.

1.5.1 Experimental

For the experimental validation of the developments, two procedures are used. The first one is the experimental collection of the necessary data from bibliographic study. The second one is directly the realization of the necessary experiments, which implies the use of the facilities and machinery for the realization of the experiments. In particular the materials laboratory of the MERI materials research center was used, at the University of Sheffield - Hallam, where the international stay was held. Specifically, the use of the Instron machine model 3369 for material testing was required for performing uniaxial tests along the three axial preferred directions of the material. For the detection of the deformations a digital image correlation was employed. These data are necessary to complement the information from the load data collected by the Instron machine. In particular, the image correlation software is the DaVis, LaVision, and for that purpose a single camera with imager M-Lite 5Mega-Pixel resolution was employed, together with the instrumentation of AF MICRO NIKKOR lens with 60 mm optical zoom.

1.5.2 Computational

The main activity of this Thesis is computational. The purpose of the developed methodology is using computational procedures for the resolution of the mechanical behavior of materials, with special contribution to those with a non-linear response, such as the soft materials. The computational activity is used mainly for the development of the extended data-driven methodology to the cases of use of compressible materials of various types such as the ones having isotropy, auxetic isotropy, orthotropy, and auxetic. Additionally the computational resources are also necessary for the extension of the procedures to different hypotheses and invariants, and generalized experimental configurations. For this purpose the employed language is MATLAB. Part of the activity is in the implementation of the derivatives of the energy functions in spline format for the FEA. The splines are required for the description of mechanical behavior of the material to be modeled. The employed code for this purpose is fortran90. The necessary lines of code were implemented in the in-house DULCINEA Finite Elements program. Likewise, MATLAB was used for the realization of complex 3D structures together with the necessary input conditions for their subsequent execution in DULCINEA, which is a finite element program oriented for research activities, and has more than 50k lines of code. It is a program capable of solving materials under different assumptions such as hyperelasticity, plasticity, damage and fracture, for different strains (small strains, Green - Lagrange, Almansi, stretches, logarithmic, etc.) and stresses, (2nd Piola Kirchhoff, Cauchy, generalized Kirchhoff, etc.), for different configurations (spatial, material), for different conditions of use (2D, 3D, axisymmetric, etc.), different topologies (isotropy, transverse isotropy, orthotropy), different formulations (Neo-Hookean, Mooney, Ogden, HGO, etc), different families of finite elements (quad of 4, 9 nodes, serendipitous, qmix, brick, etc), in addition to other additional configurations. The motivation of using the DULCINEA program against a commercial one is the possession of total control and visibility inside the FEA. This is an important

point to consider in the use of finite element software in research tasks. Specially in the case of treating results generated by finite elements, the number of data is so big that some infrastructure is required to address the interpretation of these results. To this end, the Meshplot auxiliary program developed in MATLAB for visualization is used and extended, as well as additional scripts that provide extra visualization features that further enhance the experience of viewing results, all with the aim of improving the understanding of the mechanical behavior of the materials in question.

1.6 Methodology

There are successive steps that require to be followed, which are common to all the extensions of the WYPiWYG method. Some of them are also employed in the work of the development of the fractional arithmetical hyperoperations. These steps are following ones.

- The study of the necessary bibliography that seeks the solution to the problem in question, the strengths and weaknesses of each applied method, and how the development in that work makes a significant contribution to the solution. This progress can be of quantitative, qualitative importance, or both of them.
- The development of the required procedure for the extension to be covered in the resolution of the mechanical behavior of materials.
- The theoretical verification that corroborates the coherence of the development. Once the procedure is developed, reference energy functions are used to generate pseudo-experimental tests. Then, the inverse problem requires to be solved. The pseudo-experimental data are treated to obtain the conversion to functional data, necessary for the method as a starting point. Then the procedure is applied to that problem, and the derivatives of the energy functions are recovered. Finally, the derivatives are compared with the original ones (employed for generation of the pseudo-experimental data) for the theoretical verification. Since the verification is theoretical, it does not intervene in the influence of realistic sources of errors such as the experimental noise, or the tolerance of calibration of the experimental tests. The behavior of the material strictly obeys the assumptions of the idealized material to be modeled.
- The experimental validation that certifies the reliability of the developed procedure. Once the theoretical verification is successfully completed, the method must be subjected to a real case. In a real material there are no reference energy functions available to compare with the energy functions obtained, since they are precisely the unknowns to be determined. In this case the experimental data are the reference to be compared with the model. For that purpose, the set of discrete experimental data needs to be converted to functional representation. Subsequently the method is applied to determine the functional unknowns from the experimental functional data. Finally the energy functions obtained and are used to reproduce the tests. Finally, the reproduction is contrasted with the original experimental functional data, and the differences are analyzed. In this case, there is presence of a collection of errors, such as the experimental noise errors, calibration errors, tolerance (quality) errors of the measuring instruments, etc. One important source of error is the difference

caused by the implemented assumptions in the model, which differs from reality (non-related deformations, complete anisotropy, heterogeneous behavior of the material, etc).

- The implementation of the spline-based model in finite elements to evaluate the applicability of the method. One of the objectives of the method is that the energy functions obtained with the spline format have at least the same validity, efficiency and reliability than the ones obtained with the conventional analytical format.
- The assessment of the benefits of the model in the FEA implementation. In particular the volumetric energy functions obtained via this procedure allow does not require a penalty function to calculate the pressure in the elements, since the conditions are computed naturally. This is a key improvement in quasi-incompressibility.
- The establishment of the necessary conclusions that analyze the impact of the contribution of the development of the method within the scientific community, both for the quantitative and the qualitative aspects.

1.7 Outline of the Thesis

The structure of this Thesis commences with the development of advanced techniques for modeling and then it covers progressively, according to material complexity, different configurations that our data-driven procedures aim to solve.

- **Chapter 1.** In the first chapter, from the approach of Number Theory, a novel concept of a continuum arithmetical space is devised, and the development of fractional arithmetical hyperoperations is performed. The aim of this work is to enlarge the mathematical possibilities for modeling, although very probably it is beneficial for other disciplines of science. In particular for the contribution to the Thesis the objective is to provide new tools for the functional conversion of the experimental data. This is necessary because the experimental data are a set of discrete experimental values, and it is a focus of interest the enhancement of the interpolation techniques for a continuous evaluation of the experimental curves behind the experimental points. This is because the final goal is to employ experimental functional data as inputs for data-driven methods developed in this Thesis in order to determine the mechanical characterization of the soft materials in terms of strain energy hyperelastic functions. Therefore, a practical application for this purpose is developed as a variant of Vandermonde interpolation technique. In particular it is applied to a stress-strain uniaxial data but can be employed for any experimental test.
- **Chapter 2.** The first implementation case of the data-driven procedure in this Thesis is developed for hyperelastic isotropic compressible materials. The basis of the hyperelastic formulation necessary to build the method is explained, as well as the stress-strain system of functional equations that arise from the adopted assumptions (i.e. Hyperelastic isotropic compressible material, Valanis-Landel decomposition). The required algorithm that solves the system of functional equations is developed and clarified. Theoretical verification of the procedure is performed using the following *modus operandi*: 1) Generate necessary pseudo-experimental data from a referential analytical prescribed formulation (e.g. Neo-Hookean, Ogden, Gent). 2) Assuming that the referential

stored energy functions are unknown, use the data-driven algorithms to recover the functional unknowns directly from the pseudo-experiments (functional data). 3) Compare both recovered and referential energy functions. This *modus operandi* will be done using different analytical proposals. After that, experimental validation will be done with real experimental data, even when they do not satisfy Valanis-Landel decomposition. Finally, both analytical and data-driven approaches will be implemented in FEA. Results and computational performances shall be compared, and discussed.

- **Chapter 3.** Advanced algorithms for auxetic hyperelastic isotropic compressible materials are here developed. Auxetic materials have a complex microstructure that is responsible for their special properties of negative Poisson's ratio. As a first approach, it is admissible to assume that certain auxetic materials are isotropic. In these cases, our data-driven procedure is applicable to these materials. With the aim to extend the method, in this chapter an additional data-driven procedure is devised for materials not following Valanis-Landel decompositions, but a decomposition in terms of J -invariants, which are also employed in the work by Blatz and Ko of compressible foams, and in the model of Ciambella-Saccomandi for auxetic isotropic foams. These algorithms lie no longer on inversion formulae, but on the functional refresh method. Since the method is similar for J -invariants and I -invariants, the implementation on the latter invariants is immediate. The main idea remains unchanged: generate the required algorithms that solves numerically the corresponding system of functional equations. The same methodology of previous chapter is applicable in this work, now to both J -invariant and E -logarithmic strains invariant formulations. In this case, the results are discussed and compared not only with the analytical formulation (Ciambella-Saccomandi), but with the J - and E - data-driven results each other (tests curves, and FEA studies). Since they are grounded on different assumptions, the results are different. Additionally, some stability considerations due to auxeticity are here discussed.
- **Chapter 4.** Enhancement of data-driven techniques for general invariant stored strain energy functions are here developed. In this occasion, the system comprises three stored strain energy functional unknowns to be found. J -invariant procedure based on the functional refresh method is here improved. A preliminary treatment of the functional data facilitates an efficient and faster convergence of the method. Besides that, an additional data-driven method called *matrix method* is here developed for J -invariant formulation with the same objective, namely to solve the system of functional equations.
- **Chapter 5.** Advanced functional refresh procedures for hyperelastic orthotropic moderate compressible materials are here developed. The procedure involves a system of seven functional equations to be solved. The same methodology is employed in this chapter. One of the improvements of the data-driven algorithms developed here is the generality: they are capable of solving the energies even when functional data comes from experimental tests in misalignment with preferred directions of the material.
- **Chapter 6.** Enhancement of functional refresh procedures for auxetic orthotropic compressible materials is here developed. This is the last level of complexity of materials covered with the development of data-driven procedures. Up to the author's knowledge, there is no analytical phenomenological model to compare with in this work. This development implied several challenges. One

of them is that highly non-linear, non-injective curves of functional data from the strain relation (i.e. load-wise longitudinal strain vs. transverse strain) may generate indefinite evaluations in previous developed algorithms (inverse of a non-injective function), and therefore a segmentation in branches was initially considered. Finally, a new functional refresh procedure in one of the algorithmic steps allowed the implementation in this, more general case. Since no analytical procedure for orthotropic auxetic materials was found, prescribed referential energies using the current developed formulation have been implemented in order to generate pseudo-experimental results. By virtue of the methodology developed in this Thesis, these pseudo-experimental data are employed for the theoretical verification (that is, recover the referential energies and contrast them to verify that they are successfully solved). Thereafter, a experimental validation is performed. It comprises the realization of a real experiment and the corresponding experimental data collection. After the experimental noise treatment, the functional data set is employed to solve the system of functional equations and to find the corresponding energies. In this case, since the reference are the functional data of the tests, the obtained energies are employed to reproduce the referential data. Once compared, it is observable that the obtained energies are the solution of the system of functional equations. Since in this case additional independent test data are generated, they are employed to quantify the aforementioned *assumption error*. A procedure is proposed to quantify this error. Finally, obtained energies from experimental data are employed to perform a FEA simulation of the mechanical behaviour of a tridimensional specimen with a complex topology of holes, corners and edges in order to check the corresponding generated gradients when loaded, and observe how the correct pressure is determined without the need of the implementation of a penalty function. Additionally the exercise of the FEA simulation is useful to compare computational times with other model possibilities such as the FE^2 method (our method offers FEA simulation times two or three orders of magnitude faster than the FE^2 method for a similar example).

Chapter 2

New model possibilities. Fractional arithmetical hyperoperations

2.1 Introduction

Most of scientific disciplines have the need of performing predictions and establishing patterns in order to characterize a system behaviour or to model an observed phenomenon.

In particular in the scope of characterization of mechanical behaviour of materials, rheology is the discipline that studies the flow of the matter. Phenomenological approaches focused on the characterization of the deformation of materials lie on mathematical modeling through functions that quantify the energy absorbed by the material when deformed. Usually these functions are defined analytically with certain number of so-called *material* parameters that are fitted in order to adapt the model to experimental evidences. This procedure is not unique for rheology, but it is widely used in most of disciplines of science. However, practically all analytical possibilities lie at a last extent in three arithmetical operations that keep a hierarchical and discrete (in opposition to continuous) relation between them. These operations are addition, multiplication and exponentiation.

There are preliminar advances of arithmetical operations beyond the three classical ones [38], which receive the name of *hyperoperations*. They are built upon them as a hierarchical continuation of the recurrence relation that defines them. For instance, *tetration* is the recurrence operation of exponentiation (e.g. $2 \text{ tetration } 3$ is equal to 2^{2^2}). However they are very limited in the meaning of admitting only discrete values in hyperoperations (e.g. in tetration only integers are admitted as a second argument of the binary operation, otherwise tetration is undefined). They are also limited in the hierarchical relation itself, that are implicitly defined by natural numbers (i.e. tetration (range 4), pentation (range 5), sextation (range 6), and so on), so they define a discrete range that do not conceive the possibility of an intermediate hyperoperation (e.g. an arithmetical hyperoperation of range $3/2$, between addition (range 1) and multiplication (range 2)).

The aim of this article is to open a general theory that establishes the basis of a continuous spectrum of arithmetical hyperoperations, and use the background of the theory to define the first *fractional hyperoperation* of range $3/2$. The main goal of this theory is to expand the arithmetical mathematical tools available for modeling in science. A practical example in rheology will be developed to characterize the stress-strain response of an specimen under uniaxial test conditions.

2.2 Convection of operational symbols and definition of the hyperoperational space, $\mathbb{H}$

Prior the arithmetic fractional hyperoperation $H_{3/2}$ is developed, it is required to establish a convection of symbols that cover hyperoperational functions, as well as defining the space of continuous spectrum of arithmetical hyperoperations, denoted by $\mathbb{H}$ symbol. Table 2.1 provides notational description of hyperoperations in $\mathbb{H}$. Properly detailed in the article, Table 2.2 briefly describes the set of assertions necessary to define $\mathbb{H}$.

Nature	Notation	Expression	Example
Direct	$\cdot_r$	$B \cdot_r E = R$	$2 \cdot_3 3 = 2^3 = 8$
R - Inverse	$/_r$	$R /_r E = B$	$8 /_3 3 = \sqrt[3]{8} = 2$
L - Inverse	$\backslash_r$	$R \backslash_r B = E$	$8 \backslash_3 2 = \log_2(8) = 3$

TABLE 2.1: Hyperoperational notation for $\mathbb{H}$

Assertion	Content	Expression
Def. 1	Definition of space	$\mathbb{H}$
Def. 2	Hyperoperational mean of rank r ,	$m_r(a, b) = (a \cdot_r b) /_{r+1} 2$
Def. 3	Hyperoperational sequence of rank r ,	$HS_r(\beta, n) = x_n = \beta \cdot_{r+1} n$
Def. 4	Neutral element of rank r , ε_r .	$a \cdot_r \varepsilon_r = a$
Def. 5	Recursive sequence RS.	$x_n = m_r(x_{n-1}, x_{n+1})$
Conj. 8, Lem. 9	Start of RS_r	$\left\{ \varepsilon_r, \beta, \beta \cdot_{r+1} 2 \right\}$
Lem. 10, Cond. 11	2-r-2 identity	$2 \cdot_r 2 = 4$

TABLE 2.2: Set of assertions required for $\mathbb{H}$

2.3 Definition of fractional hyperoperation $H_{3/2}$

Once the necessary prerequisites have been properly defined, it is possible to develop the fractional hyperoperation of range $r = 3/2$. Let the following set be considered,

$$\left\{ \varepsilon_{3/2}, \beta, \beta \cdot_{5/2} 2 \right\} \quad (2.1)$$

Setting $\beta = 2$ and taking into account Condition 11 it becomes,

$$\{ \varepsilon_{3/2}, 2, 4 \} \quad (2.2)$$

Due to Def. 2, Conjecture 8 and Lemma 9, in the paper the following relation between the corresponding arithmetical mean of rank $r = 3/2$, $m_{3/2}$ and its neutral element $\varepsilon_{3/2}$ is satisfied,

$$m_{3/2}(\varepsilon_{3/2}, 4) = 2 \quad (2.3)$$

Because mean of rank $r = 1$ and $r = 2$ are respectively the arithmetical and geometrical means, it is admissible consider $m_{3/2}$ as the arithmetic-geometric mean, denoted by agm . Relation between them is observable if expressing them in hyperoperational notation,

$$m_1(a, b) = (a \cdot_1 b) /_2 = (a + b) / 2 \quad (2.4)$$

$$m_{3/2}(a, b) = (a \cdot_{3/2} b) /_{5/2} = agm(a, b) \quad (2.5)$$

$$m_2(a, b) = (a \cdot_2 b) /_3 = \sqrt{ab} \quad (2.6)$$

Obviously, because they are means of ranks $r = 1, r = 3/2, r = 2$ respectively, the following relations are satisfied,

$$m_1(a, b) \leq m_{3/2}(a, b) \leq m_2(a, b) \quad (2.7)$$

$$m_1(a, a) = m_{3/2}(a, a) = m_2(a, a) = a \quad (2.8)$$

$$(2.9)$$

Neutral element $\varepsilon_{3/2}$ is found using Eq.(2.3) and the function *Arithmetic-Geometric Mean Opposite* or $agmo$, which is defined by the following two operations,

$$agmo(M, b) = a \quad (2.10)$$

$$agmo(M, a) = b \quad (2.11)$$

where $M = agm(a, b)$, so that neutral element is,

$$\varepsilon_{3/2} = agmo(agm(2, 4), 4) \approx 0.70305193814261 \quad (2.12)$$

As expected, its neutral element is comprised by corresponding ones of ranks 1 and 2, that is $\varepsilon_1 = 0$ and $\varepsilon_2 = 1$. Because Conjecture 8 and Lemma 9 are satisfied for any β , using Definition 2 of $\mathbb{H}$, the arithmetical fractional hyperoperation is finally found if setting $\beta = agm(a, b)$,

$$a \cdot_{3/2} b = agmo(agm(a, b), \varepsilon_{3/2}) \quad (2.13)$$

As in the case of $r = 1$ (addition) and $r = 2$ (multiplication) it can be observed that shares the commutative property. As expected it can be checked that,

$$x \cdot_{3/2} \varepsilon_{3/2} = \varepsilon_{3/2} \cdot_{3/2} x = x \quad (2.14)$$

Which these basis, the development behind of this article aims to expand and enhance the mathematical possibilities of adaptative modelizations in science. The following advances are included in this article,

- Definition of arithmetic continuum spectrum of hyperoperational space $\mathbb{H}$. Establishment assertions and properties included in $\mathbb{H}$.
- Determination of $agmo$ function algorithm for its computation.
- Determination of fractional hyperoperation of rank $r = 3/2$.
- Determination of fractional hyperoperation of rank $r = 5/2$.

- Applications. Development of Vandermonde-3/2 procedure. It is the enhancement of Vandermonde interpolation fitting procedure with the substitution of exponentiation in polynomials ($r = 3$) by *fractional polynomials* with rank $r = 3/2$. Improved results from comparison with convectional Vandermonde are included.
- Usage case scenario in discipline science of rheology. Application with the fitting of an experimental stress-strain curve from uniaxial test of a specimen. Also mathematical functions are employed to test the accuracy of the method.

FRACTIONAL MATHEMATICAL OPERATORS AND THEIR COMPUTATIONAL APPROXIMATION

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ABSTRACT

Usual applied mathematics employs three fundamental arithmetical operators: addition, multiplication, and exponentiation. However, for example transcendental numbers are said not to be attainable via algebraic combination with these fundamental operators. At the same time, simulation and modelling frequently have to rely on expensive numerical approximations of the exact solution. The main purpose of this article is to analyze new fractional arithmetical operators, explore some of their properties, and devise ways of computing them. These new operators may bring new possibilities, for example, in approximation theory and in obtaining closed forms of those approximations and solutions. We show some simple demonstrative examples.

Keywords Hyperoperations · Arithmetic · Modelization

1 Introduction

Science mostly hinges on mathematics which has been built on three fundamental operations: the addition, the multiplication and the exponentiation. We have become extremely used to them. However, the rigidity of these preset tools may at times make it difficult to find ways and solutions for nature problems that are not easily expressed in terms of traditional operators. For example, transcendental numbers are said not to be attainable via algebraic combination with these fundamental operators, which are a long standing human invention. At the same time, simulation and modelling have to deal with some situations in which the only solution is to compute an expensive numerical approximation of the exact solution, which frequently cannot be written in closed form in terms of traditional operators.

The purpose of this work is to present and apply some operations beyond the rigidity of the known fundamental operations, such as an intermediate operation between addition and multiplication. The ideas have some parallelism with fractional derivatives [1] which, for example, allow the accurate characterization of viscous materials with just two parameters [2], [3] rendering linear equations. We will also see possible applications of the presented operators in constitutive modelling.

Consider the classification described in Table 1.

Op. rank, r	Operational name	Conventional notation	Rank-wise notation
0	Sucessor	$S(S(a)) = (a + 1) + 1$	$a \cdot_0 a = a \cdot_1 2$
1	Addition	$a + a = a \cdot 2$	$a \cdot_1 a = a \cdot_2 2$
2	Multiplication	$a \cdot a = a^2$	$a \cdot_2 a = a \cdot_3 2$
3	Exponentiation	$a^a = a \# 2$	$a \cdot_3 a = a \cdot_4 2$

Table 1: Hierarchical classification of fundamental operations

As observed in Table 1, in the last column, exponentiation is expressed in terms of a higher operation. This operation is called *tetration* and is commonly considered as the first *hyperoperation* because it has a higher rank ($r = 4$) than exponentiation ($r = 3$). Preliminar and fundamental works in this line have been performed by Peano [4] with his *Peano Arithmetic* axioms, Ackermann [5] with their non primitive recursive funcions and the work of Goodman [6] with the *Hyperoperational sequence*, among others.

However, intermediate-rank operations are also possible and may be useful. The problem we address is how to compute a hyperoperation of rank $r = 3/2$ (from now on, $H_{3/2}$). To this respect, this was already an open question formulated by Romero & Rutsov [7] or Williams [8]. We will first set the proper environment, namely the *arithmetical continuous spectrum*. Some definitions are useful to understand some properties that are going to be necessary to compute $H_{3/2}$, as well as to establish a comfortable notation for our purposes.

2 The arithmetical continuous spectrum

The arithmetical continuous spectrum focuses on the idea of having a continuous spectrum of arithmetical operations as it occurs with real numbers. Here we note that there are many possibilities to define hyperoperations of intermediate ranks. The reader is referred to the explanation and discussion in Ref. [9]. The fractional operators that are herein defined have the purpose of seeking improved and more compact interpolations in engineering fields in general, and in constitutive modelling in particular.

In order to connect operations of different ranks, the environment *Set of Hyperoperations* $\mathbb{H}$ must be previously defined. For this purpose, a set of definitions and lemmas will facilitate the task of establishing fractional hyperoperators and their computational approximations.

Definition 1. Let $\mathbb{H}$ be the set that contains every binary hyperoperation of rank r , $r \in \mathbb{R}$. $\mathbb{H}_N \subset \mathbb{H}$ is the space of integer rank hyperoperations, and $\mathbb{H}_Q \subset \mathbb{H}$ is the space of fractional rank hyperoperations; i.e. $\mathbb{H}_N \subset \mathbb{H}_Q \subset \mathbb{H}$.

The suggested notation described in Table 2 will be employed in order to extend a universal notation for hyperoperations of rank $r \in \mathbb{R}$. Consider $B, E, R \in \mathbb{R}$, which resembles the notion of *base*, *exponent* and *result* respectively.

Operational nature	Notation	Operation	Example ($r = 3$)
Direct	$\cdot_r$	$B \cdot_r E = R$	$2 \cdot_3 3 = 2^3 = 8$
R - Inverse	$/_r$	$R /_r E = B$	$8 /_3 3 = \sqrt[3]{8} = 2$
L - Inverse	$\backslash_r$	$R \backslash_r B = E$	$8 \backslash_3 2 = \log_2(8) = 3$

Table 2: Proposed hyperoperational notation

The names of R- and L- inverses reminds those of *Root-kind inverse* and *Log-kind inverse*, but note that the notation is also such that the bar is slanted *Right* for the R-inverse operator and *Left* for the L-inverse operator. Some trivial particular cases are those for $r = 1$ and $r = 2$

$$r = 1 \Rightarrow \begin{cases} B + E = B \cdot_1 E = R \\ R /_1 E = B = R - E \\ R \backslash_1 B = E = R - B \\ \text{so } (\cdot) /_1 (\cdot) \equiv (\cdot) \backslash_1 (\cdot) \equiv (\cdot) - (\cdot) \end{cases} \quad (1)$$

$$r = 2 \Rightarrow \begin{cases} B \cdot E = B \cdot E = R \\ R / E = B = R/E \\ R \overset{2}{\setminus} B = E = R/B \\ \text{so } (\cdot) / \overset{2}{(*)} \equiv (\cdot) \overset{2}{\setminus} (*) \equiv (\cdot) / (*) \end{cases} \quad (2)$$

For instance, in the case of rank $r = 3$, the relations between the base B , the exponent E , and the result, R are as follows,

$$r = 2 \Rightarrow \begin{cases} B^E = B \cdot E = R \\ \sqrt[E]{R} = R / E = (B \cdot E) / E = B \\ \log_B R = R \overset{3}{\setminus} B = (B \overset{3}{\cdot} E) \overset{3}{\setminus} B = E \\ \text{so } (\cdot) / \overset{3}{(*)} \neq (\cdot) \overset{3}{\setminus} (*) \end{cases}$$

Definition 2 (Hyperoperational mean). *All rank- r arithmetical operation in $\mathbb{H}$ has a corresponding hyperoperational mean, which is defined the following way,*

$$m_r(x, y) = (x \cdot_r y) / \overset{r+1}{2}, \quad x > y \quad (3)$$

This definition is the natural extension of ranks $r = 1$ (arithmetical mean) and $r = 2$ (geometrical mean),

$$m_1(x, y) = \frac{x + y}{2} = (x \cdot_1 y) / \overset{2}{2} \quad (4)$$

$$m_2(x, y) = \sqrt[2]{x \cdot y} = (x \cdot_2 y) / \overset{3}{2} \quad (5)$$

Definition 3 (Hyperoperational sequence, HS). *Hyperoperational sequence of base β is a sequence $\text{HS}_r(\beta, n)$ so that the n -th term is,*

$$x_n = \beta \cdot_{r+1} n = \text{HS}_r(\beta, n) \quad (6)$$

i.e.

$$\begin{aligned} \text{HS}_r(\beta, n) &\equiv \{x_n\} = \left\{ \dots, (\beta), \left(\beta \cdot_r \beta \right), \left(\beta \cdot_r \beta \cdot_r \beta \right), \dots \right\} \\ &= \left\{ \dots, \beta \cdot_{r+1} 1, \beta \cdot_{r+1} 2, \beta \cdot_{r+1} 3, \dots \right\} \end{aligned} \quad (7)$$

Definition 4 (Neutral element). *The neutral element ε_r for hyperoperations of rank r is the number such that*

$$\beta \cdot_r \varepsilon_r = \beta \quad (8)$$

and then obviously

$$\beta / \varepsilon_r = \beta \quad (9)$$

$$\beta \overset{r}{\setminus} \beta = \varepsilon_r \quad (10)$$

Definition 5 (Recursive Sequence, RS). *Let a Recursive Sequence $\text{RS}_r(\beta, n)$, of rank r , base β and neutral element ε_r , be the sequence built by its corresponding mean, m_r , and the following pair of starting values*

$$\{x_0, x_1\} = \{\varepsilon_r, \beta\} \quad (11)$$

The sequence can be run either forwards (direct values) in this way,

$$x_2 = (\beta \cdot_{r+1} 2) / \varepsilon_r \quad (12)$$

or backwards (inverse values), in this way.

$$x_{-1} = (\varepsilon_r \cdot_r 2) \setminus_r \beta \quad (13)$$

Generally, RS is based on the relation that adjacent terms satisfy. This relation is the hyperoperational mean.

$$m_r(x_{n-1}, x_{n+1}) = x_n \quad (14)$$

$$(x_{n-1} \cdot_r x_{n+1}) /_{r+1} 2 = x_n \quad (15)$$

If solved for x_{n+1} it is obtained the forward direction of RS . On the contrary, if solved for x_{n-1} it yields the expression of backward direction.

$$x_{n+1} = (x_n \cdot_{r+1} 2) /_r x_{n-1} \quad \text{forwards} \quad (16)$$

$$x_{n-1} = (x_n \cdot_{r+1} 2) \setminus_r x_{n-1} \quad \text{backwards} \quad (17)$$

According to Def.(5), and example of rank $r = 1$ is shown. $RS_1(3, n)$ satisfy arithmetical mean, m_1 .

$$x_{-1} : m_1(x_1, x_{-1}) = x_0 = \frac{x_1 + x_{-1}}{2} \quad (18)$$

$$x_{-1} = (x_0 \cdot 2) - x_1 = (x_0 \cdot_2 2) \setminus_1 x_1 = 0 \cdot 2 - 3 = -3 \quad (19)$$

$$x_0 = \epsilon_1 = 0 \quad (20)$$

$$x_1 = \beta = 3 \quad (21)$$

$$x_2 : m_1(x_2, x_0) = x_1 = \frac{x_0 + x_2}{2} \quad (22)$$

$$x_2 = (x_1 \cdot 2) - x_0 = (x_1 \cdot_2 2) /_1 x_0 = 6 - 0 = 6 \quad (23)$$

$$x_3 = (x_2 \cdot_2 2) /_1 x_1 = 12 \cdot 2 - 3 = 9 \quad (24)$$

$$x_4 = (x_3 \cdot_2 2) /_1 x_2 = 18 \cdot 2 - 6 = 12 \quad (25)$$

$$x_5 = (x_4 \cdot_2 2) /_1 x_3 = 24 \cdot 2 - 9 = 15 \quad (26)$$

$$\dots \quad (27)$$

$$x_n = (x_{n-1} \cdot_2 2) /_1 x_{n-2} = 3 \cdot n = 3 \cdot_2 n = \beta \cdot_2 n \quad (28)$$

Now another example, this time of rank $r = 3$. $RS_3(3, n)$ must satisfy the corresponding hyperoperational mean, m_3 .

$$x_0 = \epsilon_3 = 1 \quad (29)$$

$$x_1 = \beta = 3 \quad (30)$$

$$x_2 : m_3(x_3, x_1) = x_2 \quad (31)$$

$$x_2 = (x_1 \cdot_4 2) /_3 x_0 = \sqrt[3]{x_1^{x_1}} = 3^3 = 27 = 3 \cdot_4 2 = 3^3 \quad (32)$$

$$x_3 = (x_2 \cdot_4 2) /_3 x_1 = \sqrt[3]{x_2^{x_2}} = \sqrt[3]{27^{27}} = 3 \cdot_4 3 = 3^3 \quad (33)$$

$$\dots \quad (34)$$

$$x_n = (x_{n-1} \cdot_4 2) /_3 x_{n-2} = \beta \cdot_4 n \quad (35)$$

It can be checked that this makes Recursive Sequences RS , coincide up to rank $r = 3, r \in \mathbb{N}$, with the corresponding Hyperoperational Sequences, HS . In turn, they also coincide with the Goodstein function if the neutral elements are

Figure 1: Arithmetical reflectivity illustrative example

the same for the corresponding rank of the Goodstein function, that is,

$$\begin{aligned}\varepsilon_1 &= 0 \\ \varepsilon_r &= 1, \quad r > 1, r \in \mathbb{N}\end{aligned}$$

Definition 6 (Arithmetical reflectivity). *Let $HS_r(\beta, n)$ be a hyperoperational sequence of rank r . Then it is said that hyperoperation H_r owns arithmetical reflectivity if, and only if,*

$$m_r(HS_r(n+a), HS_r(n-a)) = HS_r(\beta, n) \quad (36)$$

with $n, a, r \in \mathbb{R}$, $a \neq 1$.

Def.6 is an extension to rank r of this property, present in ranks $r = 1$ and $r = 2$,

$$\begin{aligned}m_1(HS_1(\beta, n-a), HS_1(\beta, n+a)) &= \frac{\beta(n-a) + \beta(n+a)}{2} = \beta n = HS_1(\beta, n) \\ m_2(HS_2(\beta, n-a), HS_2(\beta, n+a)) &= \sqrt{\beta^{n-a} \cdot \beta^{n+a}} = \beta^n = HS_2(\beta, n)\end{aligned}$$

An example of this property is shown in Figure 1.

Definition 7 (Arithmetical Duality or Duality RS - HS). *It is said that a hyperoperation H_r have arithmetical duality when its recursive sequence, RS_r and its hyperoperational sequence, HS_r , coincide,*

$$RS_r = HS_r$$

Conjecture 8. *Let $RS_r(\beta, n)$ be a recursive sequence of base β , with $r \in \mathbb{R}$. Then, the precedent term, ε_r , of $\{\beta, \beta_{r+1} \cdot 2\}$, is the neutral element of $RS_r(\beta, n)$, which works as right identity element of H_r .*

$$m_r(\varepsilon_r, \beta_{r+1} \cdot 2) = \beta$$

In the case of rank $r \in \mathbb{N}$, the Conjecture 8 becomes a lemma.

Lemma 9 (RS starting set). *Let $RS_r(\beta, n)$ be a recursive sequence of base β . Then, the first three terms of $RS_r(\beta, n)$ are,*

$$\{\beta_{r+1} \cdot 0, \beta_{r+1} \cdot 1, \beta_{r+1} \cdot 2\} = \{\varepsilon_r, \beta, \beta_{r+1} \cdot 2\} \quad (37)$$

being the term ε_r the right neutral element of H_r .

Proof. The right neutrality of ε_r with $r \geq 2$, is imposed to the value of $\varepsilon_r = 1$ due to multiplicative recursion, $\beta \cdot_{r+1} 1 = \beta$. According to Definition 5,

$$\begin{aligned} m_r(x_2, x_0) &= x_1 \\ x_0 &= \varepsilon_r \\ x_1 &= \beta \end{aligned}$$

Therefore,

$$\begin{aligned} (x_2 \cdot_{r+1} \varepsilon_r) / 2 &= \beta \\ x_2 \cdot_{r+1} \varepsilon_r &= \beta \cdot_{r+1} 2 \\ x_2 &= \beta \cdot_{r+1} 2 \end{aligned}$$

□

Lemma 10 (Tetric Identity for natural ranks). *All arithmetical operations in $\mathbb{H}$ with natural rank r satisfy $2 \cdot_r 2 = 4$, $\forall r \in \mathbb{N}$*

Proof. Via inductive method.

For $r = 1$, $2 \cdot_1 2 = 2 + 2 = 4$.

For $r = 2$, $2 \cdot_2 2 = 2 \cdot_1 2 = 4$.

For $r = n$, $2 \cdot_n 2 = 2 \cdot_{n-1} 2$.

Then, for every $r \in \mathbb{N}$, $2 \cdot_r 2 = 4$.

□

In the case of non integer ranks the lemma 10 must be formulated as a condition (hypothesis) to be imposed.

Condition 11 (Tetric Identity). *All arithmetical operation in $\mathbb{H}$ shall comply with $2 \cdot_r 2 = 4$, $r \in \mathbb{R}$*

Lemma 12 (About arithmetical duality on $\mathbb{H}$). *Arithmetical duality is not an inherent property of $\mathbb{H}$.*

Proof. From Definition 5, the sequence RS_r can be expressed recursively,

$$\begin{aligned} m_r(x_{n+1}, x_{n-1}) &= x_n \\ (x_{n+1} \cdot_r x_{n-1}) / 2 &= x_n \\ x_{n+1} &= (x_n \cdot_{r+1} 2) / x_{n-1} \end{aligned} \tag{38}$$

From Lemma 9,

$$\begin{aligned} x_0 &= \varepsilon_r \\ x_1 &= \beta \\ x_2 &= \beta \cdot_{r+1} 2 \end{aligned}$$

A counter-example is enough to prove the lemma. For rank $r = 4$,

$$\begin{aligned} m_4(x_3, x_1) &= x_2 \\ m_4(x_3, \beta) &= x_2 \\ (x_3 \cdot_4 \beta) / 2 &= x_2 \\ x_3 \cdot_4 \beta &= x_2 \cdot_5 2 \\ x_3 \cdot_4 \beta &= (\beta \cdot_4 2) \cdot_4 (\beta \cdot_4 2) \end{aligned}$$

Let be assumed that the lemma is not true and therefore $x_3 = \beta \cdot_5 3$. Then, for $\beta = 2$, and using Lemma 10,

$$\begin{aligned}
 (\beta \cdot_5 3) \cdot_4 \beta &\stackrel{?}{=} (\beta \cdot_4 2) \cdot_4 (\beta \cdot_4 2) \\
 (2 \cdot_5 3) \cdot_4 2 &\stackrel{?}{=} (2 \cdot_4 2) \cdot_4 (2 \cdot_4 2) \\
 (2 \cdot_4 (2 \cdot_4 2)) \cdot_4 2 &\stackrel{?}{=} 4 \cdot_4 4 \\
 (2 \cdot_4 4) \cdot_4 2 &\stackrel{?}{=} 4 \cdot_3 (4 \cdot_3 (4 \cdot_3 4)) \\
 &\dots \\
 2 \cdot_3 (2 \cdot_3 20) &\stackrel{?}{=} 2 \cdot_3 (2 \cdot_3 (1 \cdot_1 2 \cdot_3 9))
 \end{aligned}$$

Taking logarithms of base 2 twice,

$$\begin{aligned}
 ((2 \cdot_3 (2 \cdot_3 20)) \cdot_3 2) \cdot_3 2 &\stackrel{?}{=} ((2 \cdot_3 (2 \cdot_3 (1 \cdot_1 2 \cdot_3 9)) \cdot_3 2) \cdot_3 2) \cdot_3 2 \\
 20 &< 1 \cdot_1 2 \cdot_3 9
 \end{aligned}$$

In other words,

$$20 \neq 1 + 2^9 \rightarrow x_3 \neq \beta \cdot_5 3$$

Therefore, $x_n = \beta \cdot_{r+1} n$ is not a general rule for a RS of rank r . That is, arithmetical duality is not inherent to $\mathbb{H}$. $\square$

This package of definitions, conditions, and lemmas enable the proper environment for $\mathbb{H}$, and for reaching an approximation of the fractional hyperoperation $H_{3/2}$.

Williams [8] suggests a creative technique, using theory of functionals. He is even able to provide discrete numerical values. Unfortunately, the William's method does not guarantee a unique solution. Campagnolo [10] also suggests in certain way the possibility of a continuity in hyperoperational hierarchy.

In order to obtain a computable approximation of $H_{3/2}$, the gaussian mean shall be the starting point of this work. The reason behind is the close relationship between an hyperoperational mean and its direct hyperoperation, as observed in previous lemmas and definitions.

3 Approximation of $H_{3/2}$

The arithmetic-geometric mean $agm(x, y)$ is computed recursively (with very fast convergence) as

$$\begin{aligned}
 x_0 &= x, \quad y_0 = y, \\
 x_i &= \frac{x_{i-1} + y_{i-1}}{2}; \quad y_i = \sqrt{x_{i-1}y_{i-1}} \quad \text{until desired convergence}
 \end{aligned}$$

In this approximation of $H_{3/2}$ (from now on, simply $H_{3/2}$), the arithmetic-geometric mean, agm , will be the mean of $H_{3/2}$,

$$m_{3/2}(x, y) = agm(x, y)$$

It will be useful to have a definition of the function complementary to agm ,

Definition 13 (Arithmetic - Geometric Mean Opposite term function, or $agmo$). *Let $RS_r(\beta, n)$ be a recursive sequence of base β and rank r . Then, given a pair $\{x, y\}$ such as $agm(x, y) = M$, the binary function is defined as,*

$$\begin{aligned}
 agmo(M, y) &= x \\
 agmo(M, x) &= y
 \end{aligned}$$

Figure 2: Approximation of $H_{3/2}$ vs. H_1 and H_2

According to Definition 2, $m_{3/2}$ can be expressed as

$$m_{3/2}(x, y) = (x \cdot_{3/2} y) /_{5/2} 2 \quad (39)$$

This allows an explicit expression of $H_{3/2}$,

$$x \cdot_{3/2} y = m_{3/2}(x, y) \cdot_{5/2} 2 \quad (40)$$

Making use of Conjecture 8, as an extension of Lemma 9,

$$RS_{3/2}(\beta, n) = \{\epsilon_{3/2}, \beta, \beta \cdot_{5/2} 2, \dots, \} \quad (41)$$

If setting $\beta = 2$, and using Condition 11 as an extension of Lemma 10, Eq.(41) becomes,

$$RS_{3/2}(2, n) = \{\epsilon_{3/2}, 2, 4, \dots, \} \quad (42)$$

Therefore, the neutral element $\epsilon_{3/2}$ is readily obtained as

$$\epsilon_{3/2} = agmo(2, 4) \approx 0.70305193814261 \quad (43)$$

The neutral element $\epsilon_{3/2}$ is easy to test as observed in Figure (2).

If setting now $\beta = agm(x, y)$ in Eq.(41), an explicit and computable expression of the approximation of $H_{3/2}$ is obtained,

$$x \cdot_{3/2} y = agmo(agm(x, y), \epsilon_{3/2}) \quad (44)$$

In Fig.3 it can be observed the behaviour of $y = x \cdot_{3/2} 2$ for $x \in [0, 2]$.

Equation (44) facilitates the computation of an approximation of $H_{5/2}$ in the same way multiplication may be computed by addition,

$$\underbrace{x \cdot_{3/2} x \cdot_{3/2} \dots \cdot_{3/2} x}_{y \text{ times}} = x \cdot_{5/2} y \quad (45)$$

Figure 3: Approximation of $H_{3/2}$ vs. H_1 and H_2 Figure 4: Approximation of the result of some hyperoperations H_r of the form $y = x \cdot_r 2$

In Fig. 4 there are examples of hyperoperations of the form $y = x \cdot_r 2$, namely $y = x \cdot_{3/2} 2$ and $y = x \cdot_{5/2} 2$, and the result is compared to the sum, product and exponentiation.

Some properties of $H_{3/2}$ are,

- Its consistentnes and uniqueness are guaranteed by Eq. (44)
- It is consistent with its mean definition

$$(x \cdot_{3/2} y) / 2 = agm(x, y)$$

Table 3: Algorithm used to compute the function $agmo$

Agmo algorithm $y = agmo(M, x)$ such that $M = agm(x, y)$	
$x = \text{argument}, M = \text{arithmetic-geometric mean}$	
A.	If $crit = \log(x/M) < 0.6$,
A.1.	Initialize values: $M_0 = M, y_0 = M$
	Until convergence $\epsilon < tol$
A.2.	Arithmetic term: $y_a = 2M_n - x$
A.3.	Geometric term: $y_g = M_n^2/x$
A.4.	Update $y_{n+1} = (y_a + y_g)/2$
A.5.	Update $M_{n+1} = M_n (M_0/agm(x, y_{n+1}))$
A.6.	Compute relative error $\epsilon = (y_{n+1} - y_n)/y_n$
B.	else
B.1.	Initialize values $y_0 = M, f = \max(1, x/M)$
	Until convergence
B.2.	Update $y_{n+1} = y_n [M/agm(x, y_n)]^f$
B.3.	Compute relative error $\epsilon = (y_{n+1} - y_n)/y_n$

- It is commutative.

$$x \cdot_{3/2} y = y \cdot_{3/2} x$$

- It has a neutral element, see Eq. (43).
- It is not associative (although produces values of the same magnitude).
- It is not distributive with addition.

$$(a \cdot_1 b) \cdot_{3/2} c \neq a \cdot_{3/2} c \cdot_1 b \cdot_{3/2} c$$

- It is not distributive with multiplication.

$$(a \cdot_{3/2} b) \cdot_2 c \neq a \cdot_2 c \cdot_{3/2} b \cdot_2 c$$

- It is not distributive with $H_{5/2}$.

$$(a \cdot_{3/2} b) \cdot_{5/2} c \neq a \cdot_{5/2} c \cdot_{3/2} b \cdot_{5/2} c$$

- It does not have arithmetical reflectivity.

$$m_{3/2}(\text{RS}_{3/2}(\beta, n+a), \text{RS}_{3/2}(\beta, n-a)) \neq \text{RS}_{3/2}(\beta, n), a \neq 1$$

- It does not have arithmetical duality. However, from Lemma 12, it is not required to be in the $\mathbb{H}$ space.

$$\text{RS}_{3/2}(\beta, n) \neq \beta \cdot_{5/2} n$$

4 Applications

The existence of fractional hyperoperations enlarges the arithmetical tools of mathematics. Therefore, although not very intuitive (we are used to traditional operators), is apparent that fractional hyperoperations may have an impact on applications that rely on every discipline that needs mathematics, particularly interesting in the modelling of physical processes. In fact, as we show below, they may be useful in curve fitting in constitutive modelling of solids [12], [13], [14], which was one of our interests in this type of operators. In this Section we show some applications of the presented framework in this field. In the applications shown, the $agmo$ operator was needed in order to uniquely compute these intermediate hyperoperations. The algorithm we employed is shown in table 3.

In Figure 5, an example of this type of application is shown. We model the behavior of copper alloy C51100 under uniaxial true tensile stress vs. strain before and after necking. Experimental data are extracted from Ling [15] via a plot

Figure 5: Modelling curve based on experimental results from alloy C51100 under uniaxial true stress vs. strain after necking

digitizer software. In particular, the resulting curve can be analytically written as,

$$\begin{aligned}
 a &= 4E + 04 \\
 b &= 0.81 \\
 c &= 0.03 \\
 d &= 5.1E + 04 \\
 f &= 2 \\
 y(x) &= a \cdot \left(b \cdot x \cdot c \cdot \frac{f}{3/2} \right) \cdot d \cdot x
 \end{aligned}$$

where x are the true (logarithmic) strains and y are the true (Cauchy) stresses, work-conjugate of the logarithmic strains if the volumetric elastic strains are neglected (they are typically orders of magnitude smaller).

This compact expression in very close agreement with the experimental results has been obtained employing a mixed rank-parameter fitting procedure. When the rank is fixed, the procedure is simpler although the result is not so compact. For example, a possible systematic solution would be the generalization of the Vandermonde matrix to any hyperoperation of rank r . Vandermonde matrix is useful for interpolation. In order to explain how the usual Vandermonde matrix works, let consider the case of a 2-D interpolation of N experimental points with coordinates (x_i, y_i) , so that given any x as input, its interpolated image y is obtained. Then, the Vandermonde matrix is built upon the experimental points. It is the representation of a system of equations, in which the M incognitas are monomial powers of x , of a polynomial expression of grade M , for each point (x_i, y_i) .

$$\begin{aligned}
 a_0 + a_1 \cdot x_0 + a_2 \cdot x_0^2 + \cdots + a_m \cdot x_0^m &= y_0 \\
 a_1 + a_1 \cdot x_1 + a_2 \cdot x_1^2 + \cdots + a_m \cdot x_1^m &= y_1 \\
 &\vdots \\
 a_n + a_n \cdot x_n + a_2 \cdot x_n^2 + \cdots + a_m \cdot x_n^m &= y_n
 \end{aligned} \tag{46}$$

So, in matrix representation,

$$\underbrace{\begin{pmatrix} 1 & x_0 & \cdots & x_0^m \\ 1 & x_1 & \cdots & x_1^m \\ \cdots & \cdots & \cdots & \cdots \\ 1 & x_n & \cdots & x_n^m \end{pmatrix}}_{\text{Vandermonde matrix}} \begin{pmatrix} a_0 \\ a_1 \\ \cdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \cdots \\ y_n \end{pmatrix} \quad (47)$$

However, a well-known drawback of this method is that the more terms in the polynomial are included, the bigger the condition number of the resulting matrix. The reason behind this is the behaviour of x_i^m as the degree m of the polynomial increases.

However x_i^m can be re-expressed in hyperoperational notation as $x_i \cdot_3 m$. If $x_i \cdot_3 m$ is replaced by $x_i \cdot_{3/2} m$, the condition number would become lower as the number of terms, m , increases. The more accuracy in the interpolation fitting is required, the more terms the polynomial must include, and the bigger becomes the differences between using $x \cdot_{3/2} m$ and $x \cdot_3 m$. Furthermore, the method can be adjusted as desired just by setting the hyperoperational rank r of the *hypermonomials*, $x \cdot_r m$.

As an illustrative example, in Figure 6 a modified Vandermonde with *hyperpolynomial* (instead of the usual polynomial) expansion of rank $r = 3/2$ is applied in order to fit points extracted from the well-known classical Treloar [11] experiment of simple tension, from a sample cut of a simple sheet of vulcanized natural rubber. In particular, the extension has the form described in Equation (48),

$$\mathbf{y} = \sum_{i=0}^n (x \cdot_{3/2} i) \cdot_2 a_i \quad (48)$$

where the coefficients a_i come from the analogous vector in Equation (47), as described in Equation (49).

$$\underbrace{\begin{pmatrix} x_0 \cdot_{3/2} 0 & x_0 \cdot_{3/2} 1 & \cdots & x_0 \cdot_{3/2} m \\ x_1 \cdot_{3/2} 0 & x_1 \cdot_{3/2} 1 & \cdots & x_1 \cdot_{3/2} m \\ \cdots & \cdots & \cdots & \cdots \\ x_n \cdot_{3/2} 0 & x_n \cdot_{3/2} 1 & \cdots & x_n \cdot_{3/2} m \end{pmatrix}}_{r=3/2 \text{ modified Vandermonde}} \begin{pmatrix} a_0 \\ a_1 \\ \cdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \cdots \\ y_n \end{pmatrix} \quad (49)$$

As commented, as the number of terms included in the expansion increase, the differences in the condition number between the usual Vandermonde matrix and the modified one, are larger. This makes the use of fractional hyperoperations in the Vandermonde method particularly interesting when dealing with high a number of terms in the Vandermonde expansion. An important advantage of hyperoperations in the Vandermonde method is that the rank r of the hyperoperation has not necessarily to be $r = 3/2$, but a free parameter instead, in order to best fit the interpolation behaviour. In Figure 6c, for 15 terms, the hyperoperational variant ($r = 3/2$) already offers better fitting than the usual Vandermonde one ($r = 3$). For higher number of terms, the condition number of the usual Vandermonde matrix becomes so unstable that interpolation application is no longer viable. In Table 4, the evolution of the condition number with the inclusion of new terms has been represented from $n = 15$ terms up to $n = 20$ terms.

Consider a virtual experiment with the (presumably unknown) result being of the form of a logarithm (i.e. $\mathbf{y} = \log(\mathbf{x})$, or $\mathbf{y} = \mathbf{x} \setminus_3 e$ in hyperoperational notation). The result of the experiment is obtained for a vector of random x values.

The aim of this emulated experiment is to contrast the value of the two Vandermonde options of the previous example, with the known exact value for the interpolated points, see Figure 7.

For a particular example, pseudoexperimental scattered points from the analytical function $y = \log(x)$ emulates an experimental event. In this simple numerical experiment we wish to obtain a proper fit for point in the interval $x \in [1.3 : 0.1 : 7]$. This numerical experiment has been performed with two different sets of random numbers in the interval $[1.3 : 7]$. A summary of the results is presented in Tables 5 & 6, where we used $n = 15$ terms in both cases

Figure 6: Modified Vandermonde with $r = 3/2$ hyperpolynomial expansion: Vandermonde expansions with 3 terms (a), 7 terms (b) and 15 terms (c).

n terms	$r=3/2$ Vandermonde	$r=3$ Vandermonde
15	1.75E+12	4.89E+17
16	2.23E+12	1.01E+19
17	4.30E+12	2.13E+20
18	5.34E+12	4.47E+21
19	7.54E+13	1.17E+23
20	9.31E+13	2.78E+24

Table 4: Condition number for modified Vandermonde $r = 3/2$ vs. usual Vandermonde matrix

Figure 7: Pseudoexperimental logarithmic curve together with Vandermonde interpolation family results $r = 3$ and $r = 3/2$ from range $x = 1.3$ to $x = 7$

with precision of 10^{-30} . It is clearly seen that the precision using $r = 3/2$ is many orders better than that using the classical Vandermonde interpolation.

Rank of Vandermonde	Mean of $y_{vander} - y_{exact}$	Std. of $y_{vander} - y_{exact}$
3/2	3.37E-10	2.35E-09
3	2.22E-05	9.98E-05

Table 5: Mean and standard deviation of difference between Vandermonde interpolation and the exact solution

Rank of Vandermonde	Mean of $y_{vander} - y_{exact}$	Std. of $y_{vander} - y_{exact}$
3/2	6.33E-13	1.59E-10
3	1.11E-07	8.80E-07

Table 6: Mean and standard deviation of difference between Vandermonde interpolation and the exact solution

In order to further explore the applicability of the presented operators to curve fitting, we present another example. This time the number of terms used in the Vandermonde method have been increased up to 1000, and the pseudoexperimental curve employed in this example is $y(x) = \sin(x)$. As it could have been expected, the typical Vandermonde approach fails with such number of terms. In fact, in this test, non numerical NaNs have been returned by MATLAB when employing the usual Vandermonde approximation due to the extremely high condition number reached, so the required numerical precision to accomplish the task cannot be attained using this approach. Nevertheless, $h_{3/2}$ Vandermonde breaks this constrain even with practical machine precision of $1E-15$, as it is shown in figure fig.(8). Note that the 1000 points are the points employed to build the $h_{3/2}$ Vandermonde hyperpolynomial, not the interpolated points. Hence, the proposed operators clearly bring new possibilities in the use of polynomial approximations by Vandermonde-type schemes.

The last numerical example we show here is to show some additional properties of this kind of interpolation: smoothing of noisy experimental data. This is a very important problem in many engineering fields, as for example in statistics [18] or in the case of curve and surface fitting [21]. It is also of practical importance in fitting experimental data from many materials, as polymers [19] and biological tissues [20]. In this case we compare the proposed interpolation method with spline interpolation techniques [21]. Spline interpolation is used in the mentioned fields because, among other reasons, the usual Vandermonde approximation loses accuracy when a big amount of points are taken into account. However, splines have their own well known problems related to large oscillations when noisy experimental data is presented, see for example [17], [18], [21] and therein references. However, $h_{3/2}$ interpolation is global in nature and uses a Householder transformation. The interpolation is naturally not forced to pass through all the points in

Figure 8: Pseudoexperimental sinusoidal curve together with Vandermonde interpolation results. For rank $r = 3$ the process diverge completely (NaN s returned), while it remains for rank $r = 3/2$.

Figure 9: $h_{3/2}$ Vandermonde interpolation vs. splines interpolation. Distorted Treloar simple tension experimental results with experimental noise.

this case. The smoothness of the approximation can be controlled with the order of the hyperpolynomial, a desirable characteristic when dealing with noisy data. For the purpose of this example, the Treloar experimental data for rubber from the previous example have been distorted with a given amount of noise. We show the altered data presented to the approach in figure fig.(9). In this figure we also show, for comparison purposes, a piecewise cubic spline interpolation and the proposed $h_{3/2}$ Vandermonde interpolation. It is seen that the proposed global interpolation naturally filters the experimental noise, whereas the spline interpolation would need specific smoothing techniques. Furthermore, the global nature of the proposed interpolation may be interesting when addressing some desired properties of stored energy functions of hyperelastic materials as polyconvexity. The inherent local nature of the splines used in the WYPIWYG approaches [12], [13], [19] makes in principle more difficult the analysis of these properties.

Finally, in passing we just mention that there are interesting relations [16] using $H_{3/2}$, so long as they are inherent to the gaussian mean.

- The π number,

$$\pi = \lim_{x \rightarrow \infty} {}_2 \cdot (1 \cdot x) / {}_{3/2} \cdot (4/x) \setminus e$$

- Its relation with the complete elliptic integral of first kind, $K(k)$,

$$x \cdot y = (\pi / {}_2 \cdot (x \cdot y) / K(k)) \cdot {}_{5/2} 2$$

$$k = (x / y) / (x \cdot y)$$

5 Conclusions

In this paper we have presented new mathematical operations and have devised the way to compute some fractional operators. These new mathematical operators are not so intuitive because we are obviously used for some millennia to addition and multiplication. However, as for the case of fractional derivatives, these operators bring some new possibilities because they brake the usual rigidity of traditional ones. Immediate examples of application are for example the obtention of more compact closed forms for experimental curves and the capability of performing better conditioned Vandermonde interpolations. Much research is still to be done in order to obtain systematic variable-rank interpolations which may unveil the power of the new operators.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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Chapter 3

WYPiWYG data-driven method for compressible isotropic materials

3.1 Introduction

In solid mechanics, FEA modeling is paramount for the study and simulation of the mechanical behaviour of materials. In the case of complex materials with non linear stress - strain response (i.e. biological tissues, rubber), depending on the nature of the problem, FEA can be performed taking into account the microscale aspects for the simulation. In other situations a phenomenological approach entitles a macroscopic simulation of the problem. The microscopic approach can facilitate under certain circumstances, a better accuracy at expense of a computational cost. On the contrary, a macroscopic phenomenological approach offers much faster simulations, but it might incur into a loss of generality. Nevertheless, if the material shows certain simplification patterns, such as isotropic behaviour, the phenomenological approach can become the most appropriate choice.

The phenomenological approach is grounded on a mathematical relation between stresses and strains that are based in energy considerations. For the specific case of hyperelastic materials, mathematical relations lie on a conservative assumption implying the existence of a potential function. Corresponding stresses and strains arise from the evaluation of these state functions. Depending on the nature of the material (e.g. incompressible, isotropic, orthotropic), the energy potential is decomposed into different contributions.

Usually, phenomenological energies are modeled using an analytical form with adaptive *material* parameters that are fitted by means of stress-strain equations and optimization algorithms like the Levenberg-Marquardt algorithm. Penalty functions for compressibility are also included in the same procedure. These mathematical relations require referential experimental test results (i.e. uniaxial test), which are the objective of the fitting. However it does not guarantee an efficient modeling. If a oversimplifying formulation is undertaken, simulations outside the reference scenario can lead to completely unpredictable results. Another source of error is the fitting method itself. Unknown potential functions can be approximated at a certain extent and at a certain range of stress-strain, but it is just an approximation, not the functional solution of the assumption (since the unknown energies are functions, the system of stress-strain relations are functional equations to be solved). Besides that, due to the great variety of proposed formulations, it becomes difficult to determine which should be the best choice. This last difficulty has been solved with a data-driven method that aims to solve the functional equations instead of approximating them. Preliminary works have been done in this line for incompressible materials. In this chapter, a data-driven method with the same purpose has been extended

for solving stress-strain functional equations of hyperelastic isotropic compressible materials under the assumption of the Valanis - Landel decomposition.

3.2 Precursor. Logarithmic strain formulation and Sussmann - Bathe model for hyperelastic isotropic incompressible materials

In order to determine the potential energy unknown functions it is necessary to establish the formulation in which corresponding stress - strain functional equations are going to be expressed. Arguments of the energy functions must comply with principles of objectivity, such as being an invariant from the reference point of view (e.g. trace of strain tensor does not depend on the system of reference), and the relation between stresses and strains must be work conjugacy.

In this chapter, the material logarithmic strain tensor, $\mathbf{E}$ is going to be considered as a natural extension of small strains, so that compressive strains implies negative values of $\mathbf{E}$ components, and positive viceversa. The advantages of this choice is twofold. Firstly, it makes phisically intuitive and meaningful the magnitude, and secondly, the corresponding formulation shall naturally recover small strain formulation at moderate strains. The corresponding work-conjugate stress is the generalized Kirchhoff tensor $\mathbf{T}$. So that considering $\mathbf{A}$ as the Green-Lagrange strain tensor and $\mathbf{S}$ the work conjugate second Kirchhoff stress tensor, then the energy $\mathbf{W}$ can be re-expressed as,

$$\mathbf{W} = \mathbf{S} : \mathbf{A} = \mathbf{T} : \mathbf{E} \quad (3.1)$$

so that $\mathbf{E}$ can be defined using the spectral decomposition from principal stretches λ_i and the corresponding eigenvectors $\mathbf{N}_i$ for the i principal directions as,

$$\mathbf{E} = \sum_{i=1}^3 \log(\lambda_i) \mathbf{N}_i \otimes \mathbf{N}_i \quad (3.2)$$

On the other side, $\mathbf{T}$ can be expressed from Cauchy stress $\boldsymbol{\sigma}$ taking into account the following transformations,

$$\bar{\boldsymbol{\tau}} = \mathbf{R}^T \mathbf{J} \boldsymbol{\sigma} \mathbf{R} \quad (3.3)$$

$$T_{ij} = \bar{\tau}_{ij} \quad i = j \quad (3.4)$$

$$T_{ij} = \frac{\lambda_j^2 - \lambda_i^2}{2\lambda_j\lambda_i(\log(\lambda_j) - \log(\lambda_i))} \quad i \neq j \quad (3.5)$$

where $\mathbf{R}$ is the rotation matrix from material to spatial description and $\bar{\boldsymbol{\tau}}$ is material Kirchhoff stress tensor.

Sussmann and Bathe described the energy function in terms of logarithmic principal strains E_i and Valanis - Landel decomposition for an incompressible isotropic hyperelastic material. That is,

$$\mathcal{W} = \omega'(E_1) + \omega'(E_2) + \omega'(E_3) \quad (3.6)$$

Stress - strain functional equation relates

The generalized Kirchhoff stress tensor and the material logarithmic strain tensor are related through the following stress - strain tensorial equation,

$$\mathbf{T} = \sum_{i=1}^3 \omega'(E_i) \mathbf{N}_i \otimes \mathbf{N}_i + p \mathbf{I} \quad (3.7)$$

where p is the langragian pressure-like term.

Kearsley and Zapas found a way to determine the functional unknown $\omega'(E)$ directly from experimental stress - strain data. If considering an available uniaxial test data $T(E)$, then the corresponding stress - strain scalar relation is,

$$T(E_u) = \omega'(E_u) - \omega'(E_t) \quad (3.8)$$

where E_u, E_t are logarithmic strains in the load and transverse directions respectively. Since the material is incompressible, $E_t = -1/2 E_u$, and assuming that $\omega'(0) = 0$, Kearsley - Zapas inversion formula yields the exact solution of the functional unknown $\omega'(E)$ directly from the functional data $T(E)$,

$$\omega'(E) = \sum_{n=1}^{\infty} T((-1/2)^n E) \quad (3.9)$$

Therefore it is not necessary to impose an analytical predefined shape of the solution to solve the functional equation. Otherwise we would only find an approximative solution from fitting an analytical suggestion. This idea is expanded in the next article to compressible materials.

3.3 WYPiWYG data-driven extension to compressible hyper-elastic isotropic materials

As a natural extension of Eq.(3.7), langragian pressure-like incompressible term p is extended to energetic volumetric function $U'(E^v)$, whose argument is the volumetric strain E^v , logarithmic of jacobian,

$$E^v = \log(J) = \log(\lambda_1) + \log(\lambda_2) + \log(\lambda_3) = \sum_{i=1}^3 E_i \quad (3.10)$$

This extension implies a deviatoric - volumetric decomposition of the strains. Corresponding strain tensors are denoted as $\mathbf{E}^d$ and $\mathbf{E}^v$ respectively. The sum of both contributions yields the total strain tensor, $\mathbf{E} = \mathbf{E}^d + \mathbf{E}^v$. Taking into account the relation between jacobian and deviatoric stretch, $\lambda_i^d = \lambda_i J^{-1/3}$, we have for logarithmic principal strains,

$$E_i^d = E_i - 1/3 E^v \quad (3.11)$$

In this occasion, ω energy is expressed in terms of deviatoric principal strain arguments, E_i^d , and there is now a volumetric contribution that covers the compressible effects. In general the energy $\mathcal{W}$ is now,

$$\mathcal{W} = \sum_{i=1}^3 \omega(E_i^d) + \mathcal{U}(E^v) \quad (3.12)$$

These considerations make the compressible extension for the stress - strain tensorial equation be,

$$\frac{d\mathcal{W}}{d\mathbf{E}} = \frac{d\mathcal{W}}{d\mathbf{E}^d} : \frac{d\mathbf{E}^d}{d\mathbf{E}} + \frac{d\mathcal{W}}{d\mathbf{E}^v} : \frac{d\mathbf{E}^v}{d\mathbf{E}} \quad (3.13)$$

$$= \bar{\mathbf{T}}^d : \mathbb{P} + \bar{\mathbf{T}}^v : (\mathbb{I}^s - \mathbb{P}) \quad (3.14)$$

$$\mathbf{T} = \sum_{i=1}^3 \omega'(E_i^d) \mathbf{N}_i^d \otimes \mathbf{N}_i^d : \mathbb{P} - 1/3 \mathcal{U}'(E^v) \mathbf{I} \quad (3.15)$$

where $\mathbf{N}_i^d$ is the eigenvector of the deviatoric principal logarithmic strain i , $\mathbb{P}$ is the fourth order deviatoric projector tensor and $\mathbb{I}^s$ is the fourth order symmetric identity tensor. Under these considerations, if we would have available uniaxial test experimental results (functional data), then the stress-strain system of functional equations can be solved,

$$\omega'(E^d) = \sum_{n=1}^{\infty} \hat{T} \left((-1/2)^n E^d \right) \quad (3.16)$$

$$\mathcal{U}'(E^v) = 1/3 \bar{T}(E^v) \quad (3.17)$$

where, functions $\hat{T}, \bar{T}$ are built using experimental points x_i, y_i that are converted into functional representation via spline definition to $y(x)$, (i.e. $\{x_i, y_i\} \rightarrow y(x)$). That is,

$$\{[E_u - 1/3(E_u + 2E_t)], T_u\} = \{E_u^d, T_u\} \rightarrow \hat{T} \quad (3.18)$$

$$\{1/3(E_u + 2E_t), T_u\} = \{E^v, T_u\} \rightarrow \bar{T} \quad (3.19)$$

The richer experimental data points set $\{E_u, E_t, T_u\}$, the finer the spline functions $\hat{T}, \bar{T}$ become. Of course, experimental noise treatment is important for the shake of best accuracy of the method. It is important to remark that, since now there are two functional unknowns, a system of two functional equations are required, and therefore two functional data. In particular, such functional data can be the uniaxial experimental data sets of longitudinal strain vs. load set $\{E_u, T_u\}$, and longitudinal vs. transverse strains set $\{E_u, E_t\}$. Finally, it is a must that $\{E_u, E_t, T_u\}$ are synchronized for the same sample evaluation (e.g. same values of E_u for both sets, or pre-evaluation of E_t, T_u for the same common values E_u).

In the following article we include the following advances,

- Natural extension to compressible regime for hyperelastic isotropic material formulation
- WYPiWYG data-driven method for determining the functional unknowns of deviatoric contribution $\omega'(E^d)$ and volumetric one $\mathcal{U}'(E^v)$.
- Data treatment conversion of equibiaxial tests into uniaxial test and corresponding motivation to solve the system of functional equations.
- Comparison of results of the method with the conventional formulation of Neo-Hookean, Mooney - Rivlin, Ogden and Gent models. In particular, test curves predictions yielded by the models are used as reference to determine the corresponding $\omega'(E^d), \mathcal{U}'(E^v)$ unknown functions. Then WYPiWYG recovery test results are superimposed with the referential test pseudo-experimental

curves. Finally, WYPiWYG predictions are contrasted with model responses out of the referential frame (i.e. under general deformation conditions beyond referential uniaxial tests employed for WYPiWYG energy determination).

- Gradual recovery of incompressible regime and corresponding functional representation of $\omega(E^d), \mathcal{U}'(E^v)$.
- Experimental validation using experimental data of Blatz and Ko and their corresponding non Valanis - Landel formulation.
- FEA implementation of the WYPiWYG data-driven method for hyperelastic isotropic compressible materials.

WYPIWYG HYPERELASTICITY FOR ISOTROPIC, COMPRESSIBLE MATERIALS

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ABSTRACT

Nowadays the most common approach to model elastic behavior at large strains is through hyperelasticity. Hyperelastic models usually specify the shape of the stored energy function. This shape is modulated by some material parameters that are computed so the predicted stresses best fit the experimental data. Many stored energy functions have been proposed in the literature for isotropic and anisotropic materials, either compressible or incompressible. What-You-Prescribe-Is-What-You-Get (WYPIWYG) formulations present a different approach which may be considered an extension of the infinitesimal framework. The shape of the stored energy is not given beforehand but computed numerically from experimental data solving the equilibrium equations. The models exactly fit the experimental data without any material parameter. WYPIWYG procedures have comparable efficiency in finite element procedures as classical hyperelasticity. In this work we present a WYPIWYG numerical procedure for compressible isotropic materials and we motivate the formulation through an equivalent infinitesimal model.

Keywords Hyperelasticity · WYPIWYG hyperelasticity · Soft materials · Polymers · Biological tissues

1 Introduction

Rubber-like solids [1, 2, 3, 4] and soft biological materials [5, 6] are able to sustain large strains in many cases without relevant inelastic effects during loading. The behavior of these materials is frequently modelled as that of hyperelastic materials. Then, other effects may be added to the hyperelastic formulation as for example viscoelasticity or damage [1, 2, 4, 5, 6]. A hyperelastic model typically consists of an assumed stored energy function shape having some material parameters which are left free to be prescribed by the user. These material parameters are computed in such a way that the model predictions fit the available experimental data [3, 7, 8]. The typical procedure is to establish an error function between predictions and experimental data and then minimize that error employing an optimization

algorithm, for example, the Levenberg-Marquardt algorithm [7, 8]. Therefore, in the current usual procedure, a stored energy is proposed (either physically motivated or purely phenomenological) and that function is modulated as to fit experimental data from different types of tests presented to the model, see for example [8, 9, 10, 11]. The obvious purpose is to characterize the behavior of the material in any loading situation [12]. Thereafter the behavior from the resulting stored energy density is sometimes checked against the experimental data from other additional tests [13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. The models may be even modified in order to account for some experimental evidence [24]. This procedure is also employed in anisotropic materials, typically in biological tissues, see for example [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42], among many others.

The What-You-Prescribe-Is-What-You-Get (WYPIWYG) approach is very different from that employed in classical models. Instead of prescribing the shape of the stored energy, this shape is computed numerically from the presented experimental data, i.e. it is in essence a computational procedure instead of a purely analytical one. The WYPIWYG model for incompressible isotropic hyperelasticity compatible with the Valanis-Landel [43] decomposition is due to Sussman and Bathe [44]. This model uses the Kearsley and Zapas inversion formula [45] to exactly obtain the stored energy in a given number of points. Then the energy function is interpolated using piecewise cubic splines in order to have a piecewise analytical expression that may be used in a finite element program. The Sussman–Bathe WYPIWYG formulation is currently available in the commercial finite element program ADINA [46].

WYPIWYG models for incompressible transversely isotropic [47] and orthotropic materials [48] are due to Latorre and Montáns. These formulations use a generalization of the Inversion Formula and a separable form of the stored energy density similar to that of the infinitesimal framework but in functions of invariants of the logarithmic strains, which are a natural extension of the infinitesimal ones [49, 50, 51, 52]. The numerical efficiency of these procedures in finite element implementations is similar to that of traditional models, see [46] for the isochoric, isotropic formulation and [48, 53, 54] in the context of incompressible anisotropy. The WYPIWYG procedure has been extended to viscoelasticity [53, 54] and damage [55] in order to model the Mullins effect. WYPIWYG hyperelastic functions are obtained from a set of experimental data, either from true experiments or freely prescribed by the modeler. The proposed set of experimental data is a key ingredient of the procedure, because the equations from this set are solved in a numerically exact manner in order to extract the stored energy information. The experimental set must be complete so these experiments uniquely define the behavior of the material under the constitutive assumptions. This set is equivalent to the set of material constants of a comparable infinitesimal model [56, 57, 58].

The main difficulty of WYPIWYG hyperelasticity lies in the necessity of solving the differential equations of the proposed experiments. Hence the inclusion of different material symmetries or compressibility results in necessary nontrivial modifications of the overall computational procedure, i.e. WYPIWYG hyperelasticity is not a model, but a family of computational procedures. Classical hyperelasticity propose global solutions to the problem (as Rayleigh functions does in structural mechanics problems) and material parameters adapt that solution as to fit experimental data. On the contrary WYPIWYG hyperelasticity propose local interpolations (as the Galerkin method does in structural mechanics) between computed, numerically exact solutions to the problem, i.e. the energy derivatives. The point is that once the stored energy is obtained solving a complete set of experiments, it is valid and accurate (if the constitutive hypotheses are fulfilled) in any other loading situation, i.e. the material behavior is completely and uniquely determined.

The purpose of this paper is to extend the WYPIWYG approach to compressible isotropic materials. The model is capable of capturing a proper complete set of experimental data that defines the material behavior up to machine precision. Because WYPIWYG approaches are a natural extension of the infinitesimal framework, in the next section we present a comparable infinitesimal bilinear model just for motivation and to explain the number of experimental curves needed to properly define the material. Thereafter, keeping an instructive parallelism with the bilinear model, we introduce the computational procedure and describe possible experiments to practically determine the large strain hyperelastic model. We also explain how to perform the equivalence to uniaxial curves which may be set as the standard input data to the model in finite element programs.

Some demonstrative examples show that the model is capable of exactly capturing some stored energy functions published in the literature (Neohookean [59], Ogden [60, 61], Mooney [62], Hartmann–Neff [63]) using only their numerical stress-strain predictions for the uniaxial test as if they were “experimental data” of a real material. Then, the behavior of these models under any arbitrary loading conditions is also captured “exactly” (numerically speaking). This shows that if the real material were behaving as these models predict, we would also capture the behavior under any arbitrary type of loading. In another example we predict the uniaxial behavior of the stored energy from Gent [64]. We note that this model does not follow the Valanis-Landel decomposition, which is one of the assumptions of our procedure. However, because the Valanis-Landel decomposition is mathematically accurate for moderate large strains [3], we show that even in this case we are able to capture to a very high precision the behavior predicted by this model in any loading situation for those moderately large strains. To show the performance of our proposal to capture the behavior observed in actual materials, we use the experiments by Blatz and Ko [65] over compressible polyurethane

foam. The observed differences between our predictions and experimental data in a different test than those used to determine the stored energies are of the order of the measured experimental errors. We note that if that were not the case, the only possibility would be that at least one of the hypotheses (isotropy, hyperelastic behavior, Valanis-Landel) would not be applicable to this material. We thereafter verify that the incompressible WYPIWYG formulation of Sussman and Bathe is recovered as a particular case in the limit. In practical finite element implementations incompressibility is frequently enforced through penalty volumetric formulations which frequently result in numerically underconstrained problems at low strains or numerical conditioning problems at large strains. Then our procedure is also a natural way of properly enforcing quasi-incompressibility in finite element simulations at every strain level, hence circumventing this problem. We also show the performance in finite element simulations and the equivalence (even in terms of iterations and convergence values) to models based on analytical functions.

Finally we note that WYPIWYG anisotropic formulations (as any other anisotropic hyperelastic model) should recover the isotropic behavior when the experimental data presented to the model is that of an isotropic material [67]. The current proposal may be coupled to our incompressible transversely isotropic and orthotropic WYPIWYG models [47, 48] as described in [67] in order to obtain a compressible orthotropic model or to obtain a quasi-incompressible one with the incompressibility constraint adequately enforced at every strain level.

2 The infinitesimal bilinear model

As mentioned, the purpose of this section is to perform a parallelism of the nonlinear model with an infinitesimal model. To facilitate the comparisons with the large strain model we will consider initially that the material has different linear behavior in extension than in compression, because as we will see the nonlinear model evaluates functions in both ranges in the same equation. Then, of course, the linearized behavior of the nonlinear formulation at the origin is recovered if we make the slopes of both branches equal.

2.1 Basic model determination

Consider a bilinear infinitesimal isotropic and compressible material which nonlinearity simply consists in that it has different linear behavior under tension and compression. Let $\mathbf{I}$ be the second order identity tensor and $\mathbb{P}$ the fourth order projector tensor

$$\mathbb{P} := \mathbb{I}^s - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \quad (1)$$

where $\mathbb{I}^s$ is the symmetric fourth-order identity tensor. Let also $\varepsilon^v = \text{tr}(\boldsymbol{\varepsilon}) = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$ be the volumetric strain and $\varepsilon_i^d = \varepsilon_i - \frac{1}{3}\varepsilon^v$ be the principal deviatoric strains, whose principal directions are $\mathbf{N}_i$. Then the constitutive equations may be written in uncoupled volumetric-deviatoric fashion as

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^v + \boldsymbol{\sigma}^d = K_* \varepsilon^v \mathbf{I} + \boldsymbol{\sigma}^{|d} : \mathbb{P} \quad (2)$$

where $\boldsymbol{\sigma}$ is the stress tensor,

$$K_* = \begin{cases} K_t & \text{if } \varepsilon^v \geq 0 \\ K_c & \text{if } \varepsilon^v < 0 \end{cases} \quad (3)$$

is the bulk modulus and $\boldsymbol{\sigma}^{|d}$ is the modified stress tensor (generally non-deviatoric if $\mu_c \neq \mu_t$)

$$\boldsymbol{\sigma}^{|d} = \sum_{i=1}^3 \sigma_i^{|d} \mathbf{N}_i \otimes \mathbf{N}_i = \sum_{i=1}^3 (2\mu_* \varepsilon_i^d) \mathbf{N}_i \otimes \mathbf{N}_i \quad (4)$$

such that

$$\mu_* = \begin{cases} \mu_t & \text{if } \varepsilon_i^d \geq 0 \\ \mu_c & \text{if } \varepsilon_i^d < 0 \end{cases} \quad (5)$$

Thus, we take into account the possibility of different moduli in extension and compression. Note that we have four moduli to be determined. Then we need four (linear) independent semi-curves (two extension-compression curves) to determine such moduli. Assume that by some tests we can determine the behavior of the material under tension and compression, and that the experimental data is presented in the form of a uniaxial (tension-compression) test curve $\sigma_u(\varepsilon_u)$ (Young moduli Y_t and Y_c) and a uniaxial (tension-compression) test curve $\varepsilon_t(\varepsilon_u)$ (Poisson ratios ν_t and ν_c , see Figure 1) such that the slopes are—note that the subscript t means *transverse* in the strain variable ε_t but *tension* in the

Figure 1: Bilinear model. Left plot: stress-strain uniaxial bilinear behavior. Right plot: Transverse strains bilinear behavior.

material constants Y_t , ν_t , K_t and μ_t .

$$\begin{cases} Y_t = \sigma_u^+ / \varepsilon_u^+ & \text{for } \varepsilon_u^+ \geq 0 \\ Y_c = \sigma_u^- / \varepsilon_u^- & \text{for } \varepsilon_u^- < 0 \end{cases} \quad (6)$$

and

$$\begin{cases} \nu_t = -\varepsilon_t^+ / \varepsilon_u^+ & \text{for } \varepsilon_u^+ \geq 0 \\ \nu_c = -\varepsilon_t^- / \varepsilon_u^- & \text{for } \varepsilon_u^- < 0 \end{cases} \quad (7)$$

We have used $+$ and $-$ superscripts in order to emphasize the sign of the main (driving) strain ε_u . We will use this emphasizing notation when convenient. The four experimental moduli Y_t , Y_c , ν_t , ν_c determine the basic constitutive ones K_t , K_c , μ_t and μ_c .

For example, during extension in direction 1 the strains are

$$\begin{cases} \varepsilon_1 \equiv \varepsilon_u^+ > 0 & \text{and } \varepsilon_2 = \varepsilon_3 \equiv \varepsilon_t^+ < 0 \\ \varepsilon_u^{v+} = \varepsilon_1 + 2\varepsilon_2 > 0 \\ \varepsilon_u^{d+} \equiv \varepsilon_1^d = \frac{2}{3}(\varepsilon_1 - \varepsilon_2) > 0 \\ \varepsilon_2^d \equiv \varepsilon_3^d = -\frac{1}{3}(\varepsilon_1 - \varepsilon_2) < 0 \end{cases} \quad (8)$$

Then, the deviatoric stresses in compact Voigt notation are (just using the diagonal terms involved)

$$\boldsymbol{\sigma}^{|d} : \mathbb{P} = \begin{bmatrix} 2/3 & -1/3 & -1/3 \\ -1/3 & 2/3 & -1/3 \\ -1/3 & -1/3 & 2/3 \end{bmatrix} \begin{bmatrix} 2\mu_t \varepsilon_u^{d+} \\ 2\mu_c \varepsilon_t^{d+} \\ 2\mu_c \varepsilon_t^{d+} \end{bmatrix} \quad (9)$$

$$= \begin{bmatrix} \frac{2}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \\ -\frac{1}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \\ -\frac{1}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \end{bmatrix} \quad (10)$$

The equilibrium equations are

$$\begin{cases} \sigma_1 = K_t \varepsilon_u^{v+} + \frac{2}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \equiv \sigma_u^+ \\ 0 = K_t \varepsilon_u^{v+} - \frac{1}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \end{cases} \quad (11)$$

We can factor-out $K_t \varepsilon_u^{v+}$ from the second equation

$$K_t \varepsilon_u^{v+} = \frac{1}{3}(2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \quad (12)$$

and substitute in the first one to get

$$\sigma_u^+ = (2\mu_t \varepsilon_u^{d+} - 2\mu_c \varepsilon_t^{d+}) \quad \text{with } \varepsilon_u > 0 \quad (13)$$

or —note that K_t is not involved if we measure ε_t

$$\sigma_u^+ = 2\mu_t \left[\frac{2}{3} (\varepsilon_u^+ - \varepsilon_t^+) \right] - 2\mu_c \left[-\frac{1}{3} (\varepsilon_u^+ - \varepsilon_t^+) \right] \quad (14)$$

Note also that $\varepsilon_t^d = -\frac{1}{2}\varepsilon_u^d$ and

$$\sigma_u^+ = (2\mu_t + \mu_c) \varepsilon_u^{d+} \Rightarrow 2\mu_t + \mu_c = \frac{\sigma_u^+}{\varepsilon_u^{d+}} \quad (15)$$

Then combining Eqs. (11) and (12) we also have

$$K_t \varepsilon_u^{v+} = \sigma_u^+ / 3 \quad (16)$$

i.e. if the transverse strain is given by $\varepsilon_t = -\nu_t \varepsilon_u$ we obtain the expected relation

$$K_t = \frac{\sigma_u^+}{3(1-2\nu_t)\varepsilon_u^+} = \frac{Y_t}{3(1-2\nu_t)} \quad (17)$$

Since $(\varepsilon_u^+ - \varepsilon_t^+) = (1 + \nu_t) \varepsilon_u^+$, Identity (11)₁ can be written as

$$\sigma_1^+ = \left(\frac{2}{3} 2\mu_t + \frac{1}{3} 2\mu_c \right) (1 + \nu_t) \varepsilon_u^+ \equiv Y_t \varepsilon_u^+ \quad (18)$$

so we obtain

$$\frac{1}{3} (2\mu_t + \mu_c) = \frac{Y_t}{2(1 + \nu_t)} =: G_t \quad (19)$$

This relation should be familiar to the reader for the particular case $\mu_c = \mu_t$. It is evident that we need the compression part in order to fully determine the basic constitutive parameters because of the involvement of μ_c . These equations emphasize the need for the compression part to properly define the material [56].

Consider now the compression test in which the strains are

$$\left\{ \begin{array}{l} \varepsilon_1^- \equiv \varepsilon_u^- < 0 \text{ and } \varepsilon_2^- = \varepsilon_3^- \equiv \varepsilon_t^- > 0 \\ \varepsilon_u^{v-} = \varepsilon_1^- + 2\varepsilon_2^- < 0 \\ \varepsilon_u^{d-} \equiv \varepsilon_1^{d-} = \frac{2}{3} (\varepsilon_1^- - \varepsilon_2^-) < 0 \\ \varepsilon_2^{d-} \equiv \varepsilon_3^{d-} = -\frac{1}{3} (\varepsilon_1^- - \varepsilon_2^-) \equiv -\frac{1}{2} \varepsilon_1^{d-} > 0 \end{array} \right. \quad (20)$$

Performing the same algebraic manipulations as for the tension case

$$\sigma_u^- = 2\mu_c \varepsilon_u^{d-} - 2\mu_t \varepsilon_t^{d-} = (2\mu_c + \mu_t) \varepsilon_u^{d-} \quad (21)$$

and

$$K_c \varepsilon_u^{v-} = \sigma_u^- / 3 \quad (22)$$

If the transverse strain is given by $\varepsilon_t^- = -\nu_c \varepsilon_u^-$ we obtain again the expected relation for compression

$$K_c = \frac{\sigma_u^-}{3(1-2\nu_c)\varepsilon_u^-} = \frac{Y_c}{3(1-2\nu_c)} \quad (23)$$

2.2 Determination of the material constants from actual tests

Whereas the tensile test is easy to perform in soft materials, an unconfined compression test is not so reliable. An alternative in incompressible materials is to substitute the compression test by an equibiaxial test, which is completely equivalent in such incompressible case [56]. However, as we will see below, in the compressible case we need an additional test in order to present a complete, independent group of experimental data. The physical reason is that in the equibiaxial test the volume also expands as in the tensile test.

Consider the equibiaxial test equilibrium equations when the stretch is in directions 1 and 2, so —we do not need sign decoration because we will assume always an equibiaxial test in extension

$$\begin{cases} \varepsilon_1 = \varepsilon_2 \equiv \varepsilon_e > 0 \quad \text{and} \quad \varepsilon_3 \equiv \varepsilon_w < 0 \\ \varepsilon_e^v = 2\varepsilon_1 + \varepsilon_3 > 0 \\ \varepsilon_1^d \equiv \varepsilon_2^d = \frac{1}{3}(\varepsilon_1 - \varepsilon_3) \equiv \varepsilon_e^d > 0 \\ \varepsilon_3^d = -\frac{2}{3}(\varepsilon_1 - \varepsilon_3) \equiv -2\varepsilon_1^d = \varepsilon_w^d < 0 \end{cases} \quad (24)$$

Then

$$\sigma^{ld} : \mathbb{P} = \begin{bmatrix} \frac{1}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \\ \frac{1}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \\ -\frac{2}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \end{bmatrix} \quad (25)$$

So the equilibrium equations are

$$\sigma_e \equiv \sigma_1 = K_t\varepsilon_e^v + \frac{1}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \equiv B_t\varepsilon_e \quad (26)$$

$$0 = K_t\varepsilon_e^v - \frac{2}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \quad (27)$$

where B_t is the tensile equibiaxial stiffness modulus. Obviously we can again factor-out $K_t(\varepsilon_e^v)$ from the second equation

$$K_t\varepsilon_e^v = \frac{2}{3}(2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d) \quad (28)$$

and substitute in the first equation

$$\sigma_e = 2\mu_t\varepsilon_e^d - 2\mu_c\varepsilon_w^d = 2\mu_t\varepsilon_e^d - 2\mu_c(-2\varepsilon_e^d) \quad (29)$$

$$= (2\mu_t + 4\mu_c)\varepsilon_e^d \quad \text{with } \varepsilon_e > 0 \quad (30)$$

or

$$\sigma_e = \frac{2}{3}[\mu_t(\varepsilon_e - \varepsilon_w) + 2\mu_c(\varepsilon_e - \varepsilon_w)] \quad (31)$$

so —cf. Eq. (16)

$$K_t\varepsilon_e^v = 2\sigma_e/3 \quad (32)$$

i.e. using $\varepsilon_e^v = (2 - \nu_e)\varepsilon_e$, where ν_e is the Poisson-like equibiaxial ratio (with value of $\nu_e = 2$ for the incompressible case)

$$K_t = \frac{B_t}{3(1 - \nu_e/2)} = \frac{Y_t}{3(1 - 2\nu_t)} \quad (33)$$

If we compare Eq. (29) with Eq. (21) we can define the uniaxial equivalence

$$\frac{-\sigma_e}{-2\varepsilon_e^d} = 2\mu_c + \mu_t = \frac{\sigma_u^-}{\varepsilon_u^{d-}} \quad (34)$$

We now use the underline decoration to emphasize for future reference that they are functions with different dependency but with the same numerical value for equivalent arguments, i.e. underlined functions have deviatoric strains as arguments. We also use the bracketed subindex (u) to emphasize that they are uniaxial-equivalent values obtained from equibiaxial ones; i.e.

$$\underline{\sigma}_{(u)}^-(-2\varepsilon_e^d) = -\underline{\sigma}_e(\varepsilon_{(u)}^{d-}) \quad \text{with } \underline{\sigma}_e > 0 \text{ so } \underline{\sigma}_{(u)}^- < 0 \quad (35)$$

Note that $\varepsilon_{(u)}^{d-} = \varepsilon_w^d$, i.e. the uniaxial equivalent deviatoric strains are the transverse equibiaxial deviatoric deformations

$$\varepsilon_{(u)}^{d-} = \varepsilon_w^d = -2\varepsilon_e^d = -\frac{2}{3}(\varepsilon_e - \varepsilon_w) \quad \text{with } \varepsilon_{(u)} < 0 \quad (36)$$

Comparing the moduli—cf. Eq. (21)

$$\underline{\sigma}_{(u)} = -\underline{\sigma}_e = (\mu_t + 2\mu_c)(-2\varepsilon_e^d) \equiv (\mu_t + 2\mu_c)\varepsilon_{(u)}^{d-} \quad (37)$$

$$= Y_c\varepsilon_{(u)}^- = -B_t\varepsilon_e \quad (38)$$

We remark that this equivalence is established only with the deviatoric strains, i.e. $\underline{\sigma}_{(u)}^- \left(\varepsilon_{(u)}^{d-} \right)$. In order to complete the equivalence, i.e. determine $\sigma_{(u)}^- \left(\varepsilon_{(u)}^- \right)$, we need the volumetric part which we obtain below. It is immediate to show that

$$\frac{B_t}{2(1+\nu_e)} = \frac{Y_c}{2(1+\nu_c)} = G_c \quad (39)$$

which clearly explains that equibiaxial and compression tests are equivalent *in deviatoric terms*. On the contrary, in volumetric terms Eq. (33) shows that the equibiaxial test is equivalent to a tensile test. Then note that from the equibiaxial test we cannot obtain K_c . If we cannot assume that $K_c = K_t$, for the remaining needed test to compute K_c we can consider a confined compression test which can be easily performed in soft materials. In this case, if we perform the test in direction 1

$$\begin{cases} \varepsilon_1 < 0 \quad \text{and} \quad \varepsilon_2 = \varepsilon_3 = 0 \\ \varepsilon^v = \varepsilon_1 < 0 \\ \varepsilon_1^d = \frac{2}{3}\varepsilon_1 < 0 \\ \varepsilon_3^d = \varepsilon_2^d = -\frac{1}{3}\varepsilon_1 > 0 \end{cases} \quad (40)$$

and

$$\boldsymbol{\sigma}^{ld} : \mathbb{P} = \begin{bmatrix} \frac{8}{9}\varepsilon_1\mu_c + \frac{4}{9}\varepsilon_1\mu_t \\ -\frac{4}{9}\varepsilon_1\mu_c - \frac{2}{9}\varepsilon_1\mu_t \\ -\frac{4}{9}\varepsilon_1\mu_c - \frac{2}{9}\varepsilon_1\mu_t \end{bmatrix} \quad (41)$$

The equilibrium equation in the main axis is

$$\sigma_1 = \left[K_c + \frac{4}{9}2\mu_c + \frac{2}{9}2\mu_t \right] \varepsilon_1 = D_c \varepsilon_1 \quad (42)$$

where D_c is the confined compressibility modulus. Then, since we already know G_c from the equibiaxial test we can factor-out K_c

$$K_c = D_c - \frac{4}{9}(2\mu_c + \mu_t) = D_c - \frac{2}{3} \left[2\mu_c \frac{2}{3} - 2\mu_t \left(-\frac{1}{3} \right) \right] \quad (43)$$

In order to complete the equivalence to the compression branch of the uniaxial test, note that using Eq. (22) and Eq. (37), we can obtain the uniaxial equivalent volumetric strain obtained from the modulus of Eq. (43) and the equivalent stresses of the equibiaxial test

$$\varepsilon_{(u)}^{v-} = K_c^{-1} \left(\underline{\sigma}_{(u)}^- / 3 \right) \quad (44)$$

Finally the equivalence is built as follows from the pairs $(\sigma_e, \varepsilon_e)$ and $(\varepsilon_w, \varepsilon_e)$

$$\begin{aligned} & \left. \begin{aligned} \varepsilon_w \rightarrow \varepsilon_e^d &= \frac{1}{3}(\varepsilon_e - \varepsilon_w) \rightarrow \varepsilon_{(u)}^{d-} = -2\varepsilon_e^d \\ \sigma_e \rightarrow \underline{\sigma}_{(u)}^- &= -\sigma_e \rightarrow \varepsilon_{(u)}^{v-} = K_c^{-1} \underline{\sigma}_{(u)}^- / 3 \end{aligned} \right\} \\ & \Rightarrow \left\{ \begin{aligned} \varepsilon_{(u)}^- &= \frac{1}{3}\varepsilon_{(u)}^{v-} + \varepsilon_{(u)}^{d-} \\ \varepsilon_{(t)}^- &= \frac{1}{3}\varepsilon_{(u)}^{v-} - \frac{1}{2}\varepsilon_{(u)}^{d-} \end{aligned} \right\} \Rightarrow \left\{ \begin{aligned} \sigma_{(u)}^- &\left(\varepsilon_{(u)}^- \right) \\ \varepsilon_{(t)}^- &\left(\varepsilon_{(u)}^- \right) \end{aligned} \right\} \end{aligned} \quad (45)$$

In summary, we can choose to obtain μ_t , μ_c , K_t and K_c directly from the complete set of tests (tensile, equibiaxial and confined compression), or from the complete uniaxial curves. As a handy alternative for standard plotting and to unify the input to the codes, the former case can be converted to the latter using the described equivalence procedure.

We now extend these ideas to large strains by use of the inversion formula.

3 The inversion formula

The formulation we will introduce in the next section is solved through a generalization of the Kearsley and Zapas inversion formula which we introduced in Ref. [47]. Assume three functions $f(x)$, $g(x)$ and $h(x)$ related by

$$f(x) = g(x) - g(h(x)) \quad (46)$$

Then, we can also write

$$f(h(x)) = g(h(x)) - g(h(h(x))) \quad (47)$$

$$f(h(h(x))) = g(h(h(x))) - g(h(h(h(x)))) \quad (48)$$

...

$$f(h^{(k)}(x)) = g(h^{(k)}(x)) - g(h^{(k+1)}(x)) \quad (49)$$

...

where

$$h^{(k)}(x) = \underbrace{h(h(\dots h(x)))}_{k \text{ times}} \quad (50)$$

is a recursive function and we define $h^{(0)}(x) = x$. Then adding $K + 1$ equations

$$g(x) - g(h^{(K+1)}(x)) = \sum_{k=0}^K f(h^{(k)}(x)) \quad (51)$$

If $h^{(K)}(x) \rightarrow 0$ and $f(0) = 0$, the series converge up to machine precision (i.e. numerically exact) in a finite number of K addends. Equation (51) is the general inversion formula, first derived in Reference [47]. The elegant layout of the proof as given this Section is due to Sussman, which improved our original, lengthier proof. In the case $h^{(\infty)}(x) \rightarrow 0$, an alternative inversion formula is possible just considering

$$f(h^{(-1)}(x)) = g(h^{(-1)}(x)) - g(x) \quad (52)$$

where $h^{(-1)}(h(x)) = x$.

4 WYPIWYG isotropic compressible hyperelasticity

In this section we extend the previous concepts to large strain hyperelasticity within the What-You-Prescribe-Is-What-You-Get realm. The formulation is based on the Valanis-Landel decomposition and a volumetric decoupling in the form

$$\Psi(E_1, E_2, E_3) = \mathcal{U}(E^v) + \mathcal{W}(E_1^d, E_2^d, E_3^d) \quad (53)$$

$$= \mathcal{U}(E^v) + \omega(E_1^d) + \omega(E_2^d) + \omega(E_3^d) \quad (54)$$

where E_i are the principal logarithmic strains,

$$E^v := E_1 + E_2 + E_3 = \ln J \quad (55)$$

is the volumetric logarithmic strain (the logarithm of the Jacobian determinant J of the deformation gradient $\mathbf{X}$) and E_i^d are the deviatoric logarithmic strains, i.e.

$$E_i^d := E_i - \frac{1}{3}E^v \quad (56)$$

The (rotated or generalized [66]) Kirchhoff principal stresses are

$$\bar{\tau}_i \equiv T_i = \frac{\partial \Psi(E_1, E_2, E_3)}{\partial E_i} \quad (57)$$

$$= \frac{d\mathcal{U}(E^v)}{dE^v} \frac{\partial E^v}{\partial E_i} + \sum_{j=1}^3 \frac{d\omega(E_j^d)}{dE_j^d} \frac{\partial E_j^d}{\partial E_i} \quad (58)$$

where

$$\frac{\partial E^v}{\partial E_i} = 1 \quad \text{and} \quad \frac{\partial E_j^d}{\partial E_i} = \delta_{ij} - \frac{1}{3} \quad (59)$$

In tensor notation —cf. Eq. (2)

$$\mathbf{T} = \mathbf{T}^v + \mathbf{T}^d = \mathcal{U}' \mathbf{I} + \mathbf{T}^d : \mathbb{P} \quad (60)$$

Figure 2: Nonlinear compressible isotropic hyperelasticity. Left plot: nonlinear stress-strain behavior. Right plot: nonlinear relation between transverse and uniaxial strains. Compare with Figure 1.

where $\mathbf{T}^d := \mathbf{T}^{|d} : \mathbb{P}$ is the corresponding deviatoric stress tensor and $\mathbf{T}^{|d}$ is the modified stress tensor —cf. Eq. (4)

$$\mathbf{T}^{|d} := \frac{d\mathcal{W}}{d\mathbf{E}^d} = \sum_{i=1}^3 \omega'(E_i^d) \mathbf{N}_i \otimes \mathbf{N}_i = \sum_{i=1}^3 T_i^{|d} \mathbf{N}_i \otimes \mathbf{N}_i \quad (61)$$

In this equation $\mathbf{N}_i$ are the principal stress (and strain) directions, so $\mathbf{T}^{|d}$ is a second-order tensor with the same eigenvectors as $\mathbf{T}^d$, $\mathbf{T}$ and $\mathbf{E}$.

The purpose of the computational procedure is to obtain the stored energy derivative functions $\omega'(E^d)$ and $\mathcal{U}'(E^v)$ from some given stress-strain measured data. As we have seen in the previous section, we need to assume two complete “experimental” (prescribed by the modeller) “curves” (actually discrete pairs of data), namely $\tilde{\mathbf{T}}_u(\tilde{\mathbf{E}}_u) \equiv \tilde{\tau}_u(\tilde{\mathbf{E}}_u)$ and $\tilde{\mathbf{E}}_t(\tilde{\mathbf{E}}_u)$, where $\tilde{\mathbf{E}}_u$ is the array of discrete, experimental, uniaxial (logarithmic) strain measurements, $\tilde{\tau}$ is the array of corresponding Kirchhoff stresses and $\tilde{\mathbf{E}}_t$ is the array of corresponding transverse strains, see Figure 2, i.e. $\tilde{\tau}_p$ and $\tilde{E}_{tp}$ are the measured axial Kirchhoff stress and transverse strain at the uniaxial strain $\tilde{E}_{up}$, with $p = 1, \dots, P$. We will use the *tilde* decoration to denote measured experimental discrete values.

Consider the uniaxial extension test performed in direction 1 in which the driving variable is $E_u \equiv E_1$. The compatibility equations yield —cf. Eq. (8)

$$\begin{cases} E_u \equiv E_1 \quad \text{and} \quad E_t \equiv E_2 = E_3 \\ E_u^v(E_u) = E_1 + 2E_2(E_1) \\ E_u^d(E_u) \equiv E_1^d(E_1) = \frac{2}{3}(E_1 - E_2(E_1)) \\ E_t^d(E_u) = \frac{1}{3}(E_2(E_1) - E_1) = -\frac{1}{2}E_u^d(E_u) \end{cases} \quad (62)$$

so the deformation state is characterized by both the uniaxial strain E_u and the transverse strain $E_t(E_u)$, which may be a nonlinear function. The constitutive equations together with the equilibrium ones give —cf. Eq. (11)

$$\begin{cases} T_u(E_u) = \mathcal{U}'(E_u^v(E_u)) + \frac{2}{3}[\omega'(E_u^d(E_u)) - \omega'(E_t^d(E_u))] \\ 0 = \mathcal{U}'(E_u^v(E_u)) - \frac{1}{3}[\omega'(E_u^d(E_u)) - \omega'(E_t^d(E_u))] \end{cases} \quad (63)$$

Note that we are explicitly keeping in the notation the functional dependencies on the main, driving strain E_u . From Eq. (63)₂ we can factor-out $\mathcal{U}'(E_u^v(E_u))$ —cf. Eq. (12)

$$\mathcal{U}'(E_u^v(E_u)) = \frac{1}{3}[\omega'(E_u^d(E_u)) - \omega'(E_t^d(E_u))] \quad (64)$$

and substitute into Eq. (63)₁ to obtain

$$T_u(E_u) = \omega'(E_u^d(E_u)) - \omega'(E_t^d(E_u)) \quad (65)$$

Equation (65) can be compared to Eq. (13), see interpretation in Figure 3. Note that Eq. (13) is the linearized model if we take $2\mu_c = 2\mu_t = 2\mu$, i.e. the slope of ω' at the origin. In fact $\omega''/2$ presents the evolution of the instantaneous

Figure 3: Conceptual comparison of the nonlinear model with the bilinear one. The slope of ω' at the origin is the linearized modulus 2μ . The curve ω'' represents the evolution of such modulus.

shear modulus at each deviatoric strain value. Because the assumed one-to-one relation in Eq. (62)₃ between E_u^d and E_u for this test we can define the new functional dependence $\underline{T}_u(E_u^d(E_u)) = T_u(E_u)$, numerically equal for different arguments, so now we have the same dependences

$$\underline{T}_u(E_u^d(E_u)) = \omega'(E_u^d(E_u)) - \omega'(-\frac{1}{2}E_u^d(E_u)) \quad (66)$$

i.e.—cf. Eq. (13)

$$\underline{T}_u(\frac{2}{3}(E_u - E_t)) = \omega'(\frac{2}{3}(E_u - E_t)) - \omega'(-\frac{1}{3}(E_u - E_t)) \quad (67)$$

Then, we can also determine $\mathcal{U}'$ as—cf. Eq. (16)

$$\begin{aligned} \mathcal{U}'(E_u^v(E_u)) &= \frac{1}{3} [\omega'(E_u^d(E_u)) - \omega'(E_t^d(E_u))] \\ &= T_u(E_u)/3 \end{aligned} \quad (68)$$

Note that $\mathcal{U}'(E_u^v(E_u)) = \mathcal{U}'(E_u + 2E_t(E_u))$ is determined directly from $T_u(E_u)$ with the knowledge of $E_t(E_u)$. On the other hand, the function $\omega'(E^d)$ in Eq. (66) may be obtained at $E_u^d(E_u)$ from the Inversion Formula Eq. (51) as

$$\omega'(E_u^d(E_u)) = \sum_{k=0}^K \underline{T}_u\left(\left(-\frac{1}{2}\right)^k E_u^d(E_u)\right) \quad (69)$$

We have set the reference at $T_u(0) = 0$ and $\omega'(0) = 0$ —note that the actual value of $\omega'(0)$ in the previous equations is not relevant.

The relation $E_t(E_u)$ has already been used in the computation of $\underline{T}_u(E_u^d(E_u))$. Note that T_u may be obtained from the tensile-test nominal stresses P_u as $P_u = T_u/\lambda_u = T_u \exp(-E_u)$. It is also important to note that both the tension and the compression parts of the uniaxial test are needed in Eq. (69) to determine ω' , see Ref. [56]. The need for the compression data includes herein the additional data for the relation $E_t(E_u < 0)$ as to properly evaluate $E_u^d(E_u)$ for $E_u < 0$. Furthermore, this expression needs the evaluation of T_u at different values of E_u which do not necessarily are coincident with those given by the experimental (discrete) data points $\tilde{E}_u$. Hence, some kind of interpolation is needed.

We use piece-wise cubic splines in order to interpolate the data sets $\tilde{T}_u(\tilde{E}_u)$ and $\tilde{E}_t(\tilde{E}_u)$. With these interpolations we obtain smooth piecewise continuous functions $T_u(E_u)$ and $E_t(E_u)$. If the experimental data present some dispersion, but we require the functions $T_u(E_u)$ and $E_t(E_u)$ to have some degree of smoothness, the “experimental” spline functions would not necessarily pass through the truly measured data points $\tilde{T}_u(\tilde{E}_u)$ and $\tilde{E}_t(\tilde{E}_u)$. We remark that the resulting smooth functions $T_u(E_u)$ and $E_t(E_u)$ constitute the actual “experimental” data *prescribed* by the user and *gotten* by the WYPIWYG procedure. Subsequently, a new discretized domain $\bar{E}_u$ is employed (say 50 equispaced $\bar{E}_{up}$, $p = 1, \dots, 50$ points) in order to obtain the respective volumetric and deviatoric strain point sets $\bar{E}_u^d$ and $\bar{E}_u^v$ using the smoothed spline function $E_t(E_u)$, see Eqs. (62)₂ and (62)₃, and the corresponding stress point set $\bar{T}_u$ using the smoothed spline function $T_u(E_u)$. We note that the strain point sets $\bar{E}_u^d$ and $\bar{E}_u^v$ are not equispaced if $E_t(E_u)$ is non linear, so further independent discretizations may be considered. With the pairs $\{\bar{E}_u^v, \bar{T}_u/3\}$ we directly compute the discrete solution values $\bar{\mathcal{U}}'(\bar{E}_u^v)$ from Eq. (68). With the pairs $\{\bar{E}_u^d, \bar{T}_u\}$ we build the non-uniform spline $\underline{T}_u(E_u^d)$, which is to be used in the inversion formula of Eq. (69) in order to compute the discrete solution values

$\bar{\omega}'(\bar{\mathbf{E}}_u^v) \equiv \bar{\mathbf{T}}^{\prime d}(\bar{\mathbf{E}}_u^v)$. Once the data point sets $\bar{\mathbf{U}}'(\bar{\mathbf{E}}_u^v)$ and $\bar{\omega}'(\bar{\mathbf{E}}_u^d)$ are known, the piecewise spline interpolations $\mathcal{U}'(E^v)$ and $\omega'(E^d)$ are performed, which should be re-built in order to obtain the final uniform first-derivative spline functions. Note that the impact of using piecewise splines in actual finite element simulations is negligible in terms of computational time if their domain breaks are evenly spaced because the corresponding cubic spline may be directly addressed. The stored energy first-derivative functions are determined before running any finite element simulation and then their spline coefficients saved in memory. The memory needs to save the piecewise spline coefficients are the main disadvantage of WYPIWYG procedures. However, this memory necessity is a very low share of the memory used in a typical finite element problem.

The overall computational procedure is

$$\begin{aligned}
 & \left. \begin{array}{l} \text{Experim.} \\ \text{data pairs:} \\ \left\{ \bar{\mathbf{E}}_u, \bar{\mathbf{T}}_u \right\} \\ \left\{ \bar{\mathbf{E}}_u, \bar{\mathbf{E}}_t \right\} \end{array} \right\} \xrightarrow{\text{Smooth splines}} \left. \begin{array}{l} \text{Spline funct.:} \\ T_u(E_u) \\ E_t(E_u) \end{array} \right\} \xrightarrow[\text{at each } \bar{E}_{up}]{\text{Eq. (62)}} \\
 & \rightarrow \left. \begin{array}{l} \text{Resampled} \\ \text{pairs(*)} \\ \left\{ \bar{\mathbf{E}}_u, \bar{\mathbf{T}}_u \right\} \\ \left\{ \bar{\mathbf{E}}_u, \bar{\mathbf{E}}_u^v \right\} \\ \left\{ \bar{\mathbf{E}}_u, \bar{\mathbf{E}}_u^d \right\} \end{array} \right\} \xrightarrow{\text{Spline interp.}} \left. \begin{array}{l} \text{New spline funct.:} \\ \underline{T}_u(E_u^d) \end{array} \right\} \rightarrow \\
 & \xrightarrow[\text{at each } \bar{E}_{up}, \text{ using also (*)}]{\text{Eqs. (68) \& (69)}} \left. \begin{array}{l} \left\{ \bar{\mathbf{E}}_u^v, \bar{\mathbf{U}}' \right\} \\ \left\{ \bar{\mathbf{E}}_u^d, \bar{\omega}' \right\} \end{array} \right\} \xrightarrow{\text{Spline interp.}} \left. \begin{array}{l} \mathcal{U}'(E^v) \\ \omega'(E^d) \end{array} \right\}
 \end{aligned}$$

A more detailed explanation of the WYPIWYG procedures layout may be found in Ref. [48], so we omit here those details.

Note that once determined, $\mathcal{U}'(E^v)$ and $\omega'(E^d)$ uniquely define the behavior of the material in any loading situation if it fulfills the constitutive assumptions. In this general loading case, it simply suffices to obtain the stretch tensor $\mathbf{U}$ of the deformation gradient $\mathbf{X}$, extract the eigenvectors $\mathbf{N}_i$ and eigenvalues λ_i , define the logarithmic strains $E_i = \ln \lambda_i$, compute the volumetric and deviatoric parts using Eqs. (55) and (56), and apply Eq. (58) to obtain the principal stresses T_i or Eq. (60) to obtain $\mathbf{T}$.

As mentioned, since in soft materials it is usually difficult to perform accurate uniaxial compression tests, it is frequently the case when alternative tests are devised. In the next section we show how to convert data from the more convenient equibiaxial and confined uniaxial tests to the compression branch of the uniaxial tensile test.

5 Conversion of equibiaxial and confined compression test data to uniaxial data

The strains during an equibiaxial test in axes 1 and 2, with $E_1 > 0$, are

$$\begin{cases} E_e^v(E_1) = 2E_1 + E_3(E_1) > 0 \\ E_e^d(E_1) \equiv E_1^d(E_1) = \frac{1}{3}[E_1 - E_3(E_1)] > 0 \\ E_w^d(E_1) \equiv -\frac{2}{3}[E_1 - E_3(E_1)] \equiv -2E_1^d(E_1) < 0 \end{cases} \quad (70)$$

The equibiaxial test equilibrium and constitutive equations under the aforementioned hypotheses (isotropy and Valanis-Landel form) are

$$\begin{cases} T_1(E_1) = \mathcal{U}'(E_e^v(E_e)) + \frac{1}{3}[\omega'(E_e^d(E_e)) - \omega'(E_w^d(E_e))] \equiv T_e(E_e) \\ T_2(E_2) = \dots \equiv T_e(E_e) \\ T_3 \equiv 0 = \mathcal{U}'(E_e^v(E_e)) - \frac{2}{3}[\omega'(E_e^d(E_e)) - \omega'(E_w^d(E_e))] \end{cases} \quad (71)$$

Form the third equation we can factor out —cf. Eq. (28)

$$\mathcal{U}'(E_e^v(E_e)) = \frac{2}{3}[\omega'(E_e^d(E_e)) - \omega'(E_w^d(E_e))] \quad (72)$$

and using the first equation —cf. Eq. (32)

$$\mathcal{U}'(E_e^v(E_e)) = 2T_e(E_e)/3 \quad (73)$$

Note that $E_e^v(E_e)$ is computed from E_e and from the measured $E_w(E_e)$. On the other hand, Eqs. (70) and (73) also bring

$$T_e(E_e) = \omega'(E_e^d(E_e)) - \omega'(-2E_e^d(E_e)) \quad (74)$$

Compare this equation with Identity (29)₂ and note again that the linearized case is obtained for $2\mu_t = 2\mu_c = 2\mu$, where 2μ is the tangent of ω' at the origin. Defining a new function $\underline{T}_e(E_e^d(E_e)) = T_e(E_e)$,

$$\underline{T}_e(E_e^d(E_e)) = \omega'(E_e^d(E_e)) - \omega'(-2E_e^d(E_e)) \quad (75)$$

If we perform the same conversions as we did in the infinitesimal model, with $E_e \geq 0$, so $E_{(u)}^{d-} \leq 0$, we have

$$E_{(u)}^{d-}(E_e) = E_w^d(E_e) = -2E_e^d(E_e) = -\frac{2}{3}[E_e - E_w(E_e)] \quad (76)$$

and —cf. Eq. (35)

$$\underline{T}_{(u)}^-(-2E_e^d(E_e)) = -\underline{T}_e(E_{(u)}^{d-}(E_e)) \quad (77)$$

with $\underline{T}_e \geq 0$ so $\underline{T}_{(u)} < 0$. Thus can write

$$\underline{T}_{(u)}^-(E_{(u)}^{d-}(E_e)) = \omega'(E_{(u)}^{d-}(E_e)) - \omega'(-\frac{1}{2}E_{(u)}^{d-}(E_e)) \quad (78)$$

This equation can be compared to Eq. (66), which solution is given in Eq. (69), i.e. for $E_{(u)}^{d-} < 0$

$$\omega'(E_{(u)}^{d-}(E_e)) = \sum_{k=0}^K \underline{T}_{(u)}^- \left(\left(-\frac{1}{2}\right)^k E_{(u)}^{d-}(E_e) \right) \quad (79)$$

which is identical to that of the extension branch. Then, it is sufficient to apply Equivalences (76) and (77) to the experimental data and we recover the (*stem*) case of the previous section. However note that as it happened with the infinitesimal formulation, we still have not completely defined the transformation because we need the volumetric part to obtain $E_{(u)}^-$.

On the other hand we have only defined $\mathcal{U}'(E^v)$ for $E^v \geq 0$ because the sign in the volumetric change in both the tensile and equibiaxial tests is the same —recall the bilinear case, Eq. (39). For a general loading situation in which volumetric compression may be expected, we need to define $\mathcal{U}'(E^v)$ for $E^v < 0$ or otherwise make a reasonable assumption on it. We also need this correspondence to complete the transformation of the experimental data to the compression branch of the uniaxial (tensile) test.

In the confined compression test in direction 1, the strain field is given by $E_1 \equiv E_c \leq 0$ and $E_2 = E_3 = 0$. Then

$$\begin{cases} E^v(E_c) = E_c \\ E_1^d(E_c) = \frac{2}{3}E_c \\ E_2^d(E_c) \equiv -\frac{1}{3}E_c \equiv E_3^d(E_c) \end{cases} \quad (80)$$

and the first equation gives —cf. Identity (43)₂

$$\mathcal{U}'(E_c) = T_c(E_c) - \frac{2}{3}[\omega'(\frac{2}{3}E_c) - \omega'(-\frac{1}{3}E_c)] \quad (81)$$

Since the last addend is already known from the tensile and equibiaxial tests, $T_c(E_c)$ determines $\mathcal{U}'(E_c)$ for values $E_c \equiv E^v \leq 0$.

Now, with the knowledge of $\mathcal{U}'(E^v)$ for $E^v \leq 0$ we can complete the equivalence computing the uniaxial transverse strains $E_{(t)}(E_{(u)})$ for $E_{(u)} \leq 0$. Indeed Eq. (68) brings —cf. Eq. (44)

$$E_{(u)}^{v-}(E_{(u)}^-) = \mathcal{U}'^{(-1)}\left(\frac{1}{3}\underline{T}_{(u)}^-\right) \quad (82)$$

where $\mathcal{U}'^{(-1)}$ denotes the inverse function of $\mathcal{U}'$ (i.e. such that $\mathcal{U}'^{(-1)}\mathcal{U}'(*) = *$) which is easily performed within the piecewise spline context. Note the dependencies $\underline{T}_{(u)}^-(E_{(u)}^{d-})$. Using Eq. (62)₂

$$E_{(t)}^-(E_{(u)}^-) = \frac{1}{2} \left[E_{(u)}^{v-}(E_{(u)}^-) - E_{(u)}^- \right] \quad (83)$$

Then, the computational procedure is summarized as in (45)

$$\begin{aligned} & \left. \begin{aligned} E_w(E_e) &\rightarrow E_e^d = \frac{1}{3}(E_e - E_w(E_e)) \rightarrow E_{(u)}^{d-} = -2E_e^d \\ T_e(E_e) &\rightarrow \underline{T}_{(u)}^- = -T_e \rightarrow E_{(u)}^{v-} = \mathcal{U}'^{(-1)}\left(\frac{1}{3}\underline{T}_{(u)}^-\right) \end{aligned} \right\} \\ \Rightarrow & \left\{ \begin{aligned} E_{(u)}^- &= \frac{1}{3}E_{(u)}^{v-} + E_{(u)}^{d-} \\ E_{(t)}^- &= \frac{1}{3}E_{(u)}^{v-} - \frac{1}{2}E_{(u)}^{d-} \end{aligned} \right\} \Rightarrow \left\{ \begin{aligned} T_{(u)}^-(E_{(u)}^-) \\ E_{(t)}^-(E_{(u)}^-) \end{aligned} \right\} \end{aligned} \quad (84)$$

6 Tangent moduli

Once the stored energy density function derivatives $\mathcal{U}'$ and ω' have been obtained, the tangent moduli are exactly the same as in any formulation employing the compressible Valanis-Landel decomposition. The tangent moduli may be easily obtained in $\mathbf{T} - \mathbf{E}$ form and then converted to any other pair of stress-strain measures through the adequate mapping tensors [66]. In general, using Eq. (54) the stress tensor $\mathbf{T} = \mathbf{T}^v + \mathbf{T}^d$ may be obtained as in Eq. (60). Then, using —see for example [55]

$$\begin{aligned} \mathbb{C}^{ld} &:= \frac{d\mathbf{T}^{ld}}{d\mathbf{E}^d} = \frac{d^2\mathcal{W}}{d\mathbf{E}^d d\mathbf{E}^d} \\ &= \sum_{i=1}^3 \omega''(E_i^d) \mathbf{M}_i \otimes \mathbf{M}_i + \sum_{i=1}^3 \sum_{j \neq i}^3 \frac{T_j^d - T_i^d}{E_j^d - E_i^d} \mathbf{M}_{ij} \otimes \mathbf{M}_{ij} \end{aligned} \quad (85)$$

with

$$\mathbf{M}_i := \mathbf{N}_i \otimes \mathbf{N}_i \text{ and } \mathbf{M}_{ij} := \frac{1}{2}(\mathbf{N}_i \otimes \mathbf{N}_j + \mathbf{N}_j \otimes \mathbf{N}_i) \quad (86)$$

the constitutive tangent is obtained as

$$\mathbb{C} = \frac{d\mathbf{T}}{d\mathbf{E}} = \frac{d^2\Psi}{d\mathbf{E}d\mathbf{E}} = \mathcal{U}''(E^v) \mathbf{I} \otimes \mathbf{I} + \mathbb{P} : \mathbb{C}^{ld} : \mathbb{P} \quad (87)$$

Note that the derivatives of the stored energy function densities are spline derivatives (i.e. local polynomials). WYPI-WYG models have comparable efficiency to traditional hyperelastic models in finite element simulations; see Ref. [48].

7 Examples

As mentioned, the model captures to any desired numerical precision the behavior of hyperelastic materials which fulfill the separability hypothesis of the strain energy function proposed by Valanis and Landel, i.e. models fulfilling the form of Eq. (54). There are many analytical stored energy functions published in the literature which follow this assumption. For the isochoric part ω we have chosen the Neo-Hookean model [59], the Mooney model [62] and the Ogden model [60], [61]. For the volumetric part we have chosen the same function for all models which is the convex function from Hartmann and Neff [63], see arguments for the selection therein. We now show that the proposed formulation is of course capable of reproducing the behavior predicted by those models in any loading situation just employing as input the “experimental” stress-strain data that those energy functions generate for the uniaxial case. We also employ the Gent [64] model which does not follow the Valanis-Landel decomposition. We show that even in this case we are able to capture the behavior of the model to high precision in moderately large strains. Note that the Valanis-Landel decomposition is mathematically accurate for moderate large strains and has been experimentally verified in some materials [3]. Furthermore, if the real material does not follow the Valanis-Landel decomposition, additional tests are needed in order to determine the coupling between strain components at very large strains. Then we select some experimental data from Blatz and Ko [65] to show the performance of our proposal in predicting the behavior of actual materials. We also show that this formulation includes the formulation of Sussman and Bathe for

isotropic (quasi-)incompressible materials as a particular case. Finally, we present a finite element simulation to show the efficiency of the method.

7.1 Volumetric component

As mentioned, for the volumetric part to be added to all models, we have chosen the function from Hartmann and Neff [63] given by the following derivative

$$\mathcal{U}'(E^v) = \frac{K}{\beta_1} (\exp(\beta_2 E^v) - \exp(\beta_3 E^v)) \quad (88)$$

where $K = 8 \times 10^5$ Pa, $\beta_1 = 10$, $\beta_2 = 4$ and $\beta_3 = -6$. The value of K was selected to allow a high compressibility at low strain as to show the features of the model. At very large strains the volumetric term usually becomes dominant. The rest of the parameters are those given by Hartmann and Neff in Table 4 of Ref. [63].

7.2 Neo-hookean model

The compressible Neo-hookean stored energy function is frequently given by the following expression [60], [59]

$$\Psi = \mathcal{U}(E^v) + C_1 (I_1^d - 3) \quad (89)$$

where I_1^d is the first invariant of the isochoric (deviatoric) right Cauchy-Green deformation tensor obtained from the isochoric deformation gradient of Flory's decomposition. The material parameter is $C_1 = 0.4$ MPa, taken from Ref. [59].

For the uniaxial case, $\sigma_2 = \sigma_3 = 0$, and the problem is solved using a Newton-Raphson algorithm. Since the procedure is well-known we omit the details.

In Figure 4a we represent the uniaxial stress-strain curve, where we show the analytical predictions given by the Neo-hookean/Hartmann–Neff model. We have used this Neo-hookean predictions as the input data of our model, as if they were measured experimental data. In the same figure 4a we also show the numerical predictions using our proposal which are coincident with the spline interpolation, and the latter obviously with the predictions of the Neo-hookean model. In Figure 4b we show the transverse strain predictions from the Neo-hookean model (and also input data to our procedure) and the resulting numerical predictions using our proposal. In Figure 4c and Figure 4d we show, respectively, the stored energies derivatives ω' and $\mathcal{U}'$ for both the Neo-hookean/Hartmann–Neff model and the WYPIWYG model. It can be seen in this Figure that both stored energy derivatives are visually coincident. As a consequence, both predictions are also coincident. However we remark that even though the stored energy derivatives in Figures 4c and 4d look identical for both models, they are indeed different. The stored energy derivatives of the Neo-hookean/Hartmann–Neff model are those given by the derivative of Eqs. (89) and (88). On the contrary, the stored energy derivatives of the WYPIWYG procedure are piecewise third order polynomials. Both stored energy derivatives are exactly coincident at the discretization points $\bar{E}_{up}$.

Consider now the following family of deformation gradients

$$\mathbf{X} = \begin{bmatrix} (1 + \gamma)^n & & \\ \gamma & (1 + \gamma)^n & \\ & & 1 \end{bmatrix} \quad (90)$$

where γ is the main deformation variable and n is a constant. The case $n = 0$ is a simple shear case and γ is the “amount of shear”. We consider also the cases of $n = 1/3$ and $n = 1/2$, which correspond to different combinations of volumetric and isochoric parts.

The predictions for the in-plane normal stresses σ_{11} , σ_{22} and shear stress σ_{12} as a function of the “amount of shear” γ are given in Figure 5 for both models. In this figure, as well as in similar figures below, we plot in the first row of axes the predictions for $n = 0$ in Eq. (90) (simple shear case), in the second row of axes we plot the predictions for $n = 1/3$ and in the third row of axes the predictions for $n = 1/2$. The first column corresponds to the component σ_{11} of the Cauchy stress tensor for each case, the second column corresponds to the shear component σ_{12} of the Cauchy stress tensor and in the third column the component σ_{22} of the same tensor is given. Note that in this case for the WYPIWYG model we simply use the stored energy derivatives given in Figures 4c and 4d. It should be of no surprise that the predictions using both models are coincident again in all cases. In fact, since we have “exactly” computed the stored energy, both models match numerically and the predictions will be coincident *in any loading situation*. In the next

Figure 4: Compressible Neohookean/Hartmann–Neff model predictions for the uniaxial test and WYPIWYG predictions using the former ones as “experimental” data. a) Tensile Kirchhoff stresses in Pa versus uniaxial (longitudinal) logarithmic strains. b) Transverse strains versus longitudinal strains. c) Energy derivative components ω' in Pa versus deviatoric longitudinal strains: prescribed (Neohookean) and obtained (WYPIWYG) energies. d) Volumetric stored energy derivative: prescribed (Hartmann and Neff) and obtained (WYPIWYG) energies.

examples we repeat these same curves, showing that we obtain the same conclusions for any model being used if it fulfills the Valanis-Landel decomposition.

7.3 Mooney model

The Mooney stored energy function is [62]

$$\Psi = \mathcal{U}(E^v) + C_1 (I_1^d - 3) + C_2 (I_2^d - 3) \quad (91)$$

where $C_1 = 0.39 \times 10^6$ Pa and $C_2 = 0.15 \times 10^6$ Pa are the material parameters, I_2^d is the second invariant of the deviatoric right Cauchy-Green deformation tensor and $\mathcal{U}(E^v)$ is the same Hartmann–Neff volumetric stored energy.

Figure 6 shows the comparison of this model and the WYPIWYG approach for the material parameters of the Mooney model. As with the previous model, it can be verified that both models give exactly the same predictions. Figure 7 shows the predictions for the deformation pattern given by Eq. (90) following the layout already explained in the previous example. It can be seen again that both models give exactly the same predictions, i.e. the WYPIWYG model exactly (numerically speaking) replicates the material behavior in any loading situation.

Figure 5: Predictions for the deformation gradient given in Eq. (90) using the compressible NeoHookean/Hartmann–Neff model and predictions obtained using the WYPIWYG model using the stored energies of Figure 4. First row: predictions for components σ_{11} , σ_{12} , σ_{22} (Pa) versus γ for $n = 0$ (simple shear) in Eq. (4). Second row: predictions for $n = 1/3$. Third row: predictions for $n = 1/2$.

7.4 Ogden model

The Ogden stored energy function is [60], [61]

$$\Psi = \mathcal{U}(E^v) + \sum_{p=1}^M \frac{\mu_p}{\alpha_p} ((\lambda_1^d)^{\alpha_p} + (\lambda_2^d)^{\alpha_p} + (\lambda_3^d)^{\alpha_p} - 3) \quad (92)$$

where μ_i and α_i are the material parameters, M is the number of terms, typically $M = 3$, and λ_i^d are the isochoric (deviatoric) stretches. The material parameters we have used are [59] $\mu_1 = 0.62 \times 10^6$ Pa, $\mu_2 = 1.18 \times 10^3$ Pa, $\mu_3 = -9.81 \times 10^3$ Pa and $\alpha_1 = 1.3$, $\alpha_2 = 5$, $\alpha_3 = -2$.

Figures 8 and 9 show the same comparisons as before. We obtain the same conclusions as in the previous examples.

Figure 6: Compressible Mooney/Hartmann–Neff model predictions for the uniaxial test and WYPIWYG predictions using the former ones as “experimental” data. a) Tensile Kirchhoff stresses in Pa versus uniaxial (longitudinal) logarithmic strains. b) Transverse strains versus longitudinal strains. c) Energy derivative components ω' in Pa versus deviatoric longitudinal strains: prescribed (Mooney) and obtained (WYPIWYG) energies. d) Volumetric stored energy derivative: prescribed (Hartmann and Neff) and obtained (WYPIWYG) energies.

7.5 Gent model

The Gent stored energy function is [64]

$$\Psi = \mathcal{U}(E^v) + \psi(I_1^d) = \mathcal{U}(E^v) - \frac{\mu J_m}{2} \ln \left(1 - \frac{I_1^d - 3}{J_m} \right) \quad (93)$$

where $\mu = 6000$ Pa and $J_m = 80$ are the material parameter values we have chosen. This model does not admit a Valanis-Landel decomposition which is a basic hypothesis of our proposal. In Figure 10 we show the predictions of the Gent model and the associated stored energy derivatives; in the case of Gent’s model the function ψ' obtained for the uniaxial test at hand. It is seen that as in the previous cases the WYPIWYG model is capable of capturing the stress-strain behavior during the uniaxial test.

In Figure 11, the deformation gradients given by Eq. (90) are again imposed to both models. However, in this case we have limited the exponent n to $n = 1/5$ due to the asymptotic behavior of the Gent model. As mentioned the Gent model does not fulfill the Valanis-Landel decomposition. However, for moderate large deformations the Valanis-Landel decomposition is an adequate approximation. The predictions shown in Figure 11 are in line with this observation. Even though Gent’s model is not built on the Valanis-Landel decomposition, our WYPIWYG model is able to capture the deformations predicted by Gent’s model to a very high accuracy for moderately large deformations.

Figure 7: Predictions for the deformation gradient given in Eq. (90) using the compressible Mooney/Hartmann-Neff model and predictions obtained using the WYPIWYG model using the stored energies of Figure 6. First row: predictions for components σ_{11} , σ_{12} , σ_{22} (Pa) versus γ for $n = 0$ (simple shear) in Eq. (90). Second row: predictions for $n = 1/3$. Third row: predictions for $n = 1/2$.

7.6 Predictions for the Blatz and Ko experiments

We now show the performance of the WYPIWYG approach to predict the behavior measured by the experiments from Blatz-Ko [65] on a polyurethane foam, which is a highly nonlinear compressible material. For this purpose, the data from both the uniaxial tension and equibiaxial tension tests are prescribed and the energy function derivatives ω' and $\mathcal{U}'$ are computed as described in this paper. We have considered that $E_w(E_s)$ is an odd function. In Figures 12a and 12b we show the averaged values (the circles in Figure 12) given by Blatz-Ko [65] for the performed experiments, conveniently converted from Figures 13, 14, 21 and 22 of Ref. [65]. This experimental data, slightly smoothed, was captured by the computed stored energy terms, whose derivatives are given in Figures 12c and 12d. These stored energies fully determine the material behavior in any loading situation if the material fulfills the constitutive hypothesis of isotropy and Valanis-Landel decoupling.

We now proceed to predict the behavior of the material for strip-biaxial (plane strain) experiments. In this case the principal deformation is given in axis 1, i.e. $E_s \equiv E_1$. Axis 2 has a vanishing strain $E_2 = 0$ and the thickness reduction is $E_w \equiv E_3$. We can perform the predictions using a finite element. However, since this is an homogeneous deformation it is more straightforward and instructive to solve directly the nonlinear equilibrium equations. The volumetric and

Figure 8: Compressible Ogden/Hartmann–Neff model predictions for the uniaxial test and WYPIWYG predictions using the former ones as “experimental” data. a) Tensile Kirchhoff stresses in Pa versus uniaxial (longitudinal) logarithmic strains. b) Transverse strains versus longitudinal strains. c) Energy derivative components ω' in Pa versus deviatoric longitudinal strains: prescribed (Ogden) and obtained (WYPIWYG) energies. d) Volumetric stored energy derivative: prescribed (Hartmann and Neff) and obtained (WYPIWYG) energies.

deviatoric logarithmic strains are

$$\begin{cases} E^v = E_s + E_w \\ E_s^d = \frac{2}{3}E_s - \frac{1}{3}E_w \\ E_w^d = -\frac{1}{3}(E_s + E_w) \\ E_w^d = \frac{2}{3}E_w - \frac{1}{3}E_s \end{cases} \quad (94)$$

In order to determine either $E_w(E_s)$, or alternatively $E_s(E_w)$, we use the boundary condition $\tau_w = 0$ to obtain the nonlinear equation

$$\begin{aligned} & \frac{2}{3}\omega' \left(\frac{2}{3}E_w - \frac{1}{3}E_s \right) - \frac{1}{3}\omega' \left(-\frac{1}{3}(E_s + E_w) \right) \\ & - \frac{1}{3}\omega' \left(\frac{2}{3}E_s - \frac{1}{3}E_w \right) + \mathcal{U}'(E_s + E_w) = 0 \end{aligned} \quad (95)$$

which can be solved for E_w by a Newton-Raphson scheme given a value of E_s . Once the relation $E_w(E_s)$ is known, the strains in Eq. (94) are known and we can compute the main stresses by a similar equilibrium equation in Axis 1.

In Figure 13 we show the predictions given by the WYPIWYG model for the strip-biaxial experiments on the same material using the stored energy densities of Figure 12. The predictions for the strip-biaxial experiments are presented against averaged experimental data from Blatz and Ko (Figures 17 and 18 of Ref. [65]). It is seen in Figure 13a that

Figure 9: Predictions for the deformation gradient given in Eq. (90) using the compressible Ogden/Hartmann–Neff model and predictions obtained using the WYPIWYG model using the stored energies of Figure 8. First row: predictions for components σ_{11} , σ_{12} , σ_{22} (Pa) versus γ for $n = 0$ (simple shear) in Eq. (90). Second row: predictions for $n = 1/3$. Third row: predictions for $n = 1/2$.

the stresses are accurately predicted by the WYPIWYG formulation, since the error observed is of the order of the experimental errors given in Reference [65]. In Figure 13b we show the predicted transverse strains (thickness reduction) against the longitudinal ones. The observed discrepancies are also in the order of some appreciated experimental errors for these quantities, see Figures 22 and 24 of Ref. [65] and note that we plot logarithmic measures.

7.7 Recovery of the incompressible formulation

In order to show that the (quasi-)incompressible model of Sussman and Bathe is recovered as a particular case, we modify the transverse strains and set $E_2(E_1) = -\nu E_1$ with different values of ν . The case of $\nu \rightarrow 0.5$ corresponds to the incompressible formulation. In Figure 14 we show the predictions and stored energy density derivatives for the Ogden model with modified transverse strains as to obtain a constant ν for values from $\nu = 0$ to $\nu = 0.499$. It is seen in Figures 14a and 14b that the prescribed stress-strain uniaxial behavior is still captured. Remarkably Figure 14a shows that the uniaxial stress-strain behavior is exactly captured in all cases. However, it is seen in Figure 14d that the stored energy derivative approaches the values $\mathcal{U}'' \rightarrow \infty$, and the volumetric strains $E^v \rightarrow 0$ as $\nu \rightarrow 0.5$, i.e. they approach the quasi-incompressible case. Note that even though the largest change is in $\mathcal{U}'$, the function ω' also changes with ν so the predicted stress-strain curve given in Figure 14a is “exactly” the same regardless of the ν value; only the predictions in Figure 14b change to accommodate the varying Poisson ratio.

Figure 10: Compressible Gent/Hartmann–Neff model predictions for the uniaxial test and WYPIWYG predictions using the former ones as “experimental” data. a) Tensile Kirchhoff stresses in Pa versus uniaxial (longitudinal) logarithmic strains. b) Transverse strains versus longitudinal strains. c) Energy derivative components ω' or ψ' in Pa versus deviatoric longitudinal strains: prescribed (Gent) and obtained (WYPIWYG) energies. d) Volumetric stored energy derivative: prescribed (Hartmann and Neff) and obtained (WYPIWYG) energies.

It is well known that incompressibility is frequently imposed in finite element procedures through a penalty volumetric stored energy density. However, because the range of deformations is large and the change in the relative volumetric stiffness may be large, this method frequently results in a too weak imposition of the incompressibility constraint at moderate strains or in numerical conditioning problems at very large strains. The present formulation also allows for an adequate imposition of the incompressibility constraint at all deformation levels simply prescribing a constant value of ν close enough to 0.5 in the transverse strains.

7.8 Plate with a hole using the Ogden model and the WYPIWYG approach

As a demonstrative example of the possibilities of the WYPIWYG approach in finite element simulations, we analyze a plate with a hole using our in-house finite element code Dulcinea. This example, with different constitutive models has been used in Refs. [48, 53, 54, 68]. The plate has initial dimensions of $l_0 \times h_0 = 32 \times 16 \text{ mm}^2$ and an inner hole of radius $r_0 = 4 \text{ mm}$.

The material data is the same as that used in the previous Ogden example. We have performed two analyses. One using the compressible Ogden/Hartmann–Neff model and one using our WYPIWYG approach capturing the Ogden/Hartmann–Neff uniaxial data, i.e. we use the stored energy densities of Figures 8c and 8d. The finite element mesh consists of 9-node plane strain quadratic elements with full integration. The prescribed displacement using a penalty approach is of 10 mm imposed at each lateral end in 10 proportional paths (i.e. 2 mm per step).

Figure 11: Predictions for the deformation gradient given in Eq. (90) using the compressible Gent/Hartmann–Neff model and predictions obtained using the WYPIWYG model using the stored energies of Figure 10. First row: predictions for components σ_{11} , σ_{12} , σ_{22} (Pa) versus γ for $n = 0$ (simple shear) in Eq. (90). Second row: predictions for $n = 1/10$. Third row: predictions for $n = 1/5$.

In Figure 16 we show the von Mises stress distributions and the pressure distributions for both models, along with the deformed meshes at the end of the analysis. As it could have been predicted from the previous examples, no difference can be appreciated in the results given by both models. This is a consequence of the WYPIWYG model ability to capture the behavior of both the Ogden and the Hartmann–Neff models in any loading situation. Note that we have used the Ogden/Hartmann–Neff model as to clearly show that if this model were exactly predicting the behavior of a real material, we would have exactly (again, numerically speaking) captured the behavior of that material in any loading situation. Of course this conclusion applies to any other model or actual material if the hypotheses of hyperelasticity, isotropy and Valanis–Landel decomposition hold.

Furthermore, in Table 1 we present the relative convergences of both models obtained in a characteristic step. This table shows that indeed the iterations of both models are almost identical; note that only the force residual at iteration 3 and the energy residual at iteration 4 present a difference in the 5 digits shown in the numbers of the table. This should not be a surprise because as repeatedly commented throughout the paper, the numerical values of the energies of both models in any loading situation are also almost identical.

This example has been computed using one thread of a 2011 Windows-PC with Dulcinea running as a 32-bit fortran90 Pentium application. Under these conditions the Ogden/Hartmann–Neff model needed 91 seconds (elapsed time), whereas the WYPIWYG formulation needed 110 seconds. We attribute the difference mainly to the retrieval and addressing operations of the spline coefficients in order to compute the stresses and constitutive tangent. Whereas

Figure 12: Determination of the stored energies of polyurethane foam from the Blatz and Ko experimental data. The circles are the averaged data for the experimentes given by Blatz and Ko. The diamonds correspond to the WYPIWYG predictions using the computed stored energies. a) Kirchhoff stress in Pa as a function of the uniaxial strain. b) Transverse strains. c) Computed ω' in units of $J/m^3 \equiv Pa$. c) Computed volumetric stored energy derivative U' in Pa.

the material parameters for the Ogden/Hartmann–Neff model are given explicitly to the program, the WYPIWYG computational time includes also the initial determination of the stored energies from uniaxial data. However, this initial determination took less than one second.

8 Conclusions

WYPIWYG hyperelasticity differs from traditional models in that the shape of the stored energy is not assumed beforehand, in that there are no material parameters and in that no optimization algorithms to obtain those parameters are needed. The stored energies are numerically computed to the desired precision solving the differential equations of the tests. These tests uniquely (numerically speaking) define the stored energy under the constitutive assumptions. In this work we have presented a WYPIWYG procedure to numerically compute the stored energy for compressible isotropic materials fulfilling the Valanis-Landel hypothesis. We have shown that the model is capable of capturing analytical models using the Valanis-Landel decomposition and of predicting the behavior observed in the experiments of Blatz and Ko. Furthermore, we have shown that the quasi-incompressible formulation is naturally recovered.

Because we understand WYPIWYG models as a natural extension of the infinitesimal framework to large strains, we have motivated the formulation in the small strain setting and have justified the number of tests needed to uniquely define such materials, an issue frequently not clear in the literature [8], [56]. Furthermore, we have also explained the way to convert data from equibiaxial and confined compression tests to the standard data of an equivalent uniaxial

Figure 13: Predictions of the strip-biaxial experiments from Blatz and Ko using the stored energy density derivatives of Figures 12a and 12b. a) Kirchhoff stresses (Pa) versus longitudinal logarithmic strains. b) Transverse strains (thickness contraction) as a function of longitudinal strains.

Relative convergence rates of the plate-with-a-hole problem. Step 7/10		
Ogden/Hartmann–Neff model		
Iter	Force residual	Energy residual
1	$1.000E + 00$	$1.000E + 00$
2	$1.339E - 03$	$4.449E - 06$
3	$5.441E - 06$	$2.542E - 11$
4	$2.998E - 11$	$3.069E - 21$
WYPIWYG model		
Iter	Force residual	Energy residual
1	$1.000E + 00$	$1.000E + 00$
2	$1.339E - 03$	$4.449E - 06$
3	$5.443E - 06$	$2.542E - 11$
4	$2.998E - 11$	$3.071E - 21$

Table 1: Convergence rates for both the Ogden/Hartmann–Neff model and the WYPIWYG model

tension-compression curve, which can be used as the standardized input in finite element procedures. The efficiency of WYPIWYG procedures in general finite element simulations is parallel to that of traditional models not only in the case of compressible isotropy presented herein but also in the case of anisotropy [48, 54].

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Figure 14: Determination of the stored energies with modified transverse strains approaching the quasi-incompressible behavior. a) Kirchhoff stress in Pa as a function of the uniaxial strain; uniaxial data from the example using Ogden's model. b) Transverse strains (modified to obtain different ν values). c) Computed derivatives of the stored energy density components ω' in units of $J / m^3 \equiv Pa$. d) Computed volumetric stored energy density derivatives U' in Pa.

Figure 15: Rectangular plate with a concentric hole: undeformed finite element mesh employing quadratic elements with full integration.

Figure 16: Rectangular plate with a concentric hole. Deformed meshes and stresses. a) Von Mises stress distribution (Pa) for the Ogden/Harmann-Neff model. b) Pressure distribution (Pa) for the Ogden/Harmann-Neff model. c) Von Mises stress distribution for the WYPIWYG model. d) Pressure distribution for the WYPIWYG model

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Chapter 4

WYPiWYG data-driven method for auxetic isotropic materials

4.1 Introduction

Auxetic materials, from Greek $\alpha\upsilon\tilde{\xi}\eta\tau\iota\kappa\acute{o}\varsigma$, auxetikos, meaning "that grows", are materials that owns the counter-intuitive behaviour of expanding transversely when stretching out, whilst convectional materials get narrower when extending. In terms of solid mechanics, they show a negative Poisson ratio, $\nu < 0$. This family of materials show very valuable properties, such as pull-out resistance, synclastic curves when bending, resistance to indentation, resistance to fracture and crack, noise absorption, etc [39]. All these properties make them very attractive to be incorporated in different sectors such as defense [40] or biomedical applications [41].

The reason of this behaviour lies on its microstructure. Because the peculiarities of auxeticity resides in topological reasons, the most faithful way to recover the nature of the material is taking into account this microscale in FEA simulations. However this is very expensive in terms of computational costs. Because of that, phenomenological analytical proposals were developed in that line, such as the proposal of Ciambella and Saccomandi [4], that aims to recover the experimental tests of Choi and Lakes foams [24]. Lakes developed the first polyurethane foam with auxeticity, with Poisson ratio $\nu \approx -0.7$. However, analytical proposals are only able to approximate the system of stress-strain functional equations that arise from them.

Nevertheless, the WYPiWYG data-driven phenomenological approach has the advantage of being an economical alternative and, at the same time, has the capability of finding the solution of the system of the stress-strain functional equations. The solution reflects the observable experimental behaviour. In Chapter 3, a WYPiWYG method aimed for hyperelastic isotropic compressible materials was developed. Precisely because one of the main properties of isotropic auxeticity is compressibility, this procedure is suitable to undertake the goal of characterizing the mechanical behaviour of hyperelastic isotropic auxetic materials.

It is worth to mention that one of the assumptions made for that WYPiWYG procedure is the Valanis-Landel decomposition and the usage of logarithmic invariants. Because of that, in this work an alternative formulation based on J-invariants that does not obbey Valanis-Landel assumption have been developed. In order to distinguish both data-driven procedures, we will denote as J-WYPiWYG the method based on J-invariants, and E-WYPiWYG the one based on logarithmic strains and Valanis-Landel decomposition.

4.2 The J-WYPiWYG hyperelastic data-driven approach

Because a certain material does not necessarily have to follow the Valanis-Landel assumption, this proposal aims to extend WYPiWYG capabilities beyond that constrain. The motivation behind J-invariants is twofold. First, this is a proposal that aims to show that WYPiWYG capabilities are not constrained to certain choice of invariants, and second, it is a way of establish coherence with the Blatz and Ko development for compressible rubbers that were made with J-invariants. One of the goals of this chapter is to show that the procedure for WYPiWYG method is compatible to any choice of invariants, such as I-invariant, or any other suggestion, since the aim of the WYPiWYG is finding numerically the functional energy derivative unknowns from a system functional equations that relate the energy functional unknowns with an independent set of functional experimental data.

Let $\Psi(J_1, J_2, J_3)$ be considered the energy function in terms of the J-invariants, whose definition arises from invariants of left-Cauchy strain tensor $\mathbf{B}$ and Jacobean J ,

$$J_1 = \text{tr}(\mathbf{B}) = \sum_{i=1}^3 \lambda_i^2 \quad (4.1)$$

$$J_2 = \text{tr}(\mathbf{B}^{-1}) = \sum_{i=1}^3 \lambda_i^{-2} \quad (4.2)$$

$$J_3 = J = \prod_{i=1}^3 \lambda_i \quad (4.3)$$

In order to keep as simple as possible and in accordance with Blatz and Ko among other available literature [REFS], the following decomposition is assumed,

$$\Psi(J_1, J_2, J_3) = W_1(J_1) + W_2(J_2) + W_3(J_3) \quad (4.4)$$

If derived Ψ with respect to left-Cauchy strain tensor $\mathbf{B}$, the following functional tensorial equation yields,

$$\boldsymbol{\sigma} = W'_3(J_3)\mathbf{I} + \frac{2}{J} \left(W'_1(J_1)\mathbf{B} - W'_2(J_2)\mathbf{B}^{-1} \right) \quad (4.5)$$

Since now there are three energy functional unknowns, if no other assumptions made, a set of three independent functional data are necessary to solve the compatible determined system of functional equations. A possible assumption is a linear constant f that relates $W_1(J_1)$ and $W_2(J_2)$ (e.g. Blatz-Ko [3], Ciambella-Saccomandi [4]) so that,

$$W'_1(J_1) = fW'(J_1) \quad (4.6)$$

$$W'_2(J_2) = (1 - f)W'(J_2) \quad (4.7)$$

So, algebraic manipulation of Eq.(4.5) yields the following scalar functional equation in which functional unknown W must be determined

$$W'(J_1) = \frac{1/f}{\lambda_u^2 - \lambda_t^2} \left[\frac{1}{2} J_3 \sigma_u + (1 - f)W'(J_2)(\lambda_u^{-2} - \lambda_t^{-2}) \right] \quad (4.8)$$

However in this occasion the equation is going to be solved using functional refresh procedure. It implies that an initial guess of the functional unknown W must

be done (e.g. zero function). As in previous work, the set data $\{\lambda_u, \lambda_t, \sigma_u\}$ must be synchronized before solve the functional equation. The unknown is then evaluated for values $J_2 = \lambda_u^{-2} + 2\lambda_t^{-2}$. Since initial guess of W is the zero function, the first update of W comes from the spline representation of synchronized data and Eq.(4.8). That is,

$$\left\{ (\lambda_u^2 + 2\lambda_t^2), \frac{1/f}{\lambda_u^2 - \lambda_t^2} \left(\frac{1}{2} \lambda_u \lambda_t^2 \sigma_u + 0 \right) \right\} = \left\{ J_1, \frac{J_3 \sigma_u}{2f(\lambda_u^2 - \lambda_t^2)} \right\} \rightarrow W'^{[1]} \quad (4.9)$$

Note the superindex "[1]" over W' to indicate the update (first iteration) of the functional unknown. Next iteration $W'^{[2]}$ will be,

$$\left\{ J_1, \left(\frac{J_3 \sigma_u}{2f(\lambda_u^2 - \lambda_t^2)} + (1 - f) W'^{[1]}(J_2)(\lambda_u^{-2} - \lambda_t^{-2}) \right) \right\} \rightarrow W'^{[2]} \quad (4.10)$$

Functional refresh must be repeated until convergence. If no convergence is attained, the process can be reversely run (i.e. update $W'(J_2)$ from $W'(J_1)$ evaluation), or even split the data set into reversal refresh and direct refresh regions.

In the next article we show,

- The experimental results of Lakes foam, captured from the Ciambella-Saccomandi phenomenological analytical approximation of the functional unknown W by means of fitting scalar parameters $(\mu_0, \nu_0, \lambda_I)$, and the numerical solution of the functional equation using E-WYPiWYG and J-WYPiWYG data-driven procedures. All three solutions aim to recover the Lakes experimental data, and they are contrasted with Lakes referential experimental data. It is observed that both E-WYPiWYG and J-WYPiWYG recover numerically the experimental results from the obtained energies W, W_3 .
- Assuming as new reference pseudo-experimental data simulated from the model of Ciambella-Saccomandi, both E-WYPiWYG and J-WYPiWYG aim to determine new energies from pseudo-experimental reference. Once again, pseudo-experimental data are numerically recovered. Since J-WYPiWYG obtains functional unknowns W', W'_3 owns the same arguments of Ciambella-Saccomandi model energy functions, both of them are compared together in common plots, and they become visually indistinguishable. In other words, the original Ciambella-Saccomandi energies W, W_3 are fully numerically recovered directly from pseudo-experimental data.
- Since once of the drawbacks of microscale FEA is computational costs, FEA spline based energies from E- J-WYPiWYG have been developed. Since it lies on phenomenological approach, corresponding FE simulations results much faster.
- In order to study differences from assuming E-WYPiWYG (Valanis-Landel) or J-WYPiWYG ansatzes, FEA example results are compared with both procedures.
- Finally, an interesting bimodular energy study of auxetic materials is developed in appendix.

A CONTINUUM APPROACH FOR THE LARGE STRAIN FINITE ELEMENT ANALYSIS OF AUXETIC MATERIALS

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ABSTRACT

Auxetic materials are materials which present negative Poisson ratios. This unusual behavior is due to their particular microstructures. It is frequent that during large deformation processes in auxetic foams, the value of the Poisson ratio also presents large variations, with transitions from auxetic to conventional behavior. In this paper we present a procedure to perform large strain finite element analysis of energy-conservative isotropic auxetic materials from a continuum perspective. Two possible approaches are used. The first one is based on uncoupled WYPiWYG hyperelasticity. This decomposition permits a simple analysis of the behavior using also infinitesimal bi-linear models. The second approach is a novel procedure for coupled hyperelasticity based on classical invariants. This latter procedure is amenable for obtaining the stored energy of highly compressible foams, including coupling terms and generic invariants, as for example those used by the analytical Blatz-Ko model or the hyperelastic model of Ciambella and Saccomandi, which was explicitly developed for auxetic foams. The applicability and efficiency of the method is shown through finite element analyses of auxetic foams at large strains using the continuum approach.

Keywords Hyperelasticity · Auxetic materials · Foams · Poisson's ratio · Large strains

1 Introduction

The theoretical limits of the infinitesimal Poisson ratio ν for isotropic materials are $-1 < \nu \leq 0.5$, being the positive values the most usual, conventional ones. However, materials with unusual Poisson ratios may have important applications. For example, cork has a Poisson ratio close to zero and has been long used to easily and effectively seal wine bottles. There are both natural and manufactured materials that have a negative Poisson ratio. These materials are known as *auxetic* materials (from the Greek *αὐξητικός*, *auxetikos*, meaning “that grows” or *αὐξήτος*, *auxetos*, meaning “capable of growing”), named so by Evans et al [1]. Auxetic materials have been known for long [2], but have attracted considerable attention in the last three decades because of their potential applications. Most of the auxetic materials are developed using re-entrant or cellular structures. Lakes [3] has been the first one to develop a polyurethane foam with re-entrant cell structure, reaching negative Poisson ratios of the order of -0.7 . Since then, many auxetic materials in a wide range of Young moduli have been produced or discovered: cubic metals [5], bucklicrystals, α -cristobalite [4], liquid crystalline polymers [6], sintered ceramics and metals [7], [8], honeycombs and foams (both metallic and polymeric [9], [10], [11]), microporous polymers like PTFE (Polytetrafluoroethylene or teflon) [12],

UHMWPE (Ultra-High-Molecular-Weight-Polyethylene) [13] and PP (Polypropylene) [14], fiber reinforced composites and sandwich panel composites [15], [16], biological materials like cat skin, cow teat skin [17] and cancellous bones [18], isotropic granular materials with large tangential-to-normal contact stiffness [19], graphene with double-vacancy defects [10], brick assemblies for seismic safety [20], and so on [8], [20], [22].

Improved material properties explain the interest in developing structures with auxetic materials. For example, auxetic materials have enhanced pull-out resistance because stretching increases transverse dimensions. This property facilitates also the pull-out resistance of fibers in composite materials and the compliance of transverse strains between matrix and fibers [23]. In bending, auxetic materials tend to deform with synclastic curvatures [23]. Remarkably, these materials have improved resistance to indentation, important in lightweight armored vehicles or bullet-proof vests [23], [24], [25]. The shear-to-bulk G/K stiffness ratio is also large since $G/K = (3/2)(1 - 2\nu)/(1 + \nu)$, which is the opposite of what happens with usual rubbery solids. Other improved properties respect to their conventional counterparts are fracture toughness and crack resistance [23], improved noise and vibration absorption [23], improved buckling loads in pressure vessels [28]. Other applications include drug delivery [26] and biomedical implants [27]. Further details on auxetic materials and their applications can be found in the reviews [10], [11], [22], [23], [26].

The analysis of structures with auxetic materials will become more usual in engineering practice as applications become also usual. However, these structures are currently computed either with linear infinitesimal continuum models (just prescribing a negative value of the Poisson ratio) or using multiscale models accounting for the microstructure, in which linear or nonlinear kinematics of the deformation of the representative cell is taken into account, either by frames, networks, beams or multiscale finite elements; see for example the recent works [9], [16], [24], [29], [30], [31], [32], [33], [34], [35]. These multiscale models are computationally very expensive for the nonlinear analysis, specially if nonlinear large strain kinematics and cell wall contacts are taken into account, so simulations of large structures may become prohibitive even with current computational resources. Finite strains are needed in order to represent the high nonlinearity observed in experimental data [40], [27], [11], [21], [36]. Furthermore, foams have nonhomogeneous cells, so a representative cell that accurately represents the overall behaviour may be difficult to determine, specially if the nonlinearity of the material of the representative cells, including wall contacts in cells, is considered. On the contrary, the continuum scale allows for very efficient finite element analysis of most types of structures.

As it is well known from the mechanics of rubbers, in order to preserve the energy during elastic deformations at large strains, a stored energy must be considered [37]. There are hundreds of proposed stored energies for rubber-like materials. These models are frequently based on the assumption of incompressibility or quasi-incompressibility (i.e. a Poisson ratio $\nu \rightarrow 0.5$), leading to an isochoric term, frequently using the Valanis-Landel decomposition, uncoupled from a volumetric penalty function. However, auxetic materials are largely compressible. Then, models for incompressibility or quasi-incompressibility have been questioned for these type of materials [38]. Models for foams like the Hyperfoam or the Blatz and Ko model [39], although not accurate for largely varying Poisson ratios [27], may be adapted to data from auxetic materials. These data may be either experimental or obtained from finite element analysis of a representative cell. To the knowledge of the authors, the models of Ciambella and Saccomandi [21] and Ciambella et al [36] are the only nonlinear hyperelastic models developed for the continuum analysis of auxetic materials. The model of Ciambella and Saccomandi [21] is an adaption of the Blatz and Ko model [39]. They modify the form of the evolution of the Poisson ratio through a new analytical nonlinear equation for the Poisson ratio $\nu(\lambda)$ (where λ is the stretch in a tensile test), better suited for auxetic materials, in particular for the experiments of Choi and Lakes [40]. The model of Ciambella et al [36] is the modification of the Hyperfoam/Ogden model using the same analytical $\nu(\lambda)$ function as in Ciambella and Saccomandi [21]. These two models are excellent for analytical analysis of the nonlinear behavior of auxetic foams because they capture the transition from auxetic to conventional behavior. However, to date these models have not been implemented in a finite element program. Aside, the model of Ciambella and Saccomandi [21] represents well the experimental auxetic behavior, but as therein noted, stresses are accurate only up to a strain of 50%; and the model of Ciambella et al [36] has only been tested and characterized for compression behavior, which is furthermore represented well only for strains below 50%. In fact, the particular analytical expression $\nu(\lambda)$ employed in these models has been proven to fit well a class of auxetic foams, but its applicability to the already large variety of auxetic materials is an open issue, so more general procedures for the finite element analysis of auxetic materials, not tied to a specific ansatz $\nu(\lambda)$, are of major interest.

WYPiWYG (What-You-Prescribe is What-You-Get) hyperelasticity [41], [42], [43] is a novel numerical procedure for the efficient finite element analysis of continua at large strains. The procedures are based on the original idea from Sussmann and Bathe [44] of employing local spline interpolations between numerically computed discrete values of the stored energy. These discrete values are computed solving numerically the equilibrium equations of a complete set of experiments. Remarkably, the method does not *fit* a proposed analytical solution (a model), it *solves numerically* the problem of determining the stored energy directly from experimental data [45]. Hence, there are no material parameters to be obtained; it is a data-driven model-free method. The establishment of constitutive behavior directly from data seems to be a new paradigm in constitutive modelling and it is an approach currently being investigated from different

perspectives, like using neural networks [46], constitutive manifolds [47], [48], [51], or minimization of penalized potentials [49], [50].

The purpose of this paper is twofold. The first objective is to show that WYPiWYG hyperelasticity is capable of representing accurately the behaviour of auxetic materials in all the range of deformations, and it is useful to perform efficient finite element simulations of these materials; we do so performing simulations on Scott foams capturing exactly the experimental data of Choi and Lakes [40] in all the range of deformations. Since auxetic materials are highly compressible, it is possible that in some materials the uncoupled forms of Valanis-Landel and distortional-volumetric split, in which the usual WYPiWYG approach (which we name here E-WYPiWYG hyperelasticity because it is based on logarithmic invariants) was based, may not be adequate. Therefore, the second objective of this paper is to develop a new class of WYPiWYG procedures (which for distinction we name J-WYPiWYG hyperelasticity because it is based in more general invariants) for coupled energy forms which are *not* based on the Valanis-Landel decomposition *nor* on a volumetric-distortional uncoupling. To show the capabilities of the new procedure, we use the Ciambella and Saccomandi model as if it were representing an actual material. This model uses classical J -invariants and is not compliant with the Valanis-Landel decomposition, so for example, the behavior in simple shear is different from that obtained from E-WYPiWYG hyperelasticity based on the Valanis-Landel decomposition. We show that the novel J-WYPiWYG formulation herein introduced, if based on the same energy decomposition as the Blatz-Ko and Ciambella-Saccomandi models is able to capture to any desired precision the behavior of these models in any possible loading situation without specifying an analytical ansatz for the terms of the stored energy, nor the evolution of the Poisson ratio. In essence, based on this decomposition, J-WYPiWYG hyperelasticity is capable of capturing exactly three complete experimental curves in the isotropic case. Finally, we perform finite element simulations with the double purpose of verifying the robustness of the method and to compare both (coupled and uncoupled) WYPiWYG approaches in general, non-proportional loading simulations. From this comparison, the relevance of the coupling terms can be assessed. To our knowledge, the present simulations are the first large strain finite element simulations of auxetic materials treated as a continuum.

2 E-WYPiWYG hyperelasticity based on the Valanis-Landel decomposition and uncoupled volumetric energy

Let $\mathbf{X}$ be the deformation gradient and $\mathbf{X} = \mathbf{R}\mathbf{U}$ the right polar decomposition, where $\mathbf{R}$ is the rotation part and $\mathbf{U}$ is the right stretch tensor. Until now, WYPiWYG hyperelasticity for isotropic, compressible materials, was developed under the assumption of the following uncoupling of the volumetric part of the stored energy and of the distortional part

$$\Psi(\mathbf{E}) = \mathcal{U}(E^v) + \mathcal{W}(E^d) = \mathcal{U}(E^v) + \omega(E_1^d) + \omega(E_2^d) + \omega(E_3^d) \quad (1)$$

where $\mathbf{E} = \ln \mathbf{U}$ are the logarithmic referential strains, $E^v = \text{tr}(\mathbf{E}) = E_1 + E_2 + E_3 = \ln J$ is the volumetric strain, $J = \det(\mathbf{X})$, E_i are the principal logarithmic strains and $E_i^d = E_i - (1/3)E^v$ are the logarithmic deviatoric (distortional) strains. The terms $\mathcal{U}(E^v)$ and $\omega(E^d)$ correspond to the uncoupled volumetric and Valanis-Landel energy density functions. In classical hyperelasticity, analytical forms for $\mathcal{U}(E^v)$ and $\omega(E^d)$, or for the terms in any other decomposition, for example based on Rivlin's invariants, is assumed. The analytical forms employed in classical hyperelastic models have some "material parameters" which are adjusted as to *fit* the experimental data. This fitting procedure is typically performed using optimization algorithms; the Levenberg-Marquadt algorithm [52] is one classical choice. Remarkably, since the chosen analytical form may be suitable only for a given class of materials, according to Volokh, there may be as many models "as researchers which work (or worked) in the field" [53], each model with its merits and drawbacks. Furthermore, typically, different sets of material parameters may be obtained for the same material depending on the procedure employed to compute the parameters from experimental data [52], [54].

The difference of E-WYPiWYG hyperelasticity respect to classical (analytical) hyperelasticity is that the global forms of the functions $\mathcal{U}(E^v)$ and $\omega(E^d)$ are not assumed, but computed numerically. The basic idea of the procedure is to compute discrete values of the derivatives of these functions solving the nonlinear equilibrium equations of the tests from which experimental data are obtained. An interpolation function with sufficient smoothness properties is employed between the computed k discrete values for the derivatives, $\mathcal{U}'_k$ and ω'_k ; we typically use cubic piecewise splines (cubic polynomials). Since upon use of the splines, the stored energy terms $\mathcal{U}(E^v)$ and $\omega(E^d)$ are piecewise analytical functions, they can be used seemingly in finite element programs, obtaining the same computational efficiency as classical hyperelastic models. In Appendix A we summarize the computational procedure for E-WYPiWYG hyperelasticity.

Remarkably, the method does not have any material parameter because in this procedure we have not imposed the shape of the Kirchhoff stress-Logarithmic strain curve $\tau_u(E_u)$ or the transverse-to-longitudinal strain curve $E_t(E_u)$. Instead of *fitting* an assumed solution, we numerically *solve* the problem. Then, the functions $\tau_u(E_u)$ or $E_t(E_u)$ may be

arbitrary as long as they represent a physically possible material. In particular, $E_t(E_u)$ includes, without modification, the case of auxetic materials, and any possible transition from auxetic to non-auxetic behavior, as observed in auxetic foams.

However, Decomposition (1) is typical of nearly-incompressible materials, where it has been validated for moderately large strains. For compressible materials, coupled formulations are usually employed [38], [57]. Noteworthy, Decomposition (1) converges to the infinitesimal case —see also Eq. (40) in Appendix B

$$\Psi(\varepsilon^v, \varepsilon_i^d) = \frac{1}{2} \kappa (\varepsilon^v)^2 + \mu (\varepsilon_1^d)^2 + \mu (\varepsilon_2^d)^2 + \mu (\varepsilon_3^d)^2 \quad (2)$$

where ε^v and ε_i^d are the infinitesimal volumetric and deviatoric principal strains. However, Decomposition (1) is the simplest nonlinear one, including just as many functions as small-strain linear elastic constants, but it is not the only large strain energy function that converges to Eq. (2). In general, other coupled formulations, which include additional functions relevant only at large strains, also converge to Eq. (2), and may be better suited for the highly compressible behavior of foams. The model of Blatz and Ko, not compatible with Decomposition (1), has been extensively proven to properly describe the compressible behavior of foams. Not surprisingly, Ciambella and Saccomandi developed their constitutive model for auxetic materials working both in tension and compression based on the decomposition given by this model. In the following section we briefly summarize the model of Ciambella and Saccomandi. Thereafter, we will introduce a new WYPiWYG procedure to accurately compute compressible soft materials in coupled forms using classical invariants, including the special class of auxetic materials just as a particular case.

3 Analytical coupled model of Ciambella and Saccomandi [21]

As mentioned, in order to improve a previous proposal to model real auxetic foams, Ciambella and Saccomandi [21] developed a new model through a modification of the well-known Blatz and Ko model for conventional foams [39]. The Blatz and Ko model, developed from experimental work on foams, uses the following relation between longitudinal λ_u and transverse λ_t stretches in a tensile test

$$\lambda_t(\lambda_u) = \frac{1}{\lambda_u^{\nu_0}} \quad (3)$$

where ν_0 is a reference Poisson ratio. In logarithmic strains, this expression is $E_t = -\nu_0 E_u$. Since the infinitesimal strains (referred to the undeformed configuration) are $\varepsilon = \lambda - 1$, we have the following Poisson ratio relation between longitudinal ε_u and transverse ε_t infinitesimal strains

$$\nu(\lambda_u) = -\frac{\varepsilon_t(\lambda_u)}{\varepsilon_u(\lambda_u)} = -\frac{\lambda_t(\lambda_u) - 1}{\lambda_u - 1} = \frac{1 - \lambda_u^{-\nu_0}}{\lambda_u - 1} \quad (4)$$

so we can verify that

$$\lim_{\lambda_u \rightarrow 1} \frac{1 - \lambda_u^{-\nu_0}}{\lambda_u - 1} = \nu_0 \quad (5)$$

is the limiting infinitesimal Poisson ratio, and the resulting Jacobian function is

$$J(\lambda_u) = \lambda_u^{(1-2\nu_0)} \Leftrightarrow E^v = E_u - 2\nu_0 E_u \quad (6)$$

which is an invertible function. As remarked by Ciambella and Saccomandi, Expressions (3) and (4) have been proven to be quite accurate in describing the real behavior of conventional foams by a number of authors [58], [59]. This is basically a linear expression in terms of logarithmic strains, and of course it could be used with a constant negative Poisson ratio. However, as they also note, Expression (4) is not capable of describing the behavior of true auxetic foams, even qualitatively, because of the monotonicity of the function: *auxetic foams behave in an auxetic manner only up to certain deformation level*, whereas the incremental “true” Poisson ratio predicted by the model is ν_0 , constant. The Poisson ratio of auxetic foams is a nonlinear function of the strains.

To obtain a better representation of the experimentally observed behavior of auxetic foams, where a transition from auxetic to conventional behavior is observed once the cells are deformed after a critical value λ_I , Ciambella et al [36] propose the following phenomenological relation

$$\lambda_t(\lambda_u) = 1 - \frac{\nu_0(\lambda_u - 1)}{\left[1 + \pi^2 \nu_0^2 (\lambda_u - 1)^2\right]^q} \quad (7)$$

Figure 1: Compatibility strain relations given by the Ciambella–Saccomandi formulation [21]. $\lambda_I = 2$.

which results in

$$\nu(\lambda_u) = \frac{\nu_0}{[1 + \pi^2 \nu_0^2 (\lambda_u - 1)^2]^q} \quad (8)$$

and where $q \geq 1/2$ is a new material parameter which may be better written in terms of the more physically understandable λ_I . This new parameter λ_I is the critical stretch at which the material changes from auxetic to non-auxetic; i.e. when it stops expanding laterally and begins to contract incrementally, which is mathematically the value of λ_u at which $d\lambda_t/d\lambda_u = 0$. The relation between q and λ_I is

$$q = \frac{1}{2} + \frac{1}{2\pi^2 (\lambda_I - 1)^2 \nu_0^2} \quad (9)$$

so the Jacobian of the deformation is

$$J(\lambda_u) = \lambda_u \left[1 - \frac{\nu_0 (\lambda_u - 1)}{[1 + \pi^2 \nu_0^2 (\lambda_u - 1)^2]^q} \right]^2 \quad (10)$$

The relations $\nu(\lambda_u)$, $\lambda_t(\lambda_u)$ and $J(\lambda_u)$ are given in Figure 1 for several values of ν_0 and $\lambda_I = 2$. The salient feature of the Ciambella and Saccomandi model is that controlling two physical parameters λ_I and ν_0 , a good qualitative description of the behavior of auxetic foams, including the transition to non-auxetic behavior, is obtained.

Let $\mathbf{B} = \mathbf{X}^T \mathbf{X}$ be the left Cauchy–Green deformation tensor and Rivlin’s principal invariants be $I_1 = \text{tr}(\mathbf{B})$, $I_2 = \frac{1}{2}[(\text{tr}(\mathbf{B}))^2 - \text{tr}(\mathbf{B}^2)]$, $I_3 = \det(\mathbf{B})$. We can use the following modified invariants, typically known as J-invariants: $J_1 = I_1$, $J_2 = I_2/I_3$, $J_3 = \sqrt{I_3}$. The Blatz and Ko model, as well as many other compressible models are based on decompositions of the type

$$\Psi(J_1, J_2, J_3) = W_3(J_3) + W_{12}(J_1, J_2) \quad (11)$$

Note that in general this decomposition does not follow the Valanis–Landel form, and both the volumetric and distortional parts are fully coupled because J_1 and J_2 are not the isochoric invariants typical of uncoupled cases. The Cauchy stresses are

$$\boldsymbol{\sigma} = \frac{dW_3}{dJ_3} \mathbf{I} + \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_1} \mathbf{B} - \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_2} \mathbf{B}^{-1} \quad (12)$$

which in particular, for a tensile test gives

$$\sigma_u = \frac{dW_3}{dJ_3} + \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_1} \lambda_u^2 - \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_2} \lambda_u^{-2} \quad (13)$$

$$0 = \frac{dW_3}{dJ_3} + \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_1} \lambda_t^2 - \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_2} \lambda_t^{-2} \quad (14)$$

where $J_1 := \text{tr}(\mathbf{B}) = \lambda_u^2 + 2\lambda_t^2$, $J_2 := \text{tr}(\mathbf{B}^{-1}) = \lambda_u^{-2} + 2\lambda_t^{-2}$ and $J_3 := J = \lambda_u \lambda_t^2$. From the second equation

$$\frac{dW_3}{dJ_3} \equiv W'_3(J_3) = -\frac{2}{J_3} \frac{\partial W_{12}}{\partial J_1} [\lambda_t(\lambda_u(J_3))]^2 + \frac{2}{J_3} \frac{\partial W_{12}}{\partial J_2} [\lambda_t(\lambda_u(J_3))]^{-2} \quad (15)$$

which is a relation not needed in the uniaxial test, but needed in a general finite element implementation. Remarkably, upon knowledge of $\partial W_{12}/\partial J_1$ and $\partial W_{12}/\partial J_2$, this equation still needs $\lambda_t(\lambda_u(J_3))$, so Eq. (10) needs to be inverted in order to write $W'_3(J_3)$ as a function solely of J_3 , which is necessary for finite element implementation. As noted by Ciambella and Saccomandi, in general, the inversion has to be done numerically; i.e. for a given J_3 , we need to obtain the equivalent λ_u from Eq. (10), and then substitute the result in Eq. (7), which is finally employed in Eq. (15). This is one of the inconvenients of the model of Ciambella and Saccomandi.

The particular choice of the W_{12} function is given by Blatz and Ko

$$W_{12} = W_1(J_1) + W_2(J_2) = \frac{\mu_0}{2} (J_1 - 3) f + \frac{\mu_0}{2} (J_2 - 3) (1 - f) \quad (16)$$

where f and μ_0 are material parameters used to fit experimental observations. The parameter μ_0 is related to the shear modulus and the parameter f is related to the volume-fraction of voids in the material [55]. In the infinitesimal limit, μ_0 is the shear modulus. Equation (16) has the familiar form employed in other models $W_{12} = C_{10} (J_1 - 3) + C_{01} (J_2 - 3)$, where $C_{10} = f\mu_0/2$ and $C_{01} = (1 - f)\mu_0/2$.

4 Simulation of the uniaxial experiments of Choi and Lakes [40]

As mentioned, Ciambella and Saccomandi used their model to fit the uniaxial tension-compression experiments of Choi and Lakes on re-entrant foams. In order to avoid the well-known problems regarding the non-monotonicity of the Blatz and Ko model, Ciambella and Saccomandi fixed $f = 1$ in order to fit the experimental data. Thus, they are left with μ_0 , λ_I and ν_0 as material parameters, all of which may be easily obtained from experimental data. The parameters they obtained are $\mu_0 = 26.53$ kPa, $\nu_0 = -0.53$ and $\lambda_I = 1.33$. The results of this fit are shown in Figures 2a and 2b, along with experimental data. As already mentioned by Ciambella and Saccomandi, it is observed that for large strains above 50%, the model is not capable of fitting well the stress-strain experimental data. This observation is in line with the reproduced Neo-Hookean model —note that $f = 1$ forces $C_{01} = 0$ and $W_{12} = C_{10} (J_1 - 3)$. Figures 2c and 2d show the derivatives of the strain energy terms $W'_{12}(J_1)$ and $W'_3(J)$ of the model of Ciambella and Saccomandi for the foam tested by Choi and Lakes. Obviously $W'_{12}(J_1) = \mu_0/2$ is constant.

We have also employed the WYPiWYG model explained in Section 2 to capture the uniaxial tension-compression experiments of Choi and Lakes. In Figures 3a and 3b, we show the predictions by the WYPiWYG model based on the Valanis-Landel decomposition. As previously noted, the WYPiWYG procedure captures to machine precision, if desired, the experimental data. The corresponding computed stored energy derivative terms, $\omega'(E^d)$ and $\mathcal{U}'(J)$ are shown in Figs. 3c and 3d. Two observations can be made.

The first one is the V-form of the energy term $\omega'(E^d)$, which results in a non-convex $\omega(E^d)$. We remark that this does not mean that the material is unstable, because stability refers to the complete stored energy $\Psi(\mathbf{E})$ in Eq. (1), where four functions are involved. For example, even if $\omega'(E_1^d < 0) > 0$, this positive value may be compensated by the other values $\omega'(E_2^d)$ and $\omega'(E_3^d)$. In Appendix B, we elaborate on the implications of the V-form; we show that it is related to the auxetic behavior and that positive observable Young moduli are still found.

The second issue noted in Figures 3c and 3d is that the computed functions $\omega'(E^d)$ and $\mathcal{U}'(E^v)$ are noisy as a consequence of the also noisy experimental data. A smoothing of the original data can be performed (and is advisable) previously to present the data to the model, so smooth functions are obtained. We refer to Ref. [56] for a procedure to reduce experimental data guaranteeing stability conditions. For further comparisons in the examples of the next sections, in Figures 4a and 4b we use the uniaxial test predictions of the Ciambella and Saccomandi model as if they were experimental data. It is shown in the same figures that the WYPiWYG model of Section 2 is also capable of exactly capturing the “experimental” data (i.e. the predictions from the Ciambella and Saccomandi model) to machine

Figure 2: Fit of the Ciambella and Saccomandi model [21] to the experimental data from Choi and Lakes [40].

precision. In Figures 4c and 4d we show the computed functions $\omega' (E^d)$ and $U' (E^v)$, where it can be seen that, as the presented data, they are smooth functions without experimental noise.

As explained above, the E-WYPiWYG hyperelastic function and the Ciambella and Saccomandi model both converge to the infinitesimal formulation for infinitesimal strains. However, this does not mean that both models produce in general the same predictions, because they are based on different coupling ansatzes. The WYPiWYG model explained in Section 2 is based on the Valanis-Landel decomposition, typical of quasi-incompressible rubber-like solids. However, the model of Ciambella and Saccomandi, following the model of Blatz and Ko for foams, is based on a decomposition written in terms of Rivlin's invariants, which results in a coupled formulation if written in terms of principal logarithmic strains. To highlight the differences in behavior, we show in Figure 5 the predictions of both models for a simple shear test. For this case, the Ciambella-Saccomandi model parameters are $\mu_0 = 1.0$, $\nu_0 = 0.45$, $\lambda_I = 2.0$, $f = 3/4$. The corresponding E-WYPiWYG stored energy is obtained from the uniaxial curves predicted by Ciambella-Saccomandi under these parameters. Obviously also, in this case the E-WYPiWYG hyperelasticity will exactly replicate the “experimental data” from the uniaxial test. Hence, the differences are only due to the coupling terms between logarithmic strains at large deformations. In fact, it can be observed in Figure 5 that at moderate strains, both models give the same result also for the shear test, but differ substantially at very large deformations. Unfortunately, Choi and Lakes did not perform further tests as to check which solution for the shear test at large strains is closer to the actual behavior of auxetic Scott

Figure 3: Computation of the E-WYPiWYG strain energy function (based on logarithmic invariants and the Valanis-Landel decomposition) from the experimental data from Choi and Lakes [40]. a) Uniaxial Cauchy stress-stretch curves. b) Transverse-to-longitudinal stretch relation. c) Derivative of the isochoic stored energy term $\omega'(E^d)$. d) Derivative of the volumetric stored energy term $U'(E^v)$.

Figure 4: E-WYPiWYG solution obtained from the stress-strain and the longitudinal-transverse strain relations given by the Ciambella and Saccomandi model [21]. a) Uniaxial Cauchy stress-stretch relations. b) Transverse-to-longitudinal stretch relations. c) Derivative of the isochoric stored energy term $\omega(E^d)$. d) Derivative of the volumetric stored energy term $U(E^v)$.

Figure 5: Comparison of the predictions from the E-WYPiWYG stored energy of Figs. 4c and 4d with those from the Ciambella-Saccomandi model [21] for a simple shear test. Ciambella-Saccomandi model parameters are $\mu_0 = 1.0$, $\nu_0 = 0.45$, $\lambda_I = 2.0$, $f = 3/4$. It is seen that the predictions of both models are coincident for moderate strains because the Valanis-Landel decomposition is recovered in such cases, but predictions differ substantially at large strains.

foams. Nonetheless, the coupled model and decomposition of Blatz and Ko have been extensively used in simulations of highly compressible foams and are available in many finite element codes. Then, the purpose of the following section is to develop a novel WYPiWYG formulation coupled in logarithmic strains and based on Rivlin's invariants. The introduction of the new function allows to "exactly" capture an *additional* test which represents the influence of the coupling of the logarithmic strains in the stored energy, a coupling that vanishes in the infinitesimal case, but which may be relevant at large strains. Of course, the novel formulation is also valid for conventional compressible materials at very large strains.

5 J-invariant-based WYPiWYG hyperelasticity

Until now, WYPiWYG hyperelasticity was based on logarithmic invariants as a natural extension of infinitesimal strains [61] and on the use of the Valanis-Landel decomposition. However, such decomposition neglects the influence of the coupling between stretches (or equivalently, of logarithmic strains) in the stored energy. At very large strains, this assumption does not necessarily hold, specially in largely compressible foams. Models based on Rivlin's invariants have been motivated from micromechanics of chains [62] and are well-accepted and extensively used in hyperelasticity. These invariants imply a special coupling form of the stretches, and stored energies are written as a function of these invariants, as for example the energy function in Eq. (11). Without loss of generality, assuming that $W_{12} = W_1(J_1) + W_2(J_2)$ as in the cases of Blatz and Ko and Ciambella and Saccomandi, the stresses of Eq. (12) can be written as

$$\boldsymbol{\sigma} = W'_3 \mathbf{I} + \frac{2}{J_3} W'_1 \mathbf{B} - \frac{2}{J_3} W'_2 \mathbf{B}^{-1} \quad (17)$$

where W'_i are three *different* functions to be determined (note that in practice we only need the derivatives of the strain energy). These functions depend on different invariants (or invariant combinations). Equation (17) has one additional function to the uncoupled form given by Equation (1). The two functions in Equation (1) are the minimum number of functions to have consistency with the infinitesimal formulation, i.e. to recover the independent modes of that theory and the two independent constants present in the linear theory. Therefore, the extra function in Eq. (17) accounts conceptually for an additional independent deformation mode due to the effects of strain couplings. This additional function may represent, for example, how the isochoric nonlinear behavior (e.g. the effective μ) changes under different volume deformations (e.g. with E^v). In foams, this coupling term may be explained by the change in the void volume fraction [55].

Following the idea behind the WYPiWYG procedures, instead of proposing a specific form of the functions W'_i of the stored energy and then fit some “material parameters”, we *numerically solve* the nonlinear differential equations of the tests from which data are available. The number of available complete experimental curves (including the compression branch if applicable) must be, obviously, the same as the number of functions to be determined. This means that for the case at hand of auxetic materials, using the form of Equation (17), we would be able to exactly (to machine precision if desired) capture three experimental curves presented to the model. We also remark that even though in the formulation of this section we will use J -invariants, any other invariants could be equally used; for example $J_1^\alpha J_2^\beta$ is an invariant that we could use in the function dependencies. As mentioned, in order to distinguish the present proposal from the one given in Section 2, we will call this new formulation J -WYPiWYG hyperelasticity.

Without loss of generality, since available experimental data from Choi and Lakes consists only of tension-compression stress-strain and transverse-to-longitudinal strain curves, we will use these data along with the additional assumption that the following relation, given both by Blatz and Ko and Ciambella and Saccomandi, holds

$$W'_1(J_1) = fW'(J_1) \quad \text{and} \quad W'_2(J_2) = (1-f)W'(J_2) \quad (18)$$

where $W'(J_\alpha)$ is a new function to be determined and f is the parameter used by Blatz and Ko and Ciambella and Saccomandi, which accounts for the volume-fraction of voids in the foam [55]. The hypothesis given in Equation (18) substitutes the missing experimental test. In general, the functional dependency would be derived from the equilibrium equation of that missing test.

The equilibrium equations of the uniaxial tension-compression test are

$$\sigma_u = W'_3(J_3) + \frac{2}{J_3} [W'_1(J_1)\lambda_u^2 - W'_2(J_2)\lambda_u^{-2}] \quad (19)$$

$$0 = W'_3(J_3) + \frac{2}{J_3} [W'_1(J_1)\lambda_t^2 - W'_2(J_2)\lambda_t^{-2}] \quad (20)$$

The system of equations (18) to (20) constitute a system of nonlinear *functional equations* in which the unknown *functions* are $W'(J_\alpha)$, $W'_1(J_1)$, $W'_2(J_2)$ and $W'_3(J_3)$. These types of functional equations may be solved in general using different techniques; for example multidimensional spline interpolations [43]. However, in the present system of equations, as in most proposed hyperelastic models, the energy terms are real-variable functions of some general invariants. In these cases more efficient solution procedures based on unidimensional interpolations are possible. For the case at hand, Equations (18) may be directly substituted into Eqs. (19), (20), and then we can use Eq. (20) to factor-out function $W'_3(J_3)$ as

$$W'_3(J_3) = -\frac{2}{J_3} [fW'(J_1)\lambda_t^2 - (1-f)W'(J_2)\lambda_t^{-2}] \quad (21)$$

Then, Eq. (19) may be used to factor-out $W'(J_1)$

$$W'(J_1) = \frac{1/f}{\lambda_u^2 - \lambda_t^2} \left(\frac{1}{2} J_3 \sigma_u + (1-f)W'(J_2)(\lambda_u^{-2} - \lambda_t^{-2}) \right) \quad (22)$$

Noteworthy, using Eqs. (18), (22), it is seen that the particular cases $f = 0$ and $f = 1$ frequently used in the literature, only involves two functions, and an *explicit solution* is immediately found, without iterations and without the need to solve a system of nonlinear function equations

$$\begin{cases} f = 0 \implies W'(J_2) = -\frac{1}{2} \frac{J_3 \sigma_u}{1/\lambda_u^2 - 1/\lambda_t^2} \quad \text{and} \quad W'_3(J_3) = \frac{2}{J_3} \frac{W'(J_2)}{\lambda_t^2} \\ f = 1 \implies W'(J_1) = \frac{1}{2} \frac{J_3 \sigma_u}{\lambda_u^2 - \lambda_t^2} \quad \text{and} \quad W'_3(J_3) = -\frac{2}{J_3} W'(J_1)\lambda_t^2 \end{cases} \quad (23)$$

Then, it is clear that *there is no need to impose a form for these functions*, as done in analytical models. For the general case, an iterative procedure is needed. During the uniaxial test, the driving variable is λ_u , so all variables of any kind depend on λ_u . Let us write the dependencies explicitly

$$W'_3(J_3(\lambda_u)) = -2 \frac{fW'(J_1(\lambda_u))[\lambda_t(\lambda_u)]^2 - (1-f)W'(J_2(\lambda_u))[\lambda_t(\lambda_u)]^{-2}}{J_3(\lambda_u)} \quad (24)$$

$$W'(J_1(\lambda_u)) = \frac{J_3(\lambda_u) \sigma_u(\lambda_u)/2 + (1-f)W'(J_2(\lambda_u)) \left(1/\lambda_u^2 - 1/[\lambda_t(\lambda_u)]^2\right)}{f \left(\lambda_u^2 - [\lambda_t(\lambda_u)]^2\right)} \quad (25)$$

The experimental data from a uniaxial tension-compression test consists in two “curves” defined by two sets of pairs, namely $\{\lambda_{uk}, \sigma_{uk}\}$, and $\{\lambda_{uk}, \lambda_{tk}\}$, $k = 1, \dots, K$. From these data, it is straightforward to compute the pairs (“curves”) $\{\lambda_{uk}, J_{1k}\}$, $\{\lambda_{uk}, J_{2k}\}$, $\{\lambda_{uk}, J_{3k}\}$, $k = 1, \dots, K$. In order to solve the nonlinear functional equations, we can employ an iterative function refreshing algorithm. We can start with a constant function $W' = \mu_0/2$, i.e. for iteration [0] we build the pairs $\{\lambda_{uk}, W_k^{[0]}\} \equiv \{\lambda_{uk}, \mu_0/2\}$, $k = 1, \dots, K$. With these pairs, by interpolating them, we build a piecewise spline function $W'^{[0]}(J_\alpha)$, which is constant in this starting guess. Then, since this continuous function may be evaluated at any given value J_α , by use of Eq. (25) we can update

$$W_k^{[j+1]}(J_{1k}) = \frac{J_{3k} \sigma_{uk}/2 + (1-f)W'^{[j]}(J_{2k}) \left(1/\lambda_{uk}^2 - 1/\lambda_{tk}^2\right)}{f \left(\lambda_{uk}^2 - \lambda_{tk}^2\right)}, \quad k = 1, \dots, K \quad (26)$$

with $j = 0, 1, \dots$ until convergence. Note that the knowledge of the discrete values $W_k^{[j]}$ is not sufficient and the construction of the iterative function $W'^{[j]}(J_\alpha)$ is necessary because the arguments J_{2k} and J_{1k} are different (the discretizations in the arguments are different but the function itself is the same). The iterative procedure in Eq. (26) is convergent for the typical experimental curves we used. Convergence is measured as the difference between two computed functions W' ; i.e. the difference between values of consecutive iterations at the discretization points. However if convergence is not reached, Eq. (26) may be reversed to give the alternative

$$W_k^{[j+1]}(J_{2k}) = \frac{(\lambda_{uk}^2 - \lambda_{tk}^2) f W'^{[j]}(J_{1k}) - J_{3k} \sigma_{uk}/2}{(1-f) (\lambda_{uk}^{-2} - \lambda_{tk}^{-2})}, \quad k = 1, \dots, K \quad (27)$$

which brings a function refreshing algorithm in reverse order.

Once the function $W'(J_\alpha)$ has been determined and thus can be evaluated for any arbitrary argument, the function $W'_3(J_3)$ can be computed explicitly, without iterations, by interpolating the following discrete values

$$W'_{3k}(J_{3k}) = -\frac{2}{J_{3k}} \left[f W'(J_{1k}) \lambda_{tk}^2 - (1-f) W'(J_{2k}) \lambda_{tk}^{-2} \right], \quad k = 1, \dots, K \quad (28)$$

In the general case, depending on the available experimental data, a set of nonlinear functional equations may be established and solved using the proper algorithm. For computational efficiency in finite element implementations, it is advisable to discretize and rebuild the spline functions in uniform intervals so the applicable interval can be immediately computed for each function. We note that in this novel procedure we have not needed any inversion formula, so the method has wider validity than the original WYPiWYG method, which was restricted to the Valanis-Landel decomposition, logarithmic strains and the inversion formula. Remarkably, this or similar computational procedures may be employed in any decomposition ansatz, and the *prescribed set* of experimental curves will be *predicted* by the model to any desired precision, without material parameters; i.e. *What-You-Prescribe is What-You-Get*.

We also remark that it is irrelevant for finite element analysis that the (piecewise spline) functions $W'_3(J_3)$ and $W'(J_\alpha)$ (or in general any other energy derivatives) have been determined solving the differential equations of some particular tests presented to the model. Since the stored energy function is unique for a material, it is valid in any other loading situation. For instance, assume that, at the integration point of a given finite element, we have the deformation gradient $\mathbf{X}$. Then we can compute the tensor $\mathbf{B} = \mathbf{X}^T \mathbf{X}$ and its invariants J_1, J_2, J_3 . With these invariants we can evaluate the piecewise spline functions to obtain the values $W'_1(J_1)$, $W'_2(J_2)$ and $W'_3(J_3)$. Since the derivatives of the stored energy function are known, it is straightforward to obtain the stresses of that general loading case via Equation (17). The tangent moduli for finite element implementation are given in Appendix C.

6 Numerical examples

6.1 Homogeneous deformations

In this section we show that the novel procedure may be efficiently used to capture “experimental” data presented to the model, including the case of auxetic materials at hand. In Figure 6, we show that the J-invariant WYPiWYG formulation (J-WYPiWYG hyperelasticity) is also capable of capturing the experimental data of Choi and Lakes accurately. Furthermore, we show that we are able to do so for different values of the parameter f . In practice, we can

Figure 6: J-WYPiWYG stored energy derivative terms that replicate the (slightly smoothed) experimental data from Choi and Lakes [40] for different values of f , in particular $f = 3/4$, $f = 1$. a) Stress-stretch data including slightly smoothed experimental data and J-WYPiWYG predictions using either $f = 3/4$ or $f = 1$. b) Experimental and predicted longitudinal-to-transverse stretches. c) Computed J-WYPiWYG stored energy derivative terms $W'_1(J_1)$ and $W'_2(J_2)$. d) Computed stored energy derivative term $W'_3(J_3)$.

fit the experimental data with infinite different sets of the functions $W'_1(J_1)$, $W'_2(J_2)$ and $W'_3(J_3)$, because we are using three functions to just reproduce two experimental curves. As previously commented, with the three functions we would be able to reproduce to any desired precision up to three complete experimental curves. Since unfortunately less curves are available for Scott foams, in order to have the determination problem well-posed, we included the same restriction employed by Blatz and Ko and Ciambella and Saccomandi, i.e. Eqs. (18).

The J-WYPiWYG iterations of the functional refreshing algorithm described in Eq. (26) are shown in Figure 7. The resulting $W'(J_\alpha)$ function replicates the unsmoothed Choi-Lakes experimental data. Machine precision is obtained in 24 iterations, but after few iterations the solutions are visually indistinguishable.

In Section 4 we have shown that even though the E-WYPiWYG formulation based on the Valanis-Landel decomposition was capable of exactly capturing the predicted behavior of the Ciambella and Saccomandi model for the uniaxial tests of Choi and Lakes, it was not capable of capturing the behavior in a general loading case for sufficiently large

Figure 7: J-WYPiWYG iterations reaching machine precision, to determine the stored energy term $W'(J_\alpha)$ with $f = 3/4$ that replicates the unsmoothed experimental data from Choi and Lakes [40] on Scott foams (recall that for the case $f = 1$ the solution is explicit)

deformations, e.g. a simple shear case. As a numerical exercise that can be extended to real materials (but in such a case experimental errors would not allow us to arrive at this claim), we now show that the new J-WYPiWYG formulation is capable of recovering the formulation of Ciambella and Saccomandi in any loading situation, to any desired numerical precision. In fact, this observation will hold for whatever other model if the same functional decomposition is employed.

In Figure 8 we present the predictions of J-WYPiWYG hyperelasticity for the simple shear test. It is seen that the predictions of J-WYPiWYG hyperelasticity are indistinguishable from those of the model of Ciambella and Saccomandi.

To show that J-WYPiWYG hyperelasticity is capable predicting the behavior of the Ciambella and Saccomandi model in any arbitrary loading condition, we perform homogeneous deformation simulations prescribing different deformation gradients of the type

$$\mathbf{X} = \begin{bmatrix} (1 + \gamma)^n & \gamma & 0 \\ 0 & (1 + \gamma)^n & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (29)$$

where γ is the “amount of shear” and n is an exponent to include a coupled volumetric component.

In Figure 9 we show the predictions of the different components of the Cauchy stress tensor versus the amount of shear, also using different values of the volumetric deformation exponent n . It is seen in that figure that the J-WYPiWYG formulation captures accurately all components of all deformation cases.

6.2 Finite element examples

In Figure 10 we show the finite element mesh of the plate with a centered hole used in the analyses below. The dimensions of the plate are 32 mm length, 16 mm width, and the hole has a radius of 4 mm. The plane strain plate is stretched in the longitudinal direction doubling its length and imposing the displacements by means of a penalty formulation. The larger sides are left free. We use 9-node elements with quadratic interpolation (note that the material is compressible). The global equilibrium equations are solved using a plain Newton procedure. The simulations are performed with our in-house finite element code Dulcinea. The mesh is similar to that used in simulations with other constitutive models, like viscoelasticity [63] and damage [64].

In order to first remark the difference in behavior between a conventional and a purely auxetic material, we have used the previous uniaxial stress-strain experimental data, see Figure 11a, along with two fictitious constant Poisson ratios, namely $\nu = 0.4$ and $\nu = -0.8$, see Figure 11b. From these data, we have computed respective E-WYPiWYG stored energy functions, shown in Figs. 11c and 11d. In Figures 11e and 11f, we show the deformed meshes of the plate along

Figure 8: Comparison of predictions for a simple shear test. The Ciambella-Saccomandi model parameters are $\mu_0 = 1.0$, $\nu_0 = 0.45$, $\lambda_I = 2.0$, $f = 3/4$. (the value of $f = 3/4$ implies that all terms are active). Both E-WYPIWYG and J-WYPIWYG hyperelasticity replicate accurately the uniaxial test (stress-strain and longitudinal-to-transverse behavior) of the Ciambella-Saccomandi model. However, this figure shows that whereas E-WYPIWYG hyperelasticity is unable to replicate also the shear test at very large strains, J-WYPIWYG hyperelasticity does it accurately.

with band plots of the von Mises stress, whereas in Figures 11g and 11h the band plots correspond to the pressure. Regardless of having exactly the same uniaxial stress-strain curve, it is seen that the behavior is remarkably different. In the conventional case, the isochoric deformation dominates, whereas in the auxetic case, the volumetric deformation dominates. These effects are also apparent in the von Mises stress and pressure distributions.

However, as previously mentioned, the Poisson ratio of real auxetic foams $\nu(\lambda)$ is a highly nonlinear non-monotonic function with transitions from auxetic to conventional behavior.

To compare the differences between E-WYPIWYG hyperelasticity and the novel J-WYPIWYG hyperelasticity predictions, we perform simulations on the same specimen with stored energies which reproduce exactly the same uniaxial curves of Figures 4a and 4b (i.e. the prediction of Ciambella - Saccomandi model for Choi and Lakes experiments on Scott's foams).

In Figure 12 we compare the results using E-WYPIWYG hyperelasticity and J-WYPIWYG hyperelasticity at the last step. The latter results are visually identical to the ones obtained from the Ciambella-Saccomandi model, which we omit for brevity, as it should be obvious from the foregoing analysis. In Figure 12a we show, along the deformed mesh, the longitudinal logarithmic strain E_x for the model using E-WYPIWYG hyperelasticity and in Figure 12b we show the results using J-WYPIWYG hyperelasticity. In Figures 12c and 12d we show the transverse logarithmic strains E_y using both models. It is clearly seen that $E_y > 0$ in most of the plate. This positive transverse strain obtained for positive longitudinal strain indicates auxetic behavior. This effect is also observable in the deformed meshes, where it is observed that the transverse dimension of the plate and of the central passing area around the hole are slightly larger than the original, undeformed ones. For comparison purposes, we show in Figs. 12e and 12f the von Mises stresses and in Figs. 12g and 12h the pressure. The differences between the results using E-WYPIWYG hyperelasticity and J-WYPIWYG hyperelasticity are due to the coupling effects between strains. At moderate strains, both E-WYPIWYG and J-WYPIWYG formulations give similar results, but at large deformations, specially in locations where deformations are far from being considered uniaxial, both formulations show some differences. In Figure 12 both stresses and strains reach similar values, although predicted stresses are slightly smaller in the case of J-WYPIWYG hyperelasticity respect to E-WYPIWYG hyperelasticity. This is in concordance with the evidence in Figure 8. Also remarkable, the overall transverse-to-longitudinal deformation ratio of the plate in Figure 12 is an intermediate case between the plates of Figure 11 which had $\nu = -0.8$ and $\nu = 0.4$. In this example, E-WYPIWYG hyperelasticity and J-WYPIWYG hyperelasticity show few differences because the plate is loaded mainly in a uniaxial mode, and both models reproduce the same uniaxial stress-strain behavior. However, in Figure 13, we show the behavior of a simple shear test when using both E-WYPIWYG hyperelasticity (Figure 13a) and J-WYPIWYG hyperelasticity (Figure 13b). The stored energies in both

Figure 9: Demonstration of the predictive capabilities of J-WYPiWYG hyperelasticity and E-WYPiWYG hyperelasticity for auxetic foams (or highly compressible materials). Different components of the stress tensor against the amount of shear parameter γ . Results for $f = 3/4$. Deformation gradient given in Eq. (29), where $n = 1/4$ for the first row of plots, $n = 1/2$ for the second row of plots and $n = 3/4$ for the third row of plots. This figure shows that J-WYPiWYG hyperelasticity captures all cases “exactly”.

Figure 10: Finite element mesh used in the examples. Elements are Lagrangean 9-node elements with 3×3 integration.

cases have been determined as to exactly capture the uniaxial curves in Figs. 4a and 4b, so the differences observed in Figure 13 are due to the coupling terms. Noteworthy, the deformed shapes are different from those expected in a conventional material. These differences are due to the auxetic behavior.

Finally, in order to show that both E-WYPiWYG and J-WYPiWYG formulations have similar efficiency in finite element simulations as any analytical hyperelastic model, in Table 1 we show the force and energy convergence rates of both WYPiWYG formulations for a representative step. It is seen that both WYPiWYG formulations result in quadratic convergence rates, and both formulations use a similar number of iterations. The convergence values of the Ciambella and Saccomandi model are almost identical to those of the J-WYPiWYG formulation because, in fact, the stored energies are also numerically coincident, so all the iterative path followed by the finite element program is also the same.

Typical relative convergence rates of the finite element example. Step 90/100		
J-WYPiWYG		
Iter	Force residual	Energy residual
1	$1.000E + 00$	$1.000E + 00$
2	$3.971E - 05$	$1.194E - 08$
3	$3.367E - 09$	$3.053E - 18$
E-WYPiWYG		
Iter	Force residual	Energy residual
1	$1.000E + 00$	$1.000E + 00$
2	$7.667E - 05$	$3.764E - 08$
3	$4.842E - 09$	$3.793E - 17$

Table 1: Convergence rates for both the J-WYPiWYG and WYPiWYG procedures

7 Conclusions

Auxetic materials have important applications. In this work we present a framework for the finite element analysis of auxetic conservative materials at large strains using the continuum approach. Auxetic materials are highly compressible materials with negative Poisson ratio, whereas most isotropic hyperelastic energy functions proposed in the literature are for conventional rubber-like materials, typically quasi-incompressible and with positive Poisson ratios. Previous

E-WYPiWYG hyperelasticity: auxetic versus conventional behavior

Figure 11: Comparison of a conventional behavior (red) and an auxetic behavior (blue) for the same stress-strain uniaxial curve $\tau_u(E_u)$. This uniaxial curve has been obtained from the Ciambella and Saccomandi model that fits the Choi-Lakes experimental data, as shown in Figure 2a with parameters $\nu_0 = -0.53$, $\mu_0 = 26.53$, $\lambda_I = 1.33$, $f = 1$. a) Uniaxial stress-strain curve in both materials. b) Prescribed constant transverse strain relations $\lambda_t(\lambda_u) = \lambda_u^{-\nu}$ for each material. c) Computed stored energy derivatives $\omega'(E)$ for both the conventional and the auxetic material. d) Computed stored energy derivatives $U'(E)$ for both the conventional and the auxetic material. e) Deformed mesh and von Mises stress for the auxetic material. f) Deformed mesh and von Mises stress for the conventional material. g) Pressure distribution for the auxetic material. h) Pressure distribution for the conventional material.

Figure 12: Comparison of the predictions obtained from E-WYPIWYG hyperelasticity, left column, and J-WYPIWYG hyperelasticity (or the Ciambella-Saccomandi model), right column. Band plots performed over a deformed mesh, unaveraged, unsmoothed at nodes. The outline of the undeformed mesh is also shown. a), b) Longitudinal logarithmic strains E_x . c), d) Transverse logarithmic strains E_y . e), f) von Mises stress. g), h) Pressure distribution.

Figure 13: Comparison of the predictions obtained for a simple-shear test using E-WYPiWYG hyperelasticity (a) and J-WYPiWYG hyperelasticity (b). Both models reproduce exactly the uniaxial behavior of the auxetic material of Figs. 4a and 4b, but show different von Mises stresses in shear. Note that the deformed shape of the auxetic material is different from that expected from a conventional material.

WYPiWYG formulations are based on logarithmic strains and on the uncoupled Valanis-Landel decomposition. However, usual stored energies for compressible materials are based on classical principal invariants and different functional decompositions. In this work we present a novel procedure for WYPiWYG hyperelasticity using these invariants and valid for the coupled forms of the stored energy function typically employed in the analysis of highly compressible foams. We have applied the procedure to predict the behavior of auxetic Scott foams. We show that the novel proposal is in particular valid for finite element continuum modelling of auxetic foams. As a demonstrative example, we show that it recovers, under any loading condition, the stored energy of a hyperelastic analytical model explicitly designed for auxetic foams just employing pseudo-experimental data generated from the model. The finite element simulations shown in this paper are, to the authors' knowledge, the first simulations for hyperelastic auxetic materials at large strains following the continuum approach. The approach is promising in the finite element analysis of structures and devices employing auxetic materials.

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Appendix A: Computational procedure for isotropic, compressible E-WYPiWYG hyperelasticity.

The computational procedure for isotropic, compressible E-WYPiWYG hyperelasticity is as follows. Assume that the experimental data consists of (1) a number of uniaxial Kirchhoff stress-strain pairs $\{E_{uk}, \tau_{uk}\}$, $k = 1, \dots, K$, where E_{uk} is the true uniaxial strain of point k , and (2) a number of longitudinal-to-transverse strain pairs $\{E_{uk}, E_{tk}\}$, where E_{tk} is the transverse value. From these discrete values, we can build a piecewise spline (analytical) function $\tau_u(E_u)$ and a piecewise analytical function $E_t(E_u)$. With the latter function, we can build new piecewise analytical functions $E^v(E_u) = E_u + 2E_t(E_u)$ and $E_u^d(E_u) = \frac{2}{3}[E_u - E_t(E_u)]$. These analytical functions may then be used to evaluate the equilibrium equation of the volumetric part

$$\mathcal{U}'(E^v(E_u)) = \tau_u(E_u)/3 \quad (30)$$

i.e. for $k = 1, \dots, K$ values of E_{uk} , we evaluate $\tau_{uk} \equiv \tau_u(E_{uk})$ and $E_k^v \equiv E^v(E_{uk})$ and then $\mathcal{U}'_k \equiv \mathcal{U}'(E_k^v) \equiv \tau_{uk}/3$, so we have the pairs $\{E_{uk}, \tau_{uk}\}$ and $\{E_k^v, \mathcal{U}'_k\}$, from which a piecewise analytical function $\mathcal{U}'(E^v)$ may be constructed. Obviously, even though we obtain $\mathcal{U}'(E^v)$ from a tensile test, it is valid under any loading situation, because it suffices to compute the volumetric strain of any general strain tensor as $E^v = \ln J$ and evaluate $\mathcal{U}'(E^v)$.

The other equilibrium equation involving distortional components is

$$\tau_u(E_u^d(E_u)) = \omega'(E_u^d(E_u)) - \omega'(-\frac{1}{2}E_u^d(E_u)) \quad (31)$$

This nonlinear functional equation may be solved in a number of different ways, for example, using the Kearsley and Zapas formula, which consists in the following convergent series

$$\omega'(E_u^d) - \omega'(0) = \sum_{n=1}^N \tau_u \left(\left(-\frac{1}{2} \right)^n E_u^d(E_u) \right) \quad (32)$$

where N is such that the required tolerance is obtained. Without loss of generality, we can choose $\omega'(0) = 0$ and then evaluate the Kearsley and Zapas formula in as many points as desired

$$\omega'_k \equiv \omega'(E_{uk}^d) = \sum_{n=1}^N \tau_u \left(\left(-\frac{1}{2} \right)^n E_{uk}^d \right) \quad (33)$$

with $E_{uk}^d \equiv E_u^d(E_{uk})$. Thus, the pairs $\{E_k^d, \omega'_k\}$ are obtained and a piecewise spline function $\omega'(E^d)$ may be built. Obviously again, this function is valid in any loading situation; it suffices to compute the principal distortional true strains E_i^d of whatever deformation $\mathbf{X}$ and apply

$$\mathbf{T} = \bar{\boldsymbol{\tau}} = \mathcal{U}'(E^v) \mathbf{I} + \mathbf{T}^{|d|} : \mathbb{P} \quad (34)$$

with

$$\mathbf{T}^{|d|} := \frac{d\mathcal{W}}{d\mathbf{E}^d} = \sum_{i=1}^3 \omega'(E_i^d) \mathbf{N}_i \otimes \mathbf{N}_i \quad (35)$$

where $\mathbf{N}_i$ are the principal strain directions and $\mathbb{P}$ is the deviatoric projector tensor. The tensor $\mathbf{T}$ is the generalized Kirchhoff stress tensor, work-conjugate of the referential logarithmic strains $\mathbf{E}$, and coincident with the rotated (or corrotational) Kirchhoff stress tensor $\bar{\boldsymbol{\tau}}$ in the isotropic case at hand. The Cauchy stress ($\boldsymbol{\sigma}$) is immediately obtained as,

$$\boldsymbol{\sigma} = J^{-1} \mathbf{R} \bar{\boldsymbol{\tau}} \mathbf{R}^T \quad (36)$$

Since during a uniaxial tensile test $\mathbf{R} = \mathbf{I}$, and $\bar{\boldsymbol{\tau}} = \boldsymbol{\tau}$, we have $\sigma_u = J^{-1} \tau_u$. The constitutive tangent is obtained by a systematic use of the chain rule as

$$\mathbb{C} = \frac{d\mathbf{T}}{d\mathbf{E}} = \frac{d^2\Psi}{d\mathbf{E}d\mathbf{E}} = \mathcal{U}''(E^v) \mathbf{I} \otimes \mathbf{I} + \mathbb{P} : \mathbb{C}^{|d|} : \mathbb{P} \quad (37)$$

where

$$\mathbb{C}^{|d|} = \frac{d\mathbf{T}^{|d|}}{d\mathbf{E}^d} = \sum_{i=1}^3 \omega''(E_i^d) \mathbf{M}_i \otimes \mathbf{M}_i + \sum_{i=1}^3 \sum_{j \neq i} \frac{T_j^d - T_i^d}{E_j^d - E_i^d} \mathbf{M}_{ij} \otimes \mathbf{M}_{ij} \quad (38)$$

with

$$\mathbf{M}_i := \mathbf{N}_i \otimes \mathbf{N}_i \text{ and } \mathbf{M}_{ij} = \frac{1}{2} (\mathbf{N}_i \otimes \mathbf{N}_j + \mathbf{N}_j \otimes \mathbf{N}_i) \quad (39)$$

The stress-strain pair $\mathbf{T} - \mathbf{E}$ and its associated constitutive tensor $\mathbb{C}$ may be systematically converted to any other work-conjugate stress-strain pair by the use of mapping tensors [60].

Appendix B: Discussion of the V-shape of the ω' energy terms of E-WYPiWYG hyperelasticity in auxetic materials

The E-WYPiWYG formulation hinges in Decomposition (1). In fact, this decomposition is equivalent, and can be motivated from the theory of infinitesimal bi-linear materials, whose strain energy is

$$\Psi(\boldsymbol{\varepsilon}) = \frac{1}{2}\kappa^* (\varepsilon^v)^2 + \mu_1^* (\varepsilon_1^d)^2 + \mu_2^* (\varepsilon_2^d)^2 + \mu_3^* (\varepsilon_3^d)^2 \quad (40)$$

where $\boldsymbol{\varepsilon}$ is the small strain tensor, ε^v and ε_i^d are the volumetric and deviatoric quantities, κ^* is the effective bulk modulus and μ_i^* are the shear moduli, such that

$$\kappa^* = \begin{cases} \kappa^t & \text{if } \varepsilon^v > 0 \\ \kappa^c & \text{if } \varepsilon^v < 0 \end{cases} \quad (41)$$

$$\mu_i^* = \begin{cases} \mu^t & \text{if } \varepsilon_i^d > 0 \\ \mu^c & \text{if } \varepsilon_i^d < 0 \end{cases} \quad (42)$$

with the superscript t/c indicating “tension” or “compression” value. Of course if $\kappa^t = \kappa^c$ and $\mu^t = \mu^c$ we recover the linear theory. Furthermore, $\mu_i^{t/c}$ and $\kappa^{t/c}$ may be related to respective Young moduli $Y^{t/c}$ and Poisson ratios $\nu^{t/c}$. For tension,

$$Y^t = \frac{9\kappa^t(2\mu^t + \mu^c)}{2\mu^t + \mu^c + 9\kappa^t} \text{ and } \nu^t = \frac{-4\mu^t - 2\mu^c + 9\kappa^t}{4\mu^t + 2\mu^c + 18\kappa^t} \quad (43)$$

$$\mu^t = \frac{Y^t}{1 + \nu^t} - \frac{1}{2} \frac{Y^c}{1 + \nu^c} \text{ and } \kappa^t = \frac{1}{3} \frac{Y^t}{1 - 2\nu^t} \quad (44)$$

The equivalent values for compression can be obtained interchanging the superscripts t/c . This infinitesimal bi-linear formulation is extremely useful in analyzing analytically problems when using Decomposition (1), and it is simpler and more general (because it is not a particular theory restricted in the elastic constants) than recent proposals, see for example [65], [66], [67].

Apparently, the V-shape of the stored energy term $\omega'(E^d)$ in Figure 3 may seem physically incorrect, because the corresponding term $\omega(E^d)$ would not be convex. The purpose of this Appendix is to show that an equivalent behavior is obtained when using the infinitesimal bi-linear model, in which case the decomposition is exact and the theory identical to the usual infinitesimal theory, but just accounting for possible different behaviors in tension and compression.

During a uniaxial test,

$$\varepsilon^v = \varepsilon_u + 2\varepsilon_t \text{ and } \varepsilon_u^d = \frac{2}{3}(\varepsilon_u - \varepsilon_t) \text{ and } \varepsilon_t^d = -\frac{1}{3}(\varepsilon_u - \varepsilon_t) \quad (45)$$

Introducing the Poisson ratio

$$-\frac{\varepsilon_t}{\varepsilon_u} = \nu^t \text{ for } \varepsilon_u > 0 \text{ and } -\frac{\varepsilon_t}{\varepsilon_u} = \nu^c \text{ for } \varepsilon_u < 0 \quad (46)$$

we can write

$$\varepsilon_u^d = \frac{2}{3}(1 + \nu^{t/c})\varepsilon_u \text{ and } \varepsilon_t^d = -\frac{1}{3}(1 + \nu^{t/c})\varepsilon_u \text{ and } \varepsilon^v = (1 - 2\nu^{t/c})\varepsilon_u \quad (47)$$

The equilibrium equations are obtained from $\boldsymbol{\sigma} = d\Psi/d\boldsymbol{\varepsilon}$ and Eq. (40) as

$$\begin{cases} \sigma_u = \kappa^{t/c}\varepsilon^v + 2\mu^{t/c}\varepsilon_u^d \\ 0 = \kappa^{t/c}\varepsilon^v + 2\mu^{c/t}\varepsilon_t^d \end{cases} \quad (48)$$

where t/c is tension or compression depending on the sign of ε_u . Assuming $\varepsilon^v > 0$, we can use the second equation to substitute the volumetric part in the first equation to arrive at

$$\sigma_u = \left[\frac{4}{3}\mu^{t/c}(1 + \nu^{t/c}) + \frac{2}{3}\mu^{c/t}(1 + \nu^{t/c}) \right] \varepsilon_u \quad (49)$$

The measured Young modulus is

$$Y^{t/c} = \frac{4}{3}\mu^{t/c} \left(1 + \nu^{t/c}\right) + \frac{2}{3}\mu^{c/t} \left(1 + \nu^{t/c}\right) \quad (50)$$

Obviously, if $\mu^t = \mu^c$ and $\nu^t = \nu^c$, the classical expression of the linear theory is recovered. Now we are interested in the auxetic case, $\nu < 0$. Assume for simplicity $\nu^t = \nu^c < 0$. Then

$$Y^{t/c} = \frac{2}{3}(1 + \nu) \left(2\mu^{t/c} + \mu^{c/t}\right) \quad (51)$$

A stable response during the tensile test is obtained if

$$(1 + \nu) \left(2\mu^{t/c} + \mu^{c/t}\right) > 0 \quad (52)$$

Since $\nu > -1$ we have $2\mu^{t/c} + \mu^{c/t} > 0$. It is apparent that μ^c may be negative whenever $2\mu^t > -\mu^c$. Hence, since $\omega''(\varepsilon < 0) = 2\mu^c$, V-shaped curves are possible in this regard.

Furthermore, from Eq. (44) and its equivalent in compression, after some little algebra we obtain

$$\frac{\mu^t}{\mu^c} = \frac{1 - 2\eta}{\eta - 2} \quad (53)$$

where $\eta = Y^t/Y^c$. If $\eta > 2$ (a material much stiffer in tension than in compression), then $\mu^t/\mu^c < 0$ (V-shape condition), which means that regardless of the value of the Poisson ratio, if $\mu^t > 0$ we must have $\mu^c < 0$, or vice-versa. Similarly, if $\eta < 1/2$, then we also have $\mu^t/\mu^c < 0$, with the same conclusion.

Let us now assume that $\eta = 1$. Then we obtain the relation

$$\frac{\mu^t}{\mu^c} = \frac{(v^t + 1) + 2(\nu^c - \nu^t)}{(v^t + 1) - (\nu^c - \nu^t)} \quad (54)$$

Noteworthy, if $\nu^t = -1$, $\mu^t/\mu^c = -2$ (V-shape), regardless of the value of ν^c . Since $(\nu^t + 1) > 0$, then $\mu^t/\mu^c < 0$ if either

$$\nu^c > 2\nu^t + 1 \text{ or } \nu^c < \frac{\nu^t - 1}{2} \quad (55)$$

For example, assume $\nu^t = -1/2$. Then from the conditions of the previous equation, it is inferred that a V-shape is obtained either when $\nu^c > 0$ or when $\nu^c < -3/4$. Therefore, if the Poisson ratios change with strains, as experimentally observed in auxetic materials, a V-shape can be expected.

In general, the condition for ν^c in which the V-shape ($\mu^t > 0$ and $\mu^c < 0$) is found is for

$$\nu^c < 1/2 \eta (1 + \nu^t) - 1 =: \nu_{crit}^c \quad (56)$$

where ν_{crit}^c is the critical value between normal-shape and V-shape. In Figure 14, we show the zones in which the V-shape is found as a function of ν^c and ν^t , for given Young moduli ratios η .

Finally, in Figure 15 we show the influence of the nonlinearity departing from a bi-linear auxetic model obtained tying the origin with the extreme values in the experimental tests of Choi and Lakes. In such case we have $\eta = 16$, $\nu^t = -0.05$ and $\nu^c = -0.04$. Then in Figures 15a and 15b we plot

$$\begin{cases} \tau_u(E_u) = L\tau_u^{bi-lin}(E_u) + (1 - L)\tau_u^{exp}(E_u) \\ E_t(E_u) = LE_t^{bi-lin}(E_u) + (1 - L)E_t^{exp}(E_u) \end{cases} \quad (57)$$

where labels *bi-lin* and *exp* correspond to the linearized and experimental data, respectively, and L is the linear parameter that ranges from zero (experimental data) to one (linear data). In Figures 15c and 15d we show the computed WYPiWYG stored energy terms for each one of the cases given in Eq. (57), Figs. 15a and 15b.

Figure 14: Parametric analysis of η, ν^c, ν^t for V-shape condition of $\omega' (E^d)$

Appendix C: Constitutive tangent moduli for J-WYPiWYG hyperelasticity

Since the spline functions are third order polynomials, their derivatives $W_1''(J_1)$, $W_2''(J_2)$ and $W_3''(J_3)$ are also trivial. The constitutive tangent is described in terms of I-invariants, as (see for example [68])

$$\begin{aligned} \mathbb{C} &= \frac{d\mathbf{S}}{d\mathbf{A}} = 4 \frac{d^2\Psi(I_1, I_2, I_3)}{d\mathbf{C}d\mathbf{C}} \\ &= \delta_1 \mathbf{I} \otimes \mathbf{I} + \delta_2 (\mathbf{I} \otimes \mathbf{C} + \mathbf{C} \otimes \mathbf{I}) + \delta_3 (\mathbf{I} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{I}) + \\ &+ \delta_4 \mathbf{C} \otimes \mathbf{C} + \delta_5 (\mathbf{C} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{C}) + \\ &+ \delta_6 \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} + \delta_7 \mathbf{C}^{-1} \odot \mathbf{C}^{-1} + \delta_8 \mathbb{I}^S \end{aligned} \quad (58)$$

where the coefficients δ_i are,

$$\delta_1 = 4 \left(\frac{\partial^2 \Psi}{\partial I_1 \partial I_1} + 2I_1 \frac{\partial^2 \Psi}{\partial I_1 \partial I_2} + \frac{\partial \Psi}{\partial I_2} + I_1^2 \frac{\partial^2 \Psi}{\partial I_2 \partial I_2} \right) \quad (59)$$

$$\delta_2 = -4 \left(\frac{\partial^2 \Psi}{\partial I_1 \partial I_2} + I_1 \frac{\partial^2 \Psi}{\partial I_2 \partial I_2} \right) \quad (60)$$

$$\delta_3 = 4 \left(I_3 \frac{\partial^2 \Psi}{\partial I_1 \partial I_3} + I_1 I_3 \frac{\partial^2 \Psi}{\partial I_2 \partial I_3} \right) \quad (61)$$

$$\delta_4 = 4 \frac{\partial^2 \Psi}{\partial I_2 \partial I_2} \quad (62)$$

and

$$\delta_5 = -4I_3 \frac{\partial^2 \Psi}{\partial I_2 \partial I_3} \quad (63)$$

$$\delta_6 = 4 \left(I_3 \frac{\partial \Psi}{\partial I_3} + I_3^2 \frac{\partial^2 \Psi}{\partial I_3 \partial I_3} \right) \quad (64)$$

$$\delta_7 = -4I_3 \frac{\partial \Psi}{\partial I_3} \quad \text{and} \quad \delta_8 = -4 \frac{\partial \Psi}{\partial I_2} \quad (65)$$

and $\mathbb{I}^S$ is the fourth-order identity tensor with major and minor symmetries. Since these functions are written in terms of I-invariants, we apply the chain rule to use the spline-based computed derivatives in terms of J -invariants

Figure 15: Effect of the nonlinearity of the stress-strain and transverse-longitudinal strains curves of the auxetic Scott foams in the computed stored energy terms ω' and U' .

$$\frac{\partial \Psi}{\partial I_1} = \frac{\partial \Psi}{\partial J_1} = W_1'(J_1) \quad (66)$$

$$\frac{\partial \Psi}{\partial I_2} = \frac{\partial \Psi}{\partial J_2} \frac{\partial J_2}{\partial I_2} = W_2'(J_2) I_3^{-1} \quad (67)$$

$$\frac{\partial \Psi}{\partial I_3} = \frac{\partial \Psi}{\partial J_2} \frac{\partial J_2}{\partial I_3} + \frac{\partial \Psi}{\partial J_3} \frac{\partial J_3}{\partial I_3} = -W_2'(J_2) I_2 I_3^{-2} + \frac{1}{2} W_3'(J_3) I_3^{-1/2} \quad (68)$$

and

$$\frac{\partial^2 \Psi}{\partial I_1 \partial I_1} = W_1''(J_1) \quad (69)$$

$$\frac{\partial^2 \Psi}{\partial I_2 \partial I_2} = W_2''(J_2) I_3^{-2} \quad (70)$$

$$\begin{aligned} \frac{\partial^2 \Psi}{\partial I_3 \partial I_3} &= W_2''(J_2) (I_2 I_3^{-2})^2 + 2W_2'(J_2) (I_2 I_3^{-3}) + \\ &\quad + \frac{1}{4} W_3''(J_3) I_3^{-1} - \frac{1}{4} W_3'(J_3) I_3^{-3/2} \end{aligned} \quad (71)$$

$$\frac{\partial^2 \Psi}{\partial I_2 \partial I_3} = -W_2''(J_2) I_2 I_3^{-3} - W_2'(J_2) I_3^{-2} \quad (72)$$

with also $\partial^2 \Psi / \partial I_1 \partial I_2 = \partial^2 \Psi / \partial I_1 \partial I_3 = 0$.

This tangent relates second Piola-Kirchhoff stresses $\mathbf{S}$ and Green-Lagrange strains $\mathbf{A}$, and it may be converted to any other stress-strain pair by means of the proper mapping tensors [60].

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Chapter 5

Extension of data-driven solutions to obtain stored energy of conservative solids from experimental data

5.1 Introduction

In line with the previous article, this chapter is focused in the enhancement of data-driven methods to obtain stored energy functions by means of solving the stress-strain system of functional equations. In particular, the previous article elucidates the idea of using general invariants as energetic functional arguments, beyond logarithmic strains. However, in the end, only one functional unknown was determined without explicit procedures. That was because functions W_1, W_2 where melt into W establishing the following relation between them,

$$\begin{aligned} W'(J_1) &= fW'_1(J_1) \\ W'(J_2) &= (1 - f)W'_2(J_2) \end{aligned}$$

Finally, W_3 is explicitly solved without any difficulty once W' was found. In this new work, such simplification is no longer necessary. Another aspect of the article was that it showed that it is possible to find the functional unknowns beyond logarithmic strains. However it does not imply that the suggested solution is guarantee to be applicable to all possible cases. It was required further development of J-WYPiWYG to strengthen the procedures that aim to find the functional unknowns. For the shake of this, in this work an enhancement of the functional refresh method is done to guarantee the convergence of the method. Additionally, an alternative system of functional equations based on I -invariants is suggested to apply the J-WYPiWYG methods if functional unknowns $W'_i(I_i)$ with I -invariants as arguments are preferable. Finally, an alternative to functional refresh is developed for linear functional equations, namely the *matricial method*.

Therefore, the aim of this article is to advance the data-driven procedures aimed to find stored energy functional unknowns in more general circumstances. In particular, the article covers the following advances,

- One of the most efficient ways to explain a procedure and in general a problem is with a simple representative example. The notions behind functional refresh and matricial methods are here explained with detail.
- Both functional refresh and matricial J-WYPiWYG data-driven methods are enhanced to cover the problem of finding several functional unknowns from

stress-strain system of equations without the simplificative assumptions already commented.

- In particular for functional refresh, an appropriate *digest* procedure of the functional data is developed as a pre-processing treatment necessary to strengthen the convergence of the functional refresh method.
- In line with preliminar articles, in order to verify the accuracy of the method, two different analytical models are employed to generate pseudo-experimental data. In particular they are the model of Horgan-Saccomandi for deviatoric contribution plus Hartman-Neff for volumetrics, and the model of Blatz-Ko. Because the original energies for producing the pseudo-experimental data are known, they are employed as a referential check for the recovery of the energies via J-WYPiWYG. Corresponding figures of the articles shows that as a matter of fact, the energetic functional unknowns are successfully found.
- Finally, FEA is done using Dulcinea code for comparing the simulations produced using the original energies of the model with the J-WYPiWYG recovered ones. Corresponding figures shows that generic simulations produce the same outputs.

GENERAL SOLUTION PROCEDURES TO COMPUTE THE STORED ENERGY DENSITY OF CONSERVATIVE SOLIDS DIRECTLY FROM EXPERIMENTAL DATA

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ABSTRACT

Energy-conservative, hyperelastic solids assume the existence of a stored energy density which relates stresses and strains for any deformation state. The usual approach to model such materials is to impose an analytical expression of the stored energy function as a function of some invariants and material parameters. These material parameters are best-fitted to available experimental data. This approach is good for analytical derivations but less optimal for data-driven computational approaches and for accurate and efficient finite element analyses. We show in this paper that the stored energy *solution* of a solid may be accurately obtained in a general case from suitable numerical procedures, regardless of the invariants being use, without using material parameters nor *fitting* any assumed analytical form. We explain two general, simple, computational procedures to solve the problem. The numerically computed stored energies may be used in general-purpose finite element programs, yielding more general procedures that have an efficiency equivalent to that of the classical approach, which uses pre-defined analytical “models” and fitting parameters.

Keywords Hyperelasticity; Soft materials; Classical invariants; Data-driven constitutive modelling.

1 Introduction

Deformations in soft materials are mainly due to the change of entropy in the constituents, reaching large values before failing or dissipating a relevant amount of energy [41, 45, 5]. Because deformations are large, nonlinearities must be considered in the formulation. The obvious approach of just considering nonlinear elastic constants (named hypoelasticity) may produce dissipation, which is in contradiction with a truly elastic, conservative behavior [14, 25]. The reason is that some integrability conditions of the constitutive equations must be fulfilled to guarantee the existence of a potential [42, 32], but in the large strain case it is in general difficult to fulfill such compatibility equations. Hence, since the mid 20th century, it has become standard to directly propose a specific analytical form of the stored energy (hyperelastic energy function) as a function of some invariants [38, 34, 41]. This has been the way to automatically guarantee the fulfillment of the compatibility equations of the constitutive relations, and hence of conservative behavior.

Unfortunately, this analytical approach, developed before the computer era, has been passed to computational procedures as the finite element method, procedures which do not produce analytical solutions but numerical ones, so there is no relevant benefit in having analytical stored energies; more on the contrary. Commercial programs have implemented

just a few hyperelastic “models” (Ogden, Mooney, Blatz-Ko, etc) out of the thousands available and sometimes even include quite elaborate procedures to obtain the non-unique material parameters from experimental data. The user is frequently and unnecessarily confronted to several quite difficult decisions, which are: (1) the selection of the model to use [43], (2) the experimental data to employ in the fitting procedure of material parameters, (3) the selection of the non-unique set of material parameters [33, 26]. Then, it is frequent the case when experimental data are not captured to the desired accuracy.

However, thanks to the availability of computers, there is a change of paradigm in modelling solids at large strains. The usual approach to hyperelasticity based on analytical functions is not ideally suited for machine learning. In contrast, the solutions herein proposed are specially relevant in data-driven constitutive modelling, which is the mentioned change in paradigm in modelling the behavior of solids [20, 23], in which less assumptions are made and the constitutive behavior is learned directly from experimental data. This type of approach is currently a challenge being pursued from very different perspectives like neural networks [46], penalized variational methods [23, 24] or projection in constitutive manifolds [20, 19].

We remark and show in this paper that there is no need to *assume* and then *fit* any analytical expression for the stored energy terms, as done in the literature and in finite element programs. Instead, the *solution* of the stored energy may be obtained from numerical procedures as to *exactly* (up to any desired numerical precision) reproduce available experimental data. In this paper we show that this claim holds even if any general set of invariants is used. In our opinion this is the logical approach in analyzing nonlinear solids with finite elements, where accurate numerical solutions, not approximate analytical solutions, are devised. This approach is also in the line of solving Truesdell’s *Hauptproblem* [8] (see also [13, 10]), that is, the determination of the requirements to ensure the existence and well-posedness in establishing the constitutive relations [26]. This is due to the functional treatment of the problem: *functional* equilibrium equations relate *functional data* (experimental data translated into functional forms) with *functional unknowns* (the strain energy density functions). So for instance if by rational arguments [13] or by experimental evidence [41] we may assume a functional decomposition of the type $W(I_1, I_2) = W_1(I_1) + W_2(I_2)$, consisting of two independent functions, then it follows that we can obtain them from two independent sets of data, even if that can be done only by numerical techniques.

The purpose of the present manuscript is not to give a “rational” approach to the behavior of polymeric materials, nor to give an insight from the micromechanics of polymers, like in chain [41, 44, 2] or worm-like [35, 39] models, but to give solution methods for a nonparametric approach in which the specific shape of the functions are not given beforehand. These solution methods may, of course, be also used in structure-based models. Thus we further propose a change from thinking in analytical function ansatzes and (probably non-unique) material parameters to numerical functions which fulfill the differential equations of the tests. Then, the desired result is to turn the focus of the hyperelastic problem into determining (1) the invariants more suitable to (2) propose a thoughtful reduced form of the strain energy function (e.g. by micromechanics, experimental evidence, mathematical analysis, etc), whose components (3) must fulfill some conditions obtained from rational mechanics or mathematical requirements (e.g. chain extensibility or stability). Much is still to be done regarding these three points [13, 10]. For example, the understanding of the effects of the chain extensibility limit has moved the attention from initial models based on Gaussian statistics to models based on the inverse Langevin function [41, 37]. However, there is no analytical expression for this function, so approximants or numerical solutions similar to the ones herein proposed are needed [4]. In this line, the proposal from Gent [4], studied in detail by Saccomandi and co-workers [17, 18, 36], use a rational approach to include most aspects of the models based on the inverse Langevin function without the inconveniences of this function. In these works, the need for an extension including the second invariant is also emphasized, [37, 10]. Noteworthy, all these considerations may (and probably should) be employed as conditions on the numerical functions to be determined. However, as mentioned, the specific purpose of this paper is not about such conditions, but about procedures that may simplify their implementation.

Departing from the ideas by Sussman and Bathe [40], used also in anisotropic materials [27, 28], our contribution here is to present more general and applicable numerical approaches to obtain the stored energy for more general forms, without resorting to any inverse formula or uncoupled forms in terms of logarithmic strains, and using any set of independent invariants. We present herein two types of algorithms for determining the stored energy using general dependencies for isotropic, compressible stored energies: a functional refreshing algorithm and a matrix one.

2 Simple introductory examples

To explain the ideas in the simplest possible context, in this section we will employ the case of incompressible materials which follow the Valanis-Landel approach. This case was solved by Sussman and Bathe [40] using the Kearsley and Zapas (KZ) formula [22] written in terms of logarithmic strains. In this section, we solve the problem following two different alternative approaches which, in contrast to the one using the KZ formula, are generally applicable. Then,

in next sections we extend the procedures to cases where the Valanis-Landel decomposition does not apply, the use of logarithmic strains is not convenient and in which a solution using the KZ formula is not possible. To these very common cases, the novel procedures are extremely useful.

The two different approaches consist in an function-refresh algorithm and a matrix method.

2.1 Function-refresh algorithm

Assume an isotropic incompressible hyperelastic material which follows the Valanis-Landel decomposition. In this case, the reduced stored energy form is written as

$$\mathcal{W}(E_1, E_2, E_3) = \omega(E_1) + \omega(E_2) + \omega(E_3) \quad (1)$$

where $\omega(E)$ is the Valanis-Landel energy term (scalar-valued function) and E_i , $i = 1, 2, 3$ are the principal logarithmic strains; i.e. $E_i = \ln \lambda_i$ where λ_i are the principal stretches. By incompressibility we have $\lambda_1 \lambda_2 \lambda_3 = 1$ and hence $E_1 + E_2 + E_3 = 0$. The equilibrium equations of a tensile test are [40]

$$T_u(E_u) = \omega'(E_u) + p \quad (2)$$

$$0 = \omega'(E_t) + p \quad (3)$$

where $T_u(E_u)$ are the uniaxial (Cauchy or Kirchhoff) stresses as a function of the logarithmic strains, subscript u stands for the uniaxial (tensile) directions and subscript t stands for the transverse directions. The pressure-like unknown p may be factored-out from the second equation and substituted in the first one, which upon inserting the incompressibility condition $E_t = -\frac{1}{2}E_u$ gives

$$T_u(E_u) = \omega'(E_u) - \omega'(-\frac{1}{2}E_u) \quad (4)$$

where we use here the convenient notation

$$\omega'(-\frac{1}{2}E_u) = \left. \frac{d\omega(E)}{dE} \right|_{E=-\frac{1}{2}E_u} \quad (5)$$

The solution to Eq. (4) was given by Kearsley and Zapas (KZ) [22] as a function of the series (we take $\omega'(0) = 0$)

$$\omega'(E_u) = \sum_{k=0}^{K \rightarrow \infty} T_u((-\frac{1}{2})^k E_u) \quad (6)$$

If we take as reference $T(0) = 0$, the series are convergent, so a relatively small number of terms K is needed.

The problem in using the KZ formula to obtain the stored energy is that it cannot be done analytically, and furthermore, the evaluation of the addends is performed at arbitrary strain values $(-1/2)^k E_u$, which do not coincide with experimental values. Sussman and Bathe [40] proposed a spline interpolation of experimental $T_u(E_u)$ values to apply the KZ formula and obtain the strain energy derivatives $\omega'(E_u)$ in as many points of E_u as needed. These values are then interpolated also using splines to obtain a piecewise spline (polynomial) stored energy derivative function $\omega'(E_u)$. This type of procedure has been used in other works using uncoupled forms in terms of logarithmic strains and using a generalization of the KZ formula. However, the procedure lacks generality and cannot be applied using general invariants and coupled energy forms. We formulate a procedure in a more general form which can be extended to those more general cases.

Assume that we know the function $\omega'^{[0]}(E)$ (i.e. the value of $\omega'^{[0]}$ for any possible argument value E), where $[0]$ stands for iteration 0. Then, from the equilibrium Equation (4), we can write

$$\omega'^{[1]}(E_u) = T_u(E_u) + \omega'^{[0]}(-\frac{1}{2}E_u) \quad (7)$$

so a new refreshed function $\omega'^{[1]}(E_u)$, which constitutes a new iteration, is obtained. This equation may be used in a recursive manner, as

$$\omega'^{[j]}(E_u) = T_u(E_u) + \omega'^{[j-1]}(-\frac{1}{2}E_u) \quad (8)$$

If, for example, we take as initial guess $\omega'^{[0]}(E) = 0$, it is immediate to show that the KZ formula is obtained, and hence, the solution to any desired precision after sufficient iterations. At each iteration, the functions may be built using any type of interpolation.

As an example that the reader can easily verify by hand, in Table 1 we perform the computation of the function $\omega'(E)$ using a function-refresh algorithm. Experimental data pairs $\{E_{uk}, T_{uk}\}$, $k = 1, \dots, 5$ are given in the first two columns

of Table 1. The remaining columns are the results of the iterations. For simplicity of presentation, we consider linear interpolation between values. In practice, spline interpolations guarantee smooth constitutive tangents, so they are the ones we typically use with computers. It is seen in Table 1 that 4 digits of precision are obtained in just 8 refreshes and it can be verified that machine precision is obtained in 25 refreshes. Obviously it is straightforward to verify that the prescribed stress-strain data are exactly recovered; for example, using Eq. (4), $T_u(E_u = 2) = \omega'(2) - \omega'(-1) = 3.6667 - (-0.3333) = 4$. That observation holds even at interpolated values, consistently with the interpolation employed, i.e. $T_u(E_u = 0.5) = \omega'(0.5) - \omega'(-0.25) = 0.8333/2 - (-0.3333/4) = 0.5$. From this very simple example it is apparent that if we use the Valanis-Landel decomposition, there is no need to specify the shape of $\omega'(E)$, (as the Neo-Hookean, Ogden and Mooney models do, among many others), because $\omega'(E)$ can be accurately determined numerically, without ever using material parameters or fitting procedures. If the function $\omega'(E)$ is discretized in equal intervals of length ΔE , the interval k which corresponds to a given strain value E is $k = \text{int}[(E - E_0)/\Delta E]$, where E_0 is the start strain of the first interval. Then, in a finite element context, given any principal strain E_i , it is immediate to evaluate $\omega'(E_i)$ and its derivative $\omega''(E_i)$, which are the only needed quantities in a finite element simulation, so the efficiency is the same as that of analytical models.

E_u	$T_u(E_u)$	$\omega'^{[1]}(E_u)$	$\omega'^{[2]}(E_u)$	$\omega'^{[3]}(E_u)$	$\omega'^{[4]}(E_u)$	...	$\omega'^{[K>8]}(E_u)$
-2	-3	-3.0000	-2.0000	-2.1250	-2.1563	...	-2.1667
-1	-0.75	-0.7500	-0.2500	-0.3125	-0.3281	...	-0.3333
0	0	0	0	0	0	...	0
1	1	1.0000	0.8750	0.8438	0.8359	...	0.8333
2	4	4.0000	3.7500	3.6875	3.6719		3.6667

Table 1: A simple example of refreshing algorithm with linear interpolation between values. The first two columns represent the “experimental” data. Iteration [0] with $\omega'^{[0]} = 0$ is not included. After 8 iterations four digits of precision are obtained; after 25 iterations machine precision is reached (16 decimal digits of mantissa in double precision)

For further reference we define the concept of *computational nesting domains*. We note that the function refreshing procedure could be applied in principle in reverse order, that is, from Eq. (4) again

$$\omega'^{[j]}(-\tfrac{1}{2}E_u) = \omega'^{[j-1]}(E_u) - T_u(E_u) \quad (9)$$

but we find a major difficulty which relates to the computational domain. In the right hand side of Eq. (9) we need stress-strain data that expands twice the computational domain of the function on the left hand side. Hence using Eq. (9), we would be able to determine the function $\omega'(E)$ in a reduced domain, or otherwise, we would need to extrapolate experimental data. Moreover, in the right hand side, Eq. (9) requires values of $\omega'(E_u)$ which have not been computed in previous iterations, so either the valid computational domain is reduced for each iteration or extrapolations of the functions are continuously needed. The former case is useless and the latter case frequently results in divergence. Then, as it will be seen below, for robustness it is important to design the iterative algorithm in a way such that each computational domain nests the following one.

Finally, we note that in the infinitesimal incompressible case, the shear modulus is obtained from Young’s modulus $Y = 3\mu$ during a tensile test as

$$\omega'(\varepsilon) = \sum_{k=0}^{\infty} T'((-\tfrac{1}{2})^k \varepsilon) = 3\mu \sum_{k=0}^{\infty} (-\tfrac{1}{2})^k \varepsilon = 2\mu\varepsilon \quad (10)$$

i.e. $\omega'' = 2\mu$, where μ is the shear modulus. Remarkably, and in contrast to recent formulations [11, 12], this framework using infinitesimal strains allows seamlessly for the consideration of different moduli in tension and compression without imposing constraints on the elastic constants.

2.2 Matrix method

In contrast to the function-refresh method, the matrix method is a non-iterative method. This method basically consists in solving a linear system of equations. We also explain the ideas using the simplest isotropic incompressible case following the Valanis-Landel decomposition.

Using the condition $\omega'(0) = 0$ and Eq. (4), re-write the above system for the experiments in Table 1 as

$$T(E = -2) = \omega'(E = -2) - \omega'(E = 1) \quad (11)$$

$$T(E = -1) = \omega'(E = -1) - \omega'(E = \frac{1}{2}) \quad (12)$$

$$T(E = 0) = \omega'(E = 0) \quad (13)$$

$$T(E = 1) = \omega'(E = 1) - \omega'(E = -\frac{1}{2}) \quad (14)$$

$$T(E = 2) = \omega'(E = 2) - \omega'(E = -1) \quad (15)$$

We denote the discrete values by $T(E) \equiv T_E$ and $\omega'(E) \equiv \omega'_E$, and use again linear interpolation to arrive at the system of equations

$$T_{-2} = \omega'_{-2} - \omega'_1 \quad (16)$$

$$T_{-1} = \omega'_{-1} - (0.5 \omega'_1 + 0.5 \omega'_0) \quad (17)$$

$$T_0 = \omega'_0 \quad (18)$$

$$T_1 = \omega'_1 - (0.5 \omega'_0 + 0.5 \omega'_{-1}) \quad (19)$$

$$T_2 = \omega'_2 - \omega'_{-1} \quad (20)$$

which can be written in matrix form as $\mathbf{T} = (\mathbf{I} - \mathbf{P})\boldsymbol{\omega}'$ and solved for $\boldsymbol{\omega}'$, i.e.

$$\begin{bmatrix} \omega'_{-2} \\ \omega'_{-1} \\ \omega'_0 \\ \omega'_1 \\ \omega'_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & -0.5 & -0.5 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -0.5 & -0.5 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} T_{-2} \\ T_{-1} \\ T_0 \\ T_1 \\ T_2 \end{bmatrix} \quad (21)$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{P}$ is a matrix which is function only of the chosen interpolation scheme. It is immediate to verify that the solution is identical to that given in the last column of Table 1 and that, in consequence, exactly predicts the experimental data.

Of course, the number of unknowns both in the matrix method and in the function-refresh method can be less than experimental data. In such case, the solution obtained is an approximation. In the function-refresh method no changes are needed. In the matrix method, an approximation in a minimum squares sense can be obtained:

$$\boldsymbol{\omega}' = [(\mathbf{I} - \mathbf{P})^T(\mathbf{I} - \mathbf{P})]^{-1}(\mathbf{I} - \mathbf{P})^T \mathbf{T} \quad (22)$$

Finally we remark that: (1) the computational effort in considering, say, one thousand points is negligible in a finite element context, but about 25 points give already 3-4 digits of precision in all the domain, (2) the interpolation functions may have any desired smoothness properties, (3) noisy data, data from multiple specimens, and some convexity/stability conditions are easily accounted for employing penalized splines with stability conditions [29], (4) the stored energies may be extrapolated outside of the domain of available experimental data, but obviously, as when using any hyperelastic model, without experimental evidence nothing can be said about the accuracy of the guess in such part of the domain.

3 Application to general forms of the stored energy

3.1 Complete and reduced representations

The previous ideas can be extended to obtain the stored energy of hyperelastic materials in more general cases, *solving* numerically the equilibrium equations of a complete set of experiments presented to the procedure. The matrix procedure is, in fact, easily applicable to general forms of the stored energy, for example coupled forms of the type $\mathcal{W}(E_1, E_2, E_3)$ or structure-based models [1]. To guarantee isotropy in a simple manner, i.e. $\mathcal{W}(\mathbf{Q}^T \mathbf{E} \mathbf{Q}) = \mathcal{W}(\mathbf{E})$, where $\mathbf{E}$ is a strain tensor and $\mathbf{Q}$ is an orthogonal tensor, general isotropic invariants are preferred in the literature for continuum-based models. One possible set of such invariants $\mathbf{J} := \{J_1, J_2, J_3\}$ has been given by Blatz and Ko as

$$J_1 = \text{tr}(\mathbf{B}) = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \quad (23)$$

$$J_2 = \text{tr}(\mathbf{B}^{-1}) = \lambda_1^{-2} + \lambda_2^{-2} + \lambda_3^{-2} \quad (24)$$

$$J_3 = \det(\mathbf{B}^{1/2}) = \lambda_1 \lambda_2 \lambda_3 \quad (25)$$

where $\mathbf{B} = \mathbf{X}\mathbf{X}^T$ is the left Cauchy-Green deformation tensor and $\mathbf{X}$ is the deformation gradient. Then, the stored energy function may be written as $W(J_1, J_2, J_3)$, and the Cauchy stresses are obtained as

$$\boldsymbol{\sigma}(J_1(\mathbf{B}), J_2(\mathbf{B}), J_3(\mathbf{B})) = \frac{\partial W}{\partial J_3} \mathbf{I} + \frac{2}{J_3} \left(\frac{\partial W}{\partial J_1} \mathbf{B} - \frac{\partial W}{\partial J_2} \mathbf{B}^{-1} \right) \quad (26)$$

The present function-determination problem is to obtain the strain energy function $W(J_1, J_2, J_3)$ from some experimental p data sets $\{J_{1p}, J_{2p}, J_{3p}, \boldsymbol{\sigma}_p\}$ obtained from different tests. In order to do so in a general context, we can discretize the computational domain as

$$\{J_{11}, J_{12}, \dots, J_{1i}, \dots, J_{1I}\} \times \{J_{21}, J_{22}, \dots, J_{2j}, \dots, J_{2J}\} \times \{J_{31}, J_{32}, \dots, J_{3k}, \dots, J_{3K}\} \quad (27)$$

Then, using local variables $\boldsymbol{\iota} := \{\iota_1, \iota_2, \iota_3\}$, for example

$$\iota_1 = \frac{2J_1 - (J_{1i+1} + J_{1i})}{J_{1i+1} - J_{1i}}, \quad \iota_2 = \frac{2J_2 - (J_{2i+1} + J_{2i})}{J_{2i+1} - J_{2i}}, \quad \iota_3 = \frac{2J_3 - (J_{3i+1} + J_{3i})}{J_{3i+1} - J_{3i}}, \quad (28)$$

we can interpolate the strain energy density $W(J_1, J_2, J_3)$ from the $N = I \times J \times K$ nodal values $\hat{W}_n$ as

$$W(J_1, J_2, J_3) \simeq \sum_{n=1}^N N_n(\boldsymbol{\iota}(\mathbf{J})) \hat{W}_n \quad (29)$$

where $N_n(\boldsymbol{\iota}(\mathbf{J}))$ are the chosen (predefined) normalized interpolation functions, which are expressed in each subdomain, as typically done in the finite element formulations. Obviously, within this context, the derivatives are immediately obtained as

$$\frac{\partial W(J_1, J_2, J_3)}{\partial J_i} = \sum_{n=1}^N \sum_{j=1}^3 \frac{\partial N_n(\boldsymbol{\iota})}{\partial \iota_j} \frac{\partial \iota_j(\mathbf{J})}{\partial J_i} \hat{W}_n \quad (30)$$

which can be inserted in Eq. (26) to arrive at the interpolated values of the Cauchy stresses when the nodal values of the stored energy $\hat{W}_n$ are known.

For someone acquainted with the finite elements theory, it is obvious that using Eqs. (30) and Eq. (26) particularized to the specific tests employed, a linear system of equations may be constructed to determine the nodal values $\hat{W}_n$ from known experimental data sets $\{J_{1p}, J_{2p}, J_{3p}, \boldsymbol{\sigma}_p\}$. We refer to any finite element book for the ideas behind such type of procedure, e.g. [3]. Once these nodal values are known, the stored energy in Eq. (29), and obviously its derivatives, Eq. (30), and related stresses, Eq. (26), are known and can be evaluated for any deformation gradient $\mathbf{X}$ present at an integration point in a finite element program. Of course to have the problem well-posed, we must have at least as many independent experimental equations as unknowns to be able to solve the system of equations. In the case that more data than unknowns are available, a minimum squares solution is possible, see Eq. (22).

However, the most frequent case is, by large, when a limited amount of experimental data is available. An issue frequently not well understood is that the experimental data must come from a complete set of experiments *physically* capable of uniquely determining the proposed form of the stored energy, see for example [26]. In essence, the experiments must span and fill all the computational domain; i.e. all possible combinations of $\{J_1, J_2, J_3\}$ in Eq. (29). For example, a tensile and an equibiaxial test are the minimum amount of tests needed to determine a stored energy using the Valanis-Landel decomposition and the incompressibility condition [33, 26]. In the same way, an extra test is needed to determine the compressible case [9]. Therefore, the amount of experimental data from independent tests needed to determine a general fully coupled form of the stored energy given by Eq. (29) is not available in general.

Hence, from a practical point of view, simplified forms of the stored energy are imperative in order to reduce the number of tests needed in the determination of the stored energy, leaving the determination problem well-posed with available experimental data. These simplified forms reduce the "curse of dimensionality" [6] and can still reproduce exactly the available experimental data. Thus, the decision on the proposed functional decomposition of the stored energy depends mainly on the available experimental data and on the assumption about the actual relevance of some coupling terms in the observed behavior. These assumptions may also come from an understanding of the micromechanics [37] or from rational arguments [13].

The Valanis-Landel form Eq. (1) is one reduced form (the simplest, that recovers the infinitesimal case), which can be used if only data from a tensile and an equibiaxial test are available. However, it is also frequent the case when data from more experiments (e.g. strip-biaxial, pure-shear, simple-shear, etc) are available. In such cases, less reduced

expressions may be used. For example, following the work from Blatz and Ko, we may use the reduced form

$$W(J_1, J_2, J_3) \equiv W_1(J_1) + W_2(J_2) + W_3(J_3) \quad (31)$$

This reduced form involves only three scalar equations and, hence, it can be determined from three complete, independent, experimental curves, including tension and compression where applicable. Blatz and Ko motivated this form in the experimentally observed little relevance of couplings between J -invariants in their tests. In the analytical models found in the literature, these functions $W_i(J_i)$ are assumed as a function of material parameters to *fit* experimental data, but as in the cases of Section 1, the functions can instead be *computed* numerically. Of course, other functions, e.g. $W_4(J_{12})$ with, say $J_{12} := J_1 J_2$, can be added to Eq. (31), so further tests can be captured. However, for simplicity of this presentation, we consider here just the three functions involved in Eq. (31).

3.2 Functional equations for reduced representations

As long as three functional unknowns are present in Eq. (31) and thus also in Eq. (26), namely $W'(J_1)$, $W'(J_2)$, $W'(J_3)$, three different functional equations are required, and therefore three independent functional (experimental) data from $\sigma(B)$ are employed. The three curves that we consider as examples are two equations of a uniaxial tension-compression test and one from a strip-biaxial test. The procedure using other tests is similar.

From the uniaxial test, the data we use here are the stress-stretch curve $\sigma_u(\lambda_u)$, and the transverse-to-longitudinal stretch relation $\lambda_t(\lambda_u)$. Regarding the strip-biaxial test, the data we use are the stretches $\lambda_w(\lambda_p)$, with λ_p being the stretch in the loading direction and λ_w in the thickness. All these data are written in functional form employing the corresponding interpolations (e.g. spline interpolations). Using Eq. (26), three functional equations can be established from the tests in terms of available data functions,

$$\sigma_u(\lambda_u) = W'_3(J_{3u}) + \frac{2}{J_{3u}} (W'_1(J_{1u})\lambda_u^2 - W'_2(J_{2u})\lambda_u^{-2}) \quad (\text{uniaxial}) \quad (32)$$

$$0 = W'_3(J_{3u}) + \frac{2}{J_{3u}} (W'_1(J_{1u})\lambda_t^2 - W'_2(J_{2u})\lambda_t^{-2}) \quad (\text{uniaxial}) \quad (33)$$

$$0 = W'_3(J_{3p}) + \frac{2}{J_{3p}} (W'_1(J_{1p})\lambda_w^2 - W'_2(J_{2p})\lambda_w^{-2}) \quad (\text{strip-biaxial}) \quad (34)$$

In these equations we have included a subscript, either u or p , to denote respectively uniaxial or strip-biaxial tests. Note that this distinction is necessary because, for example $J_{1u}(\lambda_u) \neq J_{1p}(\lambda_p)$, since the invariant J_1 for a given uniaxial λ_u is different from that for a given strip-biaxial λ_p having both the same numerical value (because they are different tests). Thus, importantly, the *functions* in Eq. (34) are the same as those of Eqs. (32) and (33), but evaluated at different, unrelated arguments of the functions. To build the function-refreshing algorithm we must relate the arguments. We observe that $W'_3(J_3)$ is present in the three equations of the system, but particularized for both tests, namely $W'_3(J_{3u})$ and $W'_3(J_{3p})$. Without loss of generality of the method, in this particular case, if we set the dependency $J_{3u} = J_{3p} \equiv J_3$ (i.e. we choose points in both tests having the same J_3), then $W'_3(J_{3u}) = W'_3(J_{3p})$ and the system can be re-written so we can uncouple one of the equations, leaving a subsystem without the $W'_3(J_3)$ functional unknown. Note that $J_{3u} = J_{3p} \equiv J_3$ ties both tests through the functional dependencies $\lambda_u(J_3)$ and $\lambda_p(J_3)$, which in essence constitute a change of driving variable for both tests to the selected common one J_3 . Since as expected both tests show that volume increases with the test i.e. $J'_{3u}(\lambda_u) > 0$ and $J'_{3p}(\lambda_p) > 0$, there is a one-to-one correlation and the test dependencies can be uniquely expressed in terms of J_3 . That is, we can write $\lambda_u(J_{3u})$, $\lambda_t(J_{3u})$, $\sigma_u(J_{3u})$, $J_{1u}(J_{3u})$, ..., $\lambda_p(J_{3p})$, $\lambda_w(J_{3p})$, $J_{1p}(J_{3u})$ and so on. Thus, the system becomes

$$\frac{\sigma_u J_{3u}}{2} = W'_1(J_{1u})(\lambda_u^2 - \lambda_t^2) - W'_2(J_{2u})(\lambda_u^{-2} - \lambda_t^{-2}) \quad (35)$$

$$0 = W'_1(J_{1u})\lambda_t^2 - W'_2(J_{2u})\lambda_t^{-2} - W'_1(J_{1p})\lambda_w^2 + W'_2(J_{2p})\lambda_w^{-2} \quad (36)$$

$$0 = W'_3(J_{3u}) + \frac{2}{J_{3u}} (W'_1(J_{1u})\lambda_t^2 - W'_2(J_{2u})\lambda_t^{-2}) \quad (37)$$

where note that the first two equations are uncoupled from the third one. Assume now that we have some available experimental data (points marked with $\times$ in Figure 1). Then we can interpolate those points with a piece-wise spline (solid line —). This piecewise-spline is a function which can be evaluated at any arbitrary point. Hence, we can re-sample (compute) the plotted data at arbitrary points $J_{3k} \equiv J_{3uk} = J_{3pk}$, $k = 1, \dots$ ($\circ$ points). This new built dependency allows all the variables to be written as functions of J_3 (e.g. $\lambda_u(J_3)$, $\lambda_w(J_3)$, $J_1(J_3)$, ...) as shown in Table 4 below as an example. It can be further observed that once $W'_1(J_1)$ and $W'_2(J_2)$ are found from Eqs. (35) and

Figure 1: Uniaxial and strip-biaxial pseudoexperimental data from the NSHN model (see Sec. 4.1): pseudo-experimental data (points marked with $\times$), spline interpolation (solid line —), resampled data at $J_3 \equiv J_{3u} = J_{3p}$ (points marked with $\circ$). Material parameters: $\mu = 6$ kPa, $J_m^I = 90$, $K = 1$ kPa, $\beta_1 = 10$, $\beta_2 = 4$, $\beta_3 = -6$. Uniaxial stress versus longitudinal stretch $\sigma_u(\lambda_u)$ (a). Uniaxial longitudinal versus transverse stretch relation $\lambda_t(\lambda_u)$ (b). Strip-biaxial longitudinal versus thickness-wise stretch relation $\lambda_w(\lambda_p)$ (c).

(36), $W'_3(J_3)$ can be explicitly obtained from Eq. (37). Obviously, in a general case when the system cannot be further simplified, all equations are solved simultaneously.

3.3 Nested computational domains

As previously explained, the successive computational domains in the function-refresh method should include previous domains to avoid extrapolations of previously computed data. For instance, according to Figure 2 if J_{1p} (strip-biaxial test) is chosen as computational domain of $W'_1(J_1)$ then for $J_3 = 1.2$ we have $J_{1u} \approx 3.56 > \max(J_{1p}) \approx 3.48$ and therefore $W'_1(J_{1u} = 3.56)$ will need an extrapolation. A similar situation in the same example is found with $W'_2(J_2)$ as it can be inferred from the same figure. In order to avoid extrapolations, we need to define nesting computational domains for the functions $W'_1(J_1)$ and $W'_2(J_2)$ depending on the compressive or dilatant branches of the tests. As an example that we will address below in Sec. 4.4, nesting domains for the functions $W'_i(J_i)$ are given by $W'_1(J_{1p})$, $W'_2(J_{2u})$ for the case $J_3 < 1$, and $W'_1(J_{1u})$, $W'_2(J_{2p})$ for the case $J_3 > 1$.

Obviously, the invariants used in the reduced representation of Eq. (31) are just one of the possibilities. Other possibility is to use the principal invariants

$$I_1 := \text{tr}(\mathbf{B}) \quad (38)$$

$$I_2 := \frac{1}{2}[(\text{tr}(\mathbf{B}))^2 - \text{tr}(\mathbf{B}^2)] \quad (39)$$

$$I_3 := \det(\mathbf{B}) \quad (40)$$

and the reduced form

$$W(I_1, I_2, I_3) \equiv W_1(I_1) + W_2(I_2) + W_3(I_3) \quad (41)$$

so

$$\boldsymbol{\sigma} = 2I_3^{-1/2} [\mathbf{B} W'_1(I_1) + (I_2 \mathbf{I} - \mathbf{B}^{-1}) W'_2(I_2) + I_3 \mathbf{I} W'_3(I_3)] \quad (42)$$

Figure 2: Nesting domains: maximize the range of J_1 , J_2 for function definitions $W'_1(J_1)$, $W'_2(J_2)$ by means of different choices for compressive and dilatant branches of uniaxial and strip-biaxial tests.

The equivalent system of equations for the previous tests is in this case,

$$\sigma_u = 2I_3^{-1/2} ((\lambda_u^2 - \lambda_t^2)W'_1(I_{1u}) - (\lambda_u^{-2} - \lambda_t^{-2})W'_2(I_{2u})) \quad (43)$$

$$0 = \lambda_t^2 W'_1(I_{1u}) - \bar{\lambda}_w^2 W'_1(\bar{I}_{1p}) + (I_2 - \lambda_t^{-2})W'_2(I_{2u}) - (I_2 - \bar{\lambda}_w^{-2})W'_2(\bar{I}_{2p}) \quad (44)$$

$$0 = 2I_3^{-1/2} (\lambda_t^2 W'_1(I_{1u}) + (I_2 - \lambda_t^{-2})W'_2(I_{2u}) + I_3 W'_3(I_3)) \quad (45)$$

so the layout of the procedure is basically unchanged for whatever invariants may be used.

4 Examples

In this section we show some illustrative examples using reduced representations. Our objective is to show that it is possible to compute to any desired precision the stored energy density of a solid directly from the experimental data using a complete set of tests for the chosen representation, so there is no need to guess, impose and restrict the shape of the terms of the stored energy function. In order to avoid discussion about possible experimental errors and noisy data (the latter can be eliminated by spline penalizations employing stability conditions), we use analytical models to generate artificial pseudo-experimental (or *in-silico* experimental) data. Then, we can show that our procedure is capable of reproducing numerically the analytical stored energy function from which experimental data has been obtained and, hence, replicating exactly such experimental data; all of this without using material parameters nor optimization algorithms. For this purpose we choose the Horgan-Saccomandi [17] model with a volumetric Hartmann-Neff [16] contribution (thereafter HSHN model for short reference), and the Blatz-Ko [7] model. In both cases we solve for the stored energies directly from experimental data using both the functional refreshing method and then the matrix one. The first example shows the robustness of the refreshing algorithm method. To this end we force the method to perform extrapolations (i.e. not using nested domains) and we start the iterations with a very poor initial guess. It is shown that even under such conditions the solution is obtained. In the second example, we use tables with just five “experimental” points so the reader may better understand and follow both computational procedures.

4.1 Pseudo-experimental data from the HSHN model

As mentioned, this model is a combination of two models. The first contribution consists on the Horgan and Saccomandi [17] model, which propose a model similar to Gent’s model [15] with considerations based on the molecular theory of elasticity [35, 30, 31]. The second addend comes from Hartmann and Neff [16], which suggest a volumetric formulation

that fulfills (itself) polyconvexity criteria; i.e.

$$W(I_1, I_2, I_3) = \widetilde{W}(I_1, I_2, I_3) + W_V \quad (46)$$

The form of $\widetilde{W}$ implies coupled deviatoric and volumetric effects, while W_V is a purely volumetric addition. The forms of $\widetilde{W}$ and W_V herein are

$$\widetilde{W} = -\frac{\mu}{2} \left(J_m^I \ln \left(1 - \frac{I_1 - 3}{J_m^I} \right) + 2 \ln J \right) \quad (47)$$

$$W_V = \frac{K}{\beta_1} \left(\frac{J^{\beta_2+1}}{\beta_2+1} - \frac{J^{\beta_3+1}}{\beta_3+1} \right) \quad (48)$$

where $J_m^I, \mu, K, \beta_1, \beta_2, \beta_3$ are material parameters. Since they are independent of I_2 , and $I_1 = J_1$ and $J_3 = J$, we can write $W_2'(J_2) = 0$, and

$$W_1'(J_1) = \frac{\mu}{2} \left(1 - \frac{J_1 - 3}{J_m^I} \right)^{-1} \quad (49)$$

$$W_3'(J_3) = \frac{K}{\beta_1} \left(J_3^{\beta_2} - J_3^{\beta_3} \right) - \mu J_3^{-1} \quad (50)$$

The parameters chosen for the simulations in this paper are $\mu = 6$ kPa, $J_m^I = 90$, $K = 1$ kPa, $\beta_1 = 10$, $\beta_2 = 4$, $\beta_3 = -6$, resulting in the experimental curves shown in Figure 1. As mentioned, we refer to this model herein as the HSHN model for brief reference.

4.2 Function refresh method applied to data from the HSHN model

As mentioned, the use of nesting computational domains and a good initial guess facilitates a faster and more robust convergence. However, even in the case when extrapolations and a poor initial guess are used, convergence is usually obtained. In this example we use 100 points for experimental data and 25 in the stored energy terms. The computational domains for $W_1'(J_1)$, $W_2'(J_2)$ will be given by the experimental data from J_{1u} and J_{2p} respectively, so extrapolations will be needed. The function-refresh algorithmic equations are

$$W_1'^{[j]}(J_{1u}) = (\lambda_u^2 - \lambda_t^2)^{-1} \left(\frac{\sigma_u J_3}{2} + (\lambda_u^{-2} - \lambda_t^{-2}) W_2'^{[j-1]}(J_{2u}) \right) \quad (51)$$

$$W_2'^{[j]}(J_{2p}) = \lambda_w^2 \left(\lambda_w^2 W_1'^{[j-1]}(J_{1p}) - \lambda_t^2 W_1'^{[j-1]}(J_{1u}) + \lambda_t^{-2} W_2'^{[j-1]}(J_{2u}) \right) \quad (52)$$

Using $W_1'^{[0]}(J_1) = 0$, $W_2'^{[0]}(J_2) = 0$ (i.e. vanishing functions) as initial guesses in Figure 3 we show the iterations of the algorithm. The computations have been performed in MATLAB running in an Intel i7 PC. Because we did not use nested computational domains and the initial guess was very poor, quite a high number of iterations were needed (964 iterations) to reach convergence (near machine precision). However, we note that even in this case, all the computations took less than one second (PC elapsed time).

Figure 3: Several iterations of the convergence process of functional refresh applied on HSHN material with initial guess of unknown functions $W_1'(\bullet) = W_2'(\bullet) = 0$. Method performed with 25 points and cubic spline interpolations, for solving stored energy derivative functions of (a) $W_1'(J_1)$ and (b) $W_2'(J_2)$. Computational elapsed time for resolution < 0.94 seconds

Furthermore, the number of iterations can be substantially reduced with a proper initial guess of the unknown functions; for example using a linear assumption as,

$$W_1^{[0]}(J_1) = \mu_1 J_1 + c_1 \quad (53)$$

$$W_2^{[0]}(J_2) = \mu_2 J_2 + c_2 \quad (54)$$

To obtain the coefficients μ_1, μ_2, c_1, c_2 , we choose the initial i and final f points of the available experimental data; shown in Table 2. With these points, the guess is obtained solving Eqs. (35) and (36) particularized to the mentioned points. For this example it gives $\mu_1 = 34.76$ Pa, $c_1 = 2894$ Pa, $\mu_2 = 1.081$ Pa, $c_2 = -3.222$ Pa. With this initial guess, the number of iterations reduces from 964 to just 50.

HSHN model. Points i -initial and f -final of the uniaxial and strip-biaxial tests								
Point	J_3	J_{1u}	J_{2u}	λ_u	λ_t	J_{1p}	J_{2p}	λ_w
i	0.7732	2.6519	3.7656	0.7296	1.0295	2.6241	3.7164	1.0296
f	1.3831	4.1384	2.6346	1.5244	0.9525	4.0140	2.5756	0.9532

Table 2: Table of resampled uniaxial and strip-biaxial dependencies with J_3

4.3 Matrix method applied to data from the HSHN model

In this example we use piece-wise cubic interpolation with *not-a-knot* end condition (see [27]). Equations (35) and (36) can be written as

$$\tau_u = 2(\lambda_u^2 - \lambda_t^2)W_{1u}' - 2(\lambda_u^{-2} - \lambda_t^{-2})W_{2p}' \quad (55)$$

$$0 = \lambda_t^2 W_{1u}' - \lambda_t^{-2} W_{2u}' - \lambda_w^2 W_{1p}' + \lambda_w^{-2} W_{2p}' \quad (56)$$

with the following definitions $\tau_u = \sigma_u J_3$, $W_{1u}' := W_1'(J_1 = J_{1u})$, $W_{1p}' := W_1'(J_1 = J_{1p})$, $W_{2u}' := W_2'(J_2 = J_{2u})$, $W_{2p}' := W_2'(J_2 = J_{2p})$. Note that τ_u and all λ_* ($* = u, t, w$) are known experimental data, and the rest (W_{1u}' , W_{2u}' , W_{1p}' , W_{2p}') are the unknowns. As in Eq. (21), we perform the mentioned spline interpolations for the functions, which can be written in matrix form using interpolating matrices P . For example, let $W_1' = [W_1', W_2', \dots]^T$ be the array of

nodal values of the function $W'_1(J_1)$ at given (e.g. equispaced) values $J_{1k}, k = 1, \dots$. These matrices relate the values $W'_{1u} = [W'_{1u1}, W'_{1u2}, \dots]^T$ at experimental points to the nodal values $W'_1 = [W'_1, W'_2, \dots]^T$, so we can write

$$W'_{1u} = P_{1u} W'_1 \quad (57)$$

$$W'_{1p} = P_{2u} W'_1 \quad (58)$$

$$W'_{2u} = P_{1p} W'_2 \quad (59)$$

$$W'_{2p} = P_{2p} W'_2 \quad (60)$$

Define the vectors $\Lambda_*^a := [\lambda_{*1}^a, \lambda_{*2}^a, \dots]$, ($*$ = u, t, w), $T_u := [\tau_{u1}, \tau_{u2}, \dots]$, and the matrix column-wise operation $[v \diamond P]_{ij} = v_j P_{ij}$ (no sum on j). Then, in general a system of equations $W' = A^{-1}T$ can be formulated and solved; in the present case it can be written as

$$\begin{bmatrix} W'_1 \\ W'_2 \end{bmatrix} = \begin{bmatrix} 2(\Lambda_u^2 - \Lambda_t^2) \diamond P_{1u} & -2(\Lambda_u^{-2} - \Lambda_t^{-2}) \diamond P_{2u} \\ (\Lambda_t^2 \diamond P_{1u}) - (\Lambda_w^2 \diamond P_{1p}) & (\Lambda_w^{-2} \diamond P_{2p}) - (\Lambda_t^{-2} \diamond P_{2u}) \end{bmatrix}^{-1} \begin{bmatrix} T_u \\ 0 \end{bmatrix} \quad (61)$$

The results of the unknown functions $W'_1(J_1), W'_2(J_2)$ are shown in Table 3. Note that in this case the solution is not exact (it has 3 digits of precision) because of the different discretizations employed in the two equations. Obviously with more points, the solution may be accurate to any desired numerical precision.

In the appendix we include the matrices of the computations for the reader's convenience.

HSHN model. Solution of matrix method					
	Comput.	Theor.		Comput.	Theor.
J_1	$W'_1(J_1)$	$W'_{1,th}(J_1)$	J_2	$W'_2(J_2)$	$W'_{2,th}(J_2)$
2.6520	2.9916	2.9885	2.5756	-0.0010	0
2.8618	2.9956	2.9955	2.6786	0.0002	0
3.1681	3.0023	3.0057	2.8626	0.0028	0
3.5741	3.0187	3.0193	3.1697	0.0006	0
4.1384	3.0389	3.0384	3.7164	-0.0017	0

Table 3: Solution for $W'_1(J_1), W'_2(J_2)$ (kPa) using 5 points and the matrix method, compared to analytical ones $W'_{1,th}(J_1), W'_{2,th}(J_2)$ from the HSHN model.

4.4 Pseudo-experimental data from the Blatz-Ko model. Nesting computational domain

The Blatz and Ko model [7] for highly compressible foams uses the reduced form Eq. (31) along with the relation $\lambda_t = \lambda_u^{-\nu}$, where ν is a constant Poisson ratio. Blatz and Ko further assume the following specific analytical forms

$$W'_1(J_1) = f\mu/2 \quad (62)$$

$$W'_2(J_2) = (1-f)\mu/2 \quad (63)$$

$$W'_3(J_3(\lambda_u)) = -2J_3^{-1}(\lambda_u) [f\mu/2 \lambda_t^2(\lambda_u) - (1-f)\mu/2 \lambda_t^{-2}(\lambda_u)] \quad (64)$$

where the last one uses the uniaxial dependencies $J_3(\lambda_u)$ and $\lambda_t(\lambda_u)$. In these equations $f \in [0, 1]$ is a parameter frequently set to 1, μ is a constant shear modulus. As an example assume the following values typical for a foam: $f = 1$, $\mu = 26.53$ kPa, $\nu = 0.15$.

To facilitate the reader the task of following the computations, we will use here only five resampled points, shown in Table 4 (obviously in a computer hundreds of points may be used at no relevant cost). From the table it should be obvious that combining columns and using an adequate interpolation, we can immediately obtain the functions $\sigma_u(J_3)$, $\lambda_u(J_3)$, $\lambda_t(J_3)$, $\lambda_w(J_3)$, ... or even $J_{1u}(\sigma_u)$, $\lambda_w(\lambda_u)$, ... etc.

The already commented Figure 2 shows that for a given J_3 , the boundary values of J_1 and J_2 correspond to different tests. For instance, the lower bound of J_1 is found during the strip biaxial test whereas the upper one is found during the uniaxial test, so that no single test contains a computational nesting domain for J_1 . Therefore we build a nesting domain for J_1 used in $W'_1(J_1)$ that contains the values J_{1p} for the compression branch and J_{1u} for the extension branch, so extrapolations are avoided during computations. In Table 4 we have underlined the values of J_1 and J_2 which establish the nesting domain for each variable. These values need to be used with their corresponding test equilibrium equations.

Blatz-Ko model. Dependencies at evaluation points with J_3 and nesting domains									
J_3	J_{1u}	J_{2u}	λ_u	λ_t	σ_u	J_{1p}	J_{2p}	λ_p	λ_w
0.8010	2.7300	<u>3.7037</u>	0.7283	1.0487	-18.85	<u>2.6832</u>	3.6234	0.7638	1.0487
0.9010	2.8338	<u>3.2596</u>	0.8616	1.0226	-8.93	<u>2.8220</u>	3.2444	0.8811	1.0226
1.0010	<u>3.0020</u>	<u>2.9980</u>	1.0014	0.9998	0.087	<u>3.0020</u>	<u>2.9980</u>	1.0012	0.9998
1.1010	<u>3.2356</u>	<u>2.8438</u>	1.1474	0.9796	8.597	3.2228	<u>2.8337</u>	1.1239	0.9796
1.2010	<u>3.5366</u>	2.7559	1.2991	0.9615	16.856	3.4847	<u>2.7226</u>	1.2491	0.9615

Table 4: Table of dependencies with J_3 as common driving parameter: set of 5 re-sampled points from uniaxial and strip-biaxial tests. σ_u in kPa. Underlined values are the ones defining the nesting domain for J_1 and J_2 .

4.5 Function-refresh method applied to data from Blatz-Ko model

In the following computations we use the previous five points shown in Table 4 and Figure 4 so the computations may be easily followed by the reader. Obviously, in general many more points should be used (typically hundreds).

Figure 4: Resampled functional data from uniaxial and strip-biaxial tests imposing a common $J_{3u} = J_{3p}$. We show the selected five data points for the example ($\circ$) obtained from tests and the corresponding linear interpolation (- -). (a) Pseudoexperimental stress-stretch data obtained from the Blatz and Ko model with material parameters $\mu = 26.53$, $\nu = 0.15$, $f = 1$; (b) uniaxial longitudinal versus transverse stretch relation $\lambda_t(\lambda_u)$ and (c) strip-biaxial longitudinal versus thickness-wise stretch relation $\lambda_w(\lambda_p)$.

Since for this case we use nesting domains, which depend on the value of J_3 , the algorithm takes two branches depending on that value; i.e.

$J_3 < 1$; compression branch :

$$W_1^{[j]}(J_{1p}) = \lambda_w^{-2} \left(\lambda_t^2 W_1'^{[j-1]}(J_{1u}) - \lambda_t^{-2} W_2'^{[j-1]}(J_{2u}) + \lambda_w^{-2} W_2'^{[j-1]}(J_{2p}) \right) \quad (65)$$

$$W_2^{[j]}(J_{2u}) = (\lambda_u^{-2} - \lambda_t^{-2})^{-1} \left((\lambda_u^2 - \lambda_t^2) W_1'^{[j-1]}(J_{1u}) - \frac{\sigma_u J_3}{2} \right) \quad (66)$$

$J_3 > 1$; expansion branch :

$$W_1^{[j]}(J_{1u}) = (\lambda_u^2 - \lambda_t^2)^{-1} \left(\frac{\sigma_u J_3}{2} + (\lambda_u^{-2} - \lambda_t^{-2}) W_2'^{[j-1]}(J_{2u}) \right) \quad (67)$$

$$W_2^{[j-1]}(J_{2p}) = \lambda_w^2 \left(\lambda_w^2 W_1'^{[j-1]}(J_{1p}) - \lambda_t^2 W_1'^{[j-1]}(J_{1u}) + \lambda_t^{-2} W_2'^{[j-1]}(J_{2u}) \right) \quad (68)$$

The initial guess can be simply, $W_1'^{[0]}(J_{1d}) = 0$ and $W_2'^{[0]}(J_{2d}) = 0$. After refreshing the functions, the new values of $W_1'^{[1]}(J_1)$ and $W_2'^{[1]}(J_2)$ are,

$J_3 < 1$; compression branch :

$$W_1'^{[1]}(J_{1p}) = \lambda_w^{-2} \left(\lambda_t^2 W_1'^{[0]}(J_{1u}) - \lambda_t^{-2} W_2'^{[0]}(J_{2u}) + \lambda_w^{-2} W_2'^{[0]}(J_{2p}) \right) = 0 \quad (69)$$

$$W_2'^{[1]}(J_{2u}) = (\lambda_u^{-2} - \lambda_t^{-2})^{-1} \left((\lambda_u^2 - \lambda_t^2) W_1'^{[0]}(J_{1u}) - \frac{\sigma_u J_3}{2} \right) = -\frac{\sigma_u J_3}{2(\lambda_u^{-2} - \lambda_t^{-2})} \quad (70)$$

$J_3 > 1$; expansion branch :

$$W_1'^{[1]}(J_{1u}) = (\lambda_u^2 - \lambda_t^2)^{-1} \left(\frac{\sigma_u J_3}{2} + (\lambda_u^{-2} - \lambda_t^{-2}) W_2'^{[0]}(J_{2u}) \right) = \frac{\sigma_u J_3}{2(\lambda_u^2 - \lambda_t^2)} \quad (71)$$

$$W_2'^{[1]}(J_{2p}) = \lambda_w^2 \left(\lambda_w^2 W_1'^{[0]}(J_{1p}) - \lambda_t^2 W_1'^{[0]}(J_{1u}) + \lambda_t^{-2} W_2'^{[0]}(J_{2u}) \right) = 0 \quad (72)$$

Iterations 0, 1, 2 are shown in Table 5 along with the final, converged iteration. Note that the only values to be refreshed along the iterations are those corresponding to the unknown functions. That is, the nesting values W_{1d}' , W_{2d}' and the corresponding interpolated values W_{1u}' , W_{1p}' , W_{2u}' , W_{2p}' . The convergence evolution of the subsequent iterations of the algorithm is shown in Figure 5.

Blatz-Ko model. Iter. 0, 1 and 2 with functional refresh method of five points								
Iter	J_{1p}	$W_1'(J_1)$	$W_1'(J_{1u})$	$W_1'(J_{1p})$	J_{2d}	$W_2'(J_2)$	$W_2'(J_{2u})$	$W_2'(J_{2p})$
0	2.7300	0	0	0	3.6234	0	0	0
	2.8338	0	0	0	3.2444	0	0	0
	3.0020	0	0	0	2.9980	0	0	0
	3.2356	0	0	0	2.8337	0	0	0
	3.5366	0	0	0	2.7226	0	0	0
1	2.6832	0	0	0	3.7037	7.7388	7.7388	8.2015
	2.8220	0	0.8675	0	3.2596	10.2980	10.2980	9.7011
	3.0020	13.2650	13.2650	13.2649	2.9980	0	0.0000	0
	3.2356	13.2650	13.2650	13.2650	2.8337	0	0	0
	3.5366	13.2650	13.2650	13.2650	2.7226	0	0	0
2	2.6832	1.4923	2.3367	1.4923	3.7037	7.0710	7.0710	7.0673
	2.8220	3.9955	4.4147	3.9955	3.2596	7.0503	7.0503	6.8078
	3.0020	10.4054	10.4054	10.4053	2.9980	2.8666	2.8666	2.8666
	3.2356	12.7486	12.7486	12.6204	2.8337	0.5156	0.6604	0.5156
	3.5366	13.5885	13.5885	13.4436	2.7226	-0.679	-0.321	-0.679
259	2.6832	13.2650	13.2650	13.2650	3.7037	0.0000	0.0000	0.0000
	2.8220	13.2650	13.2650	13.2650	3.2596	0.0000	0.0000	0.0000
	3.0020	13.2650	13.2650	13.2650	2.9980	0.0000	0.0000	0.0000
	3.2356	13.2650	13.2650	13.2650	2.8337	0.0000	0.0000	0.0000
	3.5366	13.2650	13.2650	13.2650	2.7226	0.0000	0.0000	0.0000

Table 5: Function refresh iterations with five points applied to experimental data from the Blatz-Ko model. Iterations 0, 1, 2 and last one (at least 7 digits of precision). The values W_1' and W_2' correspond to the nesting domain.

Figure 5: Convergence evolution of (a) $W_1'(J_1)$ and (b) $W_2'(J_2)$ during functional refresh for Blatz-Ko experimental data (5 points). Iteration = 259 has 7 digits of precision.

4.6 Matrix method applied to data from the Blatz-Ko model

Following the same procedure applied in Section 4.3, using the same five points we can compute the solution for the unknown functions $W_1'(J_1)$ and $W_2'(J_2)$, shown in Table 6. We include in the appendix, for the reader's convenience, the resulting matrices in the system of equations. Note again that the solution is not exact because of the discretizations and interpolations employed, but in practical computations (using hundreds of points and piecewise interpolations) the solution may be obtained to any desired precision.

Blatz-Ko data. Solution by the matrix method					
	Comput.	Theor.		Comput.	Theor.
J_1	$W_1'(J_1)$	$W_{1,th}'(J_1)$	J_2	$W_2'(J_2)$	$W_{2,th}'(J_2)$
2.6940	13.3715	13.2650	2.7146	-0.1635	0
2.8366	13.3899	13.2650	2.8219	-0.1828	0
3.0203	13.5432	13.2650	2.9804	-0.2852	0
3.2599	13.4127	13.2650	3.2300	-0.1058	0
3.5671	13.3720	13.2650	3.6532	-0.0671	0

Table 6: Solution for $W_1'(J_1)$, $W_2'(J_2)$ (kPa) using the matrix method with linear interpolations applied to five experimental points obtained from the Blatz-Ko model. These values are compared to analytical ones $W_{1,th}'(J_1)$, $W_{2,th}'(J_2)$.

5 Comparison of finite element solutions using analytical and numerical stored energy functions

We now show that the spline-based stored energy function obtained following either the function-refresh algorithm or the matrix algorithm produce accurate results, visually indistinguishable from the analytical models from which we obtained the pseudo-experimental data. For these examples, the stored energies $W_1'(J_1)$, $W_2'(J_2)$, $W_3'(J_3)$ are discretized using 100 experimental points and 25 nodal energy values, and interpolated using piecewise cubic splines. The stored energies are computed using a wide range to avoid extrapolations (local stretches are much larger than in previous examples).

The demonstrative finite element example consists of a $32 \times 16 \text{ mm}^2$ plate with a centered hole of 8 mm diameter, which is stretched to twice its length in 100 steps using a plain Newton-Raphson algorithm for regaining global equilibrium. Since the material is compressible, the finite element formulation employed is a standard 9-node (quadratic, lagrangean) element.

Figure 6: FEM mesh employed for calculations

The comparison of the von Mises stresses and the pressure for both models are shown in Fig. 7. In Fig. 7a we show the von Mises stresses for the data-driven spline-based model, which stored energy has been obtained directly from pseudo-experimental data simulated using the HSHN model and the material data from the previous sections. This band plot should be compared to that in Fig. 7b obtained using the HSHN model directly (i.e. the *analytical* stored energy function). No relevant difference can be appreciated between both band plots nor between both deformed meshes. In Figs. 7c and 7d we perform the comparison of the pressure band plots. Again, no relevant difference can be appreciated. The comparisons are repeated in Figs. 7e to 7h for the data-driven spline-based model capturing the experimental data from the Blatz-Ko model also with the same material parameters as in the foregoing section. As in the previous example, no relevant difference can be observed between band plots of the data-driven model and the analytical one.

As for the computational efficiency, all models require essentially the same computational effort, and have similar convergence rates. For example, in Table 7 we show comparative convergence rates for the Blatz and Ko case. It is seen that very similar convergence rates are obtained.

Typical relative convergence rates of the finite element example. Blatz-Ko data. Step 90/100		
From analytical energies (Blatz-Ko model)		
Iter	Relative force residual	Relative energy residual
1	$1.000E+00$	$1.000E+00$
2	$1.686E-05$	$1.786E-09$
3	$3.599E-09$	$3.201E-20$
From data-driven spline-based energies		
Iter	Relative force residual	Relative energy residual
1	$1.000E+00$	$1.000E+00$
2	$5.564E-05$	$7.023E-09$
3	$1.870E-08$	$1.197E-16$

Table 7: Comparison of equilibrium convergence rates for the Blatz-Ko model and the data-driven spline-based model capturing the Blatz-Ko pseudo-experimental data.

Figure 7: Comparison of predictions between analytical models (right column) and data-driven spline-based models (left column) which stored energies are computed from pseudo-experimental data obtained from the HSHN model and the Blatz-Ko model. a) Von Mises band plots from simulations using the data-driven model, if data is obtained from the HSHN model. b) Von Mises band plots from simulations using the analytical HSHN energies. c), d) Pressure band plots for the same models. e) Von Mises band plots from simulations using the data-driven model, if experimental data is obtained from the Blatz-Ko model. f) Von Mises band plots from simulations using the analytical Blatz and Ko energies. g), h) Pressure band plots for the same models.

6 Conclusions

In this paper we have shown that regardless of the invariants being used and the complete or reduced representation of the stored energy function, it is possible to *compute* numerically the stored energy function for the assumed reduced representation compatible with whatever available experimental data. This approach is clearly different to the widely used approach of *assuming* both the reduced representation *and* the analytical form of the energy terms, leaving the fitting of the experimental data to some material parameters. In this sense, they are in line with Ericksen's reflexions on the mathematician's criterion [21], appraised also by Puglisi and Saccomandi [37]: "the weaker the hypothesis, the better the theorem".

Undoubtedly, analytical forms of the stored energy are important in obtaining a deep understanding of many aspects of the behavior of polymeric materials, and in many instances cannot be avoided. However, they have no relevant advantage for the widely used numerical procedures employed to predict the behavior of nonlinear solids, from which much is also learned. In contrast, computational procedures as the ones presented herein are: (1) more accurate, (2) more general, not relying on predefined shapes of the stored energy, (3) easier to use for an engineer because there is no "model" selection nor material parameters nor special procedures to obtain those parameters, and (4) more suitable for current data-driven approaches, where material behavior is learned directly from experimental data. Of course, the purpose of this paper has not been to give insight on the actual reason for the behavior of the polymers nor to impose specific conditions on those functions. These should come from rational thinking [8, 13]. Furthermore, the specific proposal of the invariants to be used together with the reduced function must be done in that framework. Regarding data-driven approaches, in order to have well-posed problems, it is important to understand that the available experimental data frequently permits only the determination of some reduced forms of the stored energy. However, if a complete set of experimental data were available, a general numerical form of the stored energy could be determined.

We have shown two types of algorithms that do not use the KZ or similar formula and are applicable to more general cases. The function-refresh algorithm is iterative but the implementation is straightforward and the solution is accurate independently of the number of points employed. The matrix method is noniterative, more systematic and more general, but a system of equations including the adequate interpolation scheme needs to be formulated, and enough points are needed to reach high precision.

In this work we demonstrated the application of the approach for general forms of the stored energy in isotropic cases. Anisotropic cases are more involved in general and are current research, but the present ideas are still applicable without relevant modifications.

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Appendix

In this appendix we include, for the reader's convenience, the matrices employed in the matrix 5-point examples.

A. HSHN example

In this example, spline interpolation with *not-a-knot* condition has been used. Therefore, interpolant matrices are full in general, except when the nodal points exactly coincide with the experimental ones, which is the case for P_{1u} and P_{2p} , which are then equal to the identity matrix I . The other two interpolation matrices P_{1p} and P_{2u} are obtained from the spline interpolation as, see for example [27]

$$P_{1p} = \begin{bmatrix} 1.2748 & -0.4971 & 0.3158 & -0.1069 & 0.0134 \\ 0.0036 & 1.0079 & -0.0150 & 0.0040 & -0.0005 \\ -0.0008 & 0.0067 & 0.9998 & -0.0065 & 0.0008 \\ 0.0033 & -0.0261 & 0.1014 & 0.9415 & -0.0200 \\ -0.0127 & 0.1019 & -0.3153 & 0.5962 & 0.6299 \end{bmatrix} \quad (73)$$

$$P_{2u} = \begin{bmatrix} 0.0086 & -0.0689 & 0.2045 & -0.3274 & 1.1832 \\ -0.0002 & 0.0019 & -0.0070 & 1.0037 & 0.0017 \\ 0.0007 & -0.0056 & 0.9999 & 0.0058 & -0.0007 \\ -0.0262 & 0.9158 & 0.1420 & -0.0361 & 0.0045 \\ 0.2313 & 1.0508 & -0.3839 & 0.1163 & -0.0145 \end{bmatrix} \quad (74)$$

The boxes A_{ij} of matrix A of the system of equations given in Eq. (61) are

$$A_{11} = \begin{bmatrix} -0.5275 & 0 & 0 & 0 & 0 \\ 0 & -0.1826 & 0 & 0 & 0 \\ 0 & 0 & 0.2121 & 0 & 0 \\ 0 & 0 & 0 & 0.7158 & 0 \\ 0 & 0 & 0 & 0 & 1.4164 \end{bmatrix} \quad (75)$$

$$A_{21} = \begin{bmatrix} -0.2917 & 0.5270 & -0.3348 & 0.1134 & -0.0142 \\ -0.0036 & -0.0080 & 0.0152 & -0.0041 & 0.0005 \\ 0.0008 & -0.0066 & 0.0001 & 0.0064 & -0.0008 \\ -0.0031 & 0.0249 & -0.0966 & 0.0554 & 0.0191 \\ 0.0116 & -0.0926 & 0.2865 & -0.5417 & 0.3350 \end{bmatrix} \quad (76)$$

$$A_{12} = \begin{bmatrix} -0.0081 & 0.0644 & -0.1912 & 0.3061 & -1.1062 \\ 0.0001 & -0.0004 & 0.0015 & -0.2170 & -0.0004 \\ 0.0001 & -0.0010 & 0.1797 & 0.0010 & -0.0001 \\ -0.0118 & 0.4124 & 0.0639 & -0.0163 & 0.0020 \\ 0.1554 & 0.7060 & -0.2579 & 0.0781 & -0.0098 \end{bmatrix} \quad (77)$$

$$A_{22} = \begin{bmatrix} -0.0081 & 0.0650 & -0.1930 & 0.3089 & -0.1731 \\ 0.0002 & -0.0019 & 0.0069 & -0.0037 & -0.0016 \\ -0.0007 & 0.0057 & 0.0001 & -0.0059 & 0.0007 \\ 0.0275 & 0.0880 & -0.1491 & 0.0379 & -0.0047 \\ 0.8456 & -1.1582 & 0.4231 & -0.1282 & 0.0160 \end{bmatrix} \quad (78)$$

6.1 B. Blatz and Ko example

In this case a nesting domain has been used to avoid extrapolations, so in contrast to the previous example, matrices P_{1u} and P_{2p} are no longer the identity matrix; it is easily verified that they are

$$P_{1u} = \begin{bmatrix} 0.7004 & 0.2996 & 0 & 0 & 0 \\ 0 & 0.9470 & 0.0530 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 \end{bmatrix} \quad (79)$$

$$P_{1p} = \begin{bmatrix} 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0.0006 & 0.9994 & 0 & 0 \\ 0 & 0 & 0.0633 & 0.9367 & 0 \\ 0 & 0 & 0 & 0.1849 & 0.8151 \end{bmatrix} \quad (80)$$

$$P_{2u} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1.0000 \\ 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0.9996 & 0.0004 & 0 \\ 0 & 0.9259 & 0.0741 & 0 & 0 \\ 0.6670 & 0.3330 & 0 & 0 & 0 \end{bmatrix} \quad (81)$$

$$P_{2p} = \begin{bmatrix} 0 & 0 & 0 & 0.1681 & 0.8319 \\ 0 & 0 & 0.0490 & 0.9510 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 \\ 1.0000 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (82)$$

where the sparse form is due to the linear interpolation used in this example. The boxes of the matrix of the system of equations are

$$A_{11} = \begin{bmatrix} -0.3830 & -0.1638 & 0 & 0 & 0 \\ 0 & -0.2628 & -0.0147 & 0 & 0 \\ 0 & 0 & 0.0331 & 0 & 0 \\ 0 & 0 & 0 & 0.3911 & 0 \\ 0 & 0 & 0 & 0 & 0.8024 \end{bmatrix} \quad (83)$$

$$A_{12} = \begin{bmatrix} 0 & 0 & 0 & 0 & -0.9122 \\ 0 & 0 & 0 & -0.3489 & 0 \\ 0 & 0 & 0.0323 & 0.0000 & 0 \\ 0 & 0.2811 & 0.0225 & 0 & 0 \\ 0.3369 & 0.1682 & 0 & 0 & 0 \end{bmatrix} \quad (84)$$

$$A_{21} = \begin{bmatrix} -0.3280 & 0.3279 & 0 & 0 & 0 \\ 0 & -0.0551 & 0.0551 & 0 & 0 \\ 0 & -0.0006 & 0.0006 & 0 & 0 \\ 0 & 0 & -0.0605 & 0.0605 & 0 \\ 0 & 0 & 0 & -0.1704 & 0.1704 \end{bmatrix} \quad (85)$$

$$A_{22} = \begin{bmatrix} 0 & 0 & 0 & 0.1536 & -0.1536 \\ 0 & 0 & 0.0470 & -0.0470 & 0 \\ 0 & 0 & 0.0004 & -0.0004 & 0 \\ 0 & 0.0775 & -0.0775 & 0 & 0 \\ 0.3613 & -0.3613 & 0 & 0 & 0 \end{bmatrix} \quad (86)$$

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Chapter 6

Extension of data-driven solution to non-linear elastic orthotropic materials

6.1 Introduction

The natural mechanical behaviour of materials is not ideally isotropic, orthotropic or monoclinic, but purely anisotropic, with non affine strains and many more properties that are simplified by means of idealizations in order to make the problem manageable. Regarding anisotropy, isotropy is the *zero order* approach to the mechanical behaviour characterization. There is certain similarity with a constant value, since the response is the same independently of the principal direction of strains. The next order of characterization would be the assumption of orthotropy.

As in the case of isotropy idealization, mechanical behaviour of materials can be covered by phenomenological approach or considering microscale aspects using FEA. Conventional phenomenological procedures imply analytical energy functions with free scalar parameters that are fitted in order to obtain an approximation of the solution of the stress-strain functional system of equations. Compressibility is not an exception in the procedure. It is usually boarded on with a penalty function, and specified by bulk modulus κ for small strains.

Using the same approach of previous articles of this Thesis, compressible orthotropic hyperelastic materials can be characterized by solving the corresponding stress-strain functional equations. Assuming the extension of Valanis-Landel decomposition in the orthotropic functions, material logarithmic strains are going to be selected as unknown function arguments. In particular,

$$\Psi = \sum_{i=1}^3 \omega_{ii}(E_{ii}^d) + \omega_{12}(E_{12}^d) + \omega_{13}(E_{13}^d) + \omega_{23}(E_{23}^d) + \mathcal{U}(E^v) \quad (6.1)$$

so that in small strains the formulation recovers the expression,

$$\Psi = \sum_{i=1}^3 \mu_{ii}(E_{ii}^d)^2 + \mu_{12}(E_{12}^d)^2 + \mu_{13}(E_{13}^d)^2 + \mu_{23}(E_{23}^d)^2 + \frac{1}{2}\kappa(E^v)^2 \quad (6.2)$$

This ansatz implies solving a system of 7 functional equations. The procedure developed here is robust enough to determine the problem even assuming that functional data comes from off-axis alignment (i.e. principal strains of the tests in misalignment with preferred orthotropic directions of the specimen).

Another procedure developed here permits orthotropic Holzapfer-Gasser-Ogden (known as *HGO*) formulation to obtain directly the energy functional unknowns defined on I -invariants.

6.2 Solving stored energy density functional unknowns from HGO formulation

Formulation of HGO is based on I -invariants. In particular, I_1 covers the influence of isotropy and I_4, I_6 account anisotropy. Thus, the energy is defined as follows,

$$\Psi(I_1, I_4, I_6) = \Psi_{iso}(I_1) + \Psi(I_4) + \Psi(I_6) \quad (6.3)$$

$$\Psi_{iso}(I_1) = \frac{c}{2}(I_1 - 3) \quad (6.4)$$

$$\Psi(I_i) = \frac{k_1}{2k_2} [\exp \{k_2(I_i - 1)^2\} - 1] \quad (6.5)$$

where

$$I_1 = \mathbf{C} : \mathbf{I} \quad (6.6)$$

$$I_i = \mathbf{C} : (\mathbf{f}_i \otimes \mathbf{f}_i) \quad (6.7)$$

and $\mathbf{f}_i$ represents the vector of the direction of the aligned fibers. What is remarked here and in all the common line of this Thesis, is that there is no necessity of imposing an analytical form to the functions ψ_{iso} and ψ . Leaving them in reduced form, the following stress-strain functional equation comes from derivation of the energy functions.

$$\boldsymbol{\sigma} = p\mathbf{I} + 2\psi'_{iso}(I_1)\mathbf{b} : \mathbb{P} + \sum_{i=4,6} \{2\psi'(I_i) {}^t\mathbf{f}_i \otimes {}^t\mathbf{f}_i : \mathbb{P}\} \quad (6.8)$$

After algebraic manipulation and particularization of Eq.(6.8) to uniaxial test, it is observed that functional unknowns ψ_{iso}, ψ can be found explicitly after the proper projection. This means that they are the solution of the system of functional scalar equations that arise from Eq.(6.8).

$$\psi'_{iso}(I_1) = \frac{\frac{1}{2}(1 - \cos 2\beta)\lambda_t^2\sigma_u}{2\lambda_t^2(\lambda_u^2 - \lambda_3^2)\sin^2(\beta) - 2\lambda_u^2(\lambda_t^2 - \lambda_3^2)\cos^2(\beta)} \quad (6.9)$$

$$\psi'(I_u) = \frac{\frac{1}{2}(\lambda_3^2 - \lambda_t^2)\sigma_u}{2\lambda_t^2(\lambda_u^2 - \lambda_3^2)\sin^2(\beta) - 2\lambda_u^2(\lambda_t^2 - \lambda_3^2)\cos^2(\beta)} \quad (6.10)$$

Since they are two functional equations, two functional data are required. In particular they are the uniaxial Cauchy stress σ_u vs. longitudinal stretch λ_u , and the uniaxial stretch relation transverse λ_t vs. longitudinal λ_u . As commented in previous chapters, it is mandatory that experimental data set be synchronized. A possible synchronization from functional data $\sigma_u(\lambda_u), \lambda_t(\lambda_u)$ is $\{\lambda_u^*, \lambda_t^*, \sigma_u^*\}$,

$$\lambda_t^* = \lambda_t(\lambda_u = \lambda_u^*)$$

$$\sigma_u^* = \sigma_u(\lambda_u = \lambda_u^*)$$

From this set, the corresponding synchronized values of $I_1^*, I_u^*, \psi_{iso}^*, \psi^*$ are obtained, and thus the spline representation of the functional unknowns ψ_{iso}, ψ ,

$$\{I_1^*, \psi_{iso}^*\} \rightarrow \psi_{iso} \quad (6.11)$$

$$\{I_u^*, \psi^*\} \rightarrow \psi \quad (6.12)$$

6.3 WYPiWYG data-driven for compressible orthotropic hyperelastic materials

Previous articles enhanced WYPiWYG data-driven techniques with different procedures (inversion formula, functional refresh method, matricial method) and for different assumptions (Valanis-Landel decomposition, J-invariant decomposition) and different functional arguments (material logarithmic strains, J-invariants, suggestion for I-invariant proposal). As common denominator, data-driven advances were all tested and employed for hyperelastic isotropic compressible materials. In this work, WYPiWYG is going to be extended to compressible hyperelastic orthotropic materials for logarithmic strains, but also for the enhancement of two I – *invariant* proposals, and for general test conditions beyond uniaxial tests along with preferred directions.

Assuming there is decoupling in logarithmic strains, the following stress-strain formulation arises from Eq.(6.1).

$$\mathbf{T} = \sum_{i=1}^3 \omega'_{ii}(E_{ii}^d) \mathbf{M}_i^d + \sum_{i \neq j}^3 \omega'_{ij}(E_{ij}^d) \mathbf{M}_{ij}^{ds} + \mathcal{U}'(E^v) \mathbf{I} \quad (6.13)$$

where,

$$\mathbf{M}_i^d = (\mathbf{N}_i \otimes \mathbf{N}_i) : \mathbb{P} \quad (6.14)$$

$$\mathbf{M}_{ij}^{ds} = \frac{1}{2} [\mathbf{N}_i \otimes \mathbf{N}_j + \mathbf{N}_j \otimes \mathbf{N}_i] : \mathbb{P} \quad (6.15)$$

$$\mathbb{P} = \mathbb{I}^s - 1/3 \mathbf{I} \otimes \mathbf{I} \quad (6.16)$$

$$E_{ij}^d = \mathbf{E} : \mathbf{M}_{ij}^{ds} \quad (6.17)$$

$$E^v = \mathbf{E} : 1/3 \mathbf{I} \otimes \mathbf{I} = \log(J^{1/3}) \quad (6.18)$$

and N_i is the strain eigenvector in direction i , $\mathbb{P}$ is the fourth order deviatoric projector tensor, $\mathbb{I}^s$ is the fourth order symmetric identity tensor, and E^v is the volumetric logarithmic strain, obtained directly from volumetric projection of strain tensor $\mathbf{E}$ or from Jacobean J .

In this article, the following advances are going to be included.

- As a preliminar approach, energies HGO and Standard Reinforced Model formulations are going to be found from pseudo-experimental results generated by them, without the need of minimization techniques. The aim of this is to recover the energies, and contrast them with the original ones employed for the pseudo-experimental data generation. Pseudo-experimental noise is also going to be included to observe the efficiency of the method when comparing the effects with and without noise.
- A WYPiWYG data-driven procedure based on the functional refresh method is developed for moderate compressible orthotropic materials. It implies that no

analytical volumetric penalty function needs to be imposed, since volumetric function $\mathcal{U}$ is considered another functional unknown more to be found. This method employs functional data from uniaxial tests performed on preferred directions.

- Because in reality uniaxial tests are not necessarily (or ideally) performed along with the preferred directions, a general E-WYPiWYG data-driven procedure based on the functional refresh method is developed for moderate compressible orthotropic materials when functional data comes from uniaxial tests in misalignment with preferred directions.
- In line with previous chapters, a section for numerical examples is included. Three different numerical examples are performed with the aim to cover progressively the different casuistry explained in this paper. The first example deals the incompressible case, the second one the quasi-incompressible one, and the third one the most general case in which uniaxial test data comes from off-axis tests.
- Finally, Appendix A is dedicated for code aimed for determination of HGO formulation. Appendix B covers different combination of input data experimental tests for E-WYPiWYG orthotropic resolution (e.g. uniaxial test stress vs. longitudinal strain in direction 1 and strain relation transverse vs. longitudinal for tests in directions 2 and 3). Appendix C attaches rotation matrix of off-axis pseudo-experimental data with respect to preferred directions.

FUNCTION-REFRESH ALGORITHMS FOR DETERMINING THE STORED ENERGY DENSITY OF NONLINEAR ELASTIC ORTHOTROPIC MATERIALS DIRECTLY FROM EXPERIMENTAL DATA

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ABSTRACT

The typical approach to hyperelasticity is to assume an analytical expression of the stored energy function in terms of invariants and some constants, named “material parameters”. A different data-driven approach is, given the available experimental data, to establish specific functional dependencies, the stored energy which can be uniquely determined in a numerical, deterministic way, exactly capturing smooth experimental data curves. In this approach the functions are not restricted to an analytical form and do not employ material parameters. Whereas the overall ideas regarding the search for a numerical solution employing proper interpolation functions are common, the actual computational procedure depends on the assumed function dependencies from available experimental data and known material symmetries. For the case of orthotropic materials, it is possible to assume a strain energy decomposition in terms of logarithmic strains which guarantees consistency with the infinitesimal theory at all deformation levels. At the same time, this energy can be determined with a minimum amount of tests. In previous works we introduced algorithms which use a generalization of the Kearsley-Zapas inversion formula for orthotropy. This approach lacks the desired generality to account for different reduced forms and possible tests available to the analyst. In this work we use a simpler approach using function-refresh algorithms, which allows us to obtain the stored energy density of orthotropic materials in more general cases.

Keywords Soft materials; data-driven hyperelasticity; orthotropy.

1 Introduction

As it is well known, due to its entropic behavior, the elastic conservative behavior of soft materials (polymers, biological tissues) occurs also at large strains [1, 2]. To guarantee conservative behavior from the outset, the existence of a potential (stored energy density) is assumed. Since this potential cannot be measured directly, unaccountable stored energy shapes have been proposed for each class of material [3, 4]. These proposals have predefined analytical functions of some deformation invariants and material constants. The constants are obtained as to best-fit available experimental data, which are captured with different success [4].

In their paper [5], Sussman and Bathe introduced a different idea: there is no need to assume the analytical form of the stored energy. As it is done in finite element procedures [6], some “nodal” values (unknowns) and some *local*

interpolation functions may be assumed. Then, the nodal values may be obtained solving numerically the equilibrium equations of available tests. Even though it is possible to establish a general procedure (e.g. [7]), the actual numerical procedure to solve the equilibrium equations depends on the available tests, the material symmetries and the assumed reduced forms. Reduced forms are needed in general to obtain a well-posed problem if a limited amount of experimental data is available, as it is almost always the case [8]. Reduced forms use decompositions (typically additive, but not necessarily) of the stored energy in functions of less variables (invariants) [3, 4, 2]. The Valanis-Landel decomposition of incompressible isotropic materials is an example which reduces the general form $\mathcal{W}(\lambda_1, \lambda_2)$ to scalar-valued functions $\omega(\lambda_i)$ of the principal stretches λ_i . Although this decomposition neglects some high-order coupling effects, the scalar-valued function $\omega(\lambda)$ can be determined from a complete tension-compression uniaxial stress-strain curve [8]. On the contrary, the determination of the complete form $\mathcal{W}(\lambda_1, \lambda_2)$ requires substantially more testing [9] (the situation is obviously much worse in compressibility and in anisotropic materials), even though in many materials the additional coupling terms are negligible at least in the range of interest [1, 9]. Of course, enhanced reduced forms including more terms (and thus high order effects) are also possible [10].

Numerical stored energies may be formulated in a hierarchical manner (introducing more and more functions), they are as efficient in the finite element context as analytical functions (even the programming is more general) and have a far-reaching advantage: they are very useful in modern data-driven techniques for machine learning, for example, to determine the behavior of soft tissues directly from medical imaging, see for example the recent works [11, 12, 13, 14, 15]. In fact, spline functions are widely used in data-driven discovery in many different fields because of their non-parametric fitting character [16], frequently substituting traditional laws, like in medicine [17], biology [18], political economy [19] and forecasting [20]. The present manuscript is a step towards the goal of data-driven, but physically-based constitutive modeling.

Sussman and Bathe solved the case of isotropic, incompressible Valanis-Landel materials [21] using the Kaersley-Zapas inversion formula [22], which are series giving $\omega'(E) \equiv d\omega(E)/dE$ (with $E = \ln \lambda$, note the abuse of notation to avoid proliferation of symbols) directly from experimental data. Unfortunately, this formula is valid only for such case. For transversely isotropic and orthotropic materials, we introduced a novel reduced form for the stored energy [23] which is compliant with the infinitesimal theory at all deformation levels [24]. For solving these cases we introduced a more general inversion formula [25]. However, these procedures have also some important inconveniences which we solve in this paper. The first one is that only some specific tests may be used because the equilibrium equations must be written in a form in which the inversion formula may be used. The second one is that the previous procedure is valid only for specific reduced forms of the stored energy.

The purpose of the present paper is (1) to show that there is no need in general to impose the analytical form of orthotropic stored energies because they can be computed numerically, and (2) how function-refresh algorithms can be successfully employed for determining reduced forms of the stored energies of orthotropic materials directly from available experimental data, without using any inversion formula. In fact we show that the inversion formula is a function-refresh algorithm restricted only to some particular cases. The function-refresh procedure can be applied to most types of decompositions available in the literature for orthotropic materials and using any type of invariants. Furthermore, the procedure is valid for most types of experiments, including off-axis experiments. The method has some resemblance to fixed-point iterations to solve a nonlinear equation, but in our case we solve nonlinear functional equations.

The method is based on spline function manipulation and it constitutes a different approach to the problem than classical methods used in the field. Hence in the following section we give a brief background on spline handling and introduce notation, highlighting the different way of approaching the problem. Thereafter we show through a simple example that in some widely-used cases, the stored energy may be obtained directly and explicitly from experimental data without using pre-defined analytical functions, material parameters or optimization algorithms. We show that the solution obtained exactly reproduces experimental data. Finally, we explain the function-refresh algorithms for more elaborate stored energy forms compatible with the infinitesimal theory at all deformation levels [24] and show some demonstrative examples.

2 Background: working with spline functions

2.1 Spline approximations and inverse spline functions

Spline functions are just one possible interpolation function employed in the procedures. We typically use cubic splines because of efficiency and because continuity can be guaranteed for stresses, tangents and even tangent derivatives if needed. Furthermore, cubic splines can be written in terms of periodic B-splines; many of their hull's properties (like convexity) are passed to the spline. Another interpolating option for nonsmooth experimental data is to use piecewise

cubic hermite interpolating polynomials (PCHIP), which avoid oscillations but lacks continuity of second derivative, so often penalized splines are preferred.

Experimental data consists usually in a set of points given by abscissae and ordinates, e.g. $\{x_i, y_i\}, i = 1, \dots, N + 1$, which we denote compactly by $\{x_i, y_i\}$; we will omit subindices unless needed to avoid confusion, i.e. we will often just write $\{x, y\}$. From these data points it is immediate to efficiently obtain a smooth piecewise cubic spline function $y(x)$ by solving a tridiagonal system of equations by the Thomas algorithm [26], whose number of operations is of the order of the number of equations. We will denote this operation by

$$\{x_i, y_i\} \rightsquigarrow y(x) \approx \eta(x) \quad (1)$$

where $\{x_i, y_i\}$ are the data points, " $\rightsquigarrow$ " implies the spline conversion operation giving the spline function $y(x)$, which represents the nature (or analytical) function $\eta(x)$. This operation is, for example, performed in Matlab by the command $pp = \text{spline}(x, y)$, where x and y are the arrays of data and pp is the pp -form (piecewise polynomial form) containing the coefficients of the polynomials. The evaluation of the spline function at $\hat{x}$ is performed in Matlab with the command $\hat{y} = \text{ppval}(pp, \hat{x})$. Multi-dimensional splines are also possible, but not used in this paper. In summary, it is quite equivalent to think in experimental data $\{x_i, y_i\}$ or in the spline function $y(x)$ which closely approximates the unknown nature function $\eta(x)$.

As a simple example consider $\eta(x) = \exp(x) - 1$. The following Matlab code (which we represent by $\{x_i, y_i\} \rightarrow \{y_i, x_i\} \rightsquigarrow x(y)$) gives the spline approximation to the inverse without employing the inverse function

```
x = [0:0.1:3]; y = exp(x) - 1; pp = spline(y,x);
```

and the accuracy may be checked with the known analytical inverse

```
1 y2 = [0:0.1:10]; x_spline = ppval(pp,y2); x_theory = log(y2+1);
2 plot(y2,x_theory,'ko'); hold on; plot(y2,x_spline,'r.');
```

As shown below, this is obviously useful for solving complex (even implicit) equations if they are monotonic (non-monotonic cases can be treated with parametric splines). In the previous example, the value of x such that $\exp(x) - 1 = 2$ is obtained by a simple evaluation of the inverse spline at 2, i.e. by $\text{ppval}(pp, 2)$. A more elaborate application of this procedure may be found in Ref. [27] for computing the inverse Langevin function (for which there is no analytical expression).

2.2 Resampling functions, synchronized data and composition of spline functions

Let us assume that we have an experiment A that observes the relation of variable x with variable y , so the observation is given as pairs of data $\{x_j, y_j\}, j = 1, \dots, N$. Assume that another experiment B relates the same variable x with another variable z , so measured data is $\{x_i, z_i\}, i = 1, \dots, M$. However, $N \neq M$ and the values x_i and x_j from both experiments have no correspondence, so we do not know the relation between y and z for a given value of x . However, if we build a spline function $y(x)$ from experiment A , and another function $z(x)$ from experiment B , we can evaluate (or *resample*) both spline functions at common values x_r so a correspondence between y_r and z_r is immediately established. We call such evaluation at x_r a "*resampling*" and we say that these values $\{x_r, y_r, z_r\}$ are now *synchronized*.

As a simple example consider that experiment A gives experimental data $\{x_i, y_i\}, i = 1, \dots, N$ which correspond to the (unknown) nature relation $\eta(x) = \exp(x) - 1$, and experiment B gives experimental data $\{x_j, z_j\}, j = 1, \dots, M$ which correspond to the (unknown) nature relation $\zeta(x) = x^2$. We now wish a function $z(y)$ representing to high accuracy the unknown nature relation $\zeta(\eta)$. The following Matlab lines give the spline in pp -form

```
1 xA = [0:0.1:3]; yA = exp(xA)-1;           % Experiment A
2 xB = [0:pi/100:3]; zB = xB.^2;           % Experiment B (not synchronized)
3 ppzx = spline(xB,zB);                   % Spline z(x)
4 xr = xA; yr = yA; zr = ppval(ppzx,xr); % Synchronization
5 ppzy = spline(yr,zr);                   % Desired approximation of z(y)
```

In general we will not know an analytical expression for the obtained relation $z(y)$, but in this case we know it should be $\zeta(\eta) = [\log(1 + \eta)]^2$, so we can test the accuracy of our procedure at some points by the following Matlab commands

```
1 y = [0:0.2:10]; z_theory = (log(1+y)).^2; z_spline = ppval(ppzy,y);
2 plot(y,z_theory,'ko'); hold on; plot(y,z_spline,'r.');
```

The reader may verify that they are visually coincident. We denote the above synchronizing operation compactly as $\{x_i, y_i\} \rightsquigarrow y(x)$, then $\{x_j, z_j\} \rightsquigarrow z(x)$, and finally $\{x_r, y_r = y(x_r), z_r = z(x_r)\}$. With this synchronization, it is immediate to obtain, for example, the spline functions $\{z_r, y_r\} \rightsquigarrow y(z)$ and $\{y_r, z_r\} \rightsquigarrow z(y)$.

3 Using spline functions to recover the energy derivatives of orthotropic materials directly from experimental data

The purpose of this section is to demonstrate that in some common cases, it is possible to recover the derivatives of the strain energy in orthotropic materials directly from experimental data, without using any iterative procedure, without using material parameters, and without using optimization algorithms. We show this through an example useful for researchers working in the mechanics of soft tissues.

In order to model nonlinear orthotropic fibre-reinforced materials, specially arteries, Holzapfel, Gasser and Ogden used a reduced, simplified form in their celebrated (HGO) model [28]. The simplifications are: (1) the material is incompressible, so $I_3 \equiv \det(\mathbf{C}) = J \equiv \det(\mathbf{X}) = 1$, where $\mathbf{X}$ is the deformation gradient and $\mathbf{C} := \mathbf{X}^T \mathbf{X}$ is the right Cauchy-Green deformation tensor, and no distinction is needed between total and isochoric invariants; (2) the influence of Rivlin-Spencer invariants I_2, I_5, I_7, I_8, I_9 is neglected; (3) the stored energy is given by the reduced form

$$\Psi(I_1, I_4, I_6) = \psi_{iso}(I_1) + \psi_{aniso}(I_4, I_6) = \psi_{iso}(I_1) + \psi(I_4) + \psi(I_6) \quad (2)$$

where $\psi_{iso}(I_1)$ is the isotropic contribution (ground matrix) and $\psi(I_i), i = 4, 6$ is the contribution of the fibers. The I -invariants are defined as usual $I_1 = \mathbf{C} : \mathbf{I}$, $I_i = \mathbf{C} : \mathbf{f}_i \otimes \mathbf{f}_i$ where $\mathbf{f}_i, i = 4, 6$ are the direction vectors of the two fibers in the reference configuration, $\mathbf{I}$ is the second-order identity tensor and “:”, “ $\otimes$ ” are the scalar (in tensors) and dyadic products. Note that in the right hand side of Eq. (2) there are only two unknown scalar-valued functions. Thereafter, Holzapfel, Gasser and Ogden constrained the possibilities to specific proposed analytical functions with material constants, namely a Neo-Hookean for the ground matrix and Fung-type exponentials for the fibers

$$\psi_{iso}(I_1) = \frac{c}{2}(I_1 - 3) \quad \text{and} \quad \psi(I_i) = \frac{k_1}{2k_2} \{\exp[k_2(I_i - 1)^2] - 1\} \quad (3)$$

where c, k_1, k_2 are the material parameters, along with the angle between fibers 2β . The fibers do not work in compression, so we take $\psi(I_i) = 0$ for $I_i \leq 1$. The material presents orthotropic symmetries with principal directions $\mathbf{a}_i$ at β and $\pi/2 - \beta$ respect to both fibers, e.g. $\mathbf{a}_1 \cdot \mathbf{f}_i = \cos \beta$. The stresses associated to the HGO stored energy are

$$\boldsymbol{\sigma} = p\mathbf{I} + 2\psi'_{iso}(I_1)\mathbf{b} : \mathbb{P} + \sum_{i=4,6} \{2\psi'(I_i) {}^t\mathbf{f}_i \otimes {}^t\mathbf{f}_i : \mathbb{P}\} \quad (4)$$

where $p, \mathbf{I}, \mathbb{P}, {}^t\mathbf{f}_i = \mathbf{X} \mathbf{f}_i$ are, respectively, a pressure-like Lagrange multiplier, the identity tensor, the usual deviatoric projector and the spatial fiber directions; the apostrophe implies derivative respect to the argument in parenthesis. A tensile test in direction $\mathbf{a}_1$ gives the following expressions

$$\sigma_u = 2\psi'_{iso}(I_1)(\lambda_u^2 - \lambda_t^2) + 4\psi'(I_u)[\lambda_u^2 \cos^2 \beta - \lambda_t^2 \sin^2 \beta] \quad (5)$$

$$0 = 2\psi'_{iso}(I_1)(\lambda_t^2 - \lambda_3^2) + 4\psi'(I_u)\lambda_t^2 \sin^2 \beta \quad (6)$$

where $I_u := I_4 = I_6 = \lambda_u^2 \cos^2 \beta + \lambda_t^2 \sin^2 \beta$. The code in Appendix A performs an “in silico” uniaxial test in this HGO material, returning the “experimental” measurements $\{\lambda_u, \sigma_u\}$ and $\{\lambda_u, \lambda_t\}$; for example using the Matlab commands

```
1 beta = 29*pi/180; c = 3; k1 = 2.3632; k2 = 0.8393; % Material parameters
2 lambda_u = [0.5:0.01:1.5];
3 [stress_u, lambda_t, I1, I4, dWdI1, dWdI4] = HGOtest(lambda_u, beta, c, k1, k2);
```

We show now that, if we accept decomposition Eq. (2), there is no need to assume the shape of the functions as done in Eq. (3), because with the single use of one tensile test, these functions may be obtained directly (in a deterministic, explicit way) from the experiment in spline format, in a way that they exactly (i.e. to any desired precision) predict the prescribed experimental data. Note that Eqs. (5) and (6) can be re-written as

$$\psi'_{iso}(I_1) = \frac{\frac{1}{2}(1 - \cos 2\beta)\lambda_t^2 \sigma_u}{2\lambda_t^2(\lambda_u^2 - \lambda_3^2) \sin^2(\beta) - 2\lambda_u^2(\lambda_t^2 - \lambda_3^2) \cos^2(\beta)} \quad (7)$$

$$\psi'(I_u) = \frac{\frac{1}{2}(\lambda_3^2 - \lambda_t^2)\sigma_u}{2\lambda_t^2(\lambda_u^2 - \lambda_3^2) \sin^2(\beta) - 2\lambda_u^2(\lambda_t^2 - \lambda_3^2) \cos^2(\beta)} \quad (8)$$

Using these general expressions, the strain energy derivatives can be recovered explicitly from experimental data, regardless of the actual analytical form of the stored energy. A Matlab function to do so is given in Appendix A. Using this function, the commands to recover and plot the derivatives of the stored energy are

```
1 ppstress_u = spline(lambda_u, stress_u); % Spline 1 of exp. data
```



```

2 pplambda_t      = spline(lambda_u,lambda_t); % Spline 2 of exp. data
3 [ppdWdI1,ppdWdI4] = HGO_recover(beta,lambda_u,ppstress_u,pplambda_t);
4 plot(I1,dWdI1,'ko'); hold on; plot(I1,ppval(ppdWdI1,I1),'r. '); figure;
5 plot(I4,dWdI4,'ko'); hold on; plot(I4,ppval(ppdWdI4,I4),'r. ');

```

where the first two lines build the spline pp-forms of the tests; i.e. perform the operations $\{\lambda_u, \sigma_u\} \rightsquigarrow \sigma_u(\lambda_u)$ and $\{\lambda_u, \lambda_t\} \rightsquigarrow \lambda_t(\lambda_u)$. The last two lines show the comparison between the values of the analytical energies used to perform the virtual test and the values obtained from the evaluation of the spline functions of the one recovered directly from experimental data. It is obvious that the recovered functions may be immediately used in a finite element code because they are, in essence, cubic polynomials. The Matlab function to retrieve the coefficients of the polynomials is `unmkpp`. Accuracy obviously depends on the points used, but near machine precision may be easily obtained. The result with a similar code (now including labels and legends) can be seen in Figure 1. It is seen that a high accuracy is obtained since both analytical and recovered plots are superposed. Obviously, in Figs. 1a and 1b it is also seen that the predictions using the recovered spline-based energies are also coincident with the original “experimental” data.

The above procedure, and the function `HGO_recover.m` are valid to recover the strain energy of any other material under the assumption that the reduced form Eq. (2) holds. For example, Fig. 2 shows the same procedure as Fig. 1 but for a modified standard reinforcing material with the strain energy

$$\Psi(I_1, I_4, I_6) = \frac{c}{2}(I_1 - 3)^2 + \frac{k_1 k_2}{2}(I_4 - 1)^2 + \frac{k_1 k_2}{2}(I_6 - 1)^2 \quad (9)$$

One of the relevant issues in data-based procedures is the possible experimental noise or the presence of multiple tests curves. In such case, a simple procedure is to obtain smoothed penalized regression splines for the experimental data; note that in these cases it is experimental data and not stored energies, what should be averaged, because average stored energies may give unphysical results [29], [30]. With the average splines of experimental data, the procedure is similar. Fig. 3 shows the recovery of the derivatives of the stored energy terms for the previous HGO model when noisy data is presented to the procedure, and Fig. 4 shows the recovery for the previous modified Standard Reinforcing Model when a similar level of noise is introduced. These noisy data may be due to experimental errors or to data from different specimens in soft tissues. It is seen in both cases that the recovered derivatives of the strain energy function have an error to the theoretical one much smaller than the uncertainties present in the experimental data. Of course, in the presence of noisy data, different data sets give different solutions. Finally, in case that we desire to impose some stability conditions on the stored energy, it is possible to use smoothing procedures that enforce them. See for example a procedure in Ref. [31] for isotropic incompressible materials.

Spline-based procedures are rather general and can be applied to many reduced forms employed in the literature, both using fiber-based invariants or symmetry-based invariants (or even a combination). In selecting the form, the main issue is how much experimental information is available on the material, because the problem must be physically well-posed. Below we apply the procedures for a simple form compatible with the infinitesimal theory at all deformation levels which has been proven to represent the behavior of many anisotropic soft tissues to some extent, e.g. [32, 33, 34]. Another important advantage is that engineering intuition may be easily applied to complete some unavailable information for the case of arteries [35].

4 Function-refresh iterations for a reduced form of the stored energy compatible the with infinitesimal theory, and connection with inversion formula

In the previous section we have used spline functions to recover, in spline format, the stored energy derivatives of materials directly from experimental data. However, in the cases addressed in the previous section, an explicit (functional) solution was possible. Unfortunately, this is not usually the case. In general, assuming a specific reduced form of the stored energy, the equilibrium equations of the experimental tests result in a set of nonlinear functional equations which solution is not as trivial as in the previous cases. However, the spline representation of functions gives an extraordinary flexibility in solving nonlinear functional equations. Then, in these cases, we show here that function-refresh algorithms over spline-based functions are a powerful and simple method to obtain the solution for those systems of functional equations. The function-refresh iterations have some conceptual connection with fixed point iterations to solve nonlinear equations, but in our case we solve functions instead of real values. As mentioned above, to keep the matter concrete and useful, we explain the procedures using a reduced form for general orthotropic materials which is fully compatible with the infinitesimal theory at all deformation levels. In this section we explain the basic procedure and the connection in some simple cases to the inversion formula.

Figure 1: In-silico uniaxial test of a Holzapfel-Gasser-Ogden material and recovery of the derivatives of the strain energy function. a) Uniaxial stress-stretch data. b) Transverse stretch-longitudinal stretch data. c) Derivative of the isotropic component of the strain energy. d) Derivative of the anisotropic component of the strain energy. In c) and d) both the analytical and the recovered strain energy derivatives are shown (superimposed). In a) and b) the predictions from the spline-based energies are also compared to the original, “experimental” data.

4.1 Proposed reduced form for orthotropic materials compatible with the infinitesimal framework at all deformation levels

The proposed reduced form for the stored energy in orthotropic materials takes the form

$$\Psi(\mathbf{E}, \mathbf{a}_1, \mathbf{a}_2) = \mathcal{U}(E^v) + \mathcal{W}(\mathbf{E}^d, \mathbf{a}_1, \mathbf{a}_2) \quad (10)$$

$$\begin{aligned} &= \mathcal{U}(E^v) + \omega(E_1^d) + \omega(E_2^d) + \omega(E_3^d) \\ &+ \omega_{11}(E_{11}^d) + \omega_{22}(E_{22}^d) + \omega_{33}(E_{33}^d) \\ &+ 2\omega_{12}(E_{12}^d) + 2\omega_{13}(E_{13}^d) + 2\omega_{23}(E_{23}^d) \end{aligned} \quad (11)$$

where $\mathbf{E} = \frac{1}{2} \ln \mathbf{C}$ are the material logarithmic strains, $\mathbf{a}_i$ are the principal material (symmetry) directions, $E^v = \mathbf{E} : \mathbf{I} = \ln J$ is the volumetric strain, $\mathbf{E}^d = \mathbf{E} - \frac{1}{3} E^v \mathbf{I}$ are the deviatoric contributions, E_i^d are the principal isochoric *invariant* strains and $E_{ij}^d := \mathbf{a}_i \cdot \mathbf{E}^d \cdot \mathbf{a}_j = \mathbf{E}^d : \mathbf{L}_{ij}$ are the orthotropic strain *invariants* for the symmetry-based structural tensors $\mathbf{L}_{ij} = \mathbf{a}_i \otimes \mathbf{a}_j$. The functions $\omega(E_i^d)$ guarantee material symmetries congruency [36] and correspond, along with the penalty function $\mathcal{U}(E^v)$, to the isotropic contribution, whereas the functions $\omega_{ij}(E_{ij}^d)$ constitute the anisotropic

Figure 2: In-silico uniaxial test of a Modified Standard Reinforcing Material and recovery of the derivatives of the strain energy function. a) Uniaxial stress-stretch data. b) Transverse stretch-longitudinal stretch data. c) Derivative of the isotropic component of the strain energy. d) Derivative of the anisotropic component of the strain energy. In c) and d) both the analytical and the recovered strain energy derivatives are shown (superimposed). In a) and b) the predictions from the spline-based energies are also compared to the original, “experimental” data.

contribution. In the case of perfect incompressibility, $\mathcal{U}(E^v)$ is not considered (we use a lagrange pressure-like multiplier) and $E_{ij}^d \equiv E_{ij}$. For $i \neq j$, since shear strains have no physical sign, we must have $\omega_{ij}(E_{ij}^d) = \omega_{ij}(-E_{ij}^d)$. The determination of the functions is usually done by tests in the principal directions, in which $\hat{\omega}_{11}(E_{11}^d) := \omega(E_1^d) + \omega_{11}(E_{11}^d)$ is the function being determined. Hence, an additional test is needed to separate the isotropic part, or otherwise it must be assumed (as for example to be equal to the softest direction).

The stresses work-conjugate to the material logarithmic strains $\mathbf{E}$, in the most general case, are the generalized Kirchhoff stresses $\mathbf{T} := d\Psi/d\mathbf{E}$. In the incompressible case, $\mathbf{T} := d\Psi/d\mathbf{E} + p\mathbf{I}$, where p is the pressure-like Lagrange multiplier and $\mathbf{I}$ is the identity tensor. These stresses are identical to the rotated Kirchhoff stresses $\bar{\tau}$ in the isotropic case, or when strains are coaxial with the material principal directions. Hence, in usual in-axis tests, the components of the generalized Kirchhoff stresses are the same as the Kirchhoff stresses, and also the Cauchy stresses in the case of incompressibility. In general, the components are related to those of $\bar{\tau}$ by [37]

$$\begin{cases} T_{ij} = \bar{\tau}_{ij} & \text{if } i = j \\ T_{ij} = \frac{\lambda_j^2 - \lambda_i^2}{2\lambda_i\lambda_j(\ln \lambda_j - \ln \lambda_i)} \bar{\tau}_{ij} & \text{if } i \neq j \end{cases} \quad (12)$$

Figure 3: In-silico uniaxial test of a Holzapfel-Gasser-Ogden material with 100% proportional noise and an additional white noise; and recovery of the derivatives of the strain energy function. a) Uniaxial stress-stretch data and cubic regression smoothed spline. b) Transverse stretch-longitudinal stretch data and cubic regression smoothed spline. c) Recovery of the derivative of the isotropic component of the strain energy and comparison with the original noiseless one. d) Recovery of the derivative of the anisotropic component of the strain energy and comparison with the original noiseless one.

which results in a very convenient and useful interpretation in the usual uniaxial and biaxial test configurations, specially in incompressible materials. Furthermore, the infinitesimal form of Eq. (11) is

$$\begin{aligned} \Psi(\boldsymbol{\varepsilon}, \mathbf{a}_1, \mathbf{a}_2) = & \frac{1}{2}\kappa(\boldsymbol{\varepsilon}^v)^2 + \mu_{11}(\boldsymbol{\varepsilon}_{11}^d)^2 + \mu_{22}(\boldsymbol{\varepsilon}_{22}^d)^2 + \mu_{33}(\boldsymbol{\varepsilon}_{33}^d)^2 \\ & + 2\mu_{12}(\boldsymbol{\varepsilon}_{12}^d)^2 + 2\mu_{13}(\boldsymbol{\varepsilon}_{13}^d)^2 + 2\mu_{23}(\boldsymbol{\varepsilon}_{23}^d)^2 \end{aligned} \quad (13)$$

which contains the six constants μ_{ij} of the infinitesimal incompressible orthotropic theory plus the penalty one κ . Obviously these constants may be easily related to Young moduli and Poisson ratios. This infinitesimal form may be used to start the iterations below to accelerate the convergence.

4.2 Introduction to function refresh algorithms

Consider the functional equation resulting from a hyperelastic orthotropic material under uniaxial testing along the preferred direction “(1)”. As we have explained above, we assume that the measured experimental data has been synchronized, so we have the set $\{T_{11}^{(1)}, E_{11}^{(1)}, E_{22}^{(1)}\}$. Note that superindex indicates the preferred direction “(1)”. In this

Figure 4: In-silico uniaxial test of a modified Standard Reinforcing Material with 100% proportional noise and an additional white noise; and recovery of the derivatives of the strain energy function. a) Uniaxial stress-stretch data and cubic regression smoothed spline. b) Transverse stretch-longitudinal stretch data and cubic regression smoothed spline. c) Recovery of the derivative of the isotropic component of the strain energy and comparison with the original noiseless one. d) Recovery of the derivative of the anisotropic component of the strain energy and comparison with the original noiseless one.

axis, the equilibrium equation during the test is [23]

$$T_{11}^{(1)} = \omega'_{11}(E_{11}^{(1)}) - \omega'_{22}(E_{22}^{(1)}) \quad (14)$$

which can be written as

$$T_{11}^{(1)} = \omega'_{11}(E_{11}^{(1)}) - \omega'_{11}(f(E_{11}^{(1)})) \quad (15)$$

where $f(E_{11}^{(1)}) = \omega_{11}^{-1}(\omega'_{22}(E_{22}^{(1)}(E_{11}^{(1)})))$ is a function relation obtained below from compatibility considerations; by $E_{22}^{(1)}(E_{11}^{(1)})$ we note that both strains in the test are related by the given experimental data and by ω_{11}^{-1} we denote the inverse function. In Eq. (15) we need to determine the unknown function $\omega'_{11}(E_{11}) := d\omega_{11}/dE_{11}$ that represents a strain energy derivative function whose argument is the logarithmic strain invariant in preferred direction “(1)”, i.e. $E_{11} = \mathbf{E} : \mathbf{a}_1 \otimes \mathbf{a}_1$. The corresponding uniaxial stress is represented in the work-conjugate generalized Kirchhoff stress along preferred direction (1), i.e. $T_{11}^{(1)}$. The function $f(x)$ is such that makes Eq.(15) compatible, and may be determined from the equilibrium equation of a uniaxial test performed along preferred direction “(3)”, in which case the compatibility requirement in the perpendicular plane is

$$\omega'_{11}(E_{11}^{(3)}) = \omega'_{22}(E_{22}^{(3)}) \quad (16)$$

Assuming we also have a set of synchronized experimental data $\{E_{11}^{(3)}, E_{22}^{(3)}\}$, then we can build a spline function $g(x)$ (e.g. in pp-form in Matlab) as $\{E_{22}^{(3)}, E_{11}^{(3)}\} \rightsquigarrow g(x)$ and with this function we can build the required spline function $\{E_{11}^{(1)}, g(E_{22}^{(1)})\} \rightsquigarrow f(E_{11}^{(1)})$. With these considerations, the following function-refresh algorithm may be established when using spline-based functions

$$\omega_{11}^{[j+1]}(E_{11}^{(1)}) = T_{11}^{(1)} + \omega_{11}^{[j]}(f(E_{11}^{(1)})) \quad (17)$$

where superindex $(\bullet)^{[j+1]}$ is the iteration counter. In a parallelism with the conditions of the fixed-point method, convergence is obtained in monotonically increasing functions if $f(E_{11}^{(1)}) < E_{11}^{(1)}$; otherwise the algorithm must be reversely run, i.e.

$$\omega_{11}^{[j+1]}(f(E_{11}^{(1)})) = \omega_{11}^{[j]}(E_{11}^{(1)}) - T_{11}^{(1)} \quad (18)$$

4.3 Connection with the inversion formula and the infinitesimal framework

The inversion formula (a generalization of the Kearsley-Zapas formula) constitutes the analytical solution in terms of infinite series. It is immediate to show that functional refreshes recover analytical solution from available test data $\{E_{11}^{(1)}, T_{11}^{(1)}\} \rightsquigarrow T_{11}(E_{11})$.

Consider recursive evaluations of Eq. (17)

$$\begin{aligned} \omega_{11}^{[0]}(E_{11}^{(1)}) &= T_{11}(E_{11}^{(1)}) \\ \omega_{11}^{[1]}(E_{11}^{(1)}) &= T_{11}(E_{11}^{(1)}) + \omega_{11}^{[0]}(f(E_{11}^{(1)})) = T_{11}(E_{11}^{(1)}) + T_{11}(f(E_{11}^{(1)})) \\ \omega_{11}^{[2]}(E_{11}^{(1)}) &= T_{11}(E_{11}^{(1)}) + \omega_{11}^{[1]}(f(E_{11}^{(1)})) = T_{11}(E_{11}^{(1)}) + (T_{11}(f(E_{11}^{(1)})) + T_{11}(f^2(E_{11}^{(1)}))) \\ &\dots \\ \omega_{11}^{[N]}(E_{11}^{(1)}) &= \sum_{n=0}^N T_{11}(f^{(n)}(E_{11}^{(1)})) \end{aligned} \quad (19)$$

which is the inversion formula, where $f^{(n)}$ means n-recursive evaluations —i.e. $f(f(f(\dots)))$. Furthermore, in the infinitesimal case, the inversion formula results in the well-known expression relating the Young modulus Y_1 , the shear modulus μ_1 and the Poisson ratios ν_{ij} . In particular for this case, denoting by ε_{ij} the small strain equivalent to E_{ij} , it is

straightforward to show that the previous relations result in the well-known relations

$$\begin{aligned}
 \varepsilon_{11}^{(3)} &= g(\varepsilon_{22}^{(3)}) = \left(\frac{\nu_{31}}{1 - \nu_{31}} \right) \varepsilon_{22}^{(3)} \\
 f(\varepsilon_{11}^{(1)}) &= g(\varepsilon_{22}^{(1)}(\varepsilon_{11}^{(1)})) = \frac{\nu_{31}\nu_{12}}{\nu_{31} - 1} \varepsilon_{11}^{(1)} \\
 \omega'_{11}(\varepsilon_{11}^{(1)}) &= 2\mu_1 \varepsilon_{11}^{(1)} = \sum_{n=0}^{\infty} Y_1 \left[\frac{\nu_{31}\nu_{12}}{\nu_{31} - 1} \right]^n \varepsilon_{11}^{(1)} = Y_1 \varepsilon_{11}^{(1)} \left(1 - \frac{\nu_{31}\nu_{12}}{\nu_{31} - 1} \right)^{-1} \\
 2\mu_1 &= Y_1 \left(1 - \frac{\nu_{31}\nu_{12}}{\nu_{31} - 1} \right)^{-1}
 \end{aligned} \tag{20}$$

5 Function-refresh algorithms for tests in preferred material directions

Unfortunately, whereas function-refresh algorithms present a quite general methodology to obtain the derivatives of the stored energy terms, a general computational layout valid for any possible test seems not obvious. The reason is that the method solves the equilibrium nonlinear functional equations of the tests, and different tests result in different equilibrium equations. The purpose of this section and the following section is to show how to derive function-refresh algorithms to solve the system of nonlinear functional equations in two cases: when tests are performed in principal material directions and when a complete set of strip-biaxial (pure shear) tests is performed in different arbitrary (misaligned) directions.

For the first case addressed in this section, there are two possibilities: (1) Incompressible materials and (2) quasi-incompressible materials.

5.1 Incompressible materials

Denoting the structure tensors by $L_{ij} = \mathbf{a}_i \otimes \mathbf{a}_j$, the following functional equations are obtained by the projections $T : (L_{11} - L_{22})$, $T : (L_{22} - L_{33})$ and $T : L_{ij}, i \neq j$

$$T : (L_{11} - L_{22}) \rightarrow T_{11} - T_{22} = \omega'_{11}(E_{11}) - \omega'_{22}(E_{22}) \tag{21}$$

$$T : (L_{22} - L_{33}) \rightarrow T_{22} - T_{33} = \omega'_{22}(E_{22}) - \omega'_{33}(E_{33}) \tag{22}$$

$$T : L_{ij} \rightarrow T : L_{ij} = T_{ij} = \omega'_{ij}(E_{ij}) \quad i \neq j \tag{23}$$

Hence, the system provides two functional equations (i.e. Eqs.(21) and (22)) that relates three axial functional unknowns ($\omega'_{11}(E_{11}), \omega'_{22}(E_{22}), \omega'_{33}(E_{33})$), and three functional equations from Eq. (23) that directly relates stress projection with corresponding shear functional unknowns ($\omega'_{ij}(E_{ij}), i \neq j$). Then, there are three axial unknown functions, but the system only provides two functional equations, namely Eqs.(21) and (22), so we cannot solve the system with a single experiment; we need two different experiments. Consider a first experiment performed along material preferred direction (1), and a second one performed along preferred direction (3). Then, the experimental data for both tests gives the spline functions $T_{11}^{(1)}(E_{11}^{(1)}), E_{22}^{(1)}(E_{11}^{(1)}), E_{11}^{(3)}(E_{33}^{(3)})$, which will be used to determine the in-axis functions through the corresponding equilibrium equations

$$T_{11}^{(1)}(E_{11}^{(1)}) - 0 = \omega'_{11}(E_{11}^{(1)}) - \omega'_{22}(E_{22}^{(1)}) \tag{24}$$

$$0 - 0 = \omega'_{22}(E_{22}^{(1)}) - \omega'_{33}(E_{33}^{(1)}) \tag{25}$$

$$0 - 0 = \omega'_{11}(E_{11}^{(3)}) - \omega'_{22}(E_{22}^{(3)}) \tag{26}$$

These equations may be solved through the following function-refresh algorithm.

Recycle until convergence: (27)

$$\text{For each } E_{11}^{(1)} : \omega_{11}^{\prime[j+1]} = T_{11}^{(1)}(E_{11}^{(1)}) + \omega_{22}^{\prime[j]}(E_{22}^{(1)}(E_{11}^{(1)})) \quad (28)$$

$$\text{Refresh of } \omega_{11}^{\prime[j+1]}(E_{11}) : \{E_{11}^{(1)}, \omega_{11}^{\prime[j+1]}\} \rightsquigarrow \omega_{11}^{\prime[j+1]}(E_{11}) \quad (29)$$

$$\text{For each } E_{22}^{(3)} : \omega_{22}^{\prime[j+1]} = \omega_{11}^{\prime[j+1]}(E_{11}^{(3)}(E_{22}^{(3)})) \quad (30)$$

$$\text{Refresh of } \omega_{22}^{\prime[j+1]}(E_{22}) : \{E_{22}^{(3)}, \omega_{22}^{\prime[j+1]}\} \rightsquigarrow \omega_{22}^{\prime[j+1]}(E_{22}) \quad (31)$$

Convergence is assessed monitoring the change of the functions during iterations. For example, Matlab commands to perform such iterations assuming known the experimental data $\{E_{11}^{(1)}, T_{11}^{(1)}\}$, $\{E_{11}^{(1)}, E_{22}^{(1)}\}$, $\{E_{22}^{(3)}, E_{11}^{(3)}\}$ are —note that to be instructive in having a spline-based thinking we keep a spline format in all equations, but it is computationally more efficient to work directly with discrete data when no function interpolations are needed:

```
1 ppT11 = spline(E11,T11); % Spline of stress-strain experimental data
2 ppE22 = spline(E11,E22); % Spline of exp. uniaxial vs. transv. strain
3 ppE11 = spline(E22_3,E11_3); % Spline of strain relations of test 2
4 %% Repeat function-refreshes until convergence is obtained:
5 ppdw11 = spline( E11 , ppval(ppT11,E11)+ppval(ppdw22,ppval(ppE22,E11)) );
6 ppdw22 = spline( E22_3, ppval(ppdw11,ppval(ppE11,E22_3)) );
```

If experimental data are synchronized (as recommended) then spline functions are only present on the unknown functions, and last two lines of code becomes even simpler,

```
1 ppdw11 = spline( E11 , T11 + ppval(ppdw22,E22) );
2 ppdw22 = spline( E22_3, ppval(ppdw11,E11_3) );
```

Once convergence is obtained, the function $\omega'_{33}(E_{33})$ can be obtained explicitly using the remaining Equation (25) and the incompressibility condition $E_{33} = -E_{11} - E_{22}$ as

$$\text{For each } E_{33}^{(1)} : \omega'_{33} = \omega'_{22}(E_{22}^{(1)}(E_{33})) \quad (32)$$

$$\text{Spline build : } \{E_{33}^{(1)}, \omega'_{33}\} \rightsquigarrow \omega'_{33}(E_{33}) \quad (33)$$

The Matlab commands are:

```
1 E33 = -E11-E22; % Incompressibility in test (1)
2 ppdw33 = spline(E33,ppval(ppdw22,E22)); % E11,E22,E33 are synchronized
```

The remaining functions are the shear functions $\omega'_{ij}, i \neq j$. In this case, the functional refresh method is not necessary for the determination of the unknown shear functions.

For the determination of the shear functions consider a pure shear experiment in plane $x - y$ at 45° with respect to preferred directions. The set of experimental data is $\{E_{xx}, T_{xx}\}$ where xx is the direction of loading. Since $E_{zz} = 0$ and it is an incompressible material, then $E_{yy} = -E_{xx}$. Attending to preferred direction (3), if we set as usual $\omega'_{33}(0) = 0$, the pressure-like lagrange multiplier is zero, and we have

$$T_{12} = T_{xx} = \omega'_{12}(E_{12}) = \omega'_{12}(E_{xx}) \quad (34)$$

Therefore the shear functions can be explicitly determined from pure shear (strip biaxial) tests. If spline form is required, then $\{E_{xx}, T_{xx}\} \rightsquigarrow \omega'_{12}(E_{12})$.

Obviously, the function-refresh algorithm is different depending on the available experimental data. In Appendix B we show different function-refresh algorithms for different sets of available experimental data.

5.2 Numerical example for the incompressible case.

In this example we show that the function-refresh algorithm is capable of reproducing the stored energy function of orthotropic incompressible materials using the function decomposition explained above. We remark here that the strain energies recovered by the procedure will in any case predict the experimental data to any desired accuracy. However, since from actual experimental data it is impossible to verify that the recovered energies correspond to the real ones (we cannot measure the energy terms, and the proposed reduced form may not be accurate), we perform this verification using an analytical model to generate virtual (in-silico) experimental data. Then, the procedure is: (1) assume an

analytical form for the stored energy of the material, (2) perform the needed virtual (in-silico) test on the material, (3) with that experimental data, *assuming that we do not know the stored energy*, recover the energy derivative functions in spline format directly from experimental data. Thereafter, (4) we can plot the spline-based energy derivatives and compare with a plot of the derivative of the analytical functions. If both stored energies are coincident, we can claim that the material behavior under any loading condition will exactly match numerically.

Since the experiments are aligned with preferred directions, the ground matrix isotropic contribution $\omega(x)$ adds to the corresponding anisotropic contributions $\omega_{ii}(x)$, and therefore only the sum of both superimposed energies $\hat{\omega}_{ii}(x)$ is recovered. That is,

$$\hat{\omega}_{11}(E_{11}) = \omega(E_{11}) + \omega_{11}(E_{11}) \quad (35)$$

$$\hat{\omega}_{22}(E_{22}) = \omega(E_{22}) + \omega_{22}(E_{22}) \quad (36)$$

$$\hat{\omega}_{33}(E_{33}) = \omega(E_{33}) \quad (37)$$

The separation of both contributions may be performed assuming, for example, that in compression only the isotropic component is active, and its contribution in tension and compression is equal. The analytical expressions chosen for this example are,

$$\omega(E) = \frac{c}{2} (\exp(2E) - 1) \quad (38)$$

$$\omega_{11}(E_{11}) = 4\{k_1[\exp(2E_{11}) - 1] \exp[k_2(\exp(2E_{11}) - 1)^2]\} \cos^2 \beta \quad (39)$$

$$\omega_{22}(E_{22}) = 4\{k_1[\exp(2E_{22}) - 1] \exp[k_2(\exp(2E_{22}) - 1)^2]\} \sin^2 \beta \quad (40)$$

with the material parameters $c = 3\text{kPa}$, $k_1 = 2.36\text{kPa}$, $k_2 = 0.84\text{kPa}$, $\beta = 29^\circ$. These reference energies are shown in

Theoretical reference strain energy derivatives

Figure 5: Orthotropic analytical stored energy derivatives ω'_{ii} (visually identical to the recovered spline-based ones $\hat{\omega}'_{ii}$). a) $\omega'_{11}(E_{11})$; b) $\omega'_{22}(E_{22})$; c) $\omega'_{33}(E_{33})$

Fig.5 . The corresponding generated pseudo-experimental data are shown in Fig.6. As aforementioned we apply the function-refresh algorithm over these experimental data in order to recover the strain energy derivatives. Convergence evolutions of the unknown functions $\hat{\omega}'_{11}$, $\hat{\omega}'_{22}$ during function refresh and the final result for $\hat{\omega}'_{33}$ are shown in Fig.7. Finally, absolute error evolution during functional refresh between referential derivative energies $\hat{\omega}'_{11}(x)$, $\hat{\omega}'_{22}(x)$ and the recovered ones are shown in Figure 8. As observed, these errors are near machine precision. Finally, we note that all these computations take less than one second using MATLAB in a laptop PC.

5.3 Quasi-incompressible case

The quasi-incompressible formulation is very important in finite element implementations. An adequate volumetric stored energy guarantees a proper penalization independent of the deformation level, avoiding a too weak penalization and a bad conditioning of the stiffness matrix. However, in this case an extra function needs to be determined. This implies that we need extra experimental data since the incompressibility condition is no longer applicable. As an example, the extra experimental data may be $\{E_{11}^{(1)}, E_{33}^{(1)}\}$. Remarkably, note that for example, we can impose directly a penalized volume change by $E_{33}^{(1)} = (10^{-3} - 1)E_{11}^{(1)} - E_{22}^{(1)}$ in order to obtain a proper penalization at all deformation

Figure 6: Input “experimental” curves. Uniaxial tension-compression test on preferred orthotropic direction 1: a) generalized Kirchhoff stress, $T_{11}^{(1)}$ [kPa] versus longitudinal logarithmic strain, $E_{11}^{(1)}$ and b) transverse logarithmic strain $E_{22}^{(1)}$ versus longitudinal logarithmic strain, $E_{11}^{(1)}$. Uniaxial tension-compression test on preferred orthotropic direction 3: c) transverse logarithmic strain $E_{33}^{(3)}$ versus longitudinal logarithmic strain, $E_{33}^{(3)}$.

Figure 7: Function refresh iterations to obtain the strain energy derivative functions: a) $\omega'_{11}(E_{11})$, b) $\omega'_{22}(E_{22})$. c) Function $\omega'_{33}(E_{33})$ is obtained explicitly once the other axial functions $\omega'_{11}(E_{11})$, $\omega'_{22}(E_{22})$ have been determined via functional refresh method.

levels. Then, consider the experimental data $\{T_{11a}^{(1)}, E_{11a}^{(1)}\}$, $\{E_{22b}^{(1)}, E_{11b}^{(1)}\}$, $\{E_{33c}^{(1)}, E_{11c}^{(1)}\}$, $\{E_{11d}^{(3)}, E_{33d}^{(3)}\}$ which after resampling data at $E_{11}^{(1)}$, results in the synchronized set

$$\{E_{11}^{(1)}, E_{22}^{(1)}, E_{33}^{(1)}, E_{11}^{d(1)}, E_{22}^{d(1)}, E_{33}^{d(1)}, E^{v(1)}, T_{11}^{(1)}\} \quad (41)$$

For the second test assume that only $\{E_{11}^{(3)}, E_{33}^{(3)}\}$ is given, so the computation of the deviatoric strains is not immediate. Then, the following computational algorithm involves more functional equations:

1. Determine $\mathcal{U}'(E^v)$ from $\mathcal{U}'(E^v) = T_{11}^{(1)}/3$
2. Set initial guess, e.g. $\omega_{11}^{[0]}(x) = 0$, $\omega_{22}^{[0]}(x) = 0$, $\omega_{33}^{[0]}(x) = 0$
3. Refresh $\omega_{11}^{[j+1]}(E_{11}^{d(1)}) = T_{11}^{(1)} + \omega_{22}^{[j]}(E_{22}^{d(2)})$ (recall that data has been synchronized)

Figure 8: Absolute error for recovered axial strain energy derivative functions $\hat{\omega}'_{11}(E_{11})$, $\hat{\omega}'_{22}(E_{22})$ measured respect to referential ones for several iterations during the function-refresh method. At the origin both energies are zero.

4. For each pair in $\{E_{11}^{(3)}, E_{33}^{(3)}\}$, find the corresponding $E^{v(3)}$ that satisfies the equilibrium equation (this can be solved using the inverse function as shown in Section 2.1)

$$0 = -\frac{1}{3}\omega_{11}^{[j+1]}(E_{11}^{(3)} - \frac{1}{3}E^{v(3)}) + \frac{2}{3}\omega_{22}^{[j]}(-E_{11}^{(3)} - E_{33}^{(3)} + \frac{2}{3}E^{v(3)}) - \frac{1}{3}\omega_{33}^{[j]}(E_{33}^{(3)} - \frac{1}{3}E^{v(3)}) + \mathcal{U}'(E^{v(3)})$$

5. Update deviatoric values $E_{11}^{d(3)} = E_{11}^{(3)} - \frac{1}{3}E^{v(3)}$ and $E_{22}^{d(3)} = -E_{11}^{(3)} - E_{33}^{(3)} + \frac{2}{3}E^{v(3)}$

6. Refresh $\omega_{22}^{[j+1]}(E_{22}^{d(3)}) = \omega_{33}^{[j]}(E_{33}^{d(3)})$ and $\omega_{33}^{[j+1]}(E_{33}^{d(1)}) = \omega_{22}^{[j+1]}(E_{22}^{d(1)})$

7. Repeat steps 3–6 until convergence.

The shear ω_{ij} , $i \neq j$ functions can be determined again, for example, from a pure shear test with the 1, 2 preferred material directions oriented at 45° . Consider the x -axis as the tensile axis and the y -axis as the free (plane stress) one. Then in preferred directions

$$[\mathbf{E}]_{x_{pr}} = \begin{bmatrix} E^v/2 & (E_{xx} - E_{yy})/2 \\ (E_{xx} - E_{yy})/2 & E^v/2 \\ 0 & 0 \end{bmatrix}_{x_{pr}} \quad (42)$$

If the experimental data is $\{E_{xx}, T_{xx}\}$, we need to compute E_{yy} . Upon knowledge of $\mathcal{U}'$ and ω'_{22} computed above, we can do so from the equation in the second axis

$$T_{22} = 0 = \mathcal{U}'(E^v) + \omega'_{22}(E^v/6) \quad (43)$$

i.e. E_{yy} is such that $\mathcal{U}'(E_{xx} + E_{yy}) = -\omega'_{22}((E_{xx} + E_{yy})/6)$, a solution which can be obtained by a Newton-Raphson algorithm or by the inversion of the resulting residual spline. Upon knowledge of $E_{yy}(E_{xx})$, we also know $E^v(E_{xx})$ and all $E_{ii}^d(E_{xx})$, and the normal stresses are immediately obtained as

$$T_{11}(E_{xx}) = \mathcal{U}'(E^v(E_{xx})) + \frac{2}{3}\omega'_{11}(E_{11}^d(E_{xx})) - \frac{1}{3}\omega'_{22}(E_{22}^d(E_{xx})) - \frac{1}{3}\omega'_{33}(E_{33}^d(E_{xx})) \quad (44)$$

and similarly for $T_{22}(E_{xx})$, $T_{33}(E_{xx})$, $T_{12}(E_{xx})$. Then in preferred material directions

$$[T]_{X_{pr}} = \begin{bmatrix} T_{11} & T_{12} & \\ T_{12} & T_{22} & \\ & & T_{33} \end{bmatrix}_{X_{pr}} \quad (45)$$

and in principal strain directions

$$[T]_{45^0} = \begin{bmatrix} \frac{1}{2}T_{11} + T_{12} + \frac{1}{2}T_{22} & \frac{1}{2}T_{22} - \frac{1}{2}T_{11} & 0 \\ \frac{1}{2}T_{22} - \frac{1}{2}T_{11} & \frac{1}{2}T_{11} - T_{12} + \frac{1}{2}T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}_{45^0} \quad (46)$$

Thus, with the previously computed functions $E_{yy}(E_{xx})$, $T_{11}(E_{xx})$ and $T_{22}(E_{xx})$, we can determine immediately ω'_{12} in an explicit manner

$$\omega'_{12} \left(\frac{E_{xx} - E_{yy}(E_{xx})}{2} \right) = T_{xx}(E_{xx}) - \frac{T_{11}(E_{xx}) + T_{22}(E_{xx})}{2} \quad (47)$$

In fact, once the axial functions are obtained, the computation of the shear ones is usually explicit.

5.4 Numerical example for the quasi-incompressible case.

In Fig. 9 we show pseudo-experimental data generated from in-silico tests using the anisotropic stored energy functions of Fig. 4 in Ref. [23] which correspond to an anisotropic calendered rubber given in [38]. In the present case, the “experimental” curves shown in Fig. 9 have been generated including predefined isotropic isochoric and volumetric energies as

$$\omega'(E^d) = \sum_{i=1}^3 \mu_i [\exp(\alpha_i - 1) - 1] \quad (48)$$

where $\mu_1 = 6.2\text{MPa}$, $\mu_2 = 0.0118\text{MPa}$, $\mu_3 = -0.0981\text{MPa}$, $\alpha_1 = 1.3$, $\alpha_2 = 5$, $\alpha_3 = -2$ and

$$\mathcal{U}'(E^v) = \frac{K}{\beta_1} [\exp(\beta_2 E^v) - \exp(\beta_3 E^v)] \quad (49)$$

where $K = 400\text{MPa}$, $\beta_1 = 10$, $\beta_2 = 4$, $\beta_3 = -6$. With the “experimental” data in spline form $T_{11}^{(1)}(E_{11}^{(1)})$, $E_{22}^{(1)}(E_{11}^{(1)})$, $E_{33}^{(3)}(E_{11}^{(1)})$ in Fig. 9, we compute the strain energies which include now the isotropic contribution given by,

$$\hat{\omega}'_{ii}(E_{ii}^d) = \omega'(E^d) + \omega'_{ii}(E^d) \quad (50)$$

The evolution of function iterations for $\hat{\omega}'_{ii}(E_{ii}^d)$ during function-refresh procedure is shown in Fig. 10 for several iterations, together with the corresponding theoretical strain energy derivative functions. It is seen that the final result includes naturally the isotropic contribution, and no difference is visually appreciable.

6 Function-refresh algorithms for tests performed in arbitrary axes

In the previous section we have assumed that the tests are performed in the principal symmetry axes. However, one of the advantages of function-refresh algorithms is that they can be used in more general situations, for example in off-axis tests. In this case we distinguish four different sets of directions in the reference configuration: material symmetry planes/directions $\mathbf{a}_i$, fiber directions $\mathbf{f}_i$, principal *strain* directions $\mathbf{N}_i$ and principal *stress* directions $\mathbf{t}_i$. The former two families are material directions (invariant) and the latter two families are deformation-dependent directions. The test directions $\mathbf{n}_i$ are not necessary aligned with any of the previous directions.

For this example, consider two pure shear experiments missaligned with preferred directions $\mathbf{a}_i$ of material symmetries, as shown schematically in Fig.11.

Figure 9: Experimental data for Example of Section 5.4. Uniaxial tension-compression test on preferred orthotropic direction 1: a) generalized Kirchhoff stress, $T_{11}^{(1)}$ [MPa] versus longitudinal logarithmic strain, $E_{11}^{(1)}$ and b) transverse-to-load logarithmic strain $E_{22}^{(1)}$ versus longitudinal logarithmic strain, $E_{11}^{(1)}$. Uniaxial tension-compression test on preferred orthotropic direction 3: c) transverse logarithmic strain $E_{11}^{(3)}$ versus longitudinal logarithmic strain, $E_{33}^{(3)}$.

Figure 10: Function-refresh iterations to obtain the strain energy derivative functions $\hat{\omega}'_{11}(E_{11}^d)$, $\hat{\omega}'_{22}(E_{22}^d)$, $\hat{\omega}'_{33}(E_{33}^d)$ for the example of Section 5.4.

Figure 11: Stresses and strains in a pure shear off-axis test

With data $\{E_{xx}, T_{xx}\}$, we could determine the orthotropic energies with Eq.(51) using data from six different misaligned tests.

$$T_{xx} - 0 = \left(\sum_{i,j,i \neq j}^3 \omega'_{ij}(E_{ij}) \mathbf{L}_{ij} + \sum_m^3 \omega'(E_m) \mathbf{M}_m \right) : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) \quad (51)$$

where $\mathbf{M}_m = \mathbf{N}_m \otimes \mathbf{N}_m$ represents the material principal strain tensorial direction. However, experimental data $\{E_{xx}, T_{xx}\}$ in the form of Generalized Kirchhoff stresses cannot be directly obtained. Instead, Cauchy stresses σ_{xx} and the corresponding stretches are the experimental data. This is because conversion from Cauchy stress σ_{xx} to the generalized Kirchhoff stress T_{xx} requires the rotated Kirchhoff stresses $\bar{\tau} = \mathbf{R}\tau\mathbf{R}^T = \mathbf{J}\mathbf{R}\sigma\mathbf{R}^T$ as an intermediate step. For the tests employed $\mathbf{R} = \mathbf{I}$ and thus $\sigma = \bar{\tau}$. Then, taking into account the mapping from the rotated Kirchhoff to the Generalized Kirchhoff tensor given in Eq. (12), we can easily write the data in generalized Kirchhoff stress and the corresponding logarithmic strains (i.e. $\{E_{xx}, T_{xx}\}$) for the six tests available.

Thus, we can use these tests to determine the orthotropic energy components of the material by means of the equation Eq. (51). This projection allows us to determine the unknown energy derivative functions without knowing the value of the incompressible pressure p because the projection is purely deviatoric,

$$\begin{aligned} \mathbf{T} : \mathbb{P} : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) &= \left[\mathbf{T} - \frac{1}{3} \text{tr}(\mathbf{T}) \mathbf{I} \right] : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) \\ &= \mathbf{T} : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) - 1/3 \text{tr}(\mathbf{T})(1 - 1) \\ &= \mathbf{T} : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) \end{aligned} \quad (52)$$

Then, taking into account that $\mathbf{L}_{xx}$ and $\mathbf{L}_{zz}$ coincide with the principal strain directions $\mathbf{M}_{xx}$ and $\mathbf{M}_{zz}$ respectively in the reference configuration, and also that $E_{xx} = -E_{zz}$, Eq. (51) results in,

$$T_{xx} = \left(\sum_{ij}^3 \omega'_{ij}(E_{ij}) \mathbf{L}_{ij} \right) : (\mathbf{L}_{xx} - \mathbf{L}_{zz}) + \omega'(E_{xx}) - \omega'(-E_{xx}) \quad (53)$$

Hence, from Eq. (53) we can establish the following function-refresh algorithm,

$$\omega_{11}^{[j+1]} = \frac{1}{\mathbf{L}_{11} : \Delta \mathbf{L}^{(1)}} \left[T_{xx}^{(1)} - \left(\sum_{i,j,i \neq 11}^3 \omega_{ij}^{[j]}(E_{ij}^{(1)}) \mathbf{L}_{ij} \right) : \Delta \mathbf{L}^{(1)} + \Delta \omega'(E_{xx}^{(1)}) \right] \quad (54)$$

$$\omega_{22}^{[j+1]} = \frac{1}{\mathbf{L}_{22} : \Delta \mathbf{L}^{(2)}} \left[T_{xx}^{(2)} - \left(\sum_{i,j,i \neq 22}^3 \omega_{ij}^{[j]}(E_{ij}^{(2)}) \mathbf{L}_{ij} \right) : \Delta \mathbf{L}^{(2)} + \Delta \omega'(E_{xx}^{(2)}) \right] \quad (55)$$

...

$$\omega_{23}^{[j+1]} = \frac{1}{\mathbf{L}_{23} : \Delta \mathbf{L}^{(6)}} \left[T_{xx}^{(6)} - \left(\sum_{i,j,i \neq 23}^3 \omega_{ij}^{[j]}(E_{ij}^{(6)}) \mathbf{L}_{ij} \right) : \Delta \mathbf{L}^{(6)} + \Delta \omega'(E_{xx}^{(6)}) \right] \quad (56)$$

where,

$$\begin{aligned} \Delta \mathbf{L}^{(e)} &= \mathbf{L}_{xx}^{(e)} - \mathbf{L}_{zz}^{(e)} \\ \Delta \omega'(E_{xx}^{(e)}) &= \omega'(E_{xx}^{(e)}) - \omega'(-E_{xx}^{(e)}) \end{aligned}$$

Finally, updated values $\omega_{ij}^{[j+1]}$ must be used to refresh the spline based functions. As shown above, the generated values $\omega_{ij}^{[j+1]}$ come from spline evaluation at synchronized data for set (e) : $\{E_{11}^{(e)}, E_{22}^{(e)}, \dots, E_{23}^{(e)}, T_{xx}^{(e)}\}$. This allows the spline constructions,

$$\{E_{11}^{(1)}, \omega_{11}^{[j+1]}\} \rightsquigarrow \omega_{11}^{[j+1]}(E_{11}) \quad (57)$$

...

$$\{E_{23}^{(6)}, \omega_{23}^{[j+1]}\} \rightsquigarrow \omega_{23}^{[j+1]}(E_{23}) \quad (58)$$

We can use this algorithm to determine orthotropic strain energy derivative functions from generic experimental results such as the ones off-axis pure shear tests proposed here, or uniaxial results in which only stress in load direction σ_u and the corresponding stretch λ_u are known. For the example, referential orthotropic energies are obtained from a modification of those in Ref. [38] with the hypothesis of $\nu_{12} = 0.7$. We assume that the isotropic strain energy function

of the ground matrix contribution is known for the calculations. In particular, it is assumed to be of the Ogden type,

$$\omega'(E) = \sum_{i=1}^3 \mu_i [\exp((\alpha_i - 1)E) - 1] \quad (59)$$

with, $\mu_1 = 620\text{kPa}$, $\mu_2 = 1.18\text{kPa}$, $\mu_3 = -9.81\text{kPa}$, $\alpha_1 = 1.3$, $\alpha_2 = 5$, $\alpha_3 = -2$. For this numerical example, data $\{\lambda_{xx}, \sigma_{xx}\}$ for the six tests are shown in Fig.12. Comparison of referential theoretical strain energy derivative functions against the corresponding recovered ones from the experimental data are shown in Fig.13. The number of points shown in this figure is small for better readability, however in Fig.14, which shows the convergence evolution along with the functional refresh iterations, it is appreciable for much more number of points that converged and reference strain energy derivative functions overlap. It is also observed specially in c) and d) of Fig.14 that first iteration is close to the solution and seems to get away, but finally converges. Rotation matrix from local to preferred axis for the six experiments are attached in Appendix C.

Figure 12: Pseudo-experimental data for six different off-axis uniaxial in-silico tests under controlled logarithmic strains $E_{xy} = E_{xz} = E_{yz} = 0$, $E_{xx} = -E_{zz}$. Uniaxial Cauchy stress σ_{xx} versus the corresponding stretch λ_x . From a) to f), corresponding tests from "(1)" to "(6)".

Figure 13: Comparison of theoretical original orthotropic strain energy derivative functions (solid red line) with the recovered spline-based functions obtained directly from experimental data (blue circles). Orthotropic strain energy derivative functions from a) to f): a) along preferred direction 11, $\omega'_{11}(E_{11})$; b) along preferred direction 22, $\omega'_{22}(E_{22})$; c) along preferred direction 33, $\omega'_{33}(E_{33})$; d) along preferred direction 12, $\omega'_{12}(E_{12})$; e) along preferred direction 13, $\omega'_{13}(E_{13})$; f) along preferred direction 23, $\omega'_{23}(E_{23})$.

Figure 14: Convergence of the orthotropic strain energy derivative functions during the functional refresh iteration process. Orthotropic strain energy derivative functions from a) to f): a) $\omega'_{11}(E_{11})$. b) $\omega'_{22}(E_{22})$. c) $\omega'_{33}(E_{33})$. d) $\omega'_{12}(E_{12})$. e) $\omega'_{13}(E_{13})$. f) $\omega'_{23}(E_{23})$.

7 Conclusions

Numerical spline-based hyperelasticity constitutes a relevant step towards physically-based data-driven constitutive modelling, because the stored energies have no predefined shape and no material parameters, are valid for a wide range of materials and may include the material structure (e.g. fiber directions or even distributions) or be formulated phenomenologically. Reduced forms of the strain energy density in terms of some invariants are typically employed in the literature when a limited amount of data is available. The reduced forms in spline-based procedures may be hierarchically enhanced to accommodate more and more available experimental data. In anisotropy, these reduced forms result in nonlinear functional equations. We have shown that spline functions are an excellent tool to solve these functional equations. However, an explicit solution is obtained only in some specific cases: when functional equations are uncoupled or when an inversion formula may be applied.

In this paper we show how function-refresh algorithms present an excellent procedure to obtain the solution of the stored energy terms in spline format, both for structure-based anisotropic models containing terms for fibers, and for phenomenological models which terms are based on material symmetry considerations. Once the stored energies are written in terms of splines, since splines are local polynomials, the derivatives are immediate and the finite element implementation is efficient and standard.

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Appendix A

The following functions have been verified in Matlab version R2011a

A.1 Matlab functions to perform an “in-silico” test of a Holzapfel-Gasser-Ogden material.

```

1 function [stress_u,lambda_t,I1,I4,dWdI1,dWdI4] = ...
2     HGOtest(lambda_u,beta,c,k1,k2)
3 % HGO test performs an in-silico uniaxial test to the
4 % Holzapfel-Gasser-Ogden (HGO) material
5 %
6 % lambda_u = prescribed stretches
7 % beta     = angle of fiber families with test direction
8 % c, k1, k2= typical HGO material parameters
9 %
10 % stress_u = uniaxial stress measurements
11 % lambda_t = transverse stretch measurements
12 % I1, I4   = isotropic and fiber invariant computations
13 % dWdI1    = derivative of isotropic energy component
14 % dWdI4    = derivative of anisotropic energy component
15 %
16 c2 = (cos(beta))^2; s2 = (sin(beta))^2;
17 for p = 1:length(lambda_u),
18     lu = lambda_u(p);
19     fun = @(lt) HGOtr(lt,lu,beta,c,k1,k2); % transv. stress
20     lt = fzero(fun,1); % solve transv. stretch
21     lu2 = lu^2; lt2 = lt^2; l32 = 1/(lu2*lt2);
22     lambda_t(p) = lt;
23     Iu = lu2*c2 + lt2*s2; % fiber invariant
24     I4(p) = Iu; % Anisotropic invariant
25     I1(p) = lu2 + lt2 + l32; % Isotropic invariant
26     dWdI1(p) = c/2; dWdI4(p) = 0;
27     if (Iu > 1), dWdI4(p) = k1*exp(k2*(Iu-1)^2)*(Iu-1); end,
28     stress_u(p) = 2*dWdI1(p)*(lu2-lt2) +...
29         4*dWdI4(p)*(lu2*c2-lt2*s2);
30 end,
31 return
32 %-----
33 function [stress_t] = HGOtr(lambda_t,lambda_u,beta,c,k1,k2)
34 %
35 % function HGOtr computes the transverse stretch in a uniaxial test of
36 % the HGO model. See HGOtest function for explanation of variables
37 %
38 lu2= lambda_u.^2; lt2 = lambda_t.^2;
39 l32= 1/(lu2*lt2); c2 = (cos(beta))^2; s2 = (sin(beta))^2;
40 I1 = lt2 + lu2 + l32; % First invariant
41 Iu = lu2 * c2 + lt2 * s2; % Fiber invariants I4 and I6
42 if (Iu < 1), Iu = 1; end, % No contribution of fibers in compression
43 % Transverse stress
44 stress_t = c*(lt2-l32) + 4*k1*exp(k2*(Iu-1)^2)*(Iu-1)*lt2*s2;
45 return

```

A.2 Matlab function to recover the strain energy derivatives from uniaxial experimental data assuming a reduced form of the type $\Psi(C) = \psi_{iso}(I_1) + \psi(I_4) + \psi(I_6)$

Independent of the specific model functions, the following code recovers the function derivatives in spline format

```

1 function [ppdWdI1,ppdWdI4] = ...
2     HGO_recover(beta,lambda_u,ppstress_u,pplambda_t)
3 %
4 % HGO_recover recovers the stored energy function derivatives from tensile
5 % test data stress_u and lambda_t in orthotropy axis for models of the type
6 % W(I1,I4,I6) = w(I1) + w(I4) + w(I6)
7 % Examples are the HGO model & the standard reinforcing models

```

```

8 % This type of models have explicit solution for this test
9 %
10 % beta      = angle of fiber families with the symmetry axes
11 % lambda_u  = uniaxial stretches used in the recovery
12 % ppstress_u = uniaxial stress data in spline pp-form
13 % pplambda_t = transverse stretch data in spline pp-form
14 %
15 % ppdWdI1 = spline pp-form strain energy der. respect to I1 invariant
16 % ppdWdI4 = spline pp-form strain energy der. respect to I4 invariant
17 %
18 c = (cos(beta))^2; s = (sin(beta))^2;
19 for i=1:length(lambda_u),
20     lu      = lambda_u(i); % for these values, next line retrieves test data
21     su      = ppval(ppstress_u,lu); lt = ppval(pplambda_t,lu);
22     l3      = 1/(lu*lt); % thickness stretch
23     l32     = l3^2; lu2 = lu^2; lt2 = lt^2; % squared stretches
24     I1(i)   = lu2 + lt2 + l32; % first invariant
25     I4(i)   = lu2*c + lt2*s; % fiber invariants
26     denominator = -2*l32*lt2*s+2*l32*lu2*c-2*lt2*lu2*c+2*lt2*lu2*s;
27     dWdI1(i) = 0.5*(1-(c-s))*su*lt2/denominator; % isotropic component
28     dWdI4(i) = su/2*(l32-lt2)/denominator; % anisotropic component
29 end,
30 ppdWdI1 = spline(I1,dWdI1); ppdWdI4 = spline(I4,dWdI4); % final splines
31 return

```

Appendix B. Algorithms for different sets of uniaxial measured data

In this appendix we briefly include, as examples, the key equations for some combinations of measured data in uniaxial tests. We show here for simplicity the incompressible material cases, but these algorithms have corresponding quasi-incompressible versions.

Measured data: $T_{11}(E_{11}^{(1)}), E_{22}^{(1)}(E_{11}^{(1)}), E_{33}^{(2)}(E_{22}^{(2)})$

The algorithm is

$$\begin{aligned}
 \{E_{11}^{(1)}, T_{11}(E_{11}^{(1)}) + \omega_{22}'^{[j]}(E_{22}^{(1)})\} &\rightsquigarrow \omega_{11}'^{[j+1]}(E_{11}) \\
 \{E_{33}^{(2)}, \omega_{13}'^{[j]}(E_{11}^{(1)})\} &\rightsquigarrow \omega_{33}'^{[j+1]}(E_{33}) \\
 \{E_{22}^{(1)}, \omega_{33}'^{[j]}(E_{33}^{(2)})\} &\rightsquigarrow \omega_{22}'^{[j+1]}(E_{22})
 \end{aligned}$$

Measured data: $T_{11}^{(1)}(E_{11}^{(1)}), E_{33}^{(2)}(E_{22}^{(2)}), E_{11}^{(3)}(E_{33}^{(3)})$

This case needs the auxiliary relation $E_{22}^{(1)}(E_{22}^{(1)})$ to be refreshed as part of the algorithm,

$$\begin{aligned}
 \{E_{11}^{(1)}, T_{11}(E_{11}^{(1)}) + \omega_{22}'^{[j]}(E_{22}^{(1)})\} &\rightsquigarrow \omega_{11}'^{[j+1]}(E_{11}) \\
 \{E_{22}^{(3)}, \omega_{11}'^{[j]}(E_{11}^{(3)})\} &\rightsquigarrow \omega_{22}'^{[j+1]}(E_{22}) \\
 \{E_{33}^{(2)}, \omega_{11}'^{[j]}(E_{11}^{(3)})\} &\rightsquigarrow \omega_{33}'^{[j+1]}(E_{33}) \\
 \{\omega_{22}'^{[j-1]}(\omega_{33}'^{[j]}(E_{33}^{(2)})) - E_{33}^{(1)}, \omega_{22}'^{[j-1]}(\omega_{33}'^{[j]}(E_{33}^{(2)}))\} &= \{-E_{22}^{(1)} - E_{33}^{(1)}, E_{22}^{(1)}\} \rightsquigarrow E_{22}^{(1)}(E_{11}^{(1)})
 \end{aligned}$$

Measured data: $T_{11}^{(1)}(E_{11}^{(1)}), E_{22}^{(1)}(E_{11}^{(1)}), E_{11}^{(3)}(E_{33}^{(3)})$

In this case determination of $\omega_{33}'(E_{33})$ is straightforward after convergence of $\omega_{11}'(E_{11})$ and $\omega_{22}'(E_{22})$. The algorithm is

$$\begin{aligned}
 \{E_{11}^{(1)}, T_{11}(E_{11}^{(1)}) + \omega_{22}'^{[j]}(E_{22}^{(1)})\} &\rightsquigarrow \omega_{11}'^{[j+1]}(E_{11}) \\
 \{E_{22}^{(3)}, \omega_{11}'^{[j]}(E_{11}^{(3)})\} &\rightsquigarrow \omega_{22}'^{[j+1]}(E_{22})
 \end{aligned}$$

Thereafter, we have the explicit solution:

$$\{E_{11}^{(3)}, \omega'_{22}(E_{22}^{(1)})\} \rightsquigarrow \omega'_{33}(E_{33})$$

Measured data: $T_{11}^{(1)}(E_{11}^{(1)}), T_{22}^{(2)}(E_{22}^{(2)}), E_{22}^{(1)}(E_{11}^{(1)})$

Auxiliar relation $E_{33}^{(2)}(E_{22}^{(2)})$ needs to be refreshed as part of the algorithm.

$$\begin{aligned} \{E_{11}^{(1)}, T_{11}(E_{11}^{(1)}) + \omega'_{22}(E_{22}^{(1)})\} &\rightsquigarrow \omega'_{11}^{[j+1]}(E_{11}) \\ \{E_{33}^{(1)}, \omega'_{22}(E_{22}^{(1)})\} &\rightsquigarrow \omega'_{33}^{[j+1]}(E_{33}) \\ \{E_{22}^{(2)}, E_{33}^{(2)}\} &= \{-E_{33}^{(2)} - \omega'_{11}^{[j]-1}(\omega'_{33}(E_{33}^{(2)})), E_{33}^{(2)}\} \rightsquigarrow E_{33}^{(2)}(E_{22}^{(2)}) \\ \{E_{22}^{(2)}, T_{22}(E_{22}^{(2)}) + \omega'_{33}(E_{33}^{(2)})\} &\rightsquigarrow \omega'_{22}^{[j+1]}(E_{22}) \end{aligned}$$

Measured data: $T_{11}^{(1)}(E_{11}^{(1)}), T_{22}^{(2)}(E_{22}^{(2)}), E_{33}^{(2)}(E_{22}^{(2)})$

Auxiliar relation $E_{22}^{(1)}(E_{11}^{(1)})$ needs to be refreshed as part of the algorithm.

$$\begin{aligned} \{E_{11}^{(2)}, \omega'_{33}(E_{33}^{(2)})\} &\rightsquigarrow \omega'_{11}^{[j+1]}(E_{11}) \\ \{E_{22}^{(2)}, T_{22}(E_{22}^{(2)}) + \omega'_{33}(E_{33}^{(2)})\} &\rightsquigarrow \omega'_{22}^{[j+1]}(E_{22}) \\ \{E_{11}^{(1)}, E_{22}^{(1)}\} &= \{-\omega'_{33}^{[j]-1}(\omega'_{22}(E_{22}^{(2)})) - E_{22}^{(1)}, E_{22}^{(1)}\} \rightsquigarrow E_{22}^{(1)}(E_{11}^{(1)}) \\ \{E_{33}^{(1)}, \omega'_{11}(E_{11}^{(1)}) - T_{11}(E_{11}^{(1)})\} &\rightsquigarrow \omega'_{33}^{[j+1]}(E_{33}) \end{aligned}$$

Measured data: $T_{11}^{(1)}(E_{11}^{(1)}), T_{22}^{(2)}(E_{22}^{(2)}), T_{33}^{(3)}(E_{33}^{(3)})$

Auxiliar relations $E_{22}^{(1)}(E_{11}^{(1)}), E_{33}^{(2)}(E_{22}^{(2)}), E_{11}^{(3)}(E_{33}^{(3)})$ need to be refreshed as part of the algorithm.

$$\begin{aligned} \{E_{11}^{(1)}, T_{11}(E_{11}^{(1)}) + \omega'_{22}(E_{22}^{(1)})\} &\rightsquigarrow \omega'_{11}^{[j+1]}(E_{11}) \\ \{E_{22}^{(2)}, T_{22}(E_{22}^{(2)}) + \omega'_{33}(E_{33}^{(2)})\} &\rightsquigarrow \omega'_{22}^{[j+1]}(E_{22}) \\ \{E_{33}^{(3)}, T_{33}(E_{33}^{(3)}) + \omega'_{11}(E_{11}^{(3)})\} &\rightsquigarrow \omega'_{33}^{[j+1]}(E_{33}) \\ \{E_{11}^{(1)}, E_{22}^{(1)}\} &= \{-\omega'_{33}^{[j]-1}(\omega'_{22}(E_{22}^{(2)})) - E_{22}^{(1)}, E_{22}^{(1)}\} \rightsquigarrow E_{22}^{(1)}(E_{11}^{(1)}) \\ \{E_{22}^{(2)}, E_{33}^{(2)}\} &= \{-\omega'_{11}^{[j]-1}(\omega'_{33}(E_{33}^{(3)})) - E_{33}^{(2)}, E_{33}^{(2)}\} \rightsquigarrow E_{33}^{(2)}(E_{22}^{(2)}) \\ \{E_{33}^{(3)}, E_{11}^{(3)}\} &= \{-\omega'_{22}^{[j]-1}(\omega'_{11}(E_{11}^{(1)})) - E_{11}^{(3)}, E_{11}^{(3)}\} \rightsquigarrow E_{11}^{(3)}(E_{33}^{(3)}) \end{aligned}$$

Appendix C. Rotation matrix from local to preferred axis of the six tests of section 6

Test (1):

$$\mathbf{R}^{(1)} = \begin{bmatrix} 9.5500E-02 & 2.9390E-01 & 9.5110E-01 \\ 8.1370E-01 & -5.7340E-01 & 9.5500E-02 \\ 5.7340E-01 & 7.6470E-01 & -2.9390E-01 \end{bmatrix}$$

Test (2):

$$\mathbf{R}^{(2)} = \begin{bmatrix} -3.0520E-01 & -9.3930E-01 & 1.5640E-01 \\ 8.8960E-01 & -3.3990E-01 & -3.0520E-01 \\ 3.3990E-01 & 4.6000E-02 & 9.3930E-01 \end{bmatrix}$$

Test (3):

$$\mathbf{R}^{(3)} = \begin{bmatrix} 6.7250E-01 & -6.7250E-01 & 3.0900E-01 \\ 7.4000E-01 & 6.0500E-01 & -2.9390E-01 \\ 1.0700E-02 & 4.2630E-01 & 9.0450E-01 \end{bmatrix}$$

Test (4):

$$\mathbf{R}^{(4)} = \begin{bmatrix} 6.7250E-01 & -2.1850E-01 & 7.0710E-01 \\ 6.9400E-01 & 5.1800E-01 & -5.0000E-01 \\ -2.5700E-01 & 8.2700E-01 & 5.0000E-01 \end{bmatrix}$$

Test (5):

$$\mathbf{R}^{(5)} = \begin{bmatrix} 5.0000E-01 & -5.0000E-01 & 7.0710E-01 \\ 8.2700E-01 & 5.1800E-01 & -2.1850E-01 \\ -2.5700E-01 & 6.9400E-01 & 6.7250E-01 \end{bmatrix}$$

Test (6):

$$\mathbf{R}^{(6)} = \begin{bmatrix} -2.9390E-01 & -9.0450E-01 & 3.0900E-01 \\ 8.7500E-01 & -3.8470E-01 & -2.9390E-01 \\ 3.8470E-01 & 1.8400E-01 & 9.0450E-01 \end{bmatrix}$$

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