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Modelado Computacional del Daño
en Materiales Blandos

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***“IF YOU CHANGE
THE WAY
YOU LOOK
AT THINGS,
THE THINGS
YOU LOOK AT
CHANGE”
CHANGE.”***

Wayne Dyer

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Resumen

Los materiales poliméricos y los tejidos biológicos son usualmente modelados como materiales hiperelásticos isocóricos. Un material hiperelástico no presenta disipación de energía durante ciclos cerrados y las tensiones son funciones de estado de las deformaciones. Sin embargo, las gomas, elastómeros, los tejidos biológicos entre otros suelen presentar un comportamiento disipativo conocido como efecto Mullins. La causa del efecto Mullins, aunque muchas veces lo relacionan con la rotura de enlaces de los materiales de relleno de los polímeros, no está completamente entendido y es usual abordarlo desde un punto de vista fenomenológico. El efecto Mullins es complejo y tiene muchos aspectos diferentes como distintas curvas de descarga-recarga asociadas al fenómeno de viscosidad, diferentes tipos de daño para pequeñas y grandes deformaciones, deformaciones residuales permanentes y anisotropía inducida. No obstante, el enfoque más sencillo es modelar el daño como un ablandamiento del material, generalmente isótropo. El enfoque usual en la mecánica del daño continuo es realizar una hipótesis sobre la función de energía sin dañar, véase por ejemplo el modelo de Ogden o el modelo Neo-Hookean, y posteriormente aplican un factor de reducción $(1 - D)$, donde $D \in [0, 1)$ es la variable de daño de Rabotnov. Sin embargo, realmente no es posible medir la función de energía almacenada sin dañar, sólo se puede medir la dañada. Para completar los modelos se suele establecer un criterio de daño y una función constitutiva para la evolución de la variable de daño que suele incluir parámetros materiales adicionales como una función de saturación o se establece una curva master de daño unidimensional. Como punto de partida, en esta tesis se ha llevado a cabo un estudio en profundidad de la literatura existente relativa a la Mecánica de Daño principalmente desde una perspectiva ingenieril, concentrándose en las principales hipótesis, modelos y diferencias entre las formulaciones propuestas. A continuación, debido a las similitudes encontradas con los algoritmos de plasticidad, se ha realizado un estudio sobre los algoritmos de plasticidad en pequeñas deformaciones. Se han analizado diversas formas de implementar los algoritmos de retorno del tipo *Proyección al Punto más Cercano* –más conocidos por su denominación en inglés *Closest Point Projection*, para demostrar la importancia que tiene una cuidadosa implementación sobre la eficiencia de los mismos y así poder concluir cuál

es la mejor estrategia de cara a proponer un nuevo modelo de daño. Posteriormente se ha planteado un nuevo enfoque para abordar el daño isótropo en materiales hiperelásticos totalmente diferente. Usualmente los modelos prescriben a priori la forma de la curva tensión-deformación y mediante parámetros del material ajustan la forma a los datos experimentales. Por el contrario, los modelos hiperelásticos basados en *splines* no requieren el uso de ningún parámetro material sino simplemente los datos experimentales y son capaces de capturar de forma exacta las curvas experimentales de comportamiento. Aunque el modelo que se propone en esta tesis puede ser utilizado con cualquier modelo hiperelástico, si bien ha sido motivado por la idea detrás de los modelos basados en splines. Finalmente se ha realizado una extensión del modelo isótropo a ortotropía, considerando que el material se daña de modo diferente en cada una de las direcciones preferentes del material. Varias simulaciones de elementos finitos muestran la gran versatilidad de estos modelos cuando se combinan con funciones hiperelásticas formadas por splines.

Abstract

Polymeric materials and biological tissues are usually modeled as hyperelastic isochoric materials. An hyperelastic material does not dissipate energy during closed cycles and the stresses are state functions of the strains. However, rubbers, carbon-filled elastomers, biological tissues etc. usually present a dissipative behavior known as Mullins effect. The cause of the Mullins effect, usually related to filler-polymer link breakages, it is not completely understood and it is usually treated from a phenomenological point of view. The Mullins effect is complex and has many different aspects as distinct curves unloading-reloading curves associated with the phenomenon of viscosity, different patterns of damage at small and large strains, permanent residual strain and induced anisotropy. Nevertheless, the simplest approach is to model the damage as a softening of the material, generally isotropic. The usual approach in continuum damage mechanics is to make an hypothesis about the shape of the undamaged stored energy function, see for example a Neo-Hookean or Ogden model, and subsequently apply a reduction factor $(1 - D)$, where $D \in [0, 1)$ it is the damage variable of Rabotnov. Nonetheless, it really is not possible to measure the undamaged stored energy function, but only the damaged one. To complete these models a damage criterion and a constitutive function which usually include additional material parameters (as for example a function of saturation or and unidimensional master damage curve). As a starting point in this thesis, a study of the literature concerning the mechanical damage mainly from an engineering perspective, focusing on the key assumptions, models and differences between the proposed formulations, has been developed. Then, because of the similarities found with plasticity, it has carried out a comparative analysis about plasticity algorithms in small strains. It has analyzed several ways to implement a return-mapping algorithm like the Closest Point Projection, in order to show the importance of a careful implementation of the efficiency of these algorithms and thus be able to conclude what is the best strategy to propose a new approach for modeling the hyperelastic material damage. Subsequently, a new approach for the damage modeling of isotropic hyperelastic materials has been postulated. In general, models usually prescribe a priori the general shape of the stress-strain curve and the material parameters simply adjust that shape to the

experimental data. By contrast, the hyperelastic *spline-based* models do not require the use of any additional material parameter but just the experimental data and also, are capable of accurately capturing the experimental stress-strain curves. Although the proposed damage model can be used with any hyperelastic model, it has been motivated by the idea behind the models based on splines. Finally an extension of the model to orthotropy has been developed, considering that the material is damaged in different degree in each of the preferred material directions. Throughout this work, several finite element simulations show the versatility and interesting characteristics of the models.

Capítulo 1

INTRODUCCIÓN

1.1. Mecánica del Continuo

La Mecánica de los Medios Continuos intenta formular, asumiendo ciertas hipótesis, las ecuaciones que gobiernan un problema físico dado [1]. En general, la solución de un problema de Mecánica de Sólidos Deformables debe satisfacer las ecuaciones de equilibrio, las condiciones de compatibilidad entre deformaciones y desplazamientos, y las relaciones de tensión-deformación o leyes constitutivas del material. El conjunto de esas ecuaciones forma un sistema de ecuaciones diferenciales (ecuaciones de campo) que se resolverá teniendo en cuenta las condiciones iniciales y de contorno. A partir de la consideración de las ecuaciones de equilibrio, se pueden relacionar las tensiones dentro de un cuerpo con las solicitaciones externas, incluidas las fuerzas de volumen y de superficie. De la misma manera, teniendo en cuenta las condiciones geométricas, se pueden relacionar las deformaciones dentro de un cuerpo con sus desplazamientos. Tanto las ecuaciones de equilibrio como las de compatibilidad son válidas independientemente del material específico del que está hecho el cuerpo. La influencia del material se expresa mediante leyes constitutivas. El planteamiento y desarrollo de dichas ecuaciones constitutivas representa un área fundamental en la Mecánica de los Medios Continuos. Bien es sabido que diferentes materiales sometidos a una misma acción pueden presentar una respuesta completamente distinta, por lo que la respuesta de cada material estará representada por una ley constitutiva concreta [2]. El objetivo de las teorías constitutivas es por tanto construir modelos matemáticos que nos permitan predecir el comportamiento de un material, de tal forma que se pueda contrastar con evidencias experimentales. Las principales leyes constitutivas son: elasticidad lineal, hiperelasticidad, plasticidad, viscoelasticidad, viscoplasticidad, entre otras.

La solución del problema físico puede ser analítica (solución exacta) o numérica

(solución aproximada). La solución analítica suele ser muy complicada o imposible de obtener por lo que se recurre a la solución numérica, no obstante, para casos sencillos es muy importante, ya que nos sirve de referencia para comprobar el grado de aproximación de la técnica numérica utilizada. Las técnicas numéricas más empleadas para resolver el sistema de ecuaciones diferenciales son: métodos de las diferencias finitas, método de los elementos finitos, método de los volúmenes finitos, métodos sin malla, entre otros. Actualmente el método de los elementos finitos es el más empleado en el ámbito de la mecánica computacional [3] y es el que se ha usado para desarrollar este trabajo. La Mecánica Computacional resuelve estos problemas físicos mediante la simulación a través de dichas técnicas numéricas implementadas en el ordenador. Se puede decir que la mecánica computacional no es un bloque independiente sino que depende de otros tres: análisis teórico (definición del problema del valor de contorno –usualmente abreviado como *PVC*), análisis experimental (laboratorio) y análisis numérico (método numérico empleado). En la Figura 1.1 se representa un posible esquema de la resolución de un problema en mecánica computacional, donde se puede apreciar el rol que desempeñan los modelos constitutivos.

El modelado del comportamiento del sólido se suele abordar siguiendo un enfoque micromecánico, macromecánico o mesomecánico. La microestructura de un material puede estar formada por distintos elementos como, por ejemplo, cristales, granos, inclusiones, vacíos, micro-cavidades, micro-defectos, fibras o partículas embebidas en una matriz, etc. Cuando se considera el entorno material infinitesimal de un medio continuo en la escala microscópica se observa que el material es heterogéneo, es decir, que está formado por distintos elementos constitutivos, cada uno de los cuales puede presentar propiedades y características morfológicas y topológicas diferentes. Además, la microestructura puede experimentar cambios durante los procesos de deformación tales como rotura de fibras, nucleación, crecimiento y coalescencia de huecos o descohesión, aparición de micro-fisuras y porosidades, deslizamientos en límites de grano y crecimiento de fases sólidas, entre otros. De este modo, las propiedades micromecánicas están definidas por las propiedades de los elementos constituyentes. Entre las propiedades de los constituyentes cabe destacar su estructura, resistencia, propiedades mecánicas, químicas y las relaciones entre los mismos. En definitiva, la micromecánica trata de establecer las variables continuas en la vecindad de un punto material, considerando la microestructura del entorno y las propiedades de las fases constituyentes. Por otra parte, las ecuaciones constitutivas se pueden plantear siguiendo una vía puramente fenomenológica sin tener en cuenta la microestructura del sólido. Según este enfoque las propiedades mecánicas asociadas a distintas direcciones en un material anisótropo se describen considerando el sólido como un medio continuo, sin necesidad de considerar la naturaleza de los componentes que originan la anisotropía y las posibles

1.1. MECÁNICA DEL CONTINUO

Figura 1.1: Esquema de un problema de mecánica computacional.

interacciones entre los mismos. En los últimos años, se ha tratado de acoplar las teorías macroscópicas y microscópicas del material compatibilizando los campos de variables dando lugar a modelos híbridos conocidos usualmente como modelos micro-macromecánicos o mesomecánicos. Estos modelos micro-macromecánicos que tratan de representar comportamientos micromecánicos frecuentemente emplean las mismas variables que se usan en el modelado macromecánico, es decir, deformaciones y tensiones.

Cabe destacar que el modelado micromecánico ha ido ganando atención en las últimas décadas ya que permite relacionar el comportamiento mecánico del sólido con los distintos mecanismos físicos existentes en el medio continuo. Sin embargo, la difícil tarea de modelar todas las interacciones existentes entre los distintos elementos constitutivos hace que las predicciones macromecánicas obtenidas mediante estas teorías, en muchas ocasiones, no sean del todo satisfactorias y además suelen llevar asociadas un alto coste computacional. La aproximación fenomenológica no permite analizar directamente la influencia de los distintos componentes (sólo indirectamente), sin embargo, permite predecir el comportamiento mecánico macroscópico del material de una forma más completa. Debido a su utilidad y eficiencia en simulaciones y análisis en ingeniería, hasta el momento, la teoría macromecánica ha sido la metodología predominante en la formulación de leyes constitutivas en el campo de la mecánica de sólidos, sobre todo en el estudio de los materiales compuestos. De este modo, todas las ecuaciones constitutivas y algoritmos computacionales desarrollados a lo largo de esta tesis han sido formulados desde un enfoque meramente fenomenológico.

1.2. Materiales blandos

Entre otros materiales, la mecánica de los medios continuos permite modelar a los materiales blandos. Los materiales blandos tales como los polímeros y los tejidos biológicos tienen muchas aplicaciones en ingeniería y en biomecánica. Estos materiales presentan un comportamiento mecánico complejo, que se caracteriza por experimentar grandes deformaciones, histéresis, efectos viscosos, ablandamiento (efecto Mullins) y plasticidad desviadora y volumétrica. La necesidad de predecir con precisión el comportamiento de estos materiales es un gran reto para los científicos e ingenieros. Tanto los tejidos blandos como los elastómeros se componen de redes tridimensionales muy estables de macromoléculas unidas mediante enlaces covalentes de van der Waals. Las similitudes entre los tejidos biológicos blandos y los elastómeros ya se habían observado alrededor de 1880 en el contexto de la mecánica de la pared arterial [4] y también en las primeras décadas de 1900 Wöhlisch [5] y Karrer [6] relacionaron la mecánica de los músculos con la de las gomas. De este modo, los fundamentos matemáticos que en un origen se desarro-

1.2. MATERIALES BLANDOS

llaron para caracterizar el comportamiento altamente no lineal de los elastómeros sin rellenos y los reforzados con partículas o fibras de carbono se han adaptado con éxito para describir la respuesta mecánica de los tejidos biológicos blandos. La respuesta mecánica de ambos materiales es cualitativamente similar. Ambos son capaces de experimentar grandes deformaciones no lineales y presentan ablandamiento durante los primeros ciclos de carga. El comportamiento termomecánico asociado a las macromoléculas es significativamente diferente del de, por ejemplo, los metales, en los que un conjunto ordenado de átomos se mantienen unidos en una estructura reticular mediante enlaces interatómicos lo que conduce a una elasticidad energética. Los metales no pueden desarrollar las grandes deformaciones características de las gomas y los tejidos biológicos blandos, por esto, Fung [7] propuso como alternativa para los tejidos biológicos blandos, la aplicación de la termodinámica de la elasticidad entrópica de la clásica teoría de gomas. Para comprender mejor este tipo de materiales se va a hacer una descripción superficial de sus características mecánicas, debido a las similitudes anteriormente planteadas, se han escogido los tejidos biológicos para su estudio. Algunos ejemplos de tejidos blandos son: tendones, ligamentos, venas, piel, cartílagos, entre otros. Los tejidos conectivos blandos de nuestro cuerpo son complejas estructuras compuestas reforzadas con fibras. Su comportamiento mecánico está fuertemente influenciado por la concentración y la disposición estructural de sus constituyentes tales como fibras de *colágeno*, *elastina* y una *matriz hidratada de proteoglicanos*, y por su correspondiente función en el organismo. Para una explicación más detallada se remite al lector a [8],[9], por ejemplo. Dichas fibras tienden a tener orientaciones preferentes por lo que se puede suponer que los tejidos blandos se comportan anisótropamente. A escala microscópica, son materiales heterogéneos, puesto que están formados por diferentes elementos constitutivos. La respuesta a tracción de estos materiales es altamente no lineal y las tensiones resultantes dependen de la tasa de deformación. A diferencia de los tejidos duros, los blandos pueden experimentar grandes deformaciones.

Se va a explicar a continuación de forma simplificada el comportamiento tensión-deformación de la piel, ya que además de ser el órgano más grande del cuerpo, constituye aproximadamente un 16 % del peso del cuerpo de una persona adulta. La piel está constituida principalmente de tejidos conectivos, en los cuales las redes tridimensionales de fibras parecen tener unas orientaciones preferentes paralelas a la superficie. Sin embargo, para prevenir cortantes fuera del plano, las orientaciones de algunas fibras tienen componentes fuera del mismo. La Figura 1.2 muestra un diagrama esquemático típico de la curva tensión-deformación de la piel [8]. Adviértase que esta curva, que es representativa de muchos tejidos blandos, difiere significativamente de las relaciones tensión-deformación de otros materiales, por ejemplo de los tejidos duros. Además, la Figura 1.2 muestra cómo las fibras de

Figura 1.2: Curva tensión-deformación típica de una muestra de piel donde se representa la morfología de las fibras de colágeno.

colágeno se van estirando con el incremento de tensión. En la zona *A* de la curva, las fibras de colágeno se encuentran onduladas y plisadas y la piel se comporta aproximadamente como si fuera isotrópica. Inicialmente se necesitan bajas tensiones para alcanzar grandes deformaciones de las fibras de colágeno sin que éstas se alarguen. Por ello en esta fase, el tejido se comporta como una lámina muy blanda de goma y las fibras de elastina son las principales responsables del alargamiento de la piel. La relación tensión-deformación correspondiente a esta zona de la curva es prácticamente lineal, con un bajo módulo elástico. En la zona *B* del diagrama, conforme la carga se va incrementando, las fibras de colágeno tienen a alinearse con la dirección de carga. Las fibras de colágeno onduladas se van alargando gradualmente y van interactuando con la matriz hidratada de proteoglicanos. En la zona *C*, a altos valores de tensión las fibras de colágeno se estiran totalmente, estando principalmente alineadas en la dirección de la carga. A partir de ese momento, las fibras de colágeno resisten casi por completo la carga y el tejido se vuelve mucho más resistente a altas tensiones. La relación tensión-deformación se vuelve lineal otra vez. Más allá de esta zona, se alcanza la tensión última y las fibras de colágeno comienzan a romperse.

Por todo lo anteriormente expuesto es mundialmente aceptado que los tejidos biológicos blandos y los elastómeros con y sin relleno pueden ser razonablemente modelados como materiales hiperelásticos [10].

1.3. Hiperelasticidad

Como se ha visto en el apartado anterior, los materiales blandos suelen exhibir un comportamiento fundamentalmente hiperelástico. Por ello en este apartado se va a mostrar la teoría básica de la hiperelasticidad.

Por sencillez expositiva, se empieza representando el estado de deformación de un sólido mediante el tensor de segundo orden $\boldsymbol{\varepsilon}$ y su estado tensional mediante el tensor de segundo orden $\boldsymbol{\sigma}$. Diremos que un material es *elástico* si su estado tensional en cada instante depende únicamente de su estado de deformación en ese instante

$$\boldsymbol{\sigma} = \mathbf{F}(\boldsymbol{\varepsilon}) \quad (1.1)$$

donde $\mathbf{F}$ representa una función tensorial de las deformaciones, sin ninguna restricción. Esta formulación implica: reversibilidad, independencia de las tensiones de la trayectoria de deformaciones (dependen sólo de valores instantáneos) y la posibilidad de generar energía en ciclos de carga y descarga. El comportamiento mecánico de este tipo de materiales se suele describir con la teoría de la elasticidad de Cauchy.

Se considera que el material es *hiperelástico* o puramente elástico si su estado tensional, además, deriva de una función de energía elástica (o de energía almacenada) $\mathcal{W}(\boldsymbol{\varepsilon})$ definida por unidad de volumen como

$$\boldsymbol{\sigma} = \frac{\partial \mathcal{W}(\boldsymbol{\varepsilon})}{\partial \boldsymbol{\varepsilon}} \quad (1.2)$$

Con esta definición, se evitan los problemas de generación de energía en ciclos cerrados de deformación. Una definición formal de hiperelasticidad fue enunciada en 1996 por Drozdov [11]: “*la teoría constitutiva que describe el comportamiento mecánico de los sólidos elásticos con el uso solamente de una función material es llamada hiperelasticidad*”. La introducción del concepto *función de energía de deformación* (o *de energía almacenada*) en elasticidad se debe a George Green [12], por eso los materiales para los que se asume que existe dicha función son llamados materiales elásticos de Green o hiperelásticos.

El trabajo mecánico interno desarrollado por las tensiones en un sólido hiperelástico de volumen unidad al pasar de un estado de deformación $\boldsymbol{\varepsilon}_1$ a otro estado de deformación $\boldsymbol{\varepsilon}_2$ es

$$\int_{t_1}^{t_2} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) : \dot{\boldsymbol{\varepsilon}} dt = \int_{t_1}^{t_2} \frac{\partial \mathcal{W}(\boldsymbol{\varepsilon})}{\partial \boldsymbol{\varepsilon}} : d\boldsymbol{\varepsilon} = \int_{t_1}^{t_2} d\mathcal{W}(\boldsymbol{\varepsilon}) = \mathcal{W}(\boldsymbol{\varepsilon}_2) - \mathcal{W}(\boldsymbol{\varepsilon}_1) \quad (1.3)$$

el cual sólo depende de los estados de deformación inicial y final y no del camino seguido entre ellos. Este último enunciado se suele tomar también como la propia definición del concepto de hiperelasticidad, cuya estructura es completamente

Figura 1.3: Ejemplo en dos dimensiones de un material elástico lineal de Cauchy que viola los principios de la Termodinámica.

conservativa. Este hecho no se puede asegurar en un material elástico de Cauchy, lo que representa la diferencia fundamental entre ambas descripciones [13]. De hecho, la conservación de la energía asociada a ecuaciones del tipo (1.1) requiere el cumplimiento de ciertas condiciones de compatibilidad o integrabilidad adicionales. A continuación se verá el caso de un material elástico lineal de Cauchy que viola los principios de la Termodinámica. Para este ejemplo se trabajará en dos dimensiones. Se propone la siguiente relación constitutiva:

$$\sigma_1 = c_{11}\varepsilon_1 + c_{12}\varepsilon_2 \quad (1.4a)$$

$$\sigma_2 = c_{21}\varepsilon_1 + c_{22}\varepsilon_2 \quad (1.4b)$$

donde c_{ij} para $i, j = \{1, 2\}$ son los coeficientes de comportamiento elástico. Se calcula el trabajo mecánico $W = \int_A^B \sigma_{ij} d\varepsilon_{ij}$ para las trayectorias ABC y ADC de la Figura 1.3. Para la trayectoria ABC resulta

$$W_{ABC} = \int_A^B (\sigma_1 d\varepsilon_1 + \sigma_2 d\varepsilon_2) + \int_B^C (\sigma_1 d\varepsilon_1 + \sigma_2 d\varepsilon_2) = \quad (1.5)$$

$$= \int_{(0,0)}^{(\varepsilon_1^*,0)} (c_{11}\varepsilon_1 + c_{12}\varepsilon_2) d\varepsilon_1 + \int_{(\varepsilon_1^*,0)}^{(\varepsilon_1^*,\varepsilon_2^*)} (c_{21}\varepsilon_1 + c_{22}\varepsilon_2) d\varepsilon_2 = \quad (1.6)$$

$$= c_{11} \frac{(\varepsilon_1^*)^2}{2} + c_{22} \frac{(\varepsilon_2^*)^2}{2} + c_{21}\varepsilon_1^*\varepsilon_2^* \quad (1.7)$$

Procediendo análogamente para la trayectoria ADC

$$W_{ADC} = c_{11} \frac{(\varepsilon_1^*)^2}{2} + c_{22} \frac{(\varepsilon_2^*)^2}{2} + c_{12}\varepsilon_1^*\varepsilon_2^* \quad (1.8)$$

Se observa que los valores del trabajo no coinciden para ambas trayectorias y por tanto, se genera una energía en el ciclo cerrado $ABCD A$

$$W_{ABCD A} = (c_{21} - c_{12})\varepsilon_1^*\varepsilon_2^* \neq 0 \quad (1.9)$$

Figura 1.4: Curva de comportamiento de un material hiperelástico típico en un ensayo uniaxial incluyendo carga y descarga bajo deformaciones finitas.

que puede ser positiva o negativa dependiendo de los valores de c_{21} y c_{12} . Sólo será nula si $c_{21} = c_{12}$ es decir, si la matriz de coeficientes elásticos es simétrica. Esta propiedad se puede generalizar a relaciones en tres dimensiones y con todas las componentes de los tensores de tensiones y deformaciones. Por tanto, para que un material sea hiperelástico la matriz de coeficientes elásticos debe ser simétrica.

En la Figura 1.4 se muestra una curva representativa del comportamiento de un sólido hiperelástico en un ensayo de tracción simple. Las deformaciones axiales ε pueden ser finitas y el comportamiento $\sigma(\varepsilon)$ altamente no lineal. La carga y descarga describen siempre la misma curva.

Los materiales poliméricos han sido tradicionalmente los más representativos del comportamiento hiperelástico. Entre los materiales compuestos más complejos y universalmente empleados se encuentran los elastómeros. Su flexibilidad y capacidad para albergar en su seno partículas como el negro de humo, la sílice o la arcilla, en diferentes cantidades pudiendo llegar a exceder su propio peso, permiten ampliar su rango de propiedades y emplearlos en múltiples aplicaciones industriales. Por ejemplo el caucho vulcanizado, reforzado con partículas o fibras de carbono o de sílice o mediante fibras de acero, es utilizado en la fabricación de neumáticos, llantas y otros muchos elementos en el campo de la automoción y desde hace muchos años incluso en la industria textil para fabricar prendas de vestir. Se han desarrollado muchos modelos hiperelásticos para representar el comportamiento mecánico de este tipo de materiales [14], [15], [87]. Frecuentemente estos materiales experimentan grandes deformaciones sin mostrar una variación apreciable de volumen, por lo que se pueden considerar incompresibles. La hipótesis de incompresibilidad se asume en este trabajo, aunque las formulaciones planteadas siguen siendo válidas para comportamientos ligeramente compresibles. La implementación práctica de

la condición de incompresibilidad se realizará mediante funciones de penalización, dando lugar a formulaciones denominadas como cuasi-incompresibles.

Otras aplicaciones en ingeniería que se aprovechan del comportamiento hiperelástico de los elastómeros, tanto isótropos como anisótropos, son: aislamiento de cables eléctricos, cintas transportadoras, tubos sometidos a altas presiones [17], absorbedores de impacto, aplicaciones más sencillas como algunos materiales de PVC rellenos de arcilla que se emplean en la fabricación de juguetes para reducir su coste, y también aplicaciones sofisticadas, como las requeridas por la industria aeroespacial, donde son necesarias altas prestaciones a elevadas temperaturas, lo que implica una formulación más cuidadosa y un mayor coste. Además, los modelos hiperelásticos han permitido, por ejemplo, el análisis de la estabilidad de estructuras de membranas [18], que es de suma importancia debido a la gran variedad de aplicaciones que desempeñan, por ejemplo, en la industria espacial: velas solares, blindajes térmicos, paneles solares, hábitats espaciales, etc., en la industria civil: diversas construcciones entre las que cabe destacar el estadio de fútbol Allianz Arena de Múnich, en la ingeniería mecánica: airbags, neumáticos, llantas, en la ingeniería aeroespacial: globos meteorológicos, paracaídas de freno, etc., en la ingeniería biomédica: catéteres para tratamientos clínicos [19], [20], implantes biomecánicos [21], [22].

Como se vio en el apartado anterior, los tejidos biológicos blandos, también pueden experimentar grandes deformaciones conservativas. En el campo de la biomecánica, las paredes arteriales, tendones, ligamentos, músculos, cartílagos o incluso el mayor órgano del cuerpo humano como es la piel, entre muchos otros, son tratados tanto analíticamente como numéricamente mediante formulaciones hiperelásticas [23], [24], [25]. La naturaleza polimérica de estos materiales junto con su gran contenido en agua, resultan en un comportamiento prácticamente incompresible. De este modo, la condición de incompresibilidad constituye una hipótesis ampliamente aceptada y empleada también en el campo de la biomecánica computacional [26], [27], [28].

Por todo lo planteado con anterioridad, parece evidente que la mecánica de medios continuos no lineal se postule como la base fundamental para el tratamiento analítico y computacional adecuado de estos materiales blandos hiperelásticos.

1.4. Grandes deformaciones

Los materiales blandos con comportamiento hiperelástico, bajo estudio, pueden experimentar grandes desplazamientos y deformaciones, de tal modo que la hipótesis inherente a la teoría infinitesimal resulta invalidada y se debe recurrir a la teoría general de deformaciones finitas.

Dado el cuerpo deformable de la Figura 1.5, a través de una suma de vectores,

Figura 1.5: Configuración inicial y actual de un sólido. Definición de las coordenadas materiales 0x y espaciales tx y del vector desplazamiento tu . Transformación del vector infinitesimal material d^0x en el vector espacial infinitesimal d^tx .

se puede escribir directamente la relación entre los vectores de posición de las partículas del cuerpo en la configuración inicial y la final. Las coordenadas de una partícula en la configuración *inicial*, *de referencia* o *no deformada*, están definidas por el vector de posición *material* o *lagrangiano* ${}^0\mathbf{x}$, mientras que las coordenadas de una partícula en la configuración *final*, *actual* o *deformada*, están definidas por el vector de posición *espacial* o *euleriano* ${}^t\mathbf{x}$. El vector desplazamiento ${}^t\mathbf{u}$ describe el desplazamiento experimentado por un punto del sólido entre los instantes inicial y final, de tal forma que

$${}^t\mathbf{x}({}^0\mathbf{x}) = {}^0\mathbf{x} + {}^t\mathbf{u}({}^0\mathbf{x}) \quad (1.10)$$

En la ecuación anterior, expresada en coordenadas materiales, se dice que ${}^t\mathbf{x}({}^0\mathbf{x})$ es el *empuje* de ${}^0\mathbf{x}$ desde la configuración de referencia a la actual. Análogamente se puede obtener la expresión inversa (espacial) donde ${}^0\mathbf{x}({}^t\mathbf{x})$ representaría el *tiro* de ${}^t\mathbf{x}$ desde la configuración final a la inicial. Las propiedades del medio continuo pueden estar descritas por unas ecuaciones que indican cómo dichas propiedades evolucionan con el transcurso del tiempo. Estas ecuaciones se pueden plantear en la configuración de referencia (lagrangiana) o en la configuración actual (euleriana). En el desarrollo de este trabajo todas las formulaciones han sido planteadas completamente siguiendo una descripción lagrangiana.

La deformación sufrida por el sólido en el entorno de la partícula ${}^0\mathbf{x}$ se puede describir mediante el gradiente de la transformación cinemática de la Ec. (1.10). Como resultado se obtiene el siguiente gradiente material de coordenadas, denominado normalmente como *gradiente de deformación material* o simplemente *gradiente de deformación*

$${}^t_0\mathbf{X} = \frac{\partial {}^t\mathbf{x}({}^0\mathbf{x})}{\partial {}^0\mathbf{x}} \quad (1.11)$$

Considérense dos puntos infinitamente próximos en la configuración de referencia 0x y 0z cuyos empujes son tx y tz , respectivamente, tal y como se muestra en la Figura 1.5. Aplicando el teorema de Taylor para el desarrollo en serie a las coordenadas espaciales tz en un entorno de la partícula ${}^0\mathbf{x}$ se obtiene

$${}^tz({}^0\mathbf{z}) = {}^tx({}^0\mathbf{x}) + \frac{\partial {}^t\mathbf{x}({}^0\mathbf{x})}{\partial {}^0\mathbf{x}} \cdot ({}^0\mathbf{z} - {}^0\mathbf{x}) + \dots \quad (1.12)$$

Si las partículas 0x y 0z están muy próximas en la configuración de referencia, los términos de orden superior pueden despreciarse, resultando

$$d{}^t\mathbf{x} = {}^t_0\mathbf{X} \cdot d{}^0\mathbf{x}$$

donde $d{}^0\mathbf{x} = {}^0\mathbf{z} - {}^0\mathbf{x}$ es el vector infinitesimal que une las partículas en la configuración de referencia y $d{}^t\mathbf{x} = {}^t\mathbf{z} - {}^t\mathbf{x}$ es dicho vector infinitesimal una vez deformado. ${}^t_0\mathbf{X}$ es el tensor de segundo orden que describe la transformación de elementos infinitesimales de línea entre ambas configuraciones. Por tanto, el gradiente de deformación es la medida fundamental de deformación en la mecánica de medios continuos para grandes deformaciones. Este tensor incluye información acerca de la deformación (cambio de forma) y la rotación del cuerpo rígido, pero no incluye información acerca de las posibles traslaciones de cuerpo rígido. Nótese que a diferencia de los desplazamientos, que son cantidades medibles, la deformación está basada en conceptos que son introducidos por conveniencia a la hora del análisis. Por lo tanto, se han propuesto en la literatura numerosas definiciones y nombres de tensores de deformación, por ello sólo vamos a introducir a continuación las medidas de deformación que se han elegido para desarrollar las formulaciones de esta tesis.

Considérese ahora, por ejemplo, la elongación uniforme de un elemento unidimensional cuya longitud inicial es 0l y su longitud final es tl , donde se define el diferencial de deformación según el eje de la barra como $d\varepsilon = dL/{}^0l$, donde dL es el diferencial de longitud de la barra. Integrando esta expresión se obtiene

$$\varepsilon = \int_{{}^0l}^{{}^tl} \frac{1}{{}^0l} dL = \ln \left(\frac{{}^tl}{{}^0l} \right) = \ln({}^t_0\lambda) \quad (1.13)$$

donde ${}^t_0\lambda := {}^tl/{}^0l$ es el *alargamiento unitario*. Esta deformación ε se denomina *deformación logarítmica* o *deformación verdadera*. Se comprueba que de haber

1.4. GRANDES DEFORMACIONES

incrementos sucesivos de desplazamientos es decir, primero de 0l a ${}^\tau l$ y posteriormente de ${}^\tau l$ a ${}^t l$, donde $0 < \tau < t$, la deformación logarítmica es aditiva

$$\begin{aligned} {}^t_0\varepsilon &= \int_{{}^0l}^{{}^t l} \frac{1}{l} dL = \int_{{}^0l}^{{}^\tau l} \frac{1}{l} dL + \int_{{}^\tau l}^{{}^t l} \frac{1}{l} dL \\ &= \ln\left(\frac{{}^\tau l}{{}^0l}\right) + \ln\left(\frac{{}^t l}{{}^\tau l}\right) = {}^\tau_0\varepsilon + {}^t_\tau\varepsilon \end{aligned} \quad (1.14)$$

Partiendo de la definición de deformación logarítmica, Ec. 1.13, podemos definir el *Tensor de Deformación Logarítmica* o *Tensor de deformación de Hencky* $\mathbf{E}$ como

$$\mathbf{E} = \ln(\mathbf{U}) \text{ and } \mathbf{U} = \sum_{i=1}^3 \ln(\lambda_i) \mathbf{N}_i \otimes \mathbf{N}_i \quad (1.15)$$

donde $\mathbf{U}$ es un tensor simétrico conocido como el *tensor derecho* (o *material*) de *alargamiento* y $\mathbf{N}_i$ son las direcciones principales de deformación. Otras características destacables del tensor de deformación logarítmico son:

- La condición de incompresibilidad adquiere la sencilla forma de $\text{tr}(\ln(\mathbf{U})) \equiv 0$.
- Las partes volumétrica e isocórica son aditivas. A veces a la hora de establecer ciertas ecuaciones constitutivas puede resultar conveniente separar la parte volumétrica de la parte isocórica (desviadora). Haciendo uso de la descomposición de Flory se puede obtener la descomposición de ${}^t_0\mathbf{X}$ en sus partes volumétrica y desviadora, del siguiente modo ${}^t_0\mathbf{X} = {}^t_0\mathbf{X}^V {}^t_0\mathbf{X}^D = {}^t_0\mathbf{X}^D {}^t_0\mathbf{X}^V$, con ${}^t_0\mathbf{X}^V = {}^t_0J^{1/3}\mathbf{I}$ y ${}^t_0\mathbf{X}^D = {}^t_0J^{-1/3} {}^t_0\mathbf{X}$, donde J representa al determinante del gradiente de deformación, ${}^t_0\mathbf{X}^D$ y ${}^t_0\mathbf{X}^V$ son las partes desviadora y volumétrica del mismo, respectivamente e $\mathbf{I}$ identifica al tensor identidad de segundo orden. Nótese que ${}^t_0\mathbf{X}^D$ es una transformación donde se preserva el volumen, es decir una transformación isocórica, $\det({}^t_0\mathbf{X}^D) = 1$, y que por el contrario ${}^t_0\mathbf{X}^V$ describe una transformación puramente volumétrica, asociada sólo con el cambio de volumen. Considerando ahora la descomposición polar del gradiente de deformaciones, se obtienen las partes desviadora y volumétrica del tensor material de alargamiento $\mathbf{U}$ del siguiente modo

$${}^t_0\mathbf{X} = {}^t_0\mathbf{R} {}^t_0\mathbf{U} = {}^t_0\mathbf{R} {}^t_0\mathbf{U}^V \begin{cases} {}^t_0\mathbf{U}^V = {}^t_0\mathbf{X}^V = {}^t_0J^{1/3}\mathbf{I} \\ {}^t_0\mathbf{X}^D = {}^t_0\mathbf{R} {}^t_0\mathbf{U}^D \\ {}^t_0\mathbf{U}^D = {}^t_0J^{-1/3} {}^t_0\mathbf{U} \end{cases} \quad (1.16)$$

donde ${}^t_0\mathbf{R}$ es el tensor de rotación. Finalmente se comprueba la propiedad aditiva de las partes volumétrica y desviadora del tensor de deformación logarítmico

$$\mathbf{E} = \ln(\mathbf{U}) = \ln(J^{-1/3}\mathbf{U} * J^{1/3}\mathbf{I}) = \ln(J^{-1/3}\mathbf{U}) + \frac{1}{3} \ln \text{tr}(\mathbf{E}) = \mathbf{E}^D + \mathbf{E}^V \quad (1.17)$$

donde $\mathbf{E}^D$ y $\mathbf{E}^V$ son la parte desviadora y volumétrica del tensor de deformación $\mathbf{E}$, respectivamente.

Sin embargo, aunque las diversas medidas de deformación tomen valores numéricos distintos, es importante comprender que todas ellas representan el mismo estado de deformación del sólido, el cual realmente viene definido por la longitud final ${}^t l$, de modo que si se conoce una medida de deformación en un instante concreto, el resto de medidas quedarán determinadas automáticamente. A las expresiones que relacionan las distintas medidas de deformación se conocen como relaciones de transformación. Señalar por último que, en un contexto de pequeñas deformaciones, todas las medidas de deformación son equivalentes (cuando los términos no lineales en ${}^t_0 \varepsilon$ son despreciables) por lo que se define una única medida de deformación, es decir la deformación ingenieril ${}^t_0 \varepsilon$, la cual se refiere indistintamente a la configuración inicial o a la final.

En Mecánica de Sólidos se busca conocer el estado tensional en cada punto de un sólido deformado. De forma similar a lo que ocurre con las medidas de deformaciones finitas, existen diversas medidas de tensión con las que evaluar el estado tensional de un cuerpo. De hecho, cada medida de deformación tiene asociada su correspondiente medida de tensión, que es su conjugada de trabajo [30]. La potencia mecánica interna por unidad de volumen deformado se obtiene a partir del producto de la tensión axial de Cauchy por el gradiente espacial de velocidades, esto es

$${}^t \sigma \frac{\partial {}^t v}{\partial {}^t x} = {}^t \sigma \frac{\partial}{\partial {}^0 x} \left(\frac{\partial {}^t x}{\partial t} \right) \frac{\partial {}^0 x}{\partial {}^t x} = {}^t \sigma \frac{\partial}{\partial t} \left(\frac{\partial {}^t x}{\partial {}^0 x} \right) \frac{\partial {}^0 x}{\partial {}^t x} = {}^t \sigma \frac{{}^t \dot{\lambda}}{{}^t_0 \lambda} \quad (1.18)$$

La transformación entre los volúmenes inicial y final viene dada por el jacobiano ${}^t_0 J = {}^t V / {}^0 V$. La potencia mecánica interna resulta

$${}^t_0 J {}^t \sigma \frac{{}^t \dot{\lambda}}{{}^t_0 \lambda} = {}^t \tau \frac{{}^t \dot{\lambda}}{{}^t_0 \lambda} \quad (1.19)$$

donde ${}^t \tau := {}^t_0 J {}^t \sigma$ define a la tensión axial de Kirchhoff. Sabiendo que, por ejemplo, ${}^t_0 E = \ln({}^t_0 \lambda)$, la potencia (1.19) se puede expresar como

$${}^t \tau \frac{{}^t \dot{\lambda}}{{}^t_0 \lambda} = {}^t T {}^t_0 \dot{E}^{(0)} \quad (1.20)$$

Ya que ambas expresiones (1.19) y (1.20) proporcionan el mismo valor de potencia mecánica, diremos que la medida de tensión ${}^t T = {}^t \tau$ es conjugada de trabajo de ${}^t_0 E$. Como la deformación logarítmica ${}^t_0 E$ es una medida material, la tensión ${}^t T$ es también una medida material. Igual que ocurre con las diferentes medidas

Figura 1.6: Ensayo de tensión cíclico de una goma con refuerzo de carbono que exhibe efecto Mullins.

de deformación, como el estado tensional es único en cada instante, si se conoce, por ejemplo, el valor tT asociado a un estado de deformación, directamente se puede obtener cualquier otra medida de tensión a través de la relación de transformación correspondiente. Se puede comprobar fácilmente que en el límite de pequeñas deformaciones, todas las medidas materiales y espaciales de tensión coinciden numéricamente, por lo que se define la tensión ingenieril de Cauchy ${}^t\sigma$ como la única medida de tensión.

1.5. Efecto Mullins

Los modelos hiperelásticos introducidos en el Apartado 1.3 no son capaces de simular el comportamiento de ciertos polímeros que se caracterizan por la pérdida de rigidez cuando se someten a grandes deformaciones. Este ablandamiento, relacionado con el daño que experimenta el material, se conoce como *efecto Mullins*, ya que Leonard Mullins es considerado el pionero en advertirlo en su trabajo publicado en 1947 [31]. Posteriormente fue estudiado en profundidad por Bueche [32], [33], Mullins [34], Johnson y Beatty [36], [37], Souza Neto et al. [35], entre otros.

Para explicar las principales características de este fenómeno de ablandamiento de tensiones se considera el ensayo uniaxial cíclico de la Figura 1.6, controlado por la deformación de una muestra de goma reforzada con partículas de carbono. El ciclo de carga y descarga parte del estado O virgen, sin tensión, y sigue la trayecto-

ria a , llamada carga primaria. Al descargar desde un punto aleatorio A , la muestra continúa por la rama b y regresa completamente al estado O sin tensión (para muestras reales esto raramente ocurre, pues suelen aparecer deformaciones remanentes). Nótese que una vez que la muestra ha sido sometida a la tensión máxima correspondiente al punto A , sus propiedades originales han cambiado permanentemente. El área encerrada por las curvas a y b representa la energía disipada por histéresis, dicha energía ya no se puede recuperar. Cuando el material es recargado el comportamiento tensión-deformación sigue la curva b otra vez hasta el punto A , donde comenzó la descarga, si a continuación se impone una deformación superior a la correspondiente a dicho punto, continuará por la curva c , que es una continuación de la curva primaria a . Nótese que para los modelos hipereelásticos clásicos, la carga se efectuaría por el camino ac y la descarga se efectuaría por el mismo camino ca .

1.6. Resolución computacional del Problema del Valor de Contorno¹

Como ya se ha visto, la solución analítica puede ser muy complicada o imposible de obtener por lo que se recurre a la solución numérica. El método numérico empleado en este trabajo es el de los elementos finitos. De este modo, los modelos computacionales y algoritmos numéricos desarrollados en esta tesis se han implementado en un código propio de elementos finitos denominado DULCINEA², programado en Fortran 90. En el programa DULCINEA se realizan las etapas de preproceso y cálculo. Las etapas de postproceso y visualización de resultados se llevan a cabo en un postprocesador implementado a tal efecto en *MATLAB*®. El programa DULCINEA permite una alta flexibilidad a la hora de incorporar nuevas subrutinas, como nuevos elementos, modelos de material y cualquier otro procedimiento, integrándose fácilmente en la estructura principal del programa. Asimismo, es especialmente práctico para el investigador, puesto que permite un control absoluto de todos los procedimientos de cálculo.

El programa DULCINEA permite la realización de análisis lineales y no lineales, tanto estáticos como dinámicos. Se incorporan distintos tipos de métodos de resolución del sistema de ecuaciones (LU , Gradiente conjugado, LDU y Bi -

¹Este apartado ha sido extraído y actualizado a partir del correspondiente apartado de la Tesis Doctoral “Métodos computacionales para visco-hiperelastividad anisótropa en grandes deformaciones”, realizada por Marcos Latorre Ferrús, dirigida también por Francisco Javier Montáns Leal.

²Programa creado por Francisco Javier Montáns Leal. El nombre DULCINEA es el acrónimo de “Dynamic Updated/total Lagrangean Code for Incremental Nonlinear Finite Element Analysis”.

1.6. RESOLUCIÓN COMPUTACIONAL DEL PROBLEMA DEL VALOR DE CONTORNO

CGSTAB) dependiendo de las características del problema (matrices simétricas/no simétricas, dimensión del sistema de ecuaciones, etc.). Para el caso no lineal, se incorpora el método de Newton-Raphson, que es un método implícito que resuelve el sistema de ecuaciones de forma iterativa. Por otra parte, también se incorporan búsquedas lineales (“line searches”), las cuales pueden activarse cuando se detecta una divergencia durante las iteraciones globales. Además, se ha implementado un procedimiento automático de subdivisión de paso de carga (“automatic time stepping”), que también presenta la opción de activarse en casos de falta de convergencia de la solución. Se espera incorporar un control mixto fuerza-desplazamiento, como el método de longitud de arco (“arc-length”), como otra herramienta para intentar evitar la divergencia de la solución ante la presencia de inestabilidades.

En este código de elementos finitos se pueden abordar análisis no lineales de varios tipos, ya sean no linealidades del material (plasticidad, viscoplasticidad, etc.) o no linealidades geoméricas (hiperelasticidad, formulación en grandes deformaciones). En el programa están implementadas diversas subrutinas de material, tanto de materiales elásticos lineales, como materiales hiperelásticos isótropos (Neo-Hookean, Ogden, Mooney-Rivlin, etc.) o modelos isótropos y anisótropos de plasticidad con endurecimiento mixto en grandes deformaciones. Además, se incorpora la hipótesis cinemática de pequeñas deformaciones y la formulación general de grandes deformaciones, ésta última implementada en dos formulaciones lagrangianas: *Updated Lagrangean* (UL) y *Total Lagrangean* (TL). En la formulación de grandes deformaciones, se incorporan medidas de deformación tanto materiales como espaciales (deformación de Green, Almansi o Hencky) y de tensión (tensiones de Cauchy, de Piola-Kirchhoff o generalizadas de Kirchhoff).

DULCINEA incorpora elementos bidimensionales, denominados *QUAD*, bajo las hipótesis de tensión plana, deformación plana y formulación axisimétrica, así como elementos tridimensionales, denominados *BRCK*. Estos elementos presentan las opciones de un número variable de nudos y de puntos de integración. Por otro lado, se incorporan elementos para formulación mixta en grandes deformaciones (formulación u/p) bidimensionales, denominados *QMIX*, y tridimensionales, denominados *BMIX*, que se utilizan en problemas con un alto grado de incompresibilidad. El programa incluye elementos que permiten distintas combinaciones de nudos de desplazamientos y de presión, con un número también variable de puntos de integración. También contiene elementos mixtos basados en modos incompatibles en grandes deformaciones *BINC* y *BENH*.

El usuario lleva a cabo el preproceso a través de un archivo de entrada que está compuesto por una serie de comandos ordenados secuencialmente. Este archivo de entrada permite la definición de parámetros, bucles, condicionales y operaciones básicas entre variables, lo cual otorga flexibilidad a la hora de automatizar la definición e implementación del mallado de elementos, condiciones de contorno y

definición de cargas.

Los resultados obtenidos en DULCINEA se exportan en archivos de texto para posteriormente visualizarlos a través de un programa desarrollado en *MATLAB*® que actúa como postprocesador. Este postprocesador consta de un menú principal interactivo, implementado en formato de ventanas, en el cual se tiene acceso las diferentes tareas programadas. Entre las funcionalidades del postprocesador cabe destacar las siguientes: visualización de elementos y su numeración, nodos y su numeración, condiciones de contorno y cargas aplicadas, configuraciones deformadas, distribución (“band plots”) de medidas de tensión y deformación personalizadas, creación de simetrías y reflexiones de la malla de elementos inicial, cambio del mapa de colores y creación de secuencias y vídeos.

Una de las tareas realizadas en este trabajo ha sido la revisión del programa DULCINEA (varias subrutinas han sido modificadas y mejoradas) y la ampliación de las funcionalidades del mismo. Se han implementado las subrutinas de material para el análisis numérico del comportamiento de materiales que presentan elasto-plasticidad anisótropa en pequeñas deformaciones. Se han implementado también las respectivas subrutinas de material para el tratamiento numérico de los materiales hiperelásticos con daño tanto isótropos como ortótropos presentados en esta tesis. Finalmente, con el fin de llevar un control sobre las distintas tareas que se van implementando en el programa DULCINEA, se ha iniciado un seguimiento de las sucesivas versiones del programa que se han ido generando.

1.7. Estructura de la tesis

Lo anteriormente expuesto constituye el marco en el que se ha desarrollado esta tesis doctoral.

En el capítulo 2, se ha realizado un estudio sobre los algoritmos de plasticidad en pequeñas deformaciones donde se han analizado diversas formas de implementar los algoritmos de retorno del tipo *Closest Point Projection*, para demostrar la importancia que tiene una cuidadosa implementación sobre la eficiencia de los mismos.

En el capítulo 3, se muestra un exhaustivo estudio del arte sobre la Mecánica del Daño, donde se realiza una revisión de diferentes modelos encontrados en la literatura y sus formulaciones.

En el capítulo 4, se introducen los fundamentos de los modelos hiperelásticos basados en *splines*, también llamados modelos *What-You-Prescribe-Is-What-You-Get* (*WYPIWYG*) tanto para el caso de hiperelasticidad isótropa como ortótropa.

En el capítulo 5, basado en la filosofía WYPIWYG, se presenta un nuevo enfoque para modelar el daño en materiales hiperelásticos incompresibles tanto isótropos como ortótropos.

1.7. ESTRUCTURA DE LA TESIS

En el capítulo 6, se exponen las conclusiones obtenidas y se plantea la línea de investigación futura.

Todos los modelos incluidos en esta tesis son fenomenológicos y han sido formulados en deformaciones materiales logarítmicas. En todos los casos se acepta la hipótesis de (cuasi-)incompresibilidad. El contenido principal se presenta a través de los diferentes trabajos (ya publicados o en proceso de revisión) a los que ha dado lugar esta tesis.

Capítulo 2

Estudio sobre la implementación de los algoritmos Closest Point Projection

2.1. Introducción

Al empezar a estudiar las formulaciones y modelos de daño existentes, que se presentarán en el Capítulo 3, se observaron bastantes similitudes con los típicos algoritmos de elastoplasticidad basados en el retorno radial, por ello se decidió realizar un análisis sobre la forma más eficiente de implementar dichos algoritmos como paso previo a poder formular e implementar un modelo de daño de la forma más eficiente posible. Con este fin, en este capítulo se va a presentar un estudio previo donde se comparó la eficiencia de tres algoritmos distintos para elastoplasticidad en pequeñas deformaciones. Los tres algoritmos seleccionados están basados en la idea de los algoritmos de *Proyección al Punto más Cercano* –más conocidos por su nombre en inglés *Closest Point Projection*, de ahora en adelante *CPP*. Por lo general, en los análisis realizados mediante el método de los elementos finitos, entre los posibles marcos de algoritmos de integración de tensiones en elastoplasticidad computacional, el algoritmo implícito CPP es probablemente el más utilizado. Estos algoritmos se basan en que todas las variables necesarias, incluidas las direcciones de flujo y de endurecimiento, se actualizan de forma iterativa y se hacen cumplir en la solución final. Por tanto, el algoritmo es totalmente implícito y la solución final es independiente de las iteraciones anteriores. Sin embargo, existen múltiples formas de llevar a cabo la implementación de este algoritmo. A pesar de que la convergencia cuadrática asintótica puede obtenerse en todas las implementaciones si el algoritmo se linealiza correctamente, estas diferentes posibilidades derivan en un número diferente de iteraciones locales y en un coste computacional

bastante distinto. Los algoritmos de integración de tensiones en pequeñas deformaciones son a menudo el núcleo iterativo de formulaciones elastoplásticas en grandes deformaciones simplemente añadiendo un preprocesador y un postprocesador no iterativos. Al mismo tiempo que son responsables de una gran parte del tiempo de cálculo global en simulaciones de elementos finitos y desempeñan un papel clave en la robustez general. En este capítulo se presenta un nuevo¹ algoritmo basado en las ideas del CPP para elastoplasticidad anisótropa con endurecimiento mixto. También se compara esta propuesta con otras posibles implementaciones del algoritmo CPP para el mismo problema, en concreto con la implementación general del CPP realizada por Simó y Hughes [38] y con la implementación de un algoritmo basado en los *Métodos de Parámetro de Gobierno* –más conocidos por su denominación en inglés *Governing Parameter Method*, de ahora en adelante *GPM*– llevada a cabo por Kojic *et al.* [39]. Se demuestra que el algoritmo propuesto es en general más eficiente.

2.2. Algoritmos de integración de tensiones

El punto de partida para cualquier relación elastoplástica en pequeñas deformaciones es la división fundamental del tensor tasa de deformación en una componente elástica $\dot{\epsilon}^e$ y una plástica $\dot{\epsilon}^p$ del siguiente modo

$$\dot{\epsilon} = \dot{\epsilon}^e + \dot{\epsilon}^p \quad (2.1)$$

Basándose en esta descomposición la relación tensión-deformación se puede escribir como

$$\dot{\sigma} = \mathbb{C}^e(\dot{\epsilon} - \dot{\epsilon}^p) \quad (2.2a)$$

La tasa de deformación plástica para plasticidad asociativa sigue una relación del siguiente tipo

$$\dot{\epsilon}^p = \dot{t} \frac{\partial f}{\partial \sigma} \quad (2.3)$$

donde f es la superficie de fluencia y $\dot{t}$ el parámetro de consistencia, el cual representa la magnitud del flujo plástico, $\frac{\partial f}{\partial \sigma}$ (a partir de ahora $\partial_\sigma f$) determina la dirección del flujo. El uso de una regla de flujo asociativa asegura que los incrementos de deformación plástica sean vectores perpendiculares a la superficie de fluencia. Las condiciones complementarias de Kuhn-Tucker y la condición de consistencia son

$$\dot{t} \geq 0, \quad f \leq 0, \quad \dot{t} f = 0 \quad \text{y} \quad \dot{t} \dot{f} = 0 \quad (2.4)$$

¹Este algoritmo fue inicialmente desarrollado en la Tesis Doctoral “Elastoplasticidad anisótropa de metales en grandes deformaciones”, realizada por Miguel Ángel Caminero Torija y dirigida por Francisco Javier Montáns Leal.

2.2. ALGORITMOS DE INTEGRACIÓN DE TENSIONES

Las técnicas para la integración de las ecuaciones constitutivas a nivel local controlan directamente la exactitud y la estabilidad de la solución numérica global. Principalmente estas técnicas se dividen en dos categorías, las técnicas explícitas (forward-Euler) y las implícitas (backward-Euler). Los esquemas implícitos fueron ampliamente usados [40], [41] hasta que en 1985 Simó y Taylor [42] propusieron el algoritmo implícito de proyección al punto más cercano, que es un tipo de algoritmo de retorno. Los algoritmos de retorno consisten en integrar primero las ecuaciones elásticas con el incremento total de deformación para obtener un predictor elástico. La tensión predicha elásticamente se relaja hasta la superficie de fluencia mediante la corrección iterativa del incremento de deformación plástica. Se puede demostrar fácilmente que el método de retorno radial propuesto por Krieg y Krieg [43] es básicamente un caso especial de CPP para plasticidad de von Mises. La exactitud y estabilidad de los algoritmos de retorno han sido examinadas por Ortiz y Popov [44]. La tasa de convergencia cuadrática asintótica hace que el enfoque sea atractivo, sin embargo los algoritmos CPP presentan tres inconvenientes significantes. En primer lugar, hay una dificultad práctica en el cálculo del módulo tangente local cuando el retorno no es radial. En segundo lugar, se necesitan calcular los gradientes de la dirección del flujo plástico (segundas derivadas) lo que además de conllevar un coste computacional extra, para modelos complejos no siempre se pueden obtener fácilmente. Por último, la convergencia de las iteraciones locales puede ser un problema, por ejemplo, para casos complejos de endurecimiento no lineal. El tercer inconveniente se presenta también en modelos simples, por ejemplo plasticidad perfecta, en los puntos de Gauss cuando las tensiones ocurren en zonas de gran curvatura de la superficie de fluencia. En estos casos el corrector plástico puede tener problemas para restablecerse en la superficie de fluencia. En [45], [46] se presentan algunas de estas dificultades. En [47] se demuestra que se debe incluir un algoritmo de búsqueda lineal para asegurar la convergencia global cuando los algoritmos CPP se combinan con un método de Newton-Raphson. En [48] y [49] se propone el uso de una técnica de búsqueda lineal incluso para las iteraciones locales. Otro algoritmo de retorno que ha recibido atención en la literatura es el algoritmo de *Planos de Corte* –más conocido por su denominación en inglés *Cutting Plane*. Este algoritmo fue presentado por Simó y Ortiz en 1985 [50], [51]. El algoritmo está basado en una estrategia de máximo descenso, la cual evita la necesidad del tratamiento implícito de las ecuaciones de gobierno. El esquema resultante implica un proceso iterativo explícito, lo que conlleva unas propiedades de convergencia mejores que las del CPP. Sin embargo, estos algoritmos no se pueden linealizar consistentemente de forma cerrada, lo que limita su uso en implementaciones de elementos finitos que emplean como estrategia de solución el método de Newton-Raphson.

Los algoritmos de retorno, como ya se ha comentado, se basan en la idea de

CAPÍTULO 2. ESTUDIO SOBRE LA IMPLEMENTACIÓN DE LOS ALGORITMOS CLOSEST POINT PROJECTION

integrar primero las ecuaciones elásticas con el incremento total de deformación para obtener un predictor elástico, que se obtiene mediante las condiciones iniciales, que son los valores convergidos del paso previo. Posteriormente se devuelve el estado tensional a la superficie de fluencia mediante una corrección plástica. Si se expresan las Ecuaciones (2.1), (2.2a) y (2.3) de forma incremental mediante la aplicación del método de backward-Euler, se obtiene

$$\boldsymbol{\varepsilon}_{n+1} = \boldsymbol{\varepsilon}_n + \Delta \boldsymbol{\varepsilon} \quad (2.5)$$

$$\boldsymbol{\varepsilon}_{n+1}^p = \boldsymbol{\varepsilon}_n^p + \Delta t \partial \boldsymbol{\sigma} f \quad (2.6)$$

$$\boldsymbol{\sigma}_{n+1} = \mathbb{C}^e(\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}_{n+1}^p) \quad (2.7)$$

Sustituyendo la Ec. (2.6) en (2.7) resulta

$$\begin{aligned} \boldsymbol{\sigma}_{n+1} &= \mathbb{C}^e(\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}_n^p - \Delta t \partial \boldsymbol{\sigma} f) \\ &= \mathbb{C}^e(\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}_n^p) - \underbrace{\mathbb{C}^e \Delta t \partial \boldsymbol{\sigma} f}_{\text{plastic corrector}} \\ &= \underbrace{\boldsymbol{\sigma}_{n+1}^{tr}}_{\text{elastic predictor}} - \underbrace{\mathbb{C}^e \Delta t \partial \boldsymbol{\sigma} f}_{\text{plastic corrector}} \end{aligned} \quad (2.8)$$

donde $\boldsymbol{\sigma}_{n+1}^{tr}$ es la tensión de prueba determinada por el predictor elástico y $\mathbb{C}^e \Delta t \frac{\partial f}{\partial \boldsymbol{\sigma}}$ es el corrector plástico, el cual devuelve la tensión de prueba a la superficie de fluencia. Durante la fase de predicción elástica la deformación plástica permanece congelada mientras que durante la corrección plástica, es la deformación total la que permanece fija.

Ambos algoritmos, Cutting Plane y CPP, son algoritmos de retorno, la diferencia entre ellos radica en cómo llevan a cabo la corrección plástica. Para exponer las ideas de forma más sencilla, se va a plantear el caso de plasticidad perfecta, sin endurecimiento. El algoritmo CPP hace cumplir la regla de la perpendicularidad de la dirección de flujo a la superficie de fluencia, al final del paso, del siguiente modo

$$\Delta \boldsymbol{\sigma}_{n+1} = -\mathbb{C}^e \Delta \boldsymbol{\varepsilon}_{n+1}^p = -\Delta t_{n+1} \mathbb{C}^e \partial \boldsymbol{\sigma} f_{n+1} \quad (2.9)$$

Se define el flujo plástico de forma residual y la función de fluencia, tal que

$$\begin{cases} \boldsymbol{R}_{n+1}^{(k)} = \boldsymbol{\varepsilon}_n^p - \boldsymbol{\varepsilon}_{n+1}^{p(k)} + \Delta t_{n+1}^{(k)} \partial \boldsymbol{\sigma} f_{n+1}^{(k)} \\ f_{n+1}^{(k)} = 0 \end{cases} \quad (2.10)$$

Este sistema de ecuaciones se resuelve aplicando el método de Newton-Raphson, el cual conlleva una linealización sistemática. Finalmente se obtiene el incremento

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del parámetro de consistencia de forma implícita

$$\Delta^2 t_{n+1}^{(k)} = \frac{f_{n+1}^{(k)} - \partial_{\sigma} f_{n+1}^{(k)} : \mathbf{A}_{n+1}^{(k)} : \mathbf{R}_{n+1}^{(k)}}{\partial_{\sigma} f_{n+1}^{(k)} : \mathbf{A}_{n+1}^{(k)} : \partial_{\sigma} f_{n+1}^{(k)}} \quad (2.11)$$

donde

$$\left[\mathbf{A}_{n+1}^{(k)} \right]^{-1} = \mathbb{C}^{e-1} + \Delta t \partial_{\sigma}^2 f_{n+1}^{(k)} \quad (2.12)$$

se puede observar que aparece el gradiente de la regla de flujo plástico, que para casos de superficies de fluencia complejas, puede resultar difícil su obtención. Una vez obtenido el incremento del parámetro de consistencia, se pueden actualizar los valores de todas las variables y proceder a la siguiente iteración, hasta que converja.

Sin embargo, el algoritmo Cutting Plane fuerza la perpendicularidad al principio de la iteración, tal que

$$\Delta \sigma^{(k)} = -\mathbb{C}^e \Delta \epsilon^{p(k)} = -\Delta t^{(k)} \mathbb{C}^e \partial_{\sigma} f^{(k)} \quad (2.13)$$

En cada iteración si la función de fluencia se linealiza en torno al valor actual de la tensión $\sigma^{(k)}$, se obtiene

$$f^{(k+1)} = f^{(k)} + \partial_{\sigma} f^{(k)} \Delta \sigma^{(k)} \quad (2.14)$$

de donde se puede despejar de forma explícita el incremento del parámetro de consistencia

$$\Delta^2 t_{n+1}^{(k)} = \frac{f_{n+1}^{(k)}}{\partial_{\sigma} f_{n+1}^{(k)} : \mathbb{C}_{n+1}^{e(k)} : \partial_{\sigma} f_{n+1}^{(k)}} \quad (2.15)$$

En las Figuras 2.1 y 2.2 se representan las interpretaciones geométricas del algoritmo CPP y Cutting Plane, respectivamente.

Una vez planteada la idea del algoritmo CPP y habiendo comparado sus propiedades con otro algoritmo de retorno (Cutting Plane), se presenta en el siguiente artículo, un estudio sobre la importancia de una cuidadosa implementación de los algoritmos CPP.

Como resumen, los puntos más importantes tratados en el siguiente artículo son:

- Presentación de un nuevo modelo para elastoplasticidad anisótropa en pequeñas deformaciones basado en la idea de los algoritmos CPP.

Figura 2.1: Interpretación geométrica del algoritmo CPP en el espacio de tensiones.

Figura 2.2: Interpretación geométrica del algoritmo Cutting Plane en el espacio de tensiones

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- Comparación entre la implementación del algoritmo que se propone con la típica implementación del algoritmo GCPP y con la de un algoritmo tipo GPM.
- Exposición de ejemplos resueltos mediante los tres algoritmos para demostrar la importancia que tiene la implementación llevada a cabo en la eficiencia y robustez de los algoritmos.

On the numerical implementation of the Closest Point Projection algorithm in anisotropic elasto-plasticity with nonlinear mixed hardening

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Abstract In finite element analysis, among the possible frameworks for stress-point integration algorithms in computational elastoplasticity, the implicit Closest Point Projection (CPP) algorithm is probably the most used one. The idea behind this algorithm is that all necessary variables, including the flow and hardening directions, are iteratively updated and enforced at the final solution. Therefore the algorithm is fully implicit and the final solution is independent of previous iterations. However, there are several possible implementations of the ideas behind the CPP algorithm. Even though asymptotic quadratic convergence may be obtained in all implementations if the algorithm is properly linearized, these different possibilities result in a different number of local iterations and in a different computational effort. Small stress-integration algorithms are frequently the only iterative core of large strain elastoplastic formulations. At the same time they are responsible for a large share of the overall computational time in finite element simulations and key in the overall robustness. In this work we present a new algorithm based on the ideas of the Closest Point Projection algorithm for anisotropic elastoplasticity with mixed hardening. We also compare our proposal with other possible implementations of the CPP algorithm for the same problem, namely the General CPP implementation and the Governing Parameter Method. We show that our proposal is in general more efficient.

Keywords Anisotropic elastoplasticity · Closest Point Projection algorithm · Mixed hardening · Radial Return Algorithm · Governing Parameter Method

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1 Introduction

The finite element simulations of plastic deformations in metals is nowadays very common in academia and industry [7], [58], [29], [12], [47], where for example there is a need for accurate predictions of the deformations produced during manufacturing processes [58] or during service of the products, as in crash-worthiness [29]. Plastic behavior is inherently nonlinear and, hence, local and global iterations are needed in general in order to fulfill simultaneously constitutive and equilibrium equations. Many current large strain models employ as the core iterative process algorithms identical or similar to those of small strains [14], [45], [42], [36], [10], so the large strain kinematics reduce to noniterative pre- and postprocessors. Therefore the efficiency of the small strains integration algorithm is very important in the overall efficiency of finite element simulations.

The radial return algorithm of Wilkins [60] and the ulterior work of Krieg and Key [31] are milestones in the currently favoured approach to the local integration of the governing equations of elastoplasticity. Even being implicit, in the case of von Mises plasticity the return direction for the stress tensor is known directly from the trial state (elastic predictor) and this flow direction does not enter in the local iterative procedure. Thus, the whole procedure may be efficiently parametrized using a single scalar as in the Governing Parameter Method (GPM) [29], [28], [54]. For the case of linear hardening the solution is obtained in closed form, i.e. in just one iteration. Nonlinear hardening models may also be easily solved using a single nonlinear scalar equation [37], [39], [33], [64], [2], [3].

The generalization of these ideas converged to those of the Closest Point Projection algorithm in optimization theory [34]: the elastoplastic solution is in essence the solution to a minimization problem [47]. Then, the extension of the algorithm of Wilkins to general plasticity models and mixed isotropic and kinematic hardening is known as the Closest Point Projection (CPP) algorithm [47], [49]. In the General Closest Point Projection (GCPP) implementation, a general framework is established for any yield function, elastic constitutive behavior and type of hardening. The main difficulty in the implementation of the CPP algorithm is in that the algorithm needs the Hessians and in that all constitutive equations are coupled, hence solved simultaneously. However the implementation is otherwise straightforward, so the procedure has been applied to different models, see for example [9], [15], [5], [25], among many others. Local and global asymptotic quadratic convergence is achieved if the algorithm is consistently linearized [48], but associated convergence difficulties are known [43]. Frequently some simplifications are considered in order to obtain more robust (but frequently less efficient) methods [30], [29], see also [62]. A usual alternative to avoid the computation of Hessians is the simpler Cutting Plane Algorithm, where part of the return to the yield surface is performed successively at each iteration. In this case asymptotic

second order convergence is usually not attained [47] and, hence, it is much less efficient. Furthermore, it may be questioned from physical grounds because the final solution should not depend on the arbitrary iterations. Both algorithms are in general first order accurate [46]. Second order accurate algorithms are also possible [46], but their second order accuracy is often not preserved in general finite element simulations [19], [13].

The General implementation of the CPP algorithm is basically the same regardless of the yield surface and hardening being considered. One simply plugs the expressions for the second derivatives of the yield surface respect to the stress, backstress and overstress and obtain seamlessly the corresponding integration algorithm. However, care must be exercised for the special cases when kinematic or isotropic hardening is small because bad conditioning is possible in the local system of equations, so different versions must be programmed in the code to account for these cases. Furthermore, because all equations are solved simultaneously without any prior reduction, the computational cost is usually higher than that obtained if the system of equations is previously reduced as much as possible. Another source of possible bad conditioning is the different nature of the variables involved.

The essence of the Governing Parameter Method (GPM) is to establish a scalar equation that can be solved using any method for nonlinear scalar equations (Newton-Raphson, bisection, regula-falsi, etc.) so local convergence is always guaranteed (if solution of the equation exists) and the mentioned properties of the parent multivariable algorithm are preserved. These scalar implementations may be more efficient and in some cases more robust than that of the nonlinear system of equations, where tensorial equations are enforced iteratively and the procedure largely depends on the type of hardening, but the large manipulations involved make it virtually impossible in many cases. For the case of anisotropic elastoplasticity using the Hill [21] yield surface, Kojić et al [30] –see also [29]– give a local robust Governing Parameter formulation in which some key approximations are considered in the algorithm. Because these approximations hold at convergence, local asymptotic quadratic convergence is preserved, but the number of preliminary iterations is larger because they do not hold during those iterations.

In this paper we present a computational procedure for small strain anisotropic elastoplasticity with mixed hardening based on Hill's 1948 criterion [21], [22]. The small strain algorithm is a modified Closest Point Projection algorithm [47] developed in the spirit of the Governing Parameter Method [29]. The efficient implementation using two scalar parameters and valid for any mixed hardening parameters is robust for large steps. All terms of both consistent local and global tangents are given so in contrast to the proposal of Kojić et al [30] global asymptotic quadratic convergence is also preserved. We herein compare the layout and resulting efficiency of the three stress integration algorithms: General Closest Point Projection (GCPP) [47], the Governing Parameter Method of Kojić et

al [30] and the algorithm proposed in this paper. This small strain algorithm may be used unmodified in the plastic correction phase of the large strain formulation of Reference [10] based on logarithmic strain measures and generalized Kirchhoff stress measures [10], [38], [32]. The algorithm of Reference [10] uses an *incremental* decomposition of logarithmic strains. Other algorithms use additive (Green) decompositions of the strain measures, plastic metrics and/or elastic isotropy in the constitutive equations, see [42], [36], [54], [33], [35], [55], [56], [16], [63] among others. Additive splits of total (versus incremental) strains have been criticized regarding the resulting constitutive equations [44], [40].

The rest of the paper is organized as follows. We first briefly summarize the continuum anisotropic elastoplastic model in order to introduce notation. Then we summarize the GCPP algorithm we used in the comparisons specialized to Hill's yield function with mixed hardening. Next we describe our proposed integration algorithm and then the GPM of [30] which can be immediately explained from our proposal. During the presentation of the algorithms we highlight the common points and the differences in order to understand their performance. Finally we show some examples to compare the performance of the proposed algorithm with the GCPP and GPM alternatives, and also to show the performance of the proposed algorithm in general finite element simulations.

2 Continuum formulation of Hill plasticity with mixed hardening.

2.1 Hill's yield function

In this paper we use Hill's anisotropic criterion of 1948 [21], see also [29]. This criterion may be written in the small strains context using Hill's original notation as

$$2\bar{f}_y(\boldsymbol{\sigma}) \equiv F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\tau_{23}^2 + 2M\tau_{31}^2 + 2N\tau_{12}^2 = 1 \quad (1)$$

where F, G, H, L, M, N are Hill's anisotropic material parameters and σ_{ij} are the components of the stress tensor in the principal orthotropic planes (symmetry planes). Defining the overstress tensor as $\mathbf{Z} = \boldsymbol{\sigma} - \boldsymbol{\beta}$, where the tensors $\boldsymbol{\sigma}$ and $\boldsymbol{\beta}$ define the stress tensor and the backstress tensor respectively, we can formulate this criterion in a more operational way from a computational standpoint as

$$f_y = \frac{1}{2} \mathbf{Z} : \mathbb{N} : \mathbf{Z} - \frac{1}{3} k^2 \quad (2)$$

where k is the effective yield stress hardened by the isotropic hardening part. If $f_y > 0$ yielding takes place. The anisotropic fourth-order tensor $\mathbb{N}$ is defined in the

directions of principal anisotropy $\mathbf{X}_{pr} = \{1, 2, 3\}$, using Voigt notation, as [29]

$$[\mathbb{N}] = \begin{bmatrix} N_1 + N_2 & -N_1 & -N_2 & 0 & 0 & 0 \\ -N_1 & N_1 + N_3 & -N_3 & 0 & 0 & 0 \\ -N_2 & -N_3 & N_2 + N_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & N_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & N_{23} & 0 \\ 0 & 0 & 0 & 0 & 0 & N_{31} \end{bmatrix} \quad (3)$$

where

$$N_1 = \frac{2}{3}H\sigma_y^2 =: \frac{2}{3}h, N_2 = \frac{2}{3}G\sigma_y^2 := \frac{2}{3}g, \dots \quad (4)$$

and the scalar σ_y is the reference yield stress (i.e. usually the initial yield stress K_0). The parameters $h = H/\sigma_y^2$, $g = G/\sigma_y^2$, .. are Hill's dimensionless parameters. Another handy form of the Hill criterion which will be used in Section 4.3 is

$$f_y > 0 \Leftrightarrow \tilde{f}_y = \sqrt{\mathbf{Z} : \mathbb{N} : \mathbf{Z}} - \sqrt{\frac{2}{3}}k > 0 \quad (5)$$

Both expressions are equivalent to check yield, but the resulting computational algorithms are different.

2.2 Flow and hardening rules

In order to obtain the flow and hardening rules, consider the stress power per unit volume

$$\mathcal{P} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_e + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p \quad (6)$$

As usual, we have assumed an additive decomposition of the total small strain tensor *rate* into an elastic and a plastic part, $\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_e + \dot{\boldsymbol{\varepsilon}}_p$. The plastic strain rate is obtained from the constitutive equation *in rate form*, according to the path-dependent nature of plastic strains. Then the total plastic strains are obtained from time integration (or load step integration) as

$$\boldsymbol{\varepsilon}_p = \int_0^t \dot{\boldsymbol{\varepsilon}}_p dt \quad (7)$$

and the elastic strains are obtained as

$$\boldsymbol{\varepsilon}_e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p \quad (8)$$

As usual, we assume a stored energy function $\mathcal{W}$ and a hardening potential $\mathcal{H}$, which for small strains are of the form

$$\begin{cases} \mathcal{W}(\boldsymbol{\varepsilon}_e) = \frac{1}{2}\boldsymbol{\varepsilon}_e : \mathbb{C}^e : \boldsymbol{\varepsilon}_e \\ \mathcal{H}(\mathbf{q}) = \frac{1}{2}\boldsymbol{\xi} : \mathbb{H} : \boldsymbol{\xi} + h(\zeta) \end{cases} \quad (9)$$

where $\mathbb{C}^e$ is the tensor of small strain elastic constants, $\mathbb{H}$ is a hardening tensor, $h(\zeta)$ is a isotropic hardening potential, for example $h(\zeta) = \frac{1}{2} (m\bar{H}) \zeta^2$ in the case of linear isotropic hardening, and $\mathbf{q} = \{\boldsymbol{\xi}, \zeta\}$ are the internal variables, where $\boldsymbol{\xi}$ is a tensor one and $\zeta \geq 0$ a scalar one such that $\dot{\zeta} \geq 0$. $(m\bar{H})$ is a material scalar. For a linear isotropic hardening, the actual yield stress is $k = K_0 + \kappa$, where K_0 is the initial yield stress and $\kappa = h' \equiv (m\bar{H}) \zeta$. We now consider a free energy function of the form $\psi = \mathcal{W} + \mathcal{H}$, but only the rate form is employed, which is consistent with the path dependency due to the plastic nature of the internal variables

$$\dot{\psi} = \dot{\mathcal{W}} + \dot{\mathcal{H}} = \frac{\partial \mathcal{W}}{\partial \boldsymbol{\varepsilon}_e} : \dot{\boldsymbol{\varepsilon}}_e + \frac{\partial \mathcal{H}}{\partial \boldsymbol{\xi}} : \dot{\boldsymbol{\xi}} + \frac{\partial \mathcal{H}}{\partial \zeta} \dot{\zeta} \quad (10)$$

Then, the dissipation equation of the commonly used theory takes the form

$$\mathcal{D} = \mathcal{P} - \dot{\psi} = \left(\boldsymbol{\sigma} - \frac{\partial \mathcal{W}}{\partial \boldsymbol{\varepsilon}_e} \right) : \dot{\boldsymbol{\varepsilon}}_e + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p - \frac{\partial \mathcal{H}}{\partial \boldsymbol{\xi}} : \dot{\boldsymbol{\xi}} - \frac{\partial \mathcal{H}}{\partial \zeta} \dot{\zeta} \geq 0 \quad (11)$$

Following the usual Coleman procedure, we obtain the sufficient conditions

$$\boldsymbol{\sigma} = \frac{\partial \mathcal{W}}{\partial \boldsymbol{\varepsilon}_e} = \mathbb{C}^e : \boldsymbol{\varepsilon}_e, \quad \boldsymbol{\beta} = \frac{\partial \mathcal{H}}{\partial \boldsymbol{\xi}} = \mathbb{H} : \boldsymbol{\xi} \quad \text{and} \quad \kappa = \frac{\partial \mathcal{H}}{\partial \zeta} \equiv h'(\zeta) \quad (12)$$

so the plastic dissipation takes the expression

$$\mathcal{D}^p = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p - \boldsymbol{\beta} : \dot{\boldsymbol{\xi}} - \kappa \dot{\zeta} \geq 0 \quad (13)$$

If the stress state is restricted to a given domain of the form $f_y(\boldsymbol{\sigma} - \boldsymbol{\beta}, \kappa)$, the Lagrangian and the Principle of Maximum Dissipation give the associative flow and hardening rules [29], [37] which we specialize to the current model

$$\mathcal{L}(\boldsymbol{\sigma}, \boldsymbol{\beta}, \kappa) = \mathcal{D}^p - \dot{t} f_y \Rightarrow \nabla \mathcal{L} = 0 \Rightarrow \begin{cases} \dot{\boldsymbol{\varepsilon}}_p = \dot{t} \partial f_y / \partial \boldsymbol{\sigma} = \dot{t} \mathbb{N} : \mathbf{Z} \\ \dot{\boldsymbol{\xi}} = -\dot{t} \partial f_y / \partial \boldsymbol{\beta} = \dot{t} \mathbb{N} : \mathbf{Z} = \dot{\boldsymbol{\varepsilon}}_p \\ \dot{\zeta} = -\dot{t} \partial f_y / \partial \kappa = \frac{2}{3} k \dot{t} \end{cases} \quad (14)$$

where as it is well known, because of the form Eq. (2), ζ takes the meaning of the effective accumulative plastic strain as it is straightforward to verify –see Equation (3.3.16) of Reference [29] and section 4.1– and hence we will also use the notation $\bar{\varepsilon}_p$. The complementary (loading/unloading) Kuhn-Tucker conditions and the consistency condition are [29], [37]

$$\dot{t} \geq 0, \quad f_y \leq 0, \quad \dot{t} f_y = 0 \quad \text{and} \quad \dot{t} \dot{f}_y = 0 \quad (15)$$

These equations result in the evolutions

$$\dot{\boldsymbol{\sigma}} = \mathbb{C}^e : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_p) = \mathbb{C}^e : \dot{\boldsymbol{\varepsilon}} - \dot{t} \mathbb{C}^e : \mathbb{N} : \mathbf{Z} \quad \text{and} \quad \dot{\boldsymbol{\beta}} = \dot{t} \mathbb{H} : \mathbb{N} : \mathbf{Z} \quad (16)$$

In the actual implementation of the theory we will use linear kinematic hardening as it is customary, but we will consider nonlinear isotropic hardening as a

yet to be prescribed nonlinear phenomenological function of the equivalent plastic strains ζ , i.e. $h'(\zeta) = \kappa(\zeta)$. This function is to be computed for the updated and implicitly obtained ζ for the final, converged, solution. This approach has some similarities to that of Hennen and Anand [20], but the actual term in the dissipative equation is different, see discussion in [20] and [38]. However this issue is not relevant in the present small strains formulation so for short we use the more compact traditional framework.

2.3 Anisotropic elasticity

In computational plasticity it is usual to consider the effect of elastic anisotropy significantly smaller than the effect of plastic anisotropy [18], [17], [23], [4]. Consequently, elastic isotropic expressions are often used for elastic stored energy functions with anisotropic yield criteria, specially at large strains [12]. However, the influence of elastic anisotropy in the elastoplastic behavior can be very important specially during elastic recovery processes. Another issue is that although the elastic strains are small compared to the plastic strains, the stored energy depends primarily on the elastic ones, and therefore the elastic strain effect on the solid behavior can be significant. Hence, the decision of neglecting elastic anisotropy depends on the specific problem at hand, but a constitutive model should include elastic anisotropy in a general case.

In the case of small strain elasticity, we can easily define a strain-stress relationship using the compliance elastic tensor $\mathbb{S}^e$ as (see for example References [29], [26])

$$\boldsymbol{\varepsilon}_e = \mathbb{S}^e : \boldsymbol{\sigma} \quad (17)$$

where $\mathbb{S}^e$ is the inverse of the elastic constitutive tensor $\mathbb{C}^e$. For an orthotropic material, the compliance elastic matrix components in terms of the engineering constants, and in principal natural directions $\mathbf{X}_{pr} = \{1, 2, 3\}$, are

$$[\mathbb{S}^e] = \begin{bmatrix} 1/E_1 & -\nu_{12}/E_2 & -\nu_{31}/E_3 & 0 & 0 & 0 \\ -\nu_{21}/E_1 & 1/E_2 & -\nu_{32}/E_3 & 0 & 0 & 0 \\ -\nu_{13}/E_1 & -\nu_{23}/E_2 & 1/E_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{23} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G_{31} \end{bmatrix} \quad (18)$$

where E_1 , E_2 and E_3 are Young's moduli in directions 1, 2 and 3 respectively; ν_{ij} are Poisson's ratios and G_{ij} are shear moduli. In summary, there are 9 independent constants which define the elastic behavior of the orthotropic solid with the principal symmetry planes. Some restrictions apply to these constants in order to ensure symmetry and positive-definiteness, see [26].

In some rolled materials, variations of elastic properties (such as the Young's modulus and the Poisson's ratio) with respect to the rolling direction may become of the same order as the variation of the plastic properties, see for example References [59], [1]. Hence, as mentioned, the consideration of elastic anisotropy is important. In other materials the variation of elastic properties is much smaller [6] and the hypothesis could be justified.

2.4 Modification for use in mixed u/p finite element formulations.

One of the problems that may appear when using anisotropic elasticity is the coupling of the pressure with the plastic flow because of the coupling present in the elastic tangent $\mathbb{C}^e$ between deviatoric and volumetric components, see Eqs. (18) and (16). This coupling prevents the use of optimal mixed u/p finite element formulations because the derivatives of the pressure are not easily obtained. One solution in this case is to use enhanced formulations as those including incompatible modes [50], [51]. These formulations are usually reliable and efficient, but care should be taken because in some cases spurious modes may be present [11], [61], [41], [53]. These problems may be present in large strain elastoplasticity because of the evolution of the effective stiffness terms. Then, another more reliable possibility is to uncouple the volumetric part to facilitate the use of the u/p formulation which is known to pass the Inf-Sup condition for u -quadratic/ p -linear elements [7], [24]. In order to do so, in Eq. (16) the pressure change during the plastic flow is taken as zero, i.e.

$$\mathbf{I} : \mathbb{C}^e : \mathbb{N} = \mathbf{0} \quad (19)$$

where $\mathbf{I}$ is the second-order identity tensor. Since $\mathbb{N}$ is given by Equation (3), this equation formulates two restrictions on the elastic material parameters. Taking the product of the non-diagonal 3×3 upper-left boxes in principal directions, the following type of conditions are obtained

$$(N_1 + N_2) C_{ii11} - N_1 C_{ii22} - N_2 C_{ii33} = 0 \quad (20)$$

which are fulfilled for any N_i values only if

$$C_{ii11} = C_{ii22} = C_{ii33} \quad (21)$$

Similar conditions are given for the kinematic hardening constants, although for this case the conditions are typically fulfilled. Equations (21) furnish the sufficient conditions for the pressure to be unaltered from trial values during plastic flow (and elastic volumetric behavior to be decoupled). Hence, an anisotropic elastic

tensor with these restrictions has $9 - 2 = 7$ constants. The general form of the deviatoric part with 6 constants is given by Equation (3); hence,

$$\mathbb{C}^e = \bar{\kappa} \mathbf{I} \otimes \mathbf{I} + \mathbb{C}^{ed} \quad (22)$$

where $\bar{\kappa}$ is the bulk modulus (the 7th constant) and

$$[\mathbb{C}^{ed}] = \begin{bmatrix} C_1^{ed} + C_2^{ed} & -C_1^{ed} & -C_2^{ed} & & & \\ -C_1^{ed} & C_1^{ed} + C_3^{ed} & -C_3^{ed} & & & \\ -C_2^{ed} & -C_3^{ed} & C_2^{ed} + C_3^{ed} & & & \\ & & & C_{12}^{ed} & & \\ & & & & C_{23}^{ed} & \\ & & & & & C_{31}^{ed} \end{bmatrix} \quad (23)$$

In order to identify these constants we can make use of the pseudo-inverses defined as

$$(\bar{\kappa} \mathbf{I} \otimes \mathbf{I})^{\sim 1} := \left(\frac{1}{3} \mathbf{I} \otimes \mathbf{I} \right) : (\bar{\kappa} \mathbf{I} \otimes \mathbf{I} + \mathbb{C}^{ed})^{-1} = \frac{1}{\bar{\kappa}} \mathbf{I} \otimes \mathbf{I} \quad (24)$$

and

$$(\mathbb{C}^{ed})^{\sim 1} := \mathbb{P} : (\bar{\kappa} \mathbf{I} \otimes \mathbf{I} + \mathbb{C}^{ed})^{-1} \quad (25)$$

where $\mathbb{P} = \mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I}$ is the fourth order deviatoric projector and $\mathbb{I}$ the fourth order identity tensor. Note that $(\mathbb{C}^{ed})^{\sim 1}$ is independent of $\bar{\kappa}$ and $\frac{1}{\bar{\kappa}} \mathbf{I} \otimes \mathbf{I}$ is independent of $\mathbb{C}^{ed}$. Also

$$(\bar{\kappa} \mathbf{I} \otimes \mathbf{I})^{\sim 1} + (\mathbb{C}^{ed})^{\sim 1} = (\bar{\kappa} \mathbf{I} \otimes \mathbf{I} + \mathbb{C}^{ed})^{-1} = \mathbb{S}^e \quad (26)$$

so we immediately identify

$$\frac{1}{\bar{\kappa}} = (\mathbf{I} \otimes \mathbf{I}) : \mathbb{S}^e \quad (27)$$

$$(\mathbb{C}^{ed})^{\sim 1} = \mathbb{P} : \mathbb{S}^e =: \mathbb{S}^{ed} \quad (28)$$

These properties hold for decoupled responses. The equivalent for (21) in terms of flexibilities is obtained using results (26) and (27)

$$S_{ii11}^e = S_{ii22}^e = S_{ii33}^e = \frac{1}{3\bar{\kappa}} \quad (29)$$

Hence, the elastic bulk modulus, which arguably may have little variation due to anisotropy in metals, is given by

$$\frac{1}{\bar{\kappa}} = \frac{1 - \nu_{21} - \nu_{13}}{E_1} + \frac{1 - \nu_{12} - \nu_{23}}{E_2} + \frac{1 - \nu_{31} - \nu_{32}}{E_3} \quad (30)$$

As for the rest of the elastic constants, two of them are given by symmetry restrictions, for example ν_{31} and ν_{32} . The constant E_3 may be obtained from a known bulk modulus, Equation (30), or from direct measurements [27]. Constants E_1 , E_2 , ν_{12} are freely prescribed, i.e., obtained from experiments.

2.5 Nonlinear hardening law

In the examples given in this paper we have used a nonlinear hardening model in which a saturation hardening term of the exponential type, as in Voce [57], is appended to the linear term. Therefore, we can define

$$\mathbb{H} = \frac{2}{3} (1 - m) \bar{H} \mathbb{P} \quad (31)$$

and

$$k(\varepsilon_p) = K_0 + m \bar{H} \bar{\varepsilon}_p + (K_\infty - K_0) [1 - e^{-\delta \bar{\varepsilon}_p}] \quad (32)$$

where $\bar{H}$ is the effective linear hardening modulus, m is a parameter that controls mixed hardening (isotropic/kinematic hardening), K_0 is the reference yield stress and $K_\infty > 0$ and $\delta \geq 0$ are saturation law parameters.

3 Generalized implementation of the Closest Point Projection Algorithm

The General Closest Point Projection (GCPP) algorithm [47], [46] is an algorithm valid for any elastoplastic model if the explicit form of the first and second derivatives are known. The advantage of this setting is that no relevant modifications are needed except for the mentioned derivatives of the yield function. The disadvantage, as we will see, is that the nonlinear system of equations is larger and then it is in general more computational intensive. Furthermore, the special cases of hardening must be taken into account in the algorithm because the dimensions of the proper nonlinear system of equations change with the different cases of hardening. We summarize the procedure we have used in the examples for the general case of mixed hardening.

Define the following arrays —consider for example Mandel's notation

$$\mathbf{E} := \begin{bmatrix} \boldsymbol{\varepsilon} \\ 0 \\ 0 \end{bmatrix}; \quad \mathbf{E}_e := \begin{bmatrix} \boldsymbol{\varepsilon}_e \\ \boldsymbol{\xi} \\ \bar{\varepsilon}_p \end{bmatrix}; \quad \mathbf{E}_p := \begin{bmatrix} \boldsymbol{\varepsilon}_p \\ -\boldsymbol{\xi} \\ -\bar{\varepsilon}_p \end{bmatrix} \quad (33)$$

Then we have

$$\dot{\mathbf{E}}_e = \dot{\mathbf{E}} - \dot{\mathbf{E}}_p \Leftrightarrow \dot{\mathbf{E}}_e (\dot{\mathbf{E}}, \dot{\mathbf{E}}_p) = \dot{\mathbf{E}}_e \Big|_{\dot{\mathbf{E}}_p=0} + \dot{\mathbf{E}}_e \Big|_{\dot{\mathbf{E}}=0} \quad (34)$$

The associative rule is

$$\dot{\mathbf{E}}_p = - \dot{\mathbf{E}}_e \Big|_{\dot{\mathbf{E}}=0} = t \nabla f \quad (35)$$

with

$$\nabla f_y \equiv \frac{df_y}{d\mathbf{S}} = \left\{ \frac{\partial f_y}{\partial \boldsymbol{\sigma}}, \frac{\partial f_y}{\partial \boldsymbol{\beta}}, \frac{\partial f_y}{\partial \kappa} \right\}^T \quad (36)$$

where the derivatives are given in Eq. (14) and we defined $\mathbf{S} := \{\boldsymbol{\sigma}, \boldsymbol{\beta}, k\}^T$. The non-dissipative rate $\dot{\mathbf{E}}_e|_{\dot{\mathbf{E}}_p=0}$ is

$$\dot{\mathbf{E}}_e|_{\dot{\mathbf{E}}_p=0} = \dot{\mathbf{E}} = {}^{tr}\mathbf{C}^{-1} \dot{\mathbf{S}}|_{\dot{\mathbf{E}}_p=0} \equiv {}^{tr}\mathbf{C}^{-1} {}^{tr}\dot{\mathbf{S}} \quad (37)$$

where ${}^{tr}\dot{\mathbf{S}}$ stands for the usual algorithmic interpretation as trial stresses of the partial rate $\dot{\mathbf{S}}|_{\dot{\mathbf{E}}_p=0}$ and ${}^{tr}\mathbf{C}^{-1} := \text{diag}(\mathbb{C}^{e-1}, \mathbb{O}, 0)$. The integration of Eq. (35) employing a backward-Euler scheme is

$$- \Delta \mathbf{E}_e|_{\dot{\mathbf{E}}=0} = {}^{t+\Delta t}\mathbf{E}_p - {}^t\mathbf{E}_p = ({}^{t+\Delta t}t - {}^tt) \nabla {}^{t+\Delta t}f_y \quad (38)$$

The purpose of the iterative algorithm is to solve the nonlinear equations in residual form, where ${}^{t+\Delta t}f_y(\boldsymbol{\sigma} - \boldsymbol{\beta}, k) = 0$ is the yield function and $\boldsymbol{\sigma}, \boldsymbol{\beta}, \kappa$ are respectively the stresses, backstresses and overstress scalar:

$${}^{t+\Delta t}\mathbf{R}^{(k)} = - {}^{t+\Delta t}\mathbf{E}_p^{(k)} + {}^t\mathbf{E}_p + \Delta t^{(k)} \nabla {}^{t+\Delta t}f_y^{(k)} \longrightarrow 0 \quad \text{with} \quad {}^{t+\Delta t}f_y^{(k)} \longrightarrow 0 \quad (39)$$

where $\Delta t^{(k)} := {}^{t+\Delta t}t^{(k)} - {}^tt$. Equation (39) means that the GCPP algorithm iterates with the full strain tensor, the backstrain tensor and the equivalent plastic strain. In contrast, in our proposal below we will use only two scalars. The GPM use only one scalar. Because little confusion is possible, we will usually omit the time step index $t + \Delta t$ when the iteration index (k) is present unless we explicitly want to remark the time step.

Then, a Newton-Raphson procedure is developed to reach $\mathbf{R}^{(k+1)} \longrightarrow 0$. Defining $\delta(\cdot)^{(k+1)} = {}^{t+\Delta t}(\cdot)^{(k+1)} - {}^{t+\Delta t}(\cdot)^{(k)}$, the updated solution is

$$\delta \mathbf{E}_e^{(k+1)} = - \left[\frac{d\mathbf{R}^{(k)}}{d\mathbf{E}_e^{(k)}} \right]^{-1} \mathbf{R}^{(k)} \quad \text{and} \quad {}^{t+\Delta t}\mathbf{E}_e^{(k+1)} = {}^{t+\Delta t}\mathbf{E}_e^{(k)} + \delta \mathbf{E}_e^{(k+1)} \quad (40)$$

where the tangent $\partial \mathbf{R}^{(k)} / \partial \mathbf{S}^{(k)}$ is obtained upon differentiation of the residual equations, and ${}^{t+\Delta t}\mathbf{E}_e^{(0)} \equiv {}^{tr}\mathbf{E}_e = {}^t\mathbf{E}_e + ({}^{t+\Delta t}\mathbf{E} - {}^t\mathbf{E})$. We can write

$$\frac{d\mathbf{R}^{(k)}}{d\mathbf{S}^{(k)}} = - \left. \frac{\partial \mathbf{E}_p^{(k)}}{\partial \mathbf{E}_e^{(k)}} \right|_{\dot{\mathbf{E}}=0} \frac{d\mathbf{E}_e^{(k)}}{d\mathbf{S}^{(k)}} + \nabla f_y^{(k)} \left[\frac{\partial \Delta t^{(k)}}{\partial \mathbf{S}^{(k)}} \right]^T + \Delta t^{(k)} \nabla^2 f_y^{(k)} \quad (41)$$

where $-\partial \mathbf{E}_p^{(k)} / \partial \mathbf{E}_e^{(k)}|_{\dot{\mathbf{E}}=0} = \mathbf{I}$, and

$$\frac{d\mathbf{E}_e^{(k)}}{d\mathbf{S}^{(k)}} \equiv [\mathbf{C}^{(k)}]^{-1} = \text{diag} \left[\mathbb{C}^{e-1}, \mathbb{H}^{-1}, \left(\frac{dk^{(k)}}{d\bar{\varepsilon}_p^{(k)}} \right)^{-1} \right] \quad (42)$$

We define the 13×13 Hessian matrix

$$\begin{aligned}
 [\mathbf{D}^{(k)}]^{-1} &= [\mathbf{C}^{(k)}]^{-1} + \Delta t^{(k)} \nabla^2 f_y^{(k)} = \delta \mathbf{E}_e^{(k)} / \delta \mathbf{S}^{(k)} \big|_{\dot{f}_y=0} \\
 &= \begin{bmatrix} \mathbb{C}^{e-1} + \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\sigma}} & \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\beta}} & \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\sigma} \partial k} \\ \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\beta}} & \mathbb{H}^{-1} + \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}} & \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\beta} \partial k} \\ \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\sigma} \partial k} & \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial \boldsymbol{\beta} \partial k} & \left(\frac{d k^{(k)}}{d \bar{\varepsilon}_p} \right)^{-1} + \Delta t^{(k)} \frac{\partial^2 f_y^{(k)}}{\partial k^2} \end{bmatrix}
 \end{aligned} \tag{43}$$

where for the Hill model

$$\frac{\partial^2 f_y}{\partial \boldsymbol{\sigma} \partial \boldsymbol{\sigma}} = \frac{\partial^2 f_y}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}} = -\frac{\partial^2 f_y}{\partial \boldsymbol{\beta} \partial \boldsymbol{\sigma}} = \mathbb{N}, \quad \frac{\partial^2 f_y}{\partial \boldsymbol{\sigma} \partial k} = \frac{\partial^2 f_y}{\partial \boldsymbol{\beta} \partial k} = \mathbf{0} \quad \text{and} \quad \frac{\partial^2 f_y}{\partial k^2} = \frac{2}{3} \tag{44}$$

It is interesting to note that in Eq. (41) we are writing

$$\dot{\mathbf{R}}(f_y, \mathbf{N}) = \dot{\mathbf{R}} \Big|_{\dot{f}=0} + \dot{\mathbf{R}} \Big|_{\dot{\mathbf{N}}=0} \quad \text{with} \quad \mathbf{N} = \nabla f_y / \sqrt{(\nabla f_y)^T \nabla f_y} \tag{45}$$

which is interpreted as the path along the equipotential $f_y^{(k)}$ direction (actually the tangent) followed by the path along the steepest descent one. Then

$$\begin{aligned}
 \delta \mathbf{R}^{(k+1)} &\simeq \frac{d \mathbf{R}^{(k)}}{d \mathbf{S}^{(k)}} \delta \mathbf{S}^{(k+1)} = \underbrace{[\mathbf{D}^{(k)}]^{-1} \delta \mathbf{S}^{(k+1)}}_{\simeq \delta \mathbf{R}^{(k+1)} \big|_{\delta f_y=0}} + \overbrace{\nabla f_y^{(k)} \left[\frac{\partial \Delta t^{(k)}}{\partial \mathbf{S}^{(k)}} \right]^T \delta \mathbf{S}^{(k+1)}}^{\simeq \delta t^{(k+1)}} \\
 &\simeq \delta \mathbf{R}^{(k+1)} \Big|_{\nabla^2 f_y^{(k)}=0}
 \end{aligned} \tag{46}$$

where

$$\delta \mathbf{S}^{(k+1)} = \frac{\partial \mathbf{S}^{(k)}}{\partial \mathbf{E}_e^{(k)}} \Big|_{\dot{\mathbf{E}}=0} \delta \mathbf{E}_e^{(k+1)} \Big|_{\dot{\mathbf{E}}=0} \tag{47}$$

Assuming $\mathbf{R}^{(k+1)} = 0$, we can factor-out $\delta \mathbf{S}^{(k+1)}$ from Eq. (46)

$$\delta \mathbf{S}^{(k+1)} = -\mathbf{D}^{(k)} [\mathbf{R}^{(k)} + \nabla f_y^{(k)} \delta t^{(k+1)}] \tag{48}$$

and

$$\delta \mathbf{E}_p^{(k+1)} = -[\mathbf{C}^{(k)}]^{-1} \delta \mathbf{S}^{(k+1)} \equiv -\delta \mathbf{E}_e \Big|_{\dot{\mathbf{E}}=0}^{(k+1)} \tag{49}$$

where $-\left[\mathbf{R}^{(k)} + \nabla f_y^{(k)} \delta t^{(k+1)}\right]$ is the change in the residual (elastic strains) along the steepest descent and $\mathbf{D}^{(k)}$ are the moduli at $f_y^{(k)}$ constant (or $\Delta t^{(k)}$ constant).

The still undetermined increment $\delta t^{(k+1)}$ may be obtained from the differentiation of the yield function

$${}^{t+\Delta t}f_y^{(k+1)} = {}^{t+\Delta t}f_y^{(k)} + [\nabla f_y^{(k)}]^T \delta \mathbf{S}^{(k+1)} \longrightarrow 0 \quad (50)$$

so using Eq. (48)

$$\delta t^{(k+1)} = \frac{{}^{t+\Delta t}f_y^{(k)} - \left(\nabla f_y^{(k)}\right)^T [\mathbf{D}^{(k)}] \mathbf{R}^{(k)}}{\left(\nabla f_y^{(k)}\right)^T [\mathbf{D}^{(k)}] \nabla f_y^{(k)}} \quad (51)$$

Then, the elastic strains are updated using Eq. (38). Only for the small strains case, because of the linearity between stresses and elastic strains, we can use Eq. (48)

$$\begin{cases} \mathbf{S}^{(k+1)} = \mathbf{S}^{(k)} + \delta \mathbf{S}^{(k)} \\ \mathbf{E}_p^{(k+1)} = \mathbf{E}_p^{(k)} + \delta \mathbf{E}_p^{(k)} \end{cases} \quad (52)$$

In the large strain case, the stresses and tangent are evaluated at the computed elastic strains using the stored energies. We also remark that the actual implementation of the GCPP algorithm must include the different possibilities in hardening because the rank of $\mathbf{D}^{(k)}$ in Eq. (43) may be zero. Furthermore, numerical problems may arise when one or both of the hardening contributions is small. The algorithm is summarized in Table 1. We note that sometimes only $\|{}^{t+\Delta t}\mathbf{R}^{(k)}\|$ has been considered to assess convergence [55] under the understanding that both $\|{}^{t+\Delta t}\mathbf{R}^{(k)}\|$ and $f_y^{(k)}$ converge simultaneously. However, we note that both should be checked in order to guarantee convergence, see Ref. [43]. In fact, during the trial state $\|{}^{t+\Delta t}\mathbf{R}^{(k)}\|$ will vanish and ${}^{t+\Delta t}f_y^{(k)} = {}^{tr}f \neq 0$. Furthermore, as it can be seen in the examples, the different nature of the variables may imply that one may have converged to a given relative tolerance while the other one has still a relevant error.

4 Stress integration algorithm proposed in this work

In anisotropic elastoplasticity with mixed hardening is not possible to pose a consistently linearized fully implicit local Newton-Raphson algorithm based on a single scalar parameter as usually done in the GPM because the plastic flow direction and the hardening are functions of the consistency parameter which depends non-linearly on the yield condition. In this case it is necessary to use approximations in order to use a GPM, as in [30]. In contrast with these procedures, the algorithm introduced below is based on a maximal reduction using only two scalar parameters. No approximation is needed in this case and a local consistently linearized fully-implicit Newton-Raphson procedure can be posed. Furthermore, we include a predictor enhancer which yields the solution for some cases in just one iteration.

Implicit small strains GCPP local algorithm

1. Compute trial values ${}^{tr}\mathbf{S}$ and ${}^{tr}f$
 2. If ${}^{tr}f \leq 0$, elastic step: $\mathbf{S} = {}^{tr}\mathbf{S}$, ${}^{t+\Delta t}\mathbb{C} = \mathbb{C}^e$, exit
 3. Step is plastic: design variables $\mathbf{E}_e^{(k)}$ or $\mathbf{E}_p^{(k)}$, Eq. (33)
 4. Compute local tangent moduli, $\mathbf{D}^{(k)}$ via Eq. (43)
 5. Compute consistency parameter increment $\delta t^{(k+1)}$ via Eq. (51)
 6. Update solution via Eqs. (48), (48) and (49)
 7. Compute new gradient (36), see Eq. (14)
 8. Build residuals, Eqs. (39) and ${}^{t+\Delta t}f_y^{(k)}$
 9. Check: If $\left| {}^{t+\Delta t}f_y^{(k)} \right| < tol_f$ and $\left\| {}^{t+\Delta t}\mathbf{R}^{(k)} \right\| < tol_R$, converged; exit
 10. Repeat from Step 4.
-

Table 1 Layout of the GCPP algorithm

4.1 Evolution of the flow direction

Using the time-left superindices to denote loading time step, Hill's yield criterion at time step $t + \Delta t$ is written as

$${}^{t+\Delta t}f_y = \frac{1}{2} {}^{t+\Delta t}\mathbf{Z} : \mathbb{N} : {}^{t+\Delta t}\mathbf{Z} - \frac{1}{3} {}^{t+\Delta t}k^2 \quad (53)$$

where ${}^{t+\Delta t}\mathbf{Z} = {}^{t+\Delta t}\boldsymbol{\sigma} - {}^{t+\Delta t}\boldsymbol{\beta}$. Another compact algorithmic notation is

$${}^{t+\Delta t}f_y = \frac{1}{2} \left\| {}^{t+\Delta t}\mathbf{Z} \right\|^2 {}^{t+\Delta t}\hat{\zeta} - \frac{1}{3} {}^{t+\Delta t}k^2 \quad (54)$$

where the anisotropy-direction-influence scalar is

$${}^{t+\Delta t}\hat{\zeta} := {}^{t+\Delta t}\hat{\mathbf{Z}} : \mathbb{N} : {}^{t+\Delta t}\hat{\mathbf{Z}} \quad (55)$$

Using $\dot{\boldsymbol{\sigma}} = \mathbb{C}^e : \dot{\boldsymbol{\epsilon}}_e$ and the additive decomposition of the small strain rate tensor $\dot{\boldsymbol{\epsilon}}$, the Cauchy stress tensor at time step $t + \Delta t$ reduces to

$${}^{t+\Delta t}\boldsymbol{\sigma} = {}^t\boldsymbol{\sigma} + \mathbb{C}^e : \Delta\boldsymbol{\epsilon} - \mathbb{C}^e : \Delta\boldsymbol{\epsilon}_p \quad (56)$$

where we use the notation $\Delta(\cdot) := {}^{t+\Delta t}(\cdot) - {}^t(\cdot)$. Defining the trial state at step $t + \Delta t$ as a state with a frozen plastic flow, we have the usual relations ${}^{tr}\boldsymbol{\sigma} = {}^t\boldsymbol{\sigma} + \mathbb{C}^e : \Delta\boldsymbol{\epsilon}$ and ${}^{tr}\boldsymbol{\beta} = {}^t\boldsymbol{\beta}$. The derivatives of ${}^{t+\Delta t}f$ are

$$\frac{\partial {}^{t+\Delta t}f_y}{\partial {}^{t+\Delta t}\boldsymbol{\sigma}} = {}^{t+\Delta t}\mathbb{N} : {}^{t+\Delta t}\mathbf{Z}; \quad \frac{\partial {}^{t+\Delta t}f_y}{\partial {}^{t+\Delta t}\boldsymbol{\beta}} = -{}^{t+\Delta t}\mathbb{N} : {}^{t+\Delta t}\mathbf{Z}; \quad \frac{\partial {}^{t+\Delta t}f_y}{\partial {}^{t+\Delta t}k} = -\frac{2}{3} {}^{t+\Delta t}k \quad (57)$$

The value of ${}^{t+\Delta t}k$ depends on the effective plastic strain. In anisotropic plasticity, the effective plastic strain should not be defined as in the isotropic case, namely $\int \sqrt{2/3 \dot{\boldsymbol{\epsilon}}_p : \dot{\boldsymbol{\epsilon}}_p} dt$, see for example [55]. In general, the effective plastic strain is

better defined as the plastic strain in an equivalent tensile test, work-conjugate to the uniaxial tensile stress, i.e.

$$\dot{\epsilon}_{px} = \frac{\mathbf{Z}}{(\sigma_x - \beta_x)} : \dot{\epsilon}_p = \begin{bmatrix} 1 & & \\ & 0 & \\ & & 0 \end{bmatrix} : \dot{\epsilon}_p = \hat{\mathbf{Z}} : \dot{\epsilon}_p \quad (58)$$

If we use the associated flow rule, Eq. (14)₁, $\dot{\epsilon}_p = \dot{t} \mathbb{N} : \mathbf{Z}$,

$$\dot{\epsilon}_{px} = \dot{t} \hat{\mathbf{Z}} : \mathbb{N} : \mathbf{Z} = \|\mathbf{Z}\| \dot{\zeta} \quad (59)$$

In the case the yield function condition is fulfilled, i.e. $f_y = 0$, if we define k as the uniaxial yield stress, then $\|\mathbf{Z}\| = k$ for this uniaxial case and it is straightforward to get the uniaxial relation

$$\dot{\epsilon}_{px} = \frac{2}{3} k \dot{t} \quad (\equiv \dot{\zeta}, \text{ see Eq. (14)}_3) \quad (60)$$

However, during the iterative process in a general loading condition the previous relation does not hold. In this case, using

$$\Delta \epsilon_p = \Delta t \mathbb{N} : {}^{t+\Delta t} \mathbf{Z} \quad (61)$$

we get

$${}^{t+\Delta t} \bar{\epsilon}_p - {}^t \bar{\epsilon}_p = \Delta \bar{\epsilon}_p = \|\| {}^{t+\Delta t} \mathbf{Z} \|\| {}^{t+\Delta t} \hat{\zeta} \Delta t \quad (62)$$

$$= {}^{t+\Delta t} \hat{\mathbf{Z}} : \Delta \epsilon_p \quad (63)$$

where ${}^{t+\Delta t} \mathbf{Z}$ also depends on Δt . The mutual dependence between ${}^{t+\Delta t} k$ and ${}^{t+\Delta t} \bar{\epsilon}_p$ and of ${}^{t+\Delta t} \mathbf{Z}$ on Δt is what makes it difficult to develop a fully implicit integration algorithm based on a single nonlinear scalar equation. From Eq. (62) it is apparent that we will need the following derivative—which note is not $\frac{2}{3} k$ when $f_y \neq 0$

$$\frac{d {}^{t+\Delta t} \bar{\epsilon}_p}{d {}^{t+\Delta t} t} = \|\| {}^{t+\Delta t} \mathbf{Z} \|\| {}^{t+\Delta t} \hat{\zeta} + \Delta t \left[2 {}^{t+\Delta t} \hat{\mathbf{Z}} : \mathbb{N} - {}^{t+\Delta t} \hat{\zeta} {}^{t+\Delta t} \hat{\mathbf{Z}} \right] : \frac{\partial {}^{t+\Delta t} \mathbf{Z}}{\partial {}^{t+\Delta t} t} \quad (64)$$

Note that there is a change of effective plastic strain because of the change of direction even when Δt remains fixed—second term of the right hand side of Eq. (64). The derivative $\partial {}^{t+\Delta t} \mathbf{Z} / \partial {}^{t+\Delta t} t$ is obtained from the algorithmic return expression:

$$\left. \begin{aligned} {}^{t+\Delta t} \boldsymbol{\sigma} &= {}^{tr} \boldsymbol{\sigma} - \mathbb{C}^e : \Delta \epsilon_p \\ {}^{t+\Delta t} \boldsymbol{\beta} &= {}^t \boldsymbol{\beta} + \mathbb{H} : \Delta \epsilon_p \end{aligned} \right\} \Rightarrow {}^{t+\Delta t} \mathbf{Z} = {}^{tr} \mathbf{Z} - \mathbb{C}^e : \Delta \epsilon_p - \mathbb{H} : \Delta \epsilon_p \quad (65)$$

where using (61)

$${}^{t+\Delta t} \mathbf{Z} = {}^{tr} \mathbf{Z} - \Delta t (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : {}^{t+\Delta t} \mathbf{Z} \quad (66)$$

i.e.

$${}^{t+\Delta t}\mathbf{Z} = {}^{t+\Delta t}\mathbb{D}^{-1} : {}^{tr}\mathbf{Z} \quad (67)$$

where

$${}^{t+\Delta t}\mathbb{D} = \mathbb{I} + \Delta t (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} \quad (68)$$

Hence, from Eq. (66), employing Eq. (67) after a little algebra we get

$$\frac{\partial {}^{t+\Delta t}\mathbf{Z}}{\partial {}^{t+\Delta t}t} = - {}^{t+\Delta t}\mathbb{D}^{-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : {}^{t+\Delta t}\mathbb{D}^{-1} : {}^{tr}\mathbf{Z} \quad (69)$$

Equation (66)–or (67)– is very important in the development of the algorithm since it gives the correct final flow direction in closed form if only the trial state and the consistency parameter (scalar) are known, so in contrast to the GCPP algorithm, Eq. (39), no residual needs to be enforced in the flow and hardening directions. In our case, this residual is always fulfilled. Hence, from the above expressions, it is possible to design a very efficient algorithm using two scalar parameters for the general nonlinear mixed hardening: Δt and ${}^{t+\Delta t}\bar{\varepsilon}_p$. This computational procedure may be consistently linearized both for the local stress integration algorithm and for the global equilibrium iterations. In fact, the global consistent tangent of this algorithm is numerically the same as that of the general implementation of the CPP algorithm because the final solution is identical, just the iterations are different. However, as seen below, advantage of the structure of this algorithm may also be taken in order to avoid special hardening cases in the derivation of the tangent.

4.2 Two-parameter computational algorithm

In a preliminary computation which we detail in Section 4.3, we obtain the consistency parameter $\Delta t^{(0)}$ that it is used as a first approximation of one of the design variables in the stress integration algorithm. Another option is to set $\Delta t^{(0)} = 0$. We define two iterative vectors: the design variables set $\mathbf{X}^{(k)}$ and the residual variables set $\mathbf{R}^{(k)}$. The design variables vector is

$$\mathbf{X}^{(k)} = \left\{ \begin{array}{c} \Delta t^{(k)} \\ \Delta \bar{\varepsilon}_p^{(k)} \end{array} \right\} \quad (70)$$

We initialize the iteration variables as follows

$$\begin{aligned} \Delta t^{(0)} &= 0 \quad \text{or} \quad \Delta t^{(0)} \leftarrow \Delta t^{(k)} \quad (\text{see Section 4.3}) \\ {}^{t+\Delta t}\mathbf{k}^{(0)} &= {}^t\mathbf{k} \\ \Delta \bar{\varepsilon}_p^{(0)} &= \frac{2}{3} {}^t\mathbf{k} : \Delta t^{(0)} \\ {}^{t+\Delta t}\bar{\varepsilon}_p^{(0)} &= {}^t\bar{\varepsilon}_p^{(0)} + \Delta \bar{\varepsilon}_p^{(0)} \end{aligned} \quad (71)$$

On the other hand, the residual vector is written as

$$\mathbf{R}^{(k)} = \begin{Bmatrix} f_y^{(k)} \\ g_y^{(k)} \end{Bmatrix} \quad (72)$$

where $f_y^{(k)}$ and $g_y^{(k)}$ are given by

$$f_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)}) = \frac{1}{2} \mathbf{Z}^{(k)}(t^{(k)}) : \mathbb{N} : \mathbf{Z}^{(k)}(t^{(k)}) - \frac{1}{3} k^{(k)2} (\bar{\varepsilon}_p^{(k)}) \quad (73)$$

and

$$g_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)}) = \Gamma \Delta \bar{\varepsilon}_p^{(k)} - \Gamma \Delta \bar{\varepsilon}_p^{(k)}(t^{(k)}) \quad (74)$$

where

$$\Delta \bar{\varepsilon}_p^{(k)} = \left\| \mathbf{Z}^{(k)} \right\| \hat{\varsigma}^{(k)} \Delta t^{(k)} \quad (75)$$

The factor Γ in the g_y -function is used to improve the conditioning of the system of equations. A handy value is σ_y^2 , where σ_y is the initial uniaxial yield stress.

Once the vector $\mathbf{R}^{(k)}$ is computed, we check convergence with a prescribed tolerance in either $\mathbf{R}^{(k)}$ or in its components separately. If this condition is satisfied, convergence is obtained and the variables are updated. Otherwise, we compute a Newton-Raphson iterative procedure in order to obtain a new solution for the design variables in the iteration $(k+1)$ as $\mathbf{X}^{(k+1)} = \left\{ \Delta t^{(k+1)}, \Delta \bar{\varepsilon}_p^{(k+1)} \right\}$. The update of the design variables vector $\mathbf{X}^{(k+1)}$ is performed as usual

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} - \left[\frac{\partial \mathbf{R}^{(k)}}{\partial \mathbf{X}^{(k)}} \right]^{-1} \mathbf{R}^{(k)} \quad (76)$$

where $\partial \mathbf{R}^{(k)} / \partial \mathbf{X}^{(k)}$ defines the local tangent matrix, which involve the following scalar components

$$\left[\frac{\partial \mathbf{R}^{(k)}}{\partial \mathbf{X}^{(k)}} \right] = \begin{bmatrix} \partial f_y^{(k)} / \partial t^{(k)} & \partial f_y^{(k)} / \partial \bar{\varepsilon}_p^{(k)} \\ \partial g_y^{(k)} / \partial t^{(k)} & \partial g_y^{(k)} / \partial \bar{\varepsilon}_p^{(k)} \end{bmatrix} \quad (77)$$

A little algebra using Eq. (69) gives

$$\frac{\partial f_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)})}{\partial t^{(k)}} = -\mathbf{Z}^{(k)} : \mathbb{N} : \mathbb{D}^{(k)-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z}^{(k)} \quad (78)$$

and

$$\frac{\partial f_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)})}{\partial \bar{\varepsilon}_p^{(k)}} = -\frac{2}{3} k^{(k)} \frac{dk^{(k)}}{d\bar{\varepsilon}_p^{(k)}} \quad (79)$$

Obviously $\partial k^{(k)}/\partial \bar{\varepsilon}_p^{(k)}$ depends on the specific isotropic hardening law employed. The other function derivatives are

$$\frac{\partial g_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)})}{\partial t^{(k)}} = -\Gamma \frac{d\bar{\varepsilon}_p^{(k)}}{dt^{(k)}} \quad \text{and} \quad \frac{\partial g_y^{(k)}(t^{(k)}, \bar{\varepsilon}_p^{(k)})}{\partial \bar{\varepsilon}_p^{(k)}} = \Gamma \quad (80)$$

where using Eq. (64)

$$\frac{d\bar{\varepsilon}_p^{(k)}}{dt^{(k)}} = \zeta^{(k)} \left\| \mathbf{Z}^{(k)} \right\| - \Delta t^{(k)} \left(2\hat{\mathbf{Z}}^{(k)} : \mathbb{N} - \zeta^{(k)} \hat{\mathbf{Z}}^{(k)} \right) : \mathbb{D}^{(k)-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z}^{(k)} \quad (81)$$

Then, the linearization of the problem brings

$$\begin{bmatrix} \Delta t^{(k+1)} \\ \Delta \bar{\varepsilon}_p^{(k+1)} \end{bmatrix} = \begin{bmatrix} \Delta t^{(k)} \\ \Delta \bar{\varepsilon}_p^{(k)} \end{bmatrix} - \begin{bmatrix} \partial f_y^{(k)}/\partial t^{(k)} & \partial f_y^{(k)}/\partial \bar{\varepsilon}_p^{(k)} \\ \partial g_y^{(k)}/\partial t^{(k)} & \partial g_y^{(k)}/\partial \bar{\varepsilon}_p^{(k)} \end{bmatrix}^{-1} \begin{bmatrix} f_y^{(k)} \\ g_y^{(k)} \end{bmatrix} \quad (82)$$

In the previous expressions we have omitted the left-superindex $t + \Delta t$ for brevity. Once the convergence is reached in the local iterative procedure, we obtain the consistency parameter Δt and the effective plastic strain $\Delta \bar{\varepsilon}_p$ at time step $t + \Delta t$. Finally, we update the iterative variables using the following sequential procedure:

$$\begin{cases} {}^{t+\Delta t}\bar{\varepsilon}_p = {}^t\bar{\varepsilon}_p + \Delta \bar{\varepsilon}_p \\ {}^{t+\Delta t}k = K_0 + m\bar{H} {}^{t+\Delta t}\bar{\varepsilon}_p + (K_\infty - K_0) \left[1 - e^{-\delta {}^{t+\Delta t}\bar{\varepsilon}_p} \right] \\ {}^{t+\Delta t}\mathbb{D} = [\mathbb{I} + \Delta t (\mathbb{C}^e + \mathbb{H}) : \mathbb{N}] \\ {}^{t+\Delta t}\mathbf{Z} = {}^{t+\Delta t}\mathbb{D}^{-1} : {}^{tr}\mathbf{Z} \\ \Delta \boldsymbol{\varepsilon}_p = \Delta t \mathbb{N} : {}^{t+\Delta t}\mathbf{Z} \\ {}^{t+\Delta t}\boldsymbol{\beta} = {}^t\boldsymbol{\beta} + \mathbb{H} : \Delta \boldsymbol{\varepsilon}_p \\ {}^{t+\Delta t}\boldsymbol{\sigma} = {}^{tr}\boldsymbol{\sigma} - \mathbb{C}^e : \Delta \boldsymbol{\varepsilon}_p \\ {}^{t+\Delta t}\boldsymbol{\varepsilon}_p = {}^t\boldsymbol{\varepsilon}_p + \Delta \boldsymbol{\varepsilon}_p \end{cases} \quad (83)$$

We note that, as in the General Closest Point Projection algorithm we can explicitly factor out the consistency parameter increment from

$$\delta \mathbf{X}^{(k+1)} := \begin{Bmatrix} \delta t^{(k)} \\ \delta \bar{\varepsilon}_p^{(k)} \end{Bmatrix} := \mathbf{X}^{(k+1)} - \mathbf{X}^{(k)} = - \left[\frac{\partial \mathbf{R}^{(k)}}{\partial \mathbf{X}^{(k)}} \right]^{-1} \mathbf{R}^{(k)} \quad (84)$$

as

$$\delta t^{(k)} = \frac{\frac{\partial f_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} g_y^{(k)} - \frac{\partial g_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} f_y^{(k)}}{\frac{\partial f_y^{(k)}}{\partial t^{(k)}} \frac{\partial g_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} - \frac{\partial g_y^{(k)}}{\partial t^{(k)}} \frac{\partial f_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}}} \quad (85)$$

Of course there is no difference with using Eq. (76) and g_y must be also checked because it is enforced iteratively. In fact, $\delta t^{(k)}$ as a variable and f_y as the related equation could also be included in the system of equations (39) of the CPP algorithm, resulting in a system of 14 equations with 14 unknowns. However, note that as a remarkable difference with the CPP algorithm, the flow and hardening directions are exactly enforced. We emphasize that in contrast with the usual implementation of the Closest Point Projection Algorithm, we need *not* to consider special cases for isotropic, kinematic or combined hardening, and no special care has to be taken in the hardening constants because of numerical difficulties, see [47] and [43]. The layout of the algorithm is given in Table 2.

Proposed implicit small strains algorithm

1. Compute trial values ${}^{tr}\boldsymbol{\sigma}$, ${}^{tr}\boldsymbol{\beta}$, ${}^{tr}\mathbf{Z}$, ${}^{tr}k$ and ${}^{tr}f$
 2. If ${}^{tr}f \leq 0$, elastic step: ${}^{t+\Delta t}(\cdot) = {}^{tr}(\cdot)$, ${}^{t+\Delta t}\mathbb{C} = \mathbb{C}^e$, exit
 3. Step is plastic: design variables $\mathbf{X}^{(k)} = \left[\Delta t^{(k)}, \bar{\varepsilon}_p^{(k)} \right]^T$.
 4. Initialize variables, Eq. (71)
 5. Obtain $\mathbb{D}^{(k)}$, Eq. (68), $\mathbf{Z}^{(k)}$, Eq. (67), $\zeta^{(k)}$, Eq. (55) and $k^{(k)}$, Eq. (32)
 6. Build $f_y^{(k)}$ and $g_y^{(k)}$ via Eqs. (53), (74), (75), and residual $\mathbf{R}^{(k)}$, Eq. (72)
 7. Check: If $\|\mathbf{R}^{(k)}\| < tol_R$, converged: update solution via Eqs. (83) and exit
 8. Compute local tangent moduli, Eq. (77) using Eqs. (78)–(81)
 9. Update solution via Eq. (82)
 10. Repeat from Step 5
-

Table 2 Layout of proposed integration algorithm. Steps 1 and 2 are only necessary if the enhanced predictor is not used

4.3 Scalar predictor enhancement

As a previous step, a consistency parameter Δt predictor algorithm may be used in order to improve the efficiency and robustness of the implicit stress integration procedure. This predictor algorithm consists of considering just the linear hardening part. We note that usually kinematic hardening is modelled as linear and the nonlinearity is assigned to the isotropic contribution, which is on its side modelled as a linear contribution plus a nonlinear one, see Eq. (32) and (2). Furthermore, in order to enhance the performance for this case in mild anisotropic cases, we reformulate this special “yield” condition for iteration (k) as

$${}^{t+\Delta t}\tilde{f}_y^{(k)} := \sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}} - \sqrt{\frac{2}{3}} {}^{t+\Delta t}\tilde{k}^{(k)} \quad (86)$$

where we define

$${}^{t+\Delta t}\tilde{k}^{(k)} := {}^tk + m\bar{H}\Delta\bar{\varepsilon}_p^{(k)} \quad (87)$$

with

$${}^tk = K_0 + m\bar{H}{}^t\bar{\varepsilon}_p + (K_\infty - K_0) \left[1 - e^{-\delta^t\bar{\varepsilon}_p} \right] \quad (88)$$

From the corresponding normality rule, using a new Lagrange multiplier γ we obtain

$$\Delta\varepsilon_p^{(k)} = \Delta\gamma^{(k)} \frac{1}{\sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}}} \mathbb{N} : \mathbf{Z}^{(k)} = \Delta t^{(k)} \mathbb{N} : \mathbf{Z}^{(k)} \quad (89)$$

i.e.

$$\Delta t^{(k)} = \frac{\Delta\gamma^{(k)}}{\sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}}} \quad (90)$$

For the iterative process we can write the uniaxial estimation

$$\Delta\bar{\varepsilon}_p^{(k)} = \sqrt{\frac{2}{3}} \Delta\gamma^{(k)} \quad (91)$$

so both iterative scalar increments Δt and $\Delta\bar{\varepsilon}_p$ from the previous procedure are related to the new one $\Delta\gamma$. Then, we can re-write Eq. (86) as

$$\tilde{f}_y^{(k)}(\Delta\gamma^{(k)}) = \sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}} - \sqrt{\frac{2}{3}} \left({}^tk + \sqrt{\frac{2}{3}} m\bar{H} \Delta\gamma^{(k)} \right) \longrightarrow 0 \quad (92)$$

This equation may be solved, to a given tolerance, by a Newton-Raphson method. The tangent is

$$\frac{d\tilde{f}_y^{(k)}}{d\gamma^{(k)}} = \mathbf{N}^{(k)} : \frac{\partial \mathbf{Z}^{(k)}}{\partial \gamma^{(k)}} - \frac{2}{3} m\bar{H} \quad (93)$$

where

$$\mathbf{N}^{(k)} = \frac{1}{\sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}}} \mathbb{N} : \mathbf{Z}^{(k)} \quad (94)$$

Using Eq. (66) and Equivalence (90) —note that the difficulty here is that $\mathbf{N}^{(k)}$ depends on $\mathbf{Z}^{(k)}$ in the nonlinear form of Eq. (94)

$$\mathbf{Z}^{(k)} = {}^{tr}\mathbf{Z} - \Delta\gamma^{(k)} (\mathbb{C}^e + \mathbb{H}) : \mathbf{N}^{(k)} \quad (95)$$

so

$$\frac{\partial \mathbf{Z}^{(k)}}{\partial \gamma^{(k)}} = -(\mathbb{C}^e + \mathbb{H}) : \mathbf{N}^{(k)} - \Delta\gamma^{(k)} (\mathbb{C}^e + \mathbb{H}) : \frac{d\mathbf{N}^{(k)}}{d\gamma^{(k)}} \quad (96)$$

where from Eq. (94)

$$\frac{d\mathbf{N}^{(k)}}{d\gamma^{(k)}} = \frac{1}{\sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}}} \left(\mathbb{N} - \mathbf{N}^{(k)} \otimes \mathbf{N}^{(k)} \right) : \frac{\partial \mathbf{Z}^{(k)}}{\partial \gamma^{(k)}} \quad (97)$$

Then we can factor-out

$$\frac{\partial \mathbf{Z}^{(k)}}{\partial \gamma^{(k)}} = -\mathbf{Z}^{(k)-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbf{N}^{(k)} \quad (98)$$

where

$$\mathbf{Z}^{(k)} = \mathbb{I} + \frac{\Delta \gamma^{(k)}}{\sqrt{\mathbf{Z}^{(k)} : \mathbb{N} : \mathbf{Z}^{(k)}}} (\mathbb{C}^e + \mathbb{H}) : \left(\mathbb{N} - \mathbf{N}^{(k)} \otimes \mathbf{N}^{(k)} \right) \quad (99)$$

The tangent of Eq. (93) is finally determined. The iterative update is

$$\Delta \gamma^{(k+1)} = \Delta \gamma^{(k)} - \frac{\tilde{f}_y^{(k)}}{d\tilde{f}_y^{(k)}/d\gamma^{(k)}} \quad (100)$$

and the direction update —note that this is a linearization which is in general an approximation

$$\mathbf{Z}^{(k+1)} = \mathbf{Z}^{(k)} + \frac{\partial \mathbf{Z}^{(k)}}{\partial \gamma^{(k)}} (\Delta \gamma^{(k+1)} - \Delta \gamma^{(k)}) \quad (101)$$

It is interesting to note the special case in which the direction of $\mathbf{Z}$ remains constant from $^{tr}\mathbf{Z}$. This happens in the case of von Mises plasticity or in the case of loading along some directions as shear in the principal anisotropy planes. Then from Eq. (94), the norm $\|\mathbf{Z}\|$ cancels-out and $\mathbf{N}$ also remains fixed, having the direction of $\mathbf{Z}$. Since $d\mathbf{N}^{(k)}/d\gamma^{(k)} = \mathbf{0}$ for this case, we get from Eq. (96)

$$\frac{\partial \mathbf{Z}}{\partial \gamma} = -(\mathbb{C}^e + \mathbb{H}) : \mathbf{N} = \left(2\mu_N + \frac{2}{3}(1-m)\bar{H}_N \right) \mathbf{N} \quad (102)$$

where $2\mu_N$ is the effective elastic modulus in direction $\mathbf{N}$, $\frac{2}{3}(1-m)\bar{H}_N$ is the kinematic hardening one and the tangent results in the *constant*

$$\frac{d\tilde{f}_y^{(k)}}{d\gamma^{(k)}} = -\mathbf{N} : (\mathbb{C}^e + \mathbb{H}) : \mathbf{N} - \frac{2}{3}m\bar{H} = -\left(2\mu_N + \frac{2}{3}(1-m)\bar{H}_N \right) - \frac{2}{3}m\bar{H} \quad (103)$$

which yields the “exact” solution *in just one iteration* because the approximations used hold. In fact for $\bar{H}_N = \bar{H}$ as taken in Eq. (31), the updated $\Delta \gamma$ for this special, particular case, has the same shape as that of von Mises plasticity

$$\Delta \gamma = \frac{\tilde{f}_y^{(k)}}{2\mu_N + \frac{2}{3}\bar{H}} \quad (104)$$

Otherwise, in few iterations we obtain an excellent predictor for the two-variable algorithm. Obviously the algorithms could have been written in terms of the form Eq. (86) applied to the nonlinear case. However note that some of the approximations taken in this section would not apply in those cases and little gain would have been obtained at the cost of a significantly more complicated framework.

The predictor enhancement algorithm is summarized in Table 3.

Note that in this case the function g_y is irrelevant because $\bar{\varepsilon}_p$ never enters explicitly the formulation.

Predictor enhancement algorithm

1. Compute trial values ${}^{tr}\boldsymbol{\sigma} = {}^t\boldsymbol{\sigma}$, ${}^{tr}\boldsymbol{\beta} = {}^t\boldsymbol{\beta}$, ${}^{tr}\mathbf{Z} = {}^t\mathbf{Z}$, ${}^{tr}k = {}^tk$
2. Compute trial ${}^{tr}\tilde{f}_y$ using Eq. (86)
3. If ${}^{tr}\tilde{f}_y \leq 0$, elastic step: ${}^{t+\Delta t}(\cdot) = {}^{tr}(\cdot)$, ${}^{t+\Delta t}\mathbb{C} = \mathbb{C}^e$, exit (*)
4. Step is plastic: $\Delta\gamma^{(0)} = 0$, $\Delta t^{(0)} = 0$, $\mathbf{Z}^{(0)} = {}^{tr}\mathbf{Z}$, $k^{(0)} \equiv {}^{tr}k$, $\tilde{f}_y^{(0)} = {}^{tr}\tilde{f}_y$
5. Compute $\mathbf{N}^{(k)}$ via Eq. (94)
6. Calculate $\mathbb{Z}^{(k)}$ by Eq. (99), $d\mathbf{Z}^{(k)}/d\gamma^{(k)}$ Eq. (98) and $d\tilde{f}_y^{(k)}/d\gamma^{(k)}$ Eq. (93)
7. Update $\Delta\gamma^{(k+1)}$ with Eq. (100) and $\mathbf{Z}^{(k+1)}$ by Eq. (101)
8. Compute $\Delta\bar{\varepsilon}_p^{(k+1)} = \sqrt{\frac{2}{3}}\Delta\gamma^{(k+1)}$ and $\tilde{k}^{(k+1)}$ using Eq. (87)
9. Compute new $\tilde{f}_y^{(k+1)}$, Eq. (86)
10. If $\left| \frac{\tilde{f}_y^{(k+1)}}{\tilde{f}_y^{(k)}} \right| / \left| \frac{{}^{tr}\tilde{f}_y}{{}^{tr}\tilde{f}_y} \right| < tol_c$ compute $\Delta t^{(k+1)}$ by Eq. (90), $\Delta\bar{\varepsilon}_p^{(k+1)}$ by Eq. (75) and exit
11. If $\left| \frac{\tilde{f}_y^{(k+1)}}{\tilde{f}_y^{(k)}} \right| / \left| \frac{{}^{tr}\tilde{f}_y}{{}^{tr}\tilde{f}_y} \right| > tol_d$ compute $\Delta t^{(k)}$ by Eq. (90), $\Delta\bar{\varepsilon}_p^{(k)}$ by Eq. (75) and exit
12. Repeat from Step 5

Table 3 Layout of proposed integration algorithm. (*) In this case there is no need to run the full algorithm because the solution is final; the trial check is needed only once

4.4 Consistent algorithmic elastoplastic tangent moduli

During global equilibrium iterations, it is necessary to obtain the 'consistent' or algorithmic elastoplastic tangent in order to preserve the second-order convergence and reduce the computational time. The elastoplastic tangent is in fact numerically identical to that of the Closest Point Projection algorithm because the final solution is also identical. However, as it happens with the local iterations, in the CPP algorithm care must be exercised for the special cases of hardening. The algorithmic tangent derived herein is valid and the derivation well-conditioned for any hardening. The algorithmic elastoplastic tangent is defined as

$${}^{t+\Delta t}\mathbb{C}_{ep} := \frac{\partial {}^{t+\Delta t}\boldsymbol{\sigma}}{\partial {}^{t+\Delta t}\boldsymbol{\varepsilon}} \quad (105)$$

where ${}^{t+\Delta t}\boldsymbol{\sigma}$ and ${}^{t+\Delta t}\boldsymbol{\varepsilon}$ are the stress and strain tensors. In the following equations all variable quantities and derivatives are assumed to be evaluated at the converged solution at $t + \Delta t$, so time-left indices are omitted. The strain derivative of the stress tensor ${}^{t+\Delta t}\boldsymbol{\sigma}$ is computed as

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} = \mathbb{C}^e - \Delta t \mathbb{C}^e : \mathbb{N} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} - \mathbb{C}^e : \mathbb{N} : \mathbf{Z} \otimes \frac{\partial t}{\partial \boldsymbol{\varepsilon}} \quad (106)$$

and

$$\frac{\partial \boldsymbol{\beta}}{\partial \boldsymbol{\varepsilon}} = \Delta t \mathbb{H} : \mathbb{N} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} + \mathbb{H} : \mathbb{N} : \mathbf{Z} \otimes \frac{\partial t}{\partial \boldsymbol{\varepsilon}} \quad (107)$$

From Eq. (66),

$$\frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} = \mathbb{D}^{-1} : \mathbb{C} - \mathbb{D}^{-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z} \otimes \frac{\partial t}{\partial \boldsymbol{\varepsilon}} \quad (108)$$

The consistency condition yields

$$\mathbf{0} = \frac{\partial f_y}{\partial \boldsymbol{\varepsilon}} = \mathbf{Z} : \mathbb{N} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} - \frac{2}{3} k \frac{dk}{d\bar{\varepsilon}_p} \frac{d\bar{\varepsilon}_p}{\partial \boldsymbol{\varepsilon}} \quad (109)$$

and the plastic strain equivalency yields

$$\mathbf{0} = \frac{\partial g_y}{\partial \boldsymbol{\varepsilon}} = -\frac{d\bar{\varepsilon}_p}{\partial \boldsymbol{\varepsilon}} + {}^{t+\Delta t}\hat{\zeta} \|\mathbf{Z}\| \frac{\partial t}{\partial \boldsymbol{\varepsilon}} + 2\Delta t \hat{\mathbf{Z}} : \mathbb{N} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} - \Delta t {}^{t+\Delta t}\hat{\zeta} \hat{\mathbf{Z}} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} \quad (110)$$

The three last equations constitute a system of three equations with three unknowns. We substitute Eq. (110) in Eq. (109) to obtain

$$\boldsymbol{\eta} : \frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} - \theta {}^{t+\Delta t}\hat{\zeta} \|\mathbf{Z}\| \frac{\partial t}{\partial \boldsymbol{\varepsilon}} = \mathbf{0} \quad (111)$$

where we defined the axillary scalar parameter θ and the axillary second-order tensor $\boldsymbol{\eta}$ as

$$\theta := \frac{2}{3} k \frac{dk}{d\bar{\varepsilon}_p} \quad (112)$$

$$\boldsymbol{\eta} := \mathbf{Z} : \mathbb{N} - 2\theta \Delta t \hat{\mathbf{Z}} : \mathbb{N} + \theta \Delta t {}^{t+\Delta t}\hat{\zeta} \hat{\mathbf{Z}} \quad (113)$$

Substituting Eq. (108) we obtain

$$\boldsymbol{\eta} : \mathbb{D}^{-1} : \mathbb{C}^e - (\boldsymbol{\eta} : \mathbb{D}^{-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z}) \frac{\partial t}{\partial \boldsymbol{\varepsilon}} - \theta {}^{t+\Delta t}\hat{\zeta} \|\mathbf{Z}\| \frac{\partial t}{\partial \boldsymbol{\varepsilon}} = \mathbf{0} \quad (114)$$

Finally, we define the scalar parameter τ as

$$\tau := (\boldsymbol{\eta} : \mathbb{D}^{-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z}) + \theta {}^{t+\Delta t}\hat{\zeta} \|\mathbf{Z}\| \quad (115)$$

and the tensors $\partial t / \partial \boldsymbol{\varepsilon}$ and $\partial \mathbf{Z} / \partial \boldsymbol{\varepsilon}$ may be determined

$$\frac{\partial t}{\partial \boldsymbol{\varepsilon}} = \frac{1}{\tau} \boldsymbol{\eta} : \mathbb{D}^{-1} : \mathbb{C}^e \quad (116)$$

$$\frac{\partial \mathbf{Z}}{\partial \boldsymbol{\varepsilon}} = \mathbb{D}^{-1} : \mathbb{C}^e - \mathbb{D}^{-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z} \otimes \frac{\partial t}{\partial \boldsymbol{\varepsilon}} \quad (117)$$

Now, all the terms in Eq. (106) are known.

5 Algorithm of Kojić et al [30].

An algorithm for anisotropic elastoplasticity with mixed hardening was proposed by Kojić et al [30]. It is easily derived in this section departing from our proposal of the previous section.

The design variable is defined in this case simply as $X^{(k)} = \{\Delta\bar{\varepsilon}_p^{(k)}\}$. Upon knowledge of this variable, we compute ${}^{t+\Delta t}k^{(k)}(\Delta\bar{\varepsilon}_p^{(k)})$ and the consistency parameter is obtained in this algorithm as if the yield condition were being fulfilled in a uniaxial case, see Eq. (60)

$$\Delta t^{(k)} = \frac{3}{2} \frac{\Delta\bar{\varepsilon}_p^{(k)}}{{}^{t+\Delta t}k^{(k)}} \quad (118)$$

The return direction is then obtained as before: $\mathbf{Z}^{(k)} = \mathbb{D}^{(k)-1} : {}^{tr}\mathbf{Z}$, where $\mathbb{D}^{(k)}$ is given by Eq. (68). The residual is written as

$$\mathbf{R}^{(k)} = \{{}^{t+\Delta t}f_y^{(k)}\} \quad (119)$$

Note that this algorithm simply proceeds as if $g_y = 0$ in all iterations. Then we compute a Newton-Raphson iterative procedure based on a single scalar parameter in order to obtain a new solution for the design variable in the iteration $(k+1)$ as $X^{(k+1)} = \{\Delta\bar{\varepsilon}_p^{(k+1)}\}$. The update of the design variable $X^{(k+1)}$ is performed as usual

$$X^{(k+1)} \equiv \Delta\bar{\varepsilon}_p^{(k+1)} = \Delta\bar{\varepsilon}_p^{(k)} - \left[\frac{\partial f_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} \right]^{-1} f_y^{(k)} \quad (120)$$

where $\partial f_y^{(k)} / \partial \bar{\varepsilon}_p^{(k)}$ defines the local tangent, which involves the following derivatives—we omit the iteration indices

$$\frac{\partial f_y^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} = \frac{\partial f_y^{(k)}}{\partial \mathbf{Z}^{(k)}} : \frac{\partial \mathbf{Z}^{(k)}}{\partial t^{(k)}} \frac{\partial t^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} + \frac{\partial f_y^{(k)}}{\partial k^{(k)}} \frac{\partial k^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} \quad (121)$$

where

$$\begin{cases} \frac{\partial f_y^{(k)}}{\partial \mathbf{Z}^{(k)}} = \mathbb{N} : \mathbf{Z}^{(k)} \\ \frac{\partial \mathbf{Z}^{(k)}}{\partial t^{(k)}} = -\mathbb{D}^{(k)-1} : (\mathbb{C}^e + \mathbb{H}) : \mathbb{N} : \mathbf{Z}^{(k)} \end{cases} \quad (122)$$

and

$$\frac{\partial t^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} = \frac{3}{2k^{(k)}}; \quad \frac{\partial f_y^{(k)}}{\partial k^{(k)}} = \frac{2}{3}k^{(k)}; \quad \frac{\partial k^{(k)}}{\partial \bar{\varepsilon}_p^{(k)}} = m\bar{H} + \delta(K_\infty - K_0)e^{-\delta\bar{\varepsilon}_p^{(k)}} \quad (123)$$

The reader should compare Eq. (123)₁ with the inverse of Eq. (64). Because of approximation Eq. (118), the influence of the change of ${}^{t+\Delta t}\hat{\zeta}$ on ${}^{t+\Delta t}\bar{\varepsilon}_p$ is also neglected during the iterations.

Upon convergence, the final update is sequentially given by Eqs. (83) with the use of Eq. (118) inserted after determining ${}^{t+\Delta t}k$, i.e. after (83)₂. Because Eq. (118) becomes increasingly true when reaching convergence, the tangent Eq. (121) will also become more accurate and the asymptotic quadratic convergence will be increasingly approached in the last iterations. The layout of the algorithm proposed by Kojić et al [30] is given in Table 4

Implicit stress integration algorithm of Kojić et al

1. Compute trial values ${}^{tr}\sigma$, ${}^{tr}\beta$, ${}^{tr}\mathbf{Z}$, ${}^{tr}k$ and ${}^{tr}f$
 2. If ${}^{tr}f \leq 0$, elastic step: $(\cdot) = {}^{tr}(\cdot)$, ${}^{t+\Delta t}\mathbb{C} = \mathbb{C}^e$, exit
 3. Step is plastic: $\Delta\bar{\varepsilon}_p^{(0)} = 0$.
 4. Compute $k^{(k)}$ via Eq. (32) and $\Delta t^{(k)}$ according to Eq. (118)
 5. Obtain $\mathbb{D}^{(k)}$, Eq. (68), $\mathbf{Z}^{(k)}$, Eq. (67)
 6. Compute ${}^{t+\Delta t}f_y^{(k)}$ via Eq. (53)
 7. Check: If $|f_y^{(k)}| < tol_R$, converged: update via Eqs. (83), (118) and exit
 8. Compute local tangent moduli, Eqs. (121)–(123)
 9. Update solution via Eq. (120)
 10. Repeat from Step 4
-

Table 4 Layout of the algorithm proposed by Kojić et al.

6 Examples

In this section we present some demonstrative examples in order to show the performance of the proposed algorithm and also in order to compare its efficiency to that of the GCPP algorithm and the GPM one. The results from the first two examples are from functions programmed in MATLAB and in obtaining the convergence rates a plain Newton-Raphson has been used. We have considered two cases, one for isotropic elasto-plasticity and one for anisotropic elastoplasticity. The results from the other examples are from our in-house finite element code DULCINEA.

6.1 Stress-point isotropic perfect plasticity

This is the simplest possible case which we employ to highlight the impact of the implementations in the efficiency of the CPP algorithm. In this example we run the

stress-point integration algorithm for isotropic perfect plasticity. It is well known that the Wilkins [60] and Krieg and Key [31] algorithms employ only one iteration to obtain the solution in the perfect plasticity and linear hardening cases. The material parameters of this example are $E = 204 \times 10^3$ MPa, $\nu = 0.3$, $\sigma_y = 235$ MPa. The amount of prescribed strain is 0.01, which is imposed in axial direction. We have employed a reduced GCPP algorithm in which hardening is not taken into account. We note here that for the cases of absence of kinematic or isotropic hardening, in the GCPP algorithm the proper set of equations for each case had to be implemented because prescribing a very low isotropic or kinematic hardening resulted in near-to-zero pivot ratios which prevented the achievement of a reasonable convergence or even reaching a solution. That was not the case for the proposed and for the Kojic algorithm because these algorithms are the same regardless of the hardening pattern. The convergence results up to machine precision are shown in Table 5. Obviously in an engineering application usually a much milder relative convergence tolerance is prescribed, but we show all convergences as to render a fully comparable table. Obviously, the final, converged solution is the same in all cases even though the iterative paths are different.

As it can be easily deduced for the isotropic case because of the lack of directional preference, loading cases in different directions and patterns (for example in shear direction and combining both shear and axial directions) show the same type of convergence and number of iterations as the one shown in Table 5, so we omit the results for these cases.

Isotropic perfect elastoplasticity. Axial loading case.					
Iter. (k)	GCPP		GPM	Proposed algorithm	
	$\ \mathbf{R}^{(k)}\ $	$f_y^{(k)}$ (MPa ²)	$f_y^{(k)}$ (MPa ²)	$f_y^{(k)}$ (MPa ²)	$g_y^{(k)}$
0	0	$8.024E + 05$	$8.024E + 05$	$8.024E + 05$	0
1	$1.951E - 03$	$1.961E + 05$	$3.519E + 05$	$4.729E - 11$	$1.197E - 14$
2	$2.190E - 03$	$4.481E + 04$	$1.518E + 05$		
3	$1.527E - 03$	$7.942E + 03$	$6.299E + 04$		
4	$3.809E - 04$	$5.985E + 02$	$2.391E + 04$		
5	$7.926E - 06$	$4.712E + 00$	$7.319E + 03$		
6	$1.147E - 09$	$3.014E - 04$	$1.310E + 03$		
7	$1.635E - 17$	$6.912E - 11$	$6.255E + 02$		
8			$1.585E - 01$		
9			$1.023E - 06$		
10			$2.547E - 11$		

Table 5 Convergences for isotropic perfect plasticity

6.2 Stress-point anisotropic example subjected to simple extension, simple shearing and combined extension and shearing.

In this example we analyze an anisotropic stress-point example. The material is anisotropic both in the elastic properties and in the plastic ones. We consider perfect plasticity so the GCPP algorithm is in the reduced, most efficient format. The set of material parameters are summarized in Table 6.

Anisotropic elastoplasticity with mixed hardening Material parameters.	
Young's Modulus in principal direction 1	$E_1 = 204 \times 10^3 \text{ MPa}$
Young's Modulus in principal direction 2	$E_2 = 190 \times 10^3 \text{ MPa}$
Young's Modulus in principal direction 3	$E_3 = 210 \times 10^3 \text{ MPa}$
Poisson ratios	$\nu_{12} = 0.3 = \nu_{23} = \nu_{13}$
Shear Modulus in principal direction 12	$G_{12} = 800 \times 10^3 \text{ MPa}$
Shear Modulus in principal direction 23	$G_{23} = 780 \times 10^3 \text{ MPa}$
Shear Modulus in principal direction 13	$G_{13} = 830 \times 10^3 \text{ MPa}$
Yield stress	$\sigma_y = K_0 = 250 \text{ MPa}$
Hill's dimensionless anisotropy parameters:	
$f = 0.4245, h = 0.5824, g = 0.4153, l = m = n = 1.175$	

Table 6 Material data. Anisotropic behaviour

As in the previous case, in order to check the performance of the algorithms, the (quite large) imposed engineering deformation is of 0.01, also in one step, either in axial direction, in shear direction or in both axial and shear directions. The convergences up to machine precision for the axial loading case are given in Table 7. The second iteration with $g_y^{(k)} = 0$ in the proposed algorithm means that the first two iterations are those of the predictor enhancement. These are slightly cheaper iterations than the two-parameter ones and usually result in an initial faster convergence. It can be observed in that table that the proposed algorithm needs less iterations than the GCPP algorithm, and half the iterations than the GPM algorithm of Kojić et al. We emphasize that all three algorithms have *asymptotic* quadratic convergence as it can be observed in the table, and of course the converged solution is exactly the same in all three cases. However, as in the isotropic case, from the table it is also clear that it does not mean that the performance of the algorithms is the same. The proposed algorithm does not obtain the solution in just one iteration because the axial deformation direction is not an eigentensor of the constitutive ones. This would be the case if, for example, anisotropy were only apparent in shear.

Anisotropic elasto-plasticity. <i>Axial</i> loading case. $f_y^{(k)}$ in units of MPa ²					
Iter. (k)	GCPP		GPM	Proposed algorithm	
	$\ \mathbf{R}^{(k)}\ $	$f_y^{(k)}$ (MPa ²)	$f_y^{(k)}$ (MPa ²)	$f_y^{(k)}$ (MPa ²)	$g_y^{(k)}$
0	0	$8.148E + 05$	$8.148E + 05$	$8.148E + 05$	0
1	$1.996E - 03$	$1.990E + 05$	$3.571E + 05$	$1.211E + 03$	0
2	$2.201E - 03$	$4.506E + 04$	$1.535E + 05$	$-6.809E + 01$	$9.94E - 02$
3	$1.484E - 03$	$7.729E + 03$	$6.326E + 04$	$1.112E - 01$	$-2.4E - 01$
4	$3.235E - 04$	$5.304E + 02$	$2.357E + 04$	$3.000E - 07$	$3.90E - 04$
5	$5.913E - 06$	$3.971E + 01$	$6.900E + 03$	$-4.72E - 11$	$1.05E - 09$
6	$1.659E - 09$	$1.854E - 03$	$1.103E + 03$		
7	$1.796E - 16$	$9.858E - 10$	$4.024E + 01$		
8			$5.814E - 02$		
9			$1.217E - 07$		
10			$1.855E - 10$		

Table 7 Anisotropic elasto-plasticity. Convergence rates for the axial loading case.

This can be more clearly seen for the anisotropic case in Table 8, where the convergence results for the shearing load are shown. Because the loading direction is an eigentensor of the material fourth order tensors, the proposed algorithm obtained the solution *in just one iteration*, as predicted above. Remarkably in this case the GCPP algorithm needs 11 iterations and the GPM 16 iterations to reach the machine precision. However, note again that both GCPP and GPM algorithms show *asymptotic* quadratic convergence.

The last loading case is the combined axial-shear loading. The convergence results up to machine precision are shown in Table 9. As in the previous cases, the proposed algorithm clearly outperforms both the GCPP and the GPM. Note again that all three algorithms have *asymptotic* quadratic convergence rate, but again this does not mean that the number of iterations they need is comparable.

6.3 Example from Kojić et al [30]

The example consists of a plate modeled by one linear three dimensional standard finite element (isoparametric element with 8 nodes and $2 \times 2 \times 2$ Gauss quadrature points in standard formulation), see Figure 1. The stress/strain state is uniform so no locking issues arise and it is not necessary to employ mixed formulations. The plate is loaded as shown in Figure 1. We note that since in both the GCPP and our proposal all terms in the linearization of the algorithm are given without simplifications, both algorithms give the same global convergence results. Hence,

Anisotropic elasto-plasticity. <i>Shear</i> loading case.					
Iter. (k)	GCPP		GPM	Proposed algorithm	
	$\ \mathbf{R}^{(k)}\ $	$f_y^{(k)}(\text{MPa}^2)$	$f_y^{(k)}(\text{MPa}^2)$	$f_y^{(k)}(\text{MPa}^2)$	$g_y^{(k)}$
0	0	$1.503E + 08$	$1.503E + 08$	$1.503E + 08$	0
1	$1.767E - 03$	$3.758E + 07$	$6.683E + 07$	$-6.91E - 10$	$-5.421E - 14$
2	$2.207E - 03$	$9.392E + 07$	$2.969E + 07$		
3	$2.312E - 03$	$2.342E + 06$	$1.319E + 07$		
4	$2.315E - 03$	$5.805E + 05$	$5.858E + 06$		
5	$2.225E - 03$	$1.401E + 05$	$2.598E + 06$		
6	$1.887E - 03$	$3.049E + 04$	$1.149E + 06$		
7	$1.017E - 03$	$4.529E + 03$	$5.055E + 05$		
8	$1.391E - 04$	$2.022E + 02$	$2.193E + 05$		
9	$8.288E - 07$	$4.856E - 01$	$9.238E + 04$		
10	$1.063E - 11$	$2.832E - 06$	$3.627E + 04$		
11	$8.674E - 19$	$0.000E + 00$	$1.206E + 04$		
12			$2.658E + 03$		
13			$2.097E + 02$		
14			$1.558E + 01$		
15			$8.736E - 05$		
16			$0.000E + 00$		

Table 8 Anisotropic elasto-plasticity. Convergence rates for the shear loading case.

we just compare now our results with those reported by Kojić et al [30] for their algorithm.

Material data corresponding to orthotropic elastic and plastic behavior are shown in Table 10. The hardening is modeled using the SPM method (see Reference [8]).

Figure 2 shows the deformed mesh and displacements for mixed hardening ($m = 0.5$) corresponding to step 2. Table 11 shows the convergence rates using two algorithms: GPM of Kojić et al [30] and the anisotropic elastoplasticity algorithm developed in this work. With GPM algorithm, the convergence rate is not truly quadratic even for the case of linear hardening, since as they explain in the derivation of elastoplastic tangent modulus, they have neglected some terms in order to develop an algorithm using only one scalar design variable in the local iterative procedure, as usual in the GPM, see References [29], [30]. As a result of the approximations employed in the method and the occasional lack of convergence, the more effective Newton-Raphson algorithm for solving the local equations is substituted by the bisection method according to Reference [30]. A local solution is granted for the problem but the efficiency of the algorithm is inferior to a

Anisotropic elasto-plasticity. <i>Combined (axial + shear) loading case.</i>					
Iter. (k)	GCPP		GPM	Proposed algorithm	
	$\ \mathbf{R}^{(k)}\ $	$f_y^{(k)}(\text{MPa}^2)$	$f_y^{(k)}(\text{MPa}^2)$	$f_y^{(k)}(\text{MPa}^2)$	$g_y^{(k)}$
0	0	$1.512E + 08$	$1.512E + 08$	$1.512E + 08$	0
1	$1.786E - 03$	$3.799E + 07$	$6.739E + 07$	$7.537E + 05$	0
2	$2.281E - 03$	$9.657E + 06$	$3.012E + 07$	$-2.03E + 03$	$2.450E + 01$
3	$2.560E - 03$	$2.529E + 06$	$1.354E + 07$	$1.168E + 01$	$-8.31E + 00$
4	$3.022E - 03$	$6.880E + 05$	$6.137E + 06$	$3.267E - 01$	$4.440E - 01$
5	$3.387E - 03$	$1.726E + 05$	$2.816E + 06$	$2.578E - 06$	$1.236E - 03$
6	$2.936E - 03$	$3.852E + 05$	$1.306E + 06$	$-4.72E - 11$	$9.753E - 09$
7	$2.022E - 03$	$6.490E + 05$	$6.056E + 05$	$-6.18E - 11$	$1.355E - 13$
8	$3.223E - 03$	$4.525E + 02$	$2.750E + 05$		
9	$1.130E - 05$	$8.288E + 00$	$1.199E + 05$		
10	$5.569E - 09$	$1.069E - 02$	$4.903E + 04$		
11	$2.852E - 15$	$6.246E - 09$	$1.757E + 04$		
12	$8.760E - 18$	$-2.80E - 10$	$4.624E + 03$		
13			$5.637E + 02$		
14			$1.099E + 01$		
15			$4.365E - 03$		
16			$6.657E - 10$		

Table 9 Anisotropic elasto-plasticity. Convergence rates for the combined loading case.

full Newton-Raphson algorithm. For the global iterations, the convergence results shown in Table 11 have been performed *using line searches*. In contrast, we do not need nor employ line searches in our algorithm for this problem, although of course the convergence rate could have been improved using them. It is seen that the global asymptotic convergence is also quadratic when using our proposal. We finally note that in [30] the authors used the split of plastic strains (SPS) method to account for mixed hardening and we used the split of plastic modulus (SPM) method. However for the case of proportional loading which obviously holds for the step shown in Table 11 both hardening procedures are identical if properly formulated [8].

6.4 Drawing of a thin circular flange

Robustness of the algorithm and applicability to more realistic problems are shown in this example. The problem is typical for the analysis of anisotropic plastic response, see for example Reference [42]. In order to simulate the drawing process without using contact elements, the inner rim is pulled radially inwards to a maxi-

Fig. 1 Plastic deformation of a elastoplastic orthotropic plate. Geometry, boundary conditions and prescribed load, see Reference [30].

num displacement of 75 mm, while the outer rim is free from restraints. Geometry and boundary conditions of the problem are shown in Figure 3.

The deformation process is displacement-driven, where displacements are prescribed, using a penalty method. In order to prevent buckling of the flange for the large strains case given later, the lower layer is supported in vertical direction. The specimen is modeled using 27-node u/p mixed Q2/P1 finite elements, named BMIX 27/27/4 in DULCINEA (elements with 27 nodes, $3 \times 3 \times 3$ Gauss integration points and 4 internal degrees of freedom of pressure), see References [7], [52]. In one case, the material is assumed to be isotropic regarding elastic properties but orthotropic in the yield properties. The hardening function is given by Equation (32). Material data corresponding to isotropic elasticity and anisotropic yielding are shown in Table 12.

Table 13 shows the analysis of the convergence rates for the Hill's elastoplastic anisotropy model presented in this work in a characteristic step of the global iterative procedure and at a characteristic local stress-point. We note again that the asymptotic quadratic convergence rate of Newton-Raphson type procedures is preserved.

Fig. 2 Small strains orthotropic elastoplasticity. Deformed and nodal displacements corresponding with step 2 with mixed hardening ($m = 0.5$)

Fig. 3 Drawing of a thin circular flange. Geometry, boundary conditions and discretization. The inner displacement is $u = 75 \text{ mm}$. Dimensions are given in mm . The problem is meshed using 27-node mixed u/p elements.

Plate loaded by in-plane loads	
Material parameters	
Young's Modulus in principal direction 1	$E_1 = 2 \times 10^{11} \text{ Pa}$
Young's Modulus in principal direction 2	$E_2 = 1 \times 10^{11} \text{ Pa}$
Young's Modulus in principal direction 3	$E_3 = 1 \times 10^{11} \text{ Pa}$
Poisson ratio in principal direction 12	$\nu_{12} = 0.3$
Poisson ratio in principal direction 23	$\nu_{23} = 0.2$
Poisson ratio in principal direction 13	$\nu_{13} = 0.15$
Shear Modulus in principal direction 12	$G_{12} = 6 \times 10^{10} \text{ Pa}$
Shear Modulus in principal direction 23	$G_{23} = 4.16 \times 10^{10} \text{ Pa}$
Shear Modulus in principal direction 13	$G_{13} = 6 \times 10^{10} \text{ Pa}$
Yield stress in principal direction 1	$\sigma_{y11} = 200 \times 10^6 \text{ Pa}$
Yield stress in principal direction 2	$\sigma_{y22} = 40 \times 10^6 \text{ Pa}$
Yield stress in principal direction 3	$\sigma_{y33} = 40 \times 10^6 \text{ Pa}$
Yield stress shear directions $i \neq j$	$\sigma_{yij} = 80 \times 10^6 \text{ Pa}$
Linear hardening modulus	$\bar{H} = 1 \times 10^9 \text{ Pa}$

Table 10 Material data. Elastoplastic orthotropic behaviour

Figure 4 shows the deformed flanges and the distribution of the effective plastic strains for different radial displacements $u = 25, 50$ and 75 mm using two sets of materials: anisotropic plasticity and the special case (uncoupled) elasto-plastic anisotropy. Material data corresponding to the uncoupled case of anisotropic elastoplasticity are shown in Table 14. In this case, the normal deviatoric stresses (in principal directions) dominate in the yield criterion. The plastic strain is expected to concentrate along the 1 and 2 axes. We compare these results with the previous one for the case of anisotropic plasticity with elastic isotropy. The distributions of effective plastic strain are slightly different due to the effect of *elastic* anisotropy.

In Figure 5 we show deformed meshes and distributions of von Mises equivalent stress for different radial displacements: $u = 25, 50$ and 75 mm using the same two sets of materials properties. The stresses are those computed at the integration points without nodal averaging in order to highlight possible band plot discontinuities. We see that the isobands of the von Mises equivalent stress are reasonably continuous and show no mesh locking.

Finally in Figure 6 we show the results of the equivalent plastic strain of the same simulation but this time *using large strain kinematics*. In this case we have linked our proposed algorithm with the large strain pre- and post-processor using Generalized Kirchhoff stresses and logarithmic strains. This algorithm is incrementally additive (i.e. it does not use plastic metrics or total additive decompositions of the strain measures). Details of how to link our proposal to large strain kine-

Fig. 4 Drawing of a circular flange using the small strains formulation. Deformed meshes and distributions of effective plastic strain for different radial displacement: (a) $u = 25$, (b) 50 and (c) 75 mm inwards using two sets of material properties: i) (on top) isotropic elasticity and anisotropic plasticity and ii) special (uncoupled) elastoplastic anisotropic behaviour. The structure is discretized using 27-node mixed u-p elements (BMIX 27/27/4)

Fig. 5 Drawing of a circular flange using the small strains formulation. Deformed meshes and distributions of von Mises stress for different radial displacement: (a) $u = 25$, (b) 50 and (c) 75 mm using two sets of materials properties: (on top) isotropic elasticity and (bottom) anisotropic plasticity behaviour and special case of elastoplastic anisotropic behaviour. The structure is discretized using 27-node mixed u-p elements (BMIX 27/27/4).

Algorithm of Kojić et al 1996 (<i>with line searches</i>)			
Step	Iteration	Unbalanced energy	
1	0	1.0000E+00	
1	1	9.1838E-01	
1	2	1.5136E-02	
1	3	2.9767E-04	
1	4	5.5054E-07	
1	5	5.1789E-10	
1	6	4.5951E-13	
Proposed algorithm (<i>no line searches</i>)			
Step	Iteration	Force	Unbalanced energy
1	0	1.000E+00	1.000E+00
1	1	1.028E+01	2.057E+01
1	2	4.729E-02	3.487E-02
1	3	5.399E-04	2.359E-05
1	4	5.461E-08	1.421E-11
1	5	1.317E-12	1.975E-23

Table 11 Convergence rates for the elastoplastic orthotropy algorithms in step 1

Drawing of a circular flange. Isotropic elasticity	
Material parameters	
Young's Modulus	$E = 206.9 \text{ GPa}$
Poisson's ratio	$\nu = 0.29$
Initial yield stress	$K_0 = 0.45 \text{ GPa}$
Saturation yield stress	$K_\infty = 0.45 \text{ GPa}$
Linear hardening modulus	$\bar{H} = 0.1 \text{ GPa}$
Hill's plastic anisotropy parameters:	
$f = h = g = 1/3, \quad l = m = n = 1/4$	

Table 12 Drawing of a flange in small strains. Material parameters

matics can be found elsewhere [10] and thus, are omitted here. The large strain effect is apparent for $u = 75 \text{ mm}$ where the necking at $\pm 45^\circ$ is larger.

7 Conclusions

In this paper we present a computational algorithm for small and large strain anisotropic elastoplasticity with mixed nonlinear isotropic-kinematic hardening. The algorithm is developed using only two scalar equations and can be considered as an efficient implementation of the idea behind the Closest Point Projection algorithm.

Relative convergence rates in local iterative algorithm			
Step	Iteration	Relative f_y and g_y residuals	
63	0	$1.0000E + 00$	$1.0000E + 00$
63	1	$0.1523E + 01$	$0.1011E + 01$
63	2	$0.5209E - 02$	$0.5606E - 03$
63	3	$0.6133E - 07$	$0.6594E - 08$
63	4	$0.7750E - 13$	$0.6308E - 13$
Relative convergence energy rate in global iterative algorithm			
Step	Iteration	Energy	
63	0	$0.1000E + 01$	
63	1	$0.1022E + 01$	
63	2	$0.2268E + 00$	
63	3	$0.2354E - 02$	
63	4	$0.1299E - 05$	
63	5	$0.2271E - 13$	

Table 13 Convergence rates for the elastoplastic orthotropy algorithm presented in this work

Drawing of a circular flange. Anisotropic elastoplasticity	
Material parameters	
Young's Modulus	$E = E_1 = E_2 = E_3 = 362.97 \text{ GPa}$
Poisson ratio	$\nu = \nu_{12} = \nu_{23} = \nu_{13} = 0.1315$
Shear Modulus	$G = G_{12} = G_{23} = G_{13} = 80.19 \text{ GPa}$
where $G \neq \frac{E}{2(1 + \nu)}$	
Initial yield stress	$K_0 = 0.45 \text{ GPa}$
Saturation yield stress	$K_\infty = 0.45 \text{ GPa}$
Linear hardening modulus	$\bar{H} = 0.1 \text{ GPa}$
Hill's plastic anisotropy parameters:	
$f = h = g = 1/3, \quad l = m = n = 1/4$	

Table 14 Drawing of a flange in small strains. Elasto-plastic anisotropy material parameters

We have analyzed and compared the efficiency of the present proposal with the General implementation of the Closest Point Projection algorithm and with the Governing Parameter Method of Kojić et al [30]. We note and have shown that different implementations of the Closest Point Projection ideas result in different iterative paths and, hence, in different convergence rates. In contrast to the GCPP algorithm, the proposed implementation is valid for the perfect plasticity case, for the purely kinematic case, for the isotropic case and for the mixed hardening case without any modification or switch. This results in a clearly more robust algorithm.

Fig. 6 Drawing of a circular flange using the large strains formulation. Deformed meshes and distributions of equivalent plastic strains for different radial displacement: (a) $u = 25$, (b) 50 and (c) 75 mm using two sets of materials properties: (on top row) isotropic elasticity and anisotropic plasticity behaviour and (bottom row) special case of elasto-plastic anisotropic behaviour.

Furthermore, a predictor enhancement procedure also results in an increased efficiency and robustness. Of course in all studied algorithms the final solution is the same because they can be understood as different implementations (iterative paths) of the backward-Euler integration. These algorithms may be employed as the only iterative component in large strain algorithms in terms of incrementally additive logarithmic strains [10].

The examples show the efficiency of the proposed algorithm. It is remarkable that in contrast to the General implementation of the Closest Point Projection algorithm and the Governing Parameter Method, the number of iterations employed for the special case of J_2 -plasticity with linear hardening and for other particular cases is just one as in that of the classical algorithms of Wilkins and Kreig and Key.

As a final conclusion we note that whereas the General implementation of the Closest Point Projection algorithm is straightforward for usual plasticity models, this implementation performs an iterative enforcement of all governing equations, leading to an increased computational effort and being more prone to numerical conditioning problems. On the contrary, a minimal implementation in terms of design variables and nonlinear equations to be solved may result in more efficient and robust procedures.

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Capítulo 3

Mecánica del daño

3.1. Introducción

En términos generales el daño de los materiales es el proceso físico progresivo por el cual éstos rompen [52]. La mecánica del daño es por tanto el estudio, a través de variables mecánicas, de los mecanismos involucrados en el deterioro de los materiales cuando éstos son sometidos a carga. A nivel de microescala este deterioro viene causado por la acumulación de microtensiones concentradas en el entorno de las intercaras y de los defectos, así como las provocadas por la rotura de enlaces. A nivel de mesoescala es originado por el crecimiento y la coalescencia de microgrietas y microporos que conjuntamente producen la iniciación de grietas. A nivel de macroescala el daño es producido por el crecimiento de esas grietas. Los dos primeros niveles pueden ser estudiados mediante variables de daño de la mecánica del medio continuo definida a nivel de mesoescala, sin embargo el tercer nivel se suele estudiar usando la mecánica de la fractura con variables definidas en este nivel.

Al estudiar algunos materiales como metales, aleaciones, polímeros, materiales compuestos, tejidos biológicos, cerámicas, rocas, hormigón, madera, etc., es muy sorprendente ver cómo dichos materiales, que poseen estructuras físicas muy diferentes, presentan un comportamiento mecánico cualitativamente similar. La mayoría suelen mostrar comportamiento elástico, fluencia, algún tipo de deformación irreversible, anisotropía inducida por deformación, histéresis, daño por carga monotónica o por fatiga y crecimiento de grietas bajo cargas estáticas o dinámicas. Ésta es la principal razón por la que es posible explicar con éxito el comportamiento de los diferentes materiales mediante la mecánica del medio continuo y la termodinámica de los procesos irreversibles, modelando los materiales sin hacer una referencia detallada a la complejidad de sus microestructuras físicas.

La mecánica de la fractura se lleva estudiando desde hace mucho tiempo, pues

ya en el siglo XV Leonardo da Vinci se interesó por la caracterización de la fractura mediante variables mecánicas. A lo largo de los años se han propuesto numerosos criterios de fallo bien conocidos: Coulomb, Rankine, Tresca, von Mises, Mohr. No obstante, el interés por la mecánica del daño es más reciente, en concreto en 1958 Kachanov [53] publicó en ruso el primer artículo en el que se introdujo una variable escalar para modelar el fallo por fluencia en metales bajo carga uniaxial. Aunque el significado físico de esta variable fue dado un año más tarde por Rabotnov [54], [55], que propuso la reducción del área de la sección transversal, debido a las microfisuras, como una medida del estado del daño interno del material. De esta idea se derivó posteriormente el concepto de tensión efectiva. Este concepto se retomó en los años setenta principalmente de la mano de Lemaitre y Chaboche [56], Odqvist y Hult [57], Leckie y Hayhurst [58], Murakami y Ohno [59], entre otros, los cuales lo extendieron a la fractura dúctil y por fatiga. Desde entonces hasta hoy, se han propuesto muchos modelos para los distintos tipos de materiales, estos modelos se pueden clasificar atendiendo a diversos aspectos. Los modelos se pueden clasificar por ejemplo, en función de cómo se define la variable de daño: escalarmente, tensorialmente, etc. La elección de esta variable es muy importante ya que representa una aproximación macroscópica para describir el proceso micromecánico subyacente. Se podría establecer otra clasificación según la definición de dicha variable de daño. Una forma muy generalizada de interpretar el daño continuo, consiste en la definición de un espacio ficticio no dañado que puede ser obtenido del espacio de tensiones y deformaciones reales a través de una transformación. Existen distintas hipótesis para definir dichas transformaciones entre el espacio dañado real y el espacio ficticio no dañado: hipótesis de equivalencia de deformaciones, hipótesis de equivalencia de tensiones, hipótesis de equivalencia de energía y una transformación de tipo cinemática.

a) Hipótesis de equivalencia de deformaciones. Físicamente la degradación de las propiedades del material es el resultado de la iniciación, crecimiento y coalescencia de microfisuras y microporos. Dentro del contexto de la mecánica del continuo se puede modelar este fenómeno introduciendo una variable interna que puede ser una cantidad escalar o tensorial. En el caso más general, se denota por $\mathbb{M}$ a un tensor de cuarto orden que caracteriza el estado de daño y transforma el tensor de tensiones de Cauchy $\boldsymbol{\sigma}$ en el tensor de tensiones de Cauchy efectivo $\bar{\boldsymbol{\sigma}}$, del siguiente modo

$$\bar{\boldsymbol{\sigma}} := \mathbb{M}^{-1} : \boldsymbol{\sigma} \quad (3.1)$$

Para el caso isótropo, el comportamiento mecánico de las microfisuras y los microporos es independiente de su orientación y depende sólo de una variable escalar D , por lo que la ecuación anterior resulta

$$\bar{\boldsymbol{\sigma}} := \frac{\boldsymbol{\sigma}}{(1 - D)} \quad (3.2)$$

Figura 3.1: Representación del concepto de tensión efectiva y del principio de equivalencia de deformaciones.

donde $D \in [0, D_c]$ es la variable de daño. El factor $(1 - D)$ es un factor de reducción asociado con la reducción de área efectiva o cantidad de daño presente en el material, en el mismo sentido que fue introducido por Kachanov y Rabotnov. Para evitar un análisis micromecánico de cada tipo de defecto y mecanismo de daño Lemaitre [60] propuso la hipótesis de equivalencia de deformación: “*la deformación asociada con un estado dañado, bajo la tensión aplicada, es equivalente a la deformación asociada con el estado no dañado bajo la tensión efectiva*”, basándose en el concepto de tensión efectiva. La Figura 3.1 ilustra el principio de equivalencia de deformación y el concepto de tensión efectiva.

A pesar de que el principio de equivalencia de deformación ha sido ampliamente utilizado, este enfoque tiene el gran inconveniente de dar lugar a tensores de rigidez y flexibilidad no simétricos, lo que deriva en la no conservación de la energía durante los procesos de descarga y recarga.

b) Hipótesis de equivalencia de tensiones. Como alternativa al concepto de tensión efectiva, se puede definir la deformación efectiva como

$$\bar{\varepsilon} := \mathbb{M} : \varepsilon \quad (\text{caso anisótropo}) \quad (3.3)$$

$$\bar{\varepsilon} := (1 - D)\varepsilon \quad (\text{caso isótropo}) \quad (3.4)$$

donde ε y $\bar{\varepsilon}$ son el tensor de deformación y el tensor de deformación efectivo respectivamente. Por analogía con la hipótesis de equivalencia de deformaciones y utilizando técnicas de homogeneización similares, Simo y Ju [61] propusieron la siguiente hipótesis de equivalencia de tensiones: “*la tensión asociada con un estado dañado bajo la deformación aplicada es equivalente a la tensión asociada con el*

Figura 3.2: Representación del concepto de deformación efectiva y del principio de equivalencia de tensiones.

estado no dañado bajo la deformación efectiva". La Figura 3.2 ilustra el principio de equivalencia de tensión y el concepto de deformación efectiva.

La hipótesis de equivalencia de tensiones tiene el mismo inconveniente teórico que la hipótesis de equivalencia de deformación, ya que da lugar a tensores de rigidez y flexibilidad no simétricos.

c) Hipótesis de equivalencia de energía (Dragon y Mroz [62], Krajcinovic y Fonseka [63], Carol *et al.* [64]). “*La energía de deformación asociada con un estado dañado bajo la tensión aplicada es equivalente a la energía de deformación asociada con el estado ficticio no dañado bajo la tensión efectiva*”. En este enfoque ni la tensión efectiva, ni la deformación efectiva coinciden con sus valores nominales. Suponiendo que las relaciones entre cantidades nominales y efectivas son lineales, quedan relacionadas por un tensor $\mathbb{M}$ de cuarto orden tal que

$$\boldsymbol{\sigma} := \mathbb{M} : \bar{\boldsymbol{\sigma}} \quad (3.5)$$

$$\bar{\boldsymbol{\epsilon}} := \mathbb{M} : \boldsymbol{\epsilon} \quad (3.6)$$

La densidad de energía elástica nominal y efectiva deben ser iguales, como se comprueba a continuación

$$\boldsymbol{\sigma} : \boldsymbol{\epsilon} = \mathbb{M} : \bar{\boldsymbol{\sigma}} : \mathbb{M}^{-1} : \bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\epsilon}} \quad (3.7)$$

De las Ecuaciones (3.5) y (3.6) se obtiene el tensor de comportamiento dañado tal que

$$\mathbb{C} = \mathbb{M} : \mathbb{C}^0 : \mathbb{M} \quad (3.8)$$

3.1. INTRODUCCIÓN

donde $\mathbb{C}^0$ representa al tensor de comportamiento no dañado. A diferencia de las hipótesis anteriores, la hipótesis de equivalencia de energía garantiza la simetría tanto del tensor de comportamiento como de su inversa.

d) Relaciones de tipo cinemático. Este enfoque está basado en una formulación matemática similar a la de la teoría de grandes deformaciones. La unificación de la formulación de daño con la de grandes deformaciones conlleva una considerable ventaja a la hora de su implementación en códigos de ordenador ya existentes que están orientados al estudio del problema de las deformaciones finitas. El daño puede interpretarse matemáticamente como una transformación cinemática entre dos espacios. Para ello se acepta que existe un espacio ficticio no dañado, que se obtiene a partir del espacio real dañado eliminando el daño. En el espacio ficticio no dañado el material se comporta como si fuese virgen. Se admite que hay una relación biunívoca entre los dos espacios que permite transformar una variable del espacio ficticio no dañado al espacio real dañado. Dicha relación puede expresarse de forma similar a una transformación cinemática, del siguiente modo

$$\boldsymbol{\sigma} = \mathbf{F} \otimes \mathbf{F}^T : \bar{\boldsymbol{\sigma}} = \mathbb{M} : \bar{\boldsymbol{\sigma}} \quad (3.9)$$

$$\boldsymbol{\varepsilon} = \mathbf{F}^{-T} \otimes \mathbf{F}^{-1} : \bar{\boldsymbol{\varepsilon}} = \mathbb{M}^{-1} : \bar{\boldsymbol{\varepsilon}} \quad (3.10)$$

En el espacio ficticio no dañado se tiene la ecuación constitutiva correspondiente al material virgen

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}} : \bar{\boldsymbol{\varepsilon}} \quad (3.11)$$

donde $\bar{\mathbb{C}} = \mathbb{C}^0$ es el tensor constitutivo elástico del material virgen (sin dañar). Despejando $\bar{\boldsymbol{\sigma}}$ y $\bar{\boldsymbol{\varepsilon}}$ de las Ecuaciones (3.9) y (3.10), respectivamente y sustituyendo en (3.11) se obtiene la ecuación constitutiva para el material dañado

$$\mathbb{M}^{-1} : \boldsymbol{\sigma} = \bar{\mathbb{C}} : \mathbb{M} : \boldsymbol{\varepsilon} \quad (3.12)$$

por lo que el tensor constitutivo dañado viene dado por

$$\mathbb{C} = \mathbb{M} : \bar{\mathbb{C}} : \mathbb{M} \quad (3.13)$$

La energía de deformación resulta por tanto

$$\mathcal{W} = \frac{1}{2} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \frac{1}{2} \mathbb{M} : \bar{\boldsymbol{\sigma}} : \mathbb{M}^{-1} : \bar{\boldsymbol{\varepsilon}} = \frac{1}{2} \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\varepsilon}} = \bar{\mathcal{W}} \quad (3.14)$$

donde se comprueba que evidentemente la energía es un invariante ante los cambios de espacio.

El tensor $\mathbf{F}$, al igual que el tensor gradiente de deformaciones, es un tensor bipuntual que vincula el espacio dañado con el espacio sin dañar.

Aunque se pueden lograr resultados satisfactorios con cualquiera de estas hipótesis, la generalización del principio de tensión efectiva del daño escalar y el principio

de equivalencia de deformaciones pueden no conducir a la existencia de un potencial elástico. Tal es el caso de la plasticidad acoplada con daño, debido a que la degradación del material está asociada a las deformaciones plásticas. Una solución generalizada consiste en reemplazar la hipótesis de equivalencia de deformaciones por una hipótesis de equivalencia de energía. De este modo, se asegura la existencia de un potencial elástico, aunque se pierde la interpretación física del daño. El daño ya no está relacionado con la densidad superficial de defectos, sino que es una variable definida por su acoplamiento con la elasticidad.

3.2. Revisión de modelos y formulaciones

En esta sección se presentará un marco teórico general que permita analizar la gran cantidad de modelos de daño existentes, no sólo desde el punto de vista de su formulación sino también teniendo en cuenta su capacidad para reproducir las evidencias experimentales correspondientes a un amplio rango de materiales.

Como resumen, los puntos más importantes tratados en el siguiente artículo son:

- La exposición de un profundo estado del arte en el que se mostrarán los modelos y formulaciones existentes en la literatura relativos a la Mecánica del Daño.
- El estudio de la representación mecánica del daño, de diversas definiciones de la variable de daño continuo y de la termodinámica asociada a los materiales dañados.
- La presentación de las distintas aplicaciones de la Mecánica del Daño Continuo en diversos tipos de materiales.

Engineering Damage Mechanics: Review of Models and Formulations

Mar Miñano · Francisco Javier Montáns

Abstract Damage mechanics is used to model a wide range of types of damage in a wide range of materials. For example, damage mechanics is used to model the deterioration of mechanical properties in classical engineering materials like steel or concrete, but it is also used for predicting bone adaptation to stimuli after, for instance, the implantation of a prosthesis (bone remodeling). Many different models have been proposed in the literature to account for damage effects. These formulations can be categorized into three main approaches: abrupt criteria, porous solid plasticity and continuum damage mechanics. The purpose of this paper is to present a review of the literature of damage mechanics mainly from an engineering perspective, aiming at the main assumptions, models and differences between the proposed formulations.

1 Introduction

The damage of materials is the gradual physical process which irreversibly deteriorates their macromechanical properties until they break. From a mechanical point of view, damage is the creation, growth and coalescence of microvoids or microcracks at the microscopic level. The theory of damage describes the evolution of the phenomena between the virgin state and macroscopic crack initiation.

Macroscopic fracture has been studied for a long time. In the XVIth century, Leonardo da Vinci was already interested in the characterization of fracture by means of mechanical variables. About one hundred years later, Galileo Galilei realized how important was the size effect in fracture and he observed that this effect placed a limit on the size of structures. However, it is much more recent

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when concern has been directed to model the progressive material deterioration preceding the macroscopic fracture. The development of damage mechanics began in 1958 when Kachanov [75] published what is considered the first paper devoted to a continuous damage variable. In this paper Kachanov introduced a scalar internal variable to model the creep failure of metals under uniaxial loads. A physical significance for this damage variable was given one year later by Rabotnov [129] who proposed the reduction of the cross-sectional area due to microcracking as a suitable measure of the state of internal damage. From this idea the concept of effective stress is derived as discussed later in this paper.

Actually, the selection of a mechanical damage variable itself presents a difficult choice. On one hand, measurements at the scale of microstructure lead to microscopic models that can be integrated over the macroscopic volume element by means of mathematical homogenization techniques. For these models it is difficult to define a macroscopic damage variable and its evolution law which are easy to use in continuum mechanics analysis. On the other hand, global physical measurements (microhardness, density, resistivity etc.) require the definition of a model to convert them into properties which characterize mechanical behavior. Finally, global mechanical measurements of the variation of elastic, plastic or viscoplastic properties, are easier to interpret in terms of damage variables using the concept of effective stress according to Rabotnov.

The simulation of these microstructural damage processes has been researched in several micromechanical and macromechanical models in the literature. According to Bonora [15] these models can be sorted into three main approaches: (i) abrupt failure criteria, (ii) porous solid plasticity and (iii) continuum damage mechanics.

For the first modelling approach, failure is predicted to occur when one chosen micromechanical variable that is uncoupled from other internal variables, reaches its critical value. These criteria are relatively simple and frequently based on experimental data. One of the pioneers in this approach was McClintock [108], who in 1968 studied the role of microvoids in ductile failure process and tried to correlate the mean radius of the cavities to the total plastic strain increment. Around the same time, in 1969, Rice and Tracey [131] proposed an approximate relation to describe growth of a spherical void in a general remote field.

In the second approach, damage is described in terms of void volume fraction that is taken into account at the macroscale, for example, by a softening term that gradually contracts the yield surface as proposed Gurson [57–59] around 1977 and Rousselier [133] in 1987. An alternative yield condition has also been proposed by Shima and Oyane [138] in 1976 for the case of powder metallurgical materials. Gurson based his work on the analysis of an isolated void developed by Rice and Tracey and on the condition for localization in elastoplastic solids studied by Rice [132]. The Gurson model contains up to ten material constants which

should be identified before application. Some of them seem to be not physically based and cannot be directly measured for a material. This complex identification entails problems in applications with a specific material for which the parameters have not been previously estimated by other authors. The main difference between Gurson's and Rousselier's models is that Rousselier based his model on thermodynamical considerations whereas Gurson derived his model from the micromechanical description of the porous material. The susceptibility to localization of the Gurson model has been studied with an emphasis on the role of heterogeneities by Yamamoto [168] in 1978. Moreover, the role of kinematic hardening was investigated by Mear and Hutchinson [110] in 1985 and together with nucleation by Tvergaard [152] in 1987. Needleman and Tvergaard [119,153] in 1984 and Koplik and Needleman [79] in 1988 modified the model proposed by Gurson in order to consider the void coalescence effect in the failure process. Needleman and Tvergaard extended McMeeking's [109] work about the initiation of crack growth. They focused on the interaction between voids closest to the crack tip and the tip itself by treating large voids as discrete entities and by modeling the much smaller voids using the Gurson relation. This modified Gurson model, commonly called Gurson-Tvergaard-Needleman model (GTN), is the most popular version of the Gurson's model. Some of these modifications were based on a cell model calculation developed by Andersson [4]. Sun et al. [146] and Brocks et al. [18] have adopted a version of the computational model proposed by Needleman and Tvergaard and have applied the model to analyze fully plastic cracking behavior of tough steels for diverse specimen geometries. Subsequently, a large number of cell models based on finite elements have been performed in order to correlate void evolution and interaction with the macroscopic material yield function. Schacht et al. [135] in 2003 used the 3D voided unit cell based approach to survey the influence of the crystallographic orientation of the void surrounding matrix, finding out that the void growth and deformation behavior on a microscopic scale significantly depend on the crystallographic orientation of an anisotropic matrix material. Tvergaard and Niordson [154] in 2004 used a non-local plasticity model as proposed by Acharya and Bassani [1] to show that the rate of void growth is significantly reduced when voids are small enough to be comparable with a characteristic material length. Bonfoh et al. [17] in 2004 used the GTN damage definition to model damage evolution initiated by intracrystalline non-shearable particles debonding in a polycrystalline material. Mahnken [100] compared the yield function of Gurson, its extensions by Tvergaard and Needleman and the yield function of Rousselier, with the single-surface yield function of Ehlers [51]. Based on the analogy for all conceptions, Mahnken proposed a new mixed model class of yield functions for simulating metallic materials with induced porosity. The GTN model, despite being widely used to study ductile failure and crack propagation (Bennani et al. [9], He et al. [66], Mahnken [99], Xia and Shih [165], Besson

et al. [11], Chen and Dong [34], Shi et al. [137]), has several known limitations. In agreement with what Bonora [15] and Chaboche [30] point out in their works, the most notable restrictions could be: (a) The identification of a large number of material constants is required; accordingly it is difficult to evaluate possible interactions between the parameters. (b) The material parameters are not physically based and cannot be directly measured for a material. Typically an iterative calibration procedure, involving finite element simulations and experimental data, is necessary. For more details the reader is referred to [52, 53, 120, 143, 144, 155]. (c) The transferability to other geometries is not always satisfactory, the standard method needs to be calibrated on specimens of different geometry. The methods using digital image processing as Broggiato et al. [19] usually only require a single test on a round-notched bar specimen to provide portability, however it is necessary a more complex experimental equipment as well as a major post-processing effort on data collected from a digital camera, and they are also limited to simple geometries. (d) The Gurson model, in the same way that other formulations with softening in the yield function, requires a length scale, see References [3, 170]. For rate-independent flow-stress formulation, the length scale is given by the element size [120]. Hence, no stable predictions can be accomplished and the damage model parameters become mesh-dependent, more references can be found in [151]. (e) Introducing anisotropic damage effects in the Gurson model is not simple. The Leblond-Gologanu-Devaux [41–43] modification introduces a cavity shape parameter. Several researchers have adopted this amendment to their models: Benzerga et al. [8], Pardoen and Hutchinson [124], Benzerga [7], Siruguet and Leblond [141], among others. A difficulty arises for the evolution equations, that must be formulated in the principal axes of the ellipsoidal voids.

For the third approach mentioned earlier, material damage and its mechanical effects are discussed in the framework of continuum mechanics. Namely, continuum damage mechanics is a branch of continuum mechanics used to describe the damage and fracture process ranging from the initiation of microcavities or microcracks to the final fracture in materials caused by the development of macrocracks. The term continuum damage mechanics (CDM) is commonly assumed [171] that was proposed in 1977 by Janson and Hult [70] although the basic idea, as already mentioned, is due to Kachanov, who introduced a damage variable to describe the microdefect density locally in a creeping material and named it *continuity*. The contribution was that damage could be measured by the volume fraction of voids, which became the foundation of CDM. One of the first papers in English describing this new theory was published by Odqvist and Hult [121] in 1961. Some authors attribute to them the physical meaning of the damage variable instead to Rabotnov since the earlier work of Rabotnov was written in Russian and was not as well known. The considered first contribution in this topic in English of Rabotnov [130] was in 1963. Since Kachanov-Rabotnov's [76] original developments, it did not take

long before the concept of internal damage was extended to three-dimensional situations by many authors. One of the best known were the contributions of Leckie and Hayhurst [86] in 1974 who exploited the theory of the effective load bearing area reduction as a scalar measure of deterioration of material properties to develop a model for creep-rupture under multiaxial stresses. The theories developed thereafter by Chaboche and Murakami and Ohno deserve particular mention. Chaboche [26] in 1981 proposed a phenomenological theory and several applications for creep damage based on thermodynamic foundations, in which due to the hypothesis of strain equivalence, the damage variable appears as a fourth-order asymmetric tensor for the most general case of anisotropy. On the other hand, Murakami and Ohno [118] in the same year, extended the effective stress concept to three dimensions for the case of orthotropic damage, through the hypothesis of the existence of a mechanically equivalent fictitious undamaged configuration. Later, Murakami [114, 115] applied this concept to the general case of anisotropic damage with special emphasis on the analysis of elastic-brittle materials.

The key issue for the CDM approach is the damage evolution law obtained from the thermodynamic and dissipation potentials. The formulation of the, as it is usually called, potential of dissipation (or function of dissipation, as a more appropriate description) has not been very well established in the literature. Lemaitre [88] in 1984 proposed one of the until now most popular damage evolution equations for ductile damage. This theory was further developed by Lemaitre, see References [89, 90], among others, and ageing effects were later incorporated by Marquis and Lemaitre [104]. Since then, several authors have proposed damage models based on the use of particular formulations for the damage dissipation potential: Tai [147] in 1990, Tai and Yang [148] in 1986, Wang [163] in 1992, Chandrakanth and Pandey [33] in 1993, Bonora [13] in 1997, Armero and Oller [5] and Dhar et al. [48] in 2000, Lin et al. [96] in 2004, among others.

The continuum damage was also applied to analyze the behavior of damage in brittle materials like rock by Shao and Khazraei [136] and Homand-Etienne et al. [68], concrete by Cipollina et al. [40], Murakami and Kamiya [117], Flórez-López [55], Peng and Meyer [126], Faming and Zongjin [95], Kuna-Ciskal and Skrzypek [82], laminates and composites by Matzenmiller et al. [105], Maire and Chaboche [102], Williams et al. [164], Edlund and Volgers [50], Maimí et al. [101], human bones by Taylor et al. [149], etc. This approach has also been used to describe fatigue processes. Janson [69] in 1978 developed a continuum theory to model fatigue crack propagation which showed good settlement with simple uniaxial tests. A general formulation including low and high-cycle fatigue and creep-fatigue interaction at arbitrary stress states has been proposed by Lemaitre [90]. Further study of these models was carried out by Chaboche [28] in 1988. In order to model the effects of fatigue, the evolution law for the damage variable is generally formulated proposing a differential equation which relates damage growth

with mean and maximum stresses and with the number of cycles. Nevertheless, as only a scalar damage variable was employed and as it involved the use of the maximum and mean stresses, under multiaxial loading conditions two fundamental problems were inevitably confronted: the definition of the multiaxial stress parameters associated with the maximum and mean values and the applicability of the models to special loading conditions including non-proportional loading for complex engineering structures. Chow and Wei [39] in 1991 proposed a new model which bypassed these problems. Throughout recent decades several authors have proposed another models to simulate fatigue processes considering damage, cf.: Wang [162] in 1992, Paas et al. [125] in 1993, Xiao et al. [166] and Bonora and Newaz [14] in 1998, Perera et al. [127] in 2000, Dattoma et al. [47] in 2006, among others.

The original notion of continuum damage mechanics was developed for an isotropic material, for which the damage variable is represented by a scalar value. At the beginning of 1980s the first efforts were done to propose realistic models to describe materials presenting anisotropic damage. To this end, Krajcinovic and Fonseka [56, 81] introduced the vector damage variables. In further attempts, two main formulations were proposed: the orthotropic model, where the damage variable is represented by a second order tensor, advocated by Murakami and Ohno [118], Chow and Wang [37], Voyiadjis and Kattan [157], Lemaitre [93], among others, and the general anisotropy model, in which the damage variable is represented by a fourth order tensor as proposed by Chaboche [27], Krajcinovic [80], Simó and Ju [139], Ju [74], Voyiadjis et al [160]. For the anisotropic damage case, the effective stress tensor is usually asymmetric. This leads to a complex theory of damage mechanics that entails micropolar media and the Cosserat continuum. To avoid such a theory, symmetrization of the effective stress tensor is used to state a continuum damage theory in the classical sense. This method was studied by Chow and Lu [36] and Voyiadjis and Park [158] among others.

Subsequent, efforts were channeled to extend the CDM approach to the study of damage modelling at large strains. In 1990 Combescure and Yin [44] proposed a generalization of the discrete Kirchhoff theory to the analysis of general shell structures subjected to large strains coupled with ductile damage. In 2001 a theory for large strain elastoplastic damage was developed by Brüning [20] who used a multiplicative decomposition of the metric transformation tensor into elastic and damage-plastic parts. The same year, Menzel and Steinmann [111] posed a theoretical and computational model for the treatment of anisotropic damage at large strains based on second order metrics. Kaliske et al. [77] established the constitutive relations for elastomeric materials presenting finite viscoelastic damage. Other models were developed by Simó and Ju [140] in 1989, Miehe [112] in 1995, Voyiadjis and Park [159] in 1999, Calvo et al. [23] in 2006, among others.

Starting from the premise that the gradient effect is significant when the characteristic dimension of the plastic deformation or damage is of the same order of the material intrinsic length scale, a set of so-called non-local theories have been developed: Pijaudier-Cabot and Bazant [6, 128] around 1987, Fleck et al. [54] in 1994, De Vree et al. [161] in 1995.

More recently, a new group of models which links the different approaches have been proposed. Chaboche et al. [31, 32] developed further interface damage mechanics (IDM) which is a numerical tool developed as a part of continuum damage mechanics, with intermediate competencies between CDM and fracture mechanics. IDM is used to model the growth of a crack at the interface between different components of the material. In 2006, Chaboche et al. [30] proposed a CDM approach with plastic compressibility. The latter model changes the classical formalism of damage mechanics so as to describe plastic compressibility for ductile damage processes. A new damage variable was used which plays the role of porosity in micromechanics based approaches like Gurson's model. Into the framework of IDM approach, Marfia et al. [103, 150] proposed a new coupled interface-body damage model for the study of the detachment process in concrete or masonry structures strengthened with fiber reinforced polymers. This latter model is developed in the framework of continuum damage mechanics and it takes into account frictional sliding. Alfano and Sacco [2] and, more recently, Sacco and Toti [134, 150] proposed a new method to combine interface damage and friction in a cohesive-zone model on the basis of a micromechanical formulation. Other interface damage models can be found in the following References: in 2000 Dobert et al. [49], in 2005 Hachemi et al. [60], in 2007 van Hal et al. [61]. On the other hand, Ladèveze et al. [46, 83–85, 98] proposed a damage mesomodel for laminates (DML) with continuous fibers based on the use of an intermediary scale related to the scale of the laminates. In this model damage mechanics and qualitative microanalysis are used to describe the degradation of mesoconstituents. One of the advantages of this procedure is that damage mechanisms, which can be very complex on the structure's scale, can be much simpler on the scale of basic constituents. Another example of this group is due to Xue [167] in 2007, who developed a new damage plasticity model which incorporates the pressure and Lode angle dependences of ductile fracture. This model has a similar formulation to that of the abrupt failure methods however as the material weakening is incorporated into the constitutive model by means of coupling the yield function and associated flow with damage, it becomes a coupled method.

The above survey is by no means a complete description of all models and formulations proposed in the literature, we have merely cited a selection of representative works of the main approaches to model damage in solids.

2 Continuum Damage Mechanics

Continuum Damage Mechanics is nowadays recognized as an effective tool to model damage, which can bridge the gap between the microscopic analysis of the internal deterioration of materials and the design of suitable engineering models. CDM is fully coupled with the constitutive law that involves the softening of the material stiffness. This approach is probably the most widely used one at present and is therefore chosen for further analysis in this work.

2.1 Mechanical representation of damage and damage variables

The proper and accurate modelling of material damage represents one of the crucial problems of CDM. It is possible to homogenize the true distribution of damage in a quasicontinuum by using properly defined internal variables that characterize damage.

Damage variables used in literature can be scalar or tensor variables. To model isotropic damage processes it suffices to consider scalar damage variables [88], whereas tensor-valued damage variables (second-, fourth- or eight-order) are required to take into account anisotropic damage. Namely, in the case of random distribution of microvoids or of isotropic distribution of spherical voids, the damage state is usually modeled as isotropic. On the other hand, when microvoids or spherical cavities have oriented distribution, the damage states are anisotropic and a tensor-valued damage variable is required. However, when void density is small, although the cavities have apparent orientation in their geometry and distribution, macroscopic mechanical properties can be considered as nearly isotropic. Besides, the scalar damage variable is much easier in its mathematical procedure than that for the tensorial variables. Thus the isotropic damage theory has been often applied to three-dimensional problems of elastoplastic, ductile, fatigue and creep damage [91].

A key issue is how to quantify the magnitude of the damage variable in a damaged body. For this purpose, many different methods have been proposed in literature. Assume a damaged body B and a representative volume element RVE at a point $P(x)$ in B , oriented by a plane defined by its normal $\mathbf{n}$ as shown in Figure 1. Let A_0 be the nominal area of the intersection of the plane with the RVE and let A be the effective load bearing area of the damaged material due to void development. In his early work on the matter, Kachanov [75] proposed (to characterize the gradual deterioration process of a microstructure) a scalar variable ψ , which he named *continuity* and defined as,

$$\psi(P, \mathbf{n}) = \frac{A}{A_0}, \quad \psi \in [0, 1] \quad (1)$$

Fig. 1 Effective area reduction due to damage

For a completely undamaged material $\psi = 1$ and for a fully damaged material without remaining load-carrying capacity $\psi = 0$. Rabotnov furthered this idea and proposed the reduction of the cross-sectional area due to microcracking as a suitable measure of the state of internal damage. In this context, a new damage variable D was introduced by Rabotnov [129]

$$D(P, \mathbf{n}) = 1 - \psi = \frac{A_0 - A}{A_0} \quad (2)$$

It follows from this definition that the value of the scalar (isotropic) variable is $D = 0$ for the virgin undamaged material and $D = 1$ for a completely damaged material. According to the Figure 1, the damage variable D depends on the position and orientation of the intersection area in the *RVE*. If the damage state may be considered as isotropic, then D is constant regardless of the orientation and position and is usually obtained as,

$$D = 1 - \frac{A}{A_0} \quad (3)$$

If damage can be considered as isotropic, the effective area A is given by Equation (3). Accordingly, the decrease in the load-carrying area increases the effect of the stress σ . Then, the effective stress $\bar{\sigma}$ [130] is obtained as,

$$\bar{\sigma} = \frac{\sigma}{1 - D} \quad (4)$$

The above definition corresponds to the effective stress on the material in tension. Instead, in compression, if some defects are closed, the area that resists the load is larger than A . For the particular case where all defects are closed, the stress in compression $\bar{\sigma}^+$ is equal to σ .

A way to avoid a micromechanical analysis for each type of defect and mechanism of damage is to postulate a principle at the mesoscale. To this end, Lemaitre

[87] proposed the hypothesis of strain equivalence based on the effective stress concept, as follows: “any strain constitutive equation for a damaged material may be derived in the same way as for a virgin material except that the usual stress is replaced by the effective stress”. In view of Equations (3) and (4), one can postulate that a damaged cylindrical bar with the cross-sectional area A_0 and subjected to a external force F is mechanically equivalent to an undamaged bar with the effective cross-sectional area A which is subjected to the same external force F . The effective stress defined by Equation (4) not only represents the effect of the decrease in the geometrical area due to damage, but also includes the effects of stress concentration at voids and the effects of interaction between them. Simó and Ju [139] proposed as an alternative to the concept of effective stress, the notion of effective strain $\bar{\epsilon} = (1 - D)\epsilon$, where ϵ is the strain tensor and $\bar{\epsilon}$ the effective strain tensor. Similarly to the strain equivalence principle and based on the concept of effective strain, they also proposed the stress equivalence principle: “the stress associated with a damaged state under the applied strain is equivalent to the stress associated with its undamaged state under the effective strain”.

For a uniaxial test, since the development of microvoids involves the reduction in stiffness of materials, the damage can be taken into account through the variation in elastic modulus [92]. As a direct result of the strain equivalence principle, Hooke’s law for the fictitious undamaged material is

$$\epsilon = \frac{\bar{\sigma}}{E} = \frac{\sigma}{E(1 - D)} = \frac{\sigma}{\bar{E}} \implies D = 1 - \frac{\bar{E}}{E} \quad (5)$$

where $\bar{E}$ is the damaged elasticity modulus and E is the undamaged one. The definition in Equation (5) of D can be extended to three dimensions and to tensorial damage variables. The modeling of damage states through the Young modulus or the elastic compliance tensor $\mathbb{C}$ have been applied also to the anisotropic damage of brittle materials like concrete.

The assumption of isotropic damage in many cases is not too far from reality or is at least a good modeling option, especially under conditions of proportional loading when the principal directions of the stresses remain constant. However, a rigorous formulation naturally leads to consider anisotropic damage by means of the definition of a damage tensor, particularly for brittle materials and for all materials under special loading conditions. Then, more general mathematical representations of anisotropic damage modeling are described below. A simple way to model anisotropic damage was proposed by Hayhurst and Leckie [65] in 1973, considering that damage occurs only in the plane normal to the maximum principal stress. In this model the damage is represented by its magnitude D and the direction of the maximum principal stress $\mathbf{n}$. For a more complex distribution of anisotropy, according to Murakami and Ohno [118] it is possible to extend the notion of the damage variable D proposed by Rabotnov by means of the Equation

(2) to a three dimensional case with orthotropic damage as follows,

$$\mathbf{A} = (\mathbf{1} - \mathbf{D}) \cdot \mathbf{n} \cdot \mathbf{A}_0 = (\mathbf{1} - \mathbf{D}) \cdot \mathbf{A}_0 \quad \text{with} \quad \mathbf{D} = \sum_{i=1}^3 D_i \mathbf{n}_i \otimes \mathbf{n}_i \quad (6)$$

where $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$ are the normals of three symmetry planes, $\mathbf{D}$ is a symmetric second-order damage tensor whereas $\mathbf{A}$ and $\mathbf{A}_0$ are the vector areas.

For a general case of anisotropy, Chaboche extended to three dimensions the notion of Equation (5) to represent the damage state in terms of the variation of the elastic modulus by defining a damage tensor $\mathcal{D}$ of fourth- or eighth-order. Let $\mathbb{C}$ and $\bar{\mathbb{C}}$ the fourth-order elasticity modulus tensor of an undamaged and a damaged material, respectively. Then the elastic constitutive equations of these materials are given by,

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}, \quad \boldsymbol{\sigma} = \bar{\mathbb{C}}(\mathcal{D}) : \boldsymbol{\varepsilon} \implies \bar{\boldsymbol{\sigma}} = \mathbb{C} : \boldsymbol{\varepsilon} \quad (7)$$

where the last identity follows from the principle of strain equivalence. Then, Equation (7) leads to,

$$\bar{\boldsymbol{\sigma}} = \mathbb{C} : [\bar{\mathbb{C}}(\mathcal{D})]^{-1} : \boldsymbol{\sigma} \quad (8)$$

Considering Equation (7), the damage tensor $\mathcal{D}$ is an eighth-order tensor which converts the fourth-order elasticity tensor $\mathbb{C}$ for an undamaged material into another fourth-order elasticity tensor $\bar{\mathbb{C}}$ for the damaged material. As the mathematical treatment and determination of eighth-order tensors is complicated, then Chaboche [26] defined an alternative fourth-order damage tensor $\mathbb{D}$ and established the following relation,

$$\mathbb{D} = \mathbb{I} - \bar{\mathbb{C}}(\mathbb{D}) : \mathbb{C}^{-1}, \quad \text{so} \quad \bar{\boldsymbol{\sigma}} = (\mathbb{I} - \mathbb{D})^{-1} : \boldsymbol{\sigma} \quad (9)$$

where $\mathbb{I}$ is the fourth-order identity tensor. In view of Equation (9), the damage tensor $\mathbb{D}$ is generally asymmetric, therefore Chaboche [29] later proposed a new fourth-order symmetric damage tensor $\bar{\mathbb{D}}$ and another alternative relation,

$$\mathbb{C}(\bar{\mathbb{D}}) = \frac{1}{2} [(\mathbb{I} - \bar{\mathbb{D}}) : \mathbb{C} + \mathbb{C} : (\mathbb{I} - \bar{\mathbb{D}})] \quad (10)$$

As a result of the Equation (9) the anisotropic damage state can be determined by the variation in the material stiffness. Therefore, several authors such as Ortiz [123] and Simo and Ju [73, 139], developed this idea further and considered the elasticity modulus tensor $\mathbb{C}$ itself as an internal variable of damage. The effective stress tensor $\bar{\boldsymbol{\sigma}}$ can be expressed in a unified form [25, 45] as

$$\bar{\boldsymbol{\sigma}} = \mathbb{M}(\mathcal{D}) : \boldsymbol{\sigma} \quad (11)$$

where $\mathbb{M}(\mathcal{D})$ is a fourth-order tensor which characterizes the state of damage and transforms the Cauchy stress tensor $\boldsymbol{\sigma}$ into an effective stress tensor $\bar{\boldsymbol{\sigma}}$ (or vice

versa) and is named as damage effect tensor. The tensor $\mathcal{D}$ is a damage tensor that may be a zero-, second-, or fourth-order tensor.

Furthermore, as already mentioned in the introduction, the damage state of a material can be described also by the void volume fraction f in the material according to Gurson [58] and Rousselier [133] is given by

$$f = \frac{V_0 - V}{V_0} = \frac{V_D}{V_0} = \frac{\rho_0 - \rho}{\rho_0} = 1 - \frac{\rho}{\rho_0}$$

where V_0 , V_D and V are the volume of *RVE*, the total volume of the voids and the effective volume of the *RVE*, respectively and ρ_0 and ρ denote the initial and the damaged density of the material, also respectively. The density form is a more convenient way to measure the void volume fraction.

In short, a simple reliable measurement of the damage state is still nowadays a defiant task.

2.2 Thermodynamics of damaged materials

A classical way to formulate the phenomena of damage is to postulate the existence of energy potentials from which one can derive the state laws and the kinetic constitutive equations. In the thermodynamics of irreversible processes, two potentials are introduced within the framework of the *State Kinetic Coupling theory* [104]: the *thermodynamic potential* and, as it is commonly named, the *dissipation potential*. The thermodynamic potential, written as a function of the state variables, defines the state laws and the variables associated with the state variables to define the power involved in each physical process. Besides, the kinetic laws of evolution of the flux dissipative variables are derived from the potential of dissipation written as function of the associated variables.

The expression of the thermodynamic potential can be determined taking into account the coupling between state variables. According to Lemaitre [91] elasticity is directly influenced by damage, since the number of atomic bonds responsible for elasticity decreases with damage. This coupling is called a *state coupling*. However damage influences plastic or irreversible strains only because the elementary area of resistance decreases as the number of bonds decreases. This indirect coupling is called *kinetic coupling*. In this way it is possible to uncouple the effects of elasticity with damage from the effects of plasticity and other internal variables. Considering the assumptions of small strains and displacements, the state variables are divided in external and internal variables. In isothermal processes the external variable is the total strain tensor $\boldsymbol{\varepsilon}$ associated with the Cauchy stress tensor $\boldsymbol{\sigma}$. On the other hand, the internal variables are: the elastic strain tensor $\boldsymbol{\varepsilon}^e$ and the plastic strain tensor $\boldsymbol{\varepsilon}^p$ both associated with the stress tensor $\boldsymbol{\sigma}$, the damage accumulated plastic strain r that is associated with the isotropic hardening variable R , the back

strain tensor $\boldsymbol{\alpha}$ which is associated with the back stress tensor $\mathbf{X}$ that represents the kinematic hardening. In this framework the Helmholtz free energy function per unit mass is given by

$$\psi = \psi^e(\boldsymbol{\varepsilon}^e, D) + \psi^p(r, \boldsymbol{\alpha}) \quad (12)$$

where the function ψ is a scalar-valued continuous function. Then, the second principle of thermodynamics written as the Clausius-Duhem inequality, focusing only on mechanical processes, provides

$$\left(\boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} \right) : \dot{\boldsymbol{\varepsilon}}^e + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \left(\rho \frac{\partial \psi}{\partial r} \dot{r} + \rho \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \dot{\boldsymbol{\alpha}} + \rho \frac{\partial \psi}{\partial D} \dot{D} \right) \geq 0 \quad (13)$$

Then, the associated conjugate variables are

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \quad R = \rho \frac{\partial \psi}{\partial r}, \quad \mathbf{X} = \rho \frac{\partial \psi}{\partial \boldsymbol{\alpha}}, \quad Y = -\rho \frac{\partial \psi}{\partial D} \quad (14)$$

where Y is the associated damage variable. The description of the change in the internal state requires the evolution equations of the internal variables. Then it is usual the introduction of a second potential from which one can derive the kinetic constitutive relations. From observation of the reduced Clausius-Duhem inequality,

$$F = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - R \cdot \dot{r} - \mathbf{X} : \dot{\boldsymbol{\alpha}} - Y \cdot \dot{D} \geq 0 \quad (15)$$

one can conclude that the dissipation inequality is expressed by the sum of the products of flux variables and their dual variables. It is frequently postulated that the kinetic laws are derived from a potential of dissipation F , which is a scalar continuous and convex function of the dual variables

$$F(\boldsymbol{\sigma}, R, \mathbf{X}, Y; \boldsymbol{\varepsilon}^e, r, \boldsymbol{\alpha}, D) \quad (16)$$

The evolution equations for the flux variables are then given by a generalized normality rule using a single positive scalar multiplier $\dot{\lambda}$. This approach implies the simultaneous evolution of inelastic deformation and damage. Within this framework, several models have been proposed, especially for modeling ductile materials [13, 15, 16, 91]. However, for usual materials, ductile damage starts after meaningful inelastic deformation, while brittle damage occurs without noticeable deformation. Therefore, postulating a single dissipation potential and a single multiplier on the standard thermodynamic approach may impose severe restrictions on the modeling of the damaged material. This limitation may be overcome by postulating a plurality of independent dissipation potentials together with their corresponding multipliers for each different damage mechanism. For models based on this approach, see References [37, 64, 73, 139, 145, 169], among others.

3 Applications of Continuum Damage Mechanics

3.1 Ductile Isotropic Damage

Ductile damage is produced by void development due to plastic deformation in materials. In the particular case of metals, this type of damage appears in a number of engineering problems, mainly in fracture of structural elements and in damage caused during plastic forming processes. Below, some representative models of ductile damage are presented. For more details on continuum damage mechanics models for ductile damage and fracture, see the exhaustive review of Besson [10].

3.1.1 The ductile isotropic damage model of Lemaitre

The first model to be reviewed herein is that of Lemaitre (1985) [89]. This model belongs to the family of models that assume simultaneous evolution of damage and plastic deformation by considering a single dissipation potential with a single multiplier. The other main feature of this model is the proportionality of the damage rate to the strain energy density release rate Y and to the accumulated plastic strain rate $\dot{p}$, once surpassed a plastic strain threshold p_0 and up to a critical level of the damage state p_{cr} . The analytical expression for ψ is chosen in the framework of the *State Kinetic Coupling Theory*. In this expression linear isotropic elasticity and state coupling of damage with elastic strain are considered:

$$\rho\psi = w_e + w_p = \frac{1}{2}\boldsymbol{\varepsilon}^e : \mathbb{C} : \boldsymbol{\varepsilon}^e(1 - D) + R \cdot r + \mathbf{X} : \boldsymbol{\alpha} \quad (17)$$

No state coupling either between elasticity and plasticity nor between plasticity and damage are assumed. Then, the energy release rate can be derived from Equations (14) and (17),

$$Y = -\rho \frac{\partial \psi}{\partial D} = \frac{1}{2}\boldsymbol{\varepsilon}^e : \mathbb{C} : \boldsymbol{\varepsilon}^e = \frac{w_e}{(1 - D)} \quad (18)$$

The strain energy density release rate Y is the principal variable which governs the damage process. Lemaitre considered interesting to interpret this parameter as an equivalent von Mises stress for plasticity. To this end, w_e is split into two parts, the shear energy corresponding to the deviatoric part and the hydrostatic energy corresponding to the spherical part, so

$$w_e = \int \sigma_{ij} d\varepsilon_{ij} = \int \sigma_{ij}^D d\varepsilon_{ij}^D + 3 \int \sigma^H d\varepsilon^H \quad (19)$$

where σ_{ij}^D and σ^H and ε_{ij}^D and ε^H are the deviatoric and hydrostatic parts of the stress and strain tensors, respectively. Solving the integral and substituting the

result in Equation (18)

$$Y = \frac{\sigma_{eq}^2}{2E(1-D)^2} \left[\frac{2}{3}(1+v) + 3(1-2v) \left(\frac{\sigma_H}{\sigma_{eq}} \right)^2 \right] = \frac{\bar{\sigma}_{eq}^2}{2E} R_v \quad (20)$$

where v is Poisson's ratio, σ_{eq} is the von Mises equivalent stress, $\bar{\sigma}_{eq}$ denotes the effective von Mises equivalent stress which is given by $\bar{\sigma}_{eq} = \sigma_{eq}/(1-D)$ and R_v is a triaxiality function.

Thus, as in plasticity, the damage equivalent stress is defined as the one-dimensional stress σ^* which, for identical damage state, yields the same value of the elastic strain energy as that of the three-dimensional case,

$$\sigma^* = \sigma_{eq} R_v^{1/2} \quad (21)$$

The damage equivalent stress differs from that of the von Mises equivalent stress by the role of triaxiality, which is a logical consequence because metal plasticity is directly related to slips, which do not depend on the hydrostatic stress. In contrast, damage is influenced by the debonding of atoms because of the hydrostatic stresses or triaxiality function.

To complete the set of constitutive equations, the evolution laws for the internal variables have to be established. From experimental observations [91] it can be concluded that plastic flow can occur without damage and likewise that damage can occur without remarkable plastic flow. Consequently, it is possible to separate the dissipation function in the damage and the plastic flow contributions, as follows

$$F = F^P(\boldsymbol{\sigma}, R, \mathbf{X}; D) + F^D(Y; p, D) \quad (22)$$

The choice of this function F^D is the key to depict the damage evolution. It is desirable to develop a unique kinetic law of damage evolution which represents the general trends of all kinds of damage in many types of materials. Lemaitre proposed:

$$F^D = \frac{Y^2}{2S(1-D)} H(p - p_D) \quad (23)$$

where S denotes a material constant which quantifies the energy strength of damage and $H(\cdot)$ represents the Heaviside step function. Then,

$$\dot{D} = \dot{\lambda} \frac{\partial F}{\partial Y} = \dot{\lambda} \frac{\partial F^D}{\partial Y} = \frac{Y}{S} \dot{p} H(p - p_D) \quad (24)$$

and the multiplier $\dot{\lambda}$ is given by $\dot{\lambda} = \dot{p}(1-D)$ where $\dot{p}$ is the accumulated plastic strain rate. In summary, the evolution of the damage variable D is obtained as,

$$\dot{D} = \frac{Y}{S} \dot{p} \quad \text{if } p \geq p_D < p_{cr} \quad \text{and} \quad \dot{D} = 0 \quad \text{if } p < p_D \quad (25)$$

Equation (24) entails a linear relation between damage development and the accumulated plastic strain. Nevertheless, depending on the material properties and the loading conditions, this linear damage model is not always suitable as it can be concluded from the experimental results of Le Roy et al. [94]. Therefore, the linear ductile damage model has been extended to describe more general ductile damage processes, see References: Tai and Yang [148], Chandrakanth and Pandey [33] and Bonora [13], among others.

3.1.2 Nonlinear ductile isotropic damage model of Bonora

The development of ductile damage is dominated not only by the strain energy release rate Y but also by the states of damage and plastic strain. Bonora also considered that the mechanical effect of damage may depend on the relative relation between the current value of damage in the material and its critical value. Accordingly, Bonora [13] proposed the following expression for the damage contribution to the dissipation function,

$$F^D = \frac{1}{2} \left(\frac{Y}{S} \right)^2 \frac{S}{1-D} \frac{(D_{cr} - D)^{(\alpha-1)/\alpha}}{p^{(2+n)/n}} \quad (26)$$

Here D_{cr} is the critical value of the damage variable for which ductile failure takes place, n is the Ramberg-Osgood material hardening exponent and α is the damage exponent that characterizes the shape of the damage evolution curve and is related to the nature of the matrix-inclusion bond that induces voids nucleation and growth. Then, the evolution of the damage variable results,

$$\dot{D} = \dot{\lambda} \frac{\partial F^D}{\partial Y} = \frac{K^2}{2ES} R_v (D_{cr} - D)^{(\alpha-1)/\alpha} \frac{\dot{p}}{p} H(p - p_D) \quad (27)$$

For a ductile material, the effective equivalent von Mises stress can be formulated using a Ramberg-Osgood power law as,

$$\frac{\sigma_{eq}}{(1-D)} = K p^{1/n} \quad (28)$$

where K is a material constant.

The kinetic law of damage evolution can be analytically integrated in the simple cases of uniaxial loading, for which $R_v = 1$, or in the case of proportional loading where R_v remains constant through the complete deformation process.

The CDM model of Bonora, as those of Lemaitre, Chandrakanth and Pandey, requires the knowledge of the values of the effective accumulated plastic strains p_D and p_{cr} in order to represent the damage evolution for general loading conditions. It is well known that stress triaxiality plays an important role in the failure process. Rice and Tracey [131] analytically found an exponential decrease of strain at failure

with the increase of triaxiality ratio. Later, Hancock and Mackenzie [63], who have researched extensively on the subject, discovered that the relation between ductility at failure and triaxiality are nonlinear and inverse. As it was enunciated by Lemaitre [91]: “high triaxiality makes materials brittle”. According to the work of Bonora, the linear damage model proposed by Lemaitre overestimates the effective strain at failure in multiaxial states of stress.

3.1.3 Ductile Isotropic Damage Model of Simó and Ju

This model belongs to the family of models that employ distinct independent dissipation potentials together with the corresponding multipliers for particular physical mechanisms of deformation and damage. Then, the dissipation potential of Equation (16) is assumed to be divided into two independent potentials F^P and F^D for plastic deformation and damage, respectively. Accordingly, for rate independent materials the evolution of plastic deformation and damage are derived from the following dissipation potentials with their corresponding criteria,

$$F^P = F^P(\boldsymbol{\sigma}, R, \mathbf{X}; D) \quad \text{and} \quad F^D = F^D(Y, p; D) \quad (29)$$

Then, the evolution equations for plastic strain and damage are given by,

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\lambda} \frac{\partial F^P}{\partial \boldsymbol{\sigma}}, \quad \dot{r} = \dot{\lambda} \frac{\partial F^P}{\partial R}, \quad \dot{\boldsymbol{\alpha}} = \dot{\lambda} \frac{\partial F^P}{\partial \mathbf{X}} \quad \text{and} \quad \dot{D} = \dot{\mu} \frac{\partial F^D}{\partial Y} \quad (30)$$

Simó and Ju [139] proposed the definition of an undamaged energy norm $\bar{\tau}$ of the strain tensor. This definition is at odds with that used by Mazars and Lemaitre [106] as the J_2 -norm of the strain tensor. The main difference between these two definitions is that the first one leads to symmetric elastic-damage moduli while the second one entails a lack of symmetry. Simó and Ju set,

$$\bar{\tau} := \sqrt{2\Psi^0(\boldsymbol{\varepsilon})} \quad (31)$$

Thereby, Simó and Ju described the state of damage in the material through the following damage criterion formulated in strain space as

$$f^D(\bar{\tau}, p) := \bar{\tau}_t - p_t \leq 0 \quad (32)$$

where p_t is the damage threshold and the subscript $t \in \mathbb{R}_+$ means the value at the actual time. This criterion establishes that damage in the material is started when the energy norm of the strain tensor $\bar{\tau}_t$ exceeds the initial damage threshold p_0 . For the isotropic case, they defined the damage evolution as

$$\dot{D} = \dot{\mu} H(\bar{\tau}_t, D_t), \quad \dot{p} = \dot{\mu} \quad (33)$$

where $\dot{\mu} \geq 0$ is a damage consistency parameter such that,

$$\dot{\mu} \geq 0, \quad f^D(\bar{\tau}, p) \leq 0, \quad \dot{\mu} f^D(\bar{\tau}, p) = 0 \quad (34)$$

3.2 Brittle Damage

Damage is generally referred to as brittle when it occurs by decohesion without any sensible plastic strain at the mesoscale. For some kinds of materials such as ceramics, concrete, rocks, bones or high-strength quenched steels, which are widely employed in engineering practice, there is no considerable plastic strain at the mesoscale up to failure. In brittle materials the irreversible deformation is caused mainly by the creation and development of microcracks in the material and involves a significant reduction in the elastic stiffness. The damage of brittle materials is generally accompanied by anisotropy and unilateral effects.

The unilateral effect or crack closure is one of the most complicated tasks in the modeling of damage in brittle materials. Cracks in a brittle material are effective only when they are open and have no mechanical effects when they are completely closed. Namely, when the state of load is such that the microcracks and microcavities are completely closed, the area that effectively carries the load is no longer the effective area but the total area. The state of the cracks that are open is named *active*, whereas the state of the cracks that are completely closed is referred as *passive*. A phenomenon in which the damage effect differs depending on the sign of stress or strain is called unilateral. The opening or closing of a crack depends on whether the normal stress which acts on the crack plane is tensile or compressive. The decrease of damage effects due to microcrack closure is generally named *damage deactivation*.

3.2.1 Elastic-brittle isotropic damage model of Mazars and Pijaudier-Cabot

As mentioned above, brittle damage is accompanied by considerable anisotropy, however isotropic damage can be considered suitably in an early stage of damage or in the particular case of proportional loading. Assuming that the material is elastic-brittle and that the damage state can be represented by a scalar damage variable D . In order to capture the differences of mechanical responses of the material in tension and compression, the damage variable D is divided into two independent scalars, D_t due to a tensile stress and D_c due to a compressive stress,

$$D = \alpha_t D_t + \alpha_c D_c \quad (35)$$

where α_t and α_c are the weighting coefficients ($\alpha_t + \alpha_c = 1$) which are functions of the strain state.

For the same purpose, the stress tensor $\boldsymbol{\sigma}$ is divided into a positive part of the principal stress $\boldsymbol{\sigma}^+$ and a negative part $\boldsymbol{\sigma}^-$ as follows,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^- \quad \text{such that} \quad \boldsymbol{\sigma}^+ = \mathbb{P}^+(\boldsymbol{\sigma}) : \boldsymbol{\sigma} \quad \text{and} \quad \boldsymbol{\sigma}^- = \boldsymbol{\sigma} - \boldsymbol{\sigma}^+ \quad (36)$$

where $\mathbb{P}^+(\boldsymbol{\sigma})$ is a positive orthotropic projection tensor which components are given by $[\mathbb{P}^+(\boldsymbol{\sigma})]_{ijkl} = H(\sigma_i)H(\sigma_j)\delta_{ij}\delta_{kl}$, where σ_i are the principal components of $\boldsymbol{\sigma}$. As the material is considered to remain elastic, the elastic potential $\rho\psi^e$ is

$$\begin{aligned} \rho\psi^e = \rho\psi^e(\boldsymbol{\sigma}^+) + \rho\psi^e(\boldsymbol{\sigma}^-) = & \frac{1}{2} \frac{1}{E_0(1-D_t)} [(1+v_0)(\boldsymbol{\sigma}^+ : \boldsymbol{\sigma}^+) - v_0(tr\boldsymbol{\sigma}^+)^2] + \\ & + \frac{1}{2} \frac{1}{E_0(1-D_c)} [(1+v_0)(\boldsymbol{\sigma}^- : \boldsymbol{\sigma}^-) - v_0(tr\boldsymbol{\sigma}^-)^2] \end{aligned} \quad (37)$$

where ρ , E_0 and v_0 are the mas density, Young's modulus and Poisson's ratio of the undamaged material, respectively. In the Clausium-Duhem inequality two damage energy release rates related to each damage scalar variable appear,

$$F^D = Y_t \dot{D}_t + Y_c \dot{D}_c \quad \text{and} \quad Y_t = -\rho \frac{\partial \psi^e}{\partial D_t}, \quad Y_c = -\rho \frac{\partial \psi^e}{\partial D_c} \quad (38)$$

On the basis of the experimental results, Mazars and Pijaudier-Cabot [107] derived the following equations for the damage variables,

$$D_t = F_t(\tilde{\epsilon}); \quad D_c = F_c(\tilde{\epsilon}) \quad \text{with} \quad F_i(\tilde{\epsilon}) = 1 - \frac{(1-A_i)K_0}{\tilde{\epsilon}} - \frac{A_i}{\exp[B_i(\tilde{\epsilon} - K_0)]} \quad (i = t, c) \quad (39a)$$

$$\alpha_t = \sum_{i=1}^3 H(\varepsilon_{ti}) \frac{\varepsilon_{ti}(\varepsilon_{ti} + \varepsilon_{ci})}{\tilde{\epsilon}}, \quad \alpha_c = \sum_{i=1}^3 H(\varepsilon_{ci}) \frac{\varepsilon_{ci}(\varepsilon_{ti} + \varepsilon_{ci})}{\tilde{\epsilon}} \quad (39b)$$

where K_0 , A_t , B_t , A_c and B_c are material parameters which can be obtained from compression tests on cylinders, and bending tests on beams and $\tilde{\epsilon}$ is the *equivalent strain* and is defined as

$$\tilde{\epsilon} = [(H(\varepsilon_i)\varepsilon_i)^2]^{\frac{1}{2}} = [tr(\mathbb{P}^+(\boldsymbol{\epsilon}) : \boldsymbol{\epsilon})^2]^{\frac{1}{2}} \quad (40)$$

Mazars and Pijaudier-Cabot proposed to use for each variable a different damage loading surface,

$$f_t(\boldsymbol{\epsilon}, \mathbb{C}, K_0) = Y_t - K_t(D_t) \quad \text{and} \quad f_c(\boldsymbol{\epsilon}, \mathbb{C}, K_0) = Y_c - K_c(D_c) \quad (41)$$

where K_t and K_c are the hardening-softening parameters which correspond to the largest value of the equivalent strain ever reached by the material.

3.2.2 Anisotropic brittle damage theory based on a second-order damage tensor

Although the representative model reviewed above is simple and understandable, it can not be applied to the cases of remarkable anisotropy. Thus a number of theories have been proposed to model the anisotropy of damage through damage variables ranging from a vector to higher order tensors [12, 116, 118, 122]. Among them, second order symmetric damage tensors are commonly used [35, 38, 78, 97, 156] because they are mathematically easier than higher rank tensors. However they can still depict the fundamental features of anisotropic damage. In these models, the damage state can be described by the damage tensor of Equation (6), which, as already explained, can not represent more complicated damage states than orthotropic ones. In this framework, the model of Murakami and Kamiya [117] is chosen to be analyzed below as a representative model of this family.

Assuming an isothermal anisotropic damage process of an elastic-brittle material, the Helmholtz free energy function per unit mass is stated as $\psi = \psi(\boldsymbol{\varepsilon}, \mathbf{D}, \beta)$ where $\boldsymbol{\varepsilon}$, $\mathbf{D}$ and β are the elastic strains, a second-order symmetric damage tensor and a damage-strengthening internal variable, respectively. Namely, besides the damage effects represented by $\mathbf{D}$, an additional effect may be also required to depict the damage state which is responsible for the further development of damage, thus another scalar damage variable β is introduced.

Murakami and Kamiya proposed the division of the free energy function into the energy $\psi^e(\boldsymbol{\varepsilon}, \mathbf{D})$ due to elastic deformation but also affected by damage and $\psi^D(\beta)$, exclusively related to the damage development, $\psi = \psi^e(\boldsymbol{\varepsilon}, \mathbf{D}) + \psi^D(\beta)$. After taking into account several mathematical, micromechanical and thermodynamic considerations, they finally arrived at the following expression for the free energy per unit mass,

$$\psi(\boldsymbol{\varepsilon}, \mathbf{D}, \beta) = \frac{1}{2}\bar{\lambda}(tr\boldsymbol{\varepsilon})^2 + \mu tr(\boldsymbol{\varepsilon}^2) + \eta_2(tr\mathbf{D})tr(\boldsymbol{\varepsilon}^+)^2 + \eta_4 tr[(\boldsymbol{\varepsilon}^+)^2 \mathbf{D}] + \frac{1}{2}K_d\beta^2 \quad (42)$$

where $\bar{\lambda}$, μ are the Lamé parameters and η_2 , η_4 and K_d are material constants. $\boldsymbol{\varepsilon}^+$ is the positive-valued strain tensor $\boldsymbol{\varepsilon}^+ = \mathbb{P}^+(\boldsymbol{\varepsilon}) : \boldsymbol{\varepsilon}$ and is introduced in the free energy function in order to take into account the unilateral effect. For a detailed explanation refer to [117]. Accordingly, the elastic constitutive equation results,

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \rho \frac{\partial \psi^e}{\partial \boldsymbol{\varepsilon}} = \lambda(tr\boldsymbol{\varepsilon})\mathbf{I} + 2\mu\boldsymbol{\varepsilon} + 2\eta_2(tr\mathbf{D})\boldsymbol{\varepsilon}^+ + 2\eta_4\boldsymbol{\varepsilon}^+\mathbf{D} \quad (43)$$

and the variables $\mathbf{Y}$ and B associated with the internal variables $\mathbf{D}$ and β , respectively, are given by

$$\mathbf{Y} = -\rho \frac{\partial \psi^e}{\partial \mathbf{D}} = -\eta_2[tr(\boldsymbol{\varepsilon}^+)^2]\mathbf{I} - \eta_4(\boldsymbol{\varepsilon}^+)^2; \quad B = \rho \frac{\partial \psi^D}{\partial \beta} = K_d\beta \quad (44)$$

In order to derive the evolution equations of the damage variable $\mathbf{D}$ and the damage strengthening internal variable β , it is necessary to establish the damage dissipation function:

$$F^D(\mathbf{Y}, B) = Y_{eq} - (B_0 + B) \quad \text{with} \quad Y_{eq} = \sqrt{\left(\frac{1}{2}\mathbf{Y} : \mathbf{Y}\right)} \quad (45)$$

where B_0 is a material constant which represents the initial threshold of the damage evolution.

Finally the evolution equations are obtained from the damage dissipation function as follows,

$$\dot{\mathbf{D}} = \dot{\lambda}^D \frac{\partial F^D}{\partial \mathbf{Y}} = \dot{\lambda}^D \frac{\mathbf{Y}}{2Y_{eq}}, \quad \dot{\beta} = -\dot{\lambda}^D \frac{\partial F^D}{\partial \mathbf{Y}} = \dot{\lambda}^D \quad (46)$$

where $\dot{\lambda}^D$ is a damage consistency parameter.

With this model, the different behavior depending on the condition of loading due to the unilateral effect can be described by use of a single set of equations and material constants, without any extra assumptions for each loading condition.

In the elastic-brittle damage produced by the development of microcracks, additional to the anisotropic damage and the unilateral effect, the effect of frictional slip between the surfaces of microcracks can also be considerable. To overcome this problem, Halm and Dragon in 1998 extended the free energy function of Equation (42) by introducing a new internal variable to represent the slipped state. For further details, refer to [62].

3.2.3 Anisotropic brittle damage theory using the elastic modulus tensor as damage variable

The model of Ju [73] based on a fourth-order symmetric damage tensor is developed below. This model covers more complex cases of anisotropy than the orthotropy. Ju postulated that the damage state of the material can be represented by its elasticity tensor $\mathbb{C}$. Accordingly, the constitutive equation and the damage-associated variable $\mathbb{Y}$ are obtained as,

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \mathbb{C} : \boldsymbol{\varepsilon}^e; \quad \mathbb{Y} = -\rho \frac{\partial \psi}{\partial \mathbb{C}} = -\frac{1}{2} \boldsymbol{\varepsilon}^e \otimes \boldsymbol{\varepsilon}^e \quad (47)$$

He also proposed the following damage dissipation function,

$$F^D(\mathbb{Y}, B) = g(\mathbb{Y}) - B \quad (48)$$

where B is the threshold for the damage initiation. Consequently, the evolution equation of the damage variable $\mathbb{C}$ results,

$$\dot{\mathbb{C}} = \dot{\lambda}^D \frac{\partial F^D}{\partial \mathbb{Y}} \quad (49)$$

where $\dot{\lambda}^D$ is a damage consistency parameter. In order to take into account the unilateral effect on damage development, a new scalar variable ξ instead the damage associated variable $\mathbb{Y}$ is introduced. The variable ξ represents the magnitude of the dissipation due to active damage and takes the form

$$\xi \equiv \text{tr}(\mathbb{Y} : \mathbb{C}_{AC}) \quad \text{where} \quad \mathbb{C}_{AC} = \mathbb{P}_\varepsilon^+ : \mathbb{C}_0 : \mathbb{P}_\varepsilon^+ \quad (50)$$

where $\mathbb{C}_{AC}$ denotes the activated elastic modulus tensor. By substituting the variable $\mathbb{Y}$ by ξ in Equation (48), the following expression is obtained,

$$\bar{F}^D(\xi, B) = \bar{g}(\xi) - B \quad (51)$$

where $\bar{F}^D$ and $\bar{g}(\xi)$ are new functions resulting from rewriting F^D and g . Then, the evolution of the damage hardening variable is defined as,

$$\dot{B} = \dot{\lambda}^D H \quad \text{with} \quad H \equiv \frac{\partial \bar{g}(\xi)}{\partial \xi} \quad (52)$$

From the consistency condition $\bar{F}^D = 0$, it is obtained $\dot{\xi} = \dot{\lambda}^D$. Finally, the evolution of anisotropic brittle damage of Equation (49) results into

$$\dot{\mathbb{C}} = \dot{\lambda}^D \frac{\partial F^D}{\partial \mathbb{Y}} = \dot{\lambda}^D \frac{\partial \bar{F}^D}{\partial \xi} \frac{\partial \xi}{\partial \mathbb{Y}} = \dot{\xi} H \mathbb{P}_\varepsilon^+ : \mathbb{C}_0 : \mathbb{P}_\varepsilon^+ \quad (53)$$

3.3 Hyperelastic materials with isotropic damage

Many rubber-like materials consist of a crosslinked elastomeric substance with a distribution of carbon particles as fillers. A specimen of filler-loaded rubber subjected to a number of loadings generally exhibits a marked stress softening due to damage, known as the Mullins effect. This effect was noticed in the pioneering research of Mullins [113] in 1948. For a detailed description refer to Johnson and Beatty [71, 72]. Most practical engineering rubbers contain carbon particles as fillers and consequently show some degree of Mullins effect.

There are several theories in the literature that attempt to explain the mechanism of microscopic damage. They can mainly be sorted into two groups: the first group is based on the idea that internal damage is produced by debonding of rubber molecular chains attached between the filler particles, for example refer to Bueche [21, 22], among others. The second group of theories proposed that at first the filler-loaded rubber is in a so-called hard phase that degrades into a soft phase with the increasing strain.

In practice several other inelastic effects appear under extensional loading-unloading cycles. From experimental observations it is well known that the shape of the stress-strain curves is also rate and temperature dependent. Furthermore, the

shape of a specimen of carbon-black filled rubber after unloading differs considerably from its original shape. This significant effect produced by reinforcement entails residual strains. For more details, refer to the model of Holzapfel et al. [67], which considers these residual strains.

For simplicity, herein it will be only considered the Mullins effect, the rate and temperature dependency as well as residual strains are neglected. Moreover, in the phenomenological model the presence of carbon-black fillers is not considered. It has been chosen a Lagrangian description. Assuming an isothermal elastic process, the Helmholtz free energy function in the coupled form, is

$$\Psi(\mathbf{C}, D) = (1 - D)\Psi_0(\mathbf{C}) \quad (54)$$

where Ψ_0 is the effective strain-energy function of the hypothetical undamaged material, D is the scalar damage variable and $\mathbf{C}$ is the right Cauchy-Green metric tensor. In order to derive the stress relation, Equation (54) is differentiated with respect to time. From the Clausius-Planck inequality,

$$\mathcal{F} = \left(\mathbf{S} - (1 - D)2\frac{\partial\Psi_0(\mathbf{C})}{\partial\mathbf{C}} \right) : \frac{\dot{\mathbf{C}}}{2} + \Psi_0(\mathbf{C})\dot{D} \geq 0 \quad (55)$$

The second Piola-Kirchoff stress tensor $\mathbf{S}$ and the internal dissipation $\mathcal{F}$ can be obtained as,

$$\mathbf{S} = (1 - D)2\frac{\partial\Psi_0(\mathbf{C})}{\partial\mathbf{C}} \quad \text{and} \quad \mathcal{F} = Y\dot{D} \geq 0 \quad \text{with} \quad Y = \Psi_0(\mathbf{C}) \geq 0 \quad (56)$$

where $\mathbf{S}/(1 - D)$ denotes the effective second Piola-Kirchoff stress tensor and Y is the thermodynamic force which governs the damage evolution. Y has the meaning of the effective strain energy released Ψ_0 and is given by $Y = \Psi_0(\mathbf{C}) = -\partial\Psi/\partial D$.

Adopting the function $D = D(\alpha)$ as the damage variable, with $D(0) = 0$ and $D(\infty) \in [0, 1]$, the phenomenological variable α describes the discontinuous damage. Miehe [112] proposed an exponential saturation expression for $D(\alpha)$. The discontinuous damage variable α can be obtained as $\alpha(t) = \max_{\tau \in (0, t)} \Psi_0(\tau)$ where $\tau \in (0, t)$ is the history variable. This definition has been used by, among others, Souza Neto et al. [142].

In addition, the damage criterion in the strain space is established as,

$$f^D(\mathbf{C}, \alpha) = Y(\mathbf{C}) - \alpha \leq 0 \quad (57)$$

where for $f^D < 0$ no evolution of damage takes place. Finally, the evolution of the maximum thermodynamic force α is determined as,

$$\dot{\alpha} = \dot{Y} = \frac{\mathbf{S}}{(1 - D)} : \frac{\dot{\mathbf{C}}}{2} \quad \text{if } f^D = 0 \text{ and } \dot{Y} > 0; \quad \dot{\alpha} = 0 \quad \text{otherwise}$$

4 Conclusions

In this paper we have made a literature survey on the main contributions to damage modelling. First, we have briefly reviewed the different approaches to model the diverse macroscopic observations of microscopic material damage: abrupt failure criteria, porous plasticity and continuum damage models. Then, to make this survey brief, we have focused on the continuum damage models, which are probably the ones that have been more extensively used in engineering-oriented computational mechanics.

As a closing remark we can say that the variety of available approaches to model damage and the extensive amount of ongoing research on the topic may be interpreted as a confirmation that a satisfactory simple, general purpose, yet accurate approach is still to be found.

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Capítulo 4

Hiperelasticidad WYPIWYG

4.1. Introducción

Como se ha visto en el capítulo anterior, los tejidos blandos son modelados usualmente como materiales hiperelásticos. Tradicionalmente el comportamiento hiperelástico se modela asumiendo la forma de la función de energía almacenada. Esta función depende de algunos parámetros del material, los cuales son obtenidos mediante un algoritmo de optimización, típicamente el algoritmo de Levenberg-Marquardt, de tal modo que las predicciones representen lo mejor posible los datos experimentales. Suele ocurrir que un modelo representa bien los ensayos para ciertos niveles de deformación y combinaciones de deformación pero sin embargo no tan bien en otras condiciones diferentes. Diversos estudios sobre modelos de hiperelasticidad y algunas de sus limitaciones se pueden encontrar en las Referencias [65], [66], [67], [68], [69], [70], [71], [93], entre otras. Por otro lado, existen unos modelos basados en la interpolación mediante *splines* que no requieren parámetros del material para representar exactamente los datos experimentales. El principal requerimiento de estos modelos es el conocimiento del comportamiento a compresión aunque sí que necesitan la rama de compresión de la curva. Este requisito no representa ningún tipo de desventaja puesto que más adelante se demuestra que para caracterizar adecuadamente el comportamiento de un material hiperelástico no es suficiente con la parte de tracción sino que se necesita también la parte de compresión de un ensayo uniaxial (u otros ensayos alternativos válidos). Estos últimos modelos son los denominados *What-You-Prescribe-Is-What-You-Get* —para abreviar *WYPIWYG*. El modelo WYPIWYG para materiales isótropos incompresibles, el cual está basado en la fórmula de inversión de Kearsley y Zapas [70], se debe a Sussmann y Bathe [74] y actualmente está disponible en el código de elementos finitos comercial ADINA. La extensión del modelo a isotropía transversal y ortotropía es debida a Latorre y Montáns [73],[76]. Estos modelos presentan una

aproximación al problema puramente fenomenológica y principalmente numérica.

4.2. Modelo WYPIWYG isótropo de Sussman y Bathe

En este apartado se presenta un modelo hiperelástico isótropo para materiales incompresibles en el que la función de energía no tiene una forma predefinida que depende de unos parámetros sino que directamente se interpola mediante splines cúbicos. Su forma final se determina resolviendo las ecuaciones de equilibrio derivadas del ensayo experimental usado para la caracterización del material. Este modelo está basado en la descomposición aditiva, originalmente propuesta por Mooney [67] y desarrollada por Valanis-Landel [69], en este caso en función de las deformaciones logarítmicas principales $E_i = \ln \lambda_i$ con $i = 1, 2, 3$ resulta

$$\mathcal{W} = \omega(E_1) + \omega(E_2) + \omega(E_3) \quad (4.1)$$

donde $\omega(E)$ no tiene una forma predefinida. Se ha demostrado que la descomposición anterior de la función de energía es aplicable a muchos materiales blandos [93],[94]. La condición de incompresibilidad se impone mediante la siguiente restricción

$$\ln J = \text{tr} E = \mathbf{E} : \mathbf{I} = E_1 + E_2 + E_3 = 0 \quad (4.2)$$

Para determinar la función $\omega(E)$ se realiza un ensayo uniaxial de tracción y compresión sobre una probeta del material que se desea caracterizar. La ecuación de equilibrio planteada en la dirección de aplicación de la carga, denotada mediante el subíndice 1, es

$$\sigma_1(E_1) = \frac{d\mathcal{W}}{dE_1} = \frac{d\omega}{dE_1} + p = \omega'(E_1) + p \quad (4.3)$$

donde p es la presión hidrostática requerida para mantener incompresibilidad y se calcula a través de las ecuaciones de equilibrio y las condiciones de contorno restantes. Como se vio en el Capítulo 1, las tensiones conjugadas de trabajo de las deformaciones logarítmicas $\mathbf{E}$ son las tensiones generalizadas de Kirchhoff $\mathbf{T}$, sin embargo, al presentar comportamiento isótropo, $\mathbf{T} = \boldsymbol{\tau}$, y si además el material es incompresible resulta que $\mathbf{T} = \boldsymbol{\tau} = J\boldsymbol{\sigma}$. Como el material es isótropo, el material se comporta idénticamente en las direcciones transversales 2 y 3. Planteando la ecuación de equilibrio en la dirección 2, por ejemplo, se obtiene

$$\sigma_2(E_2) = \frac{d\omega}{dE_2} + p = \omega'(E_2) + p = 0 \implies p = -\omega'(E_2) \quad (4.4)$$

Teniendo en cuenta que $E_2 = E_3$ (debido a la isotropía del material), de la condición de incompresibilidad de la Ec. (4.2) se determina $E_2 = -E_1/2$. Sustituyendo los valores anteriores en la ecuación de equilibrio (4.3), resulta

$$\sigma_1(E_1) = \omega'(E_1) - \omega'\left(\frac{1}{2}E_1\right) \quad (4.5)$$

La ecuación (4.5) se puede invertir y resolver exactamente para cualquier función continua $\sigma_1(E_1)$ desarrollando la siguiente serie infinita (en la práctica es finita, puesto que es convergente) propuesta por Kearsley y Zapas [70]

$$\omega'(E_1) = \sum_{k=0}^{\infty} \sigma_1 \left(\left(\frac{1}{4} \right)^k E_1 \right) + \sigma_1 \left(-\frac{1}{2} \left(\frac{1}{4} \right)^k E_1 \right) \quad (4.6)$$

A esta expresión se le suele denominar *fórmula de inversión* [73]. No obstante, lo habitual es disponer de los puntos experimentales $\tilde{\sigma}_1(\tilde{E}_1)$, los cuales se interpolan mediante splines cúbicos para dar como resultado la función continua $\sigma_1(E_1)$, como se muestra en la Figura 4.1b. Posteriormente, el intervalo de deformaciones $[E_{\min}, E_{\max}]$ se discretiza de forma uniforme mediante los puntos E_k , $k = 1, \dots, n$. A continuación, la fórmula de inversión se evalúa en esos puntos, obteniendo $\bar{\omega}'(\bar{E}_1)$, tal y como se muestra en la Figura 4.1c. Finalmente, los puntos $\bar{\omega}'(\bar{E}_1)$ se interpolan a su vez también mediante splines cúbicos para poder obtener la función continua buscada $\omega'(E_1)$, véase Figura 4.1d. La función resultante $\omega'(E_1)$ reproduce los datos experimentales originales de forma exacta, como se puede observar en la Referencia [74]. Se usan splines cúbicos para interpolar con el fin de garantizar la continuidad de la primera y segunda derivadas [75], de este modo las funciones $\omega''(E)$ y $\omega'''(E)$ son continuas en el rango de interés $[E_{\min}, E_{\max}]$.

4.3. Modelo WYPIWYG ortótropo de Latorre y Montáns

Como se ha comentado en el Capítulo 1, los refuerzos (fibras y partículas de carbono, sílice, etc.) que se añaden a los materiales poliméricos y las fibras de colágeno en los tejidos y otros tipos de materiales biológicos transfieren a dichos materiales cierto grado de anisotropía. Se puede encontrar en la literatura varios modelos que asumen la forma de la función de energía, para materiales transversalmente isótropos véanse, por ejemplo, Referencias [77], [114] y para materiales ortótropos [79], [80], [81], entre otros. Pero estos modelos no son tan óptimos como los existentes para isotropía, por ello la contribución de los modelos WYPIWYG para estos dos tipos de materiales es importante ya que los datos tensión-deformación de los experimentos son reproducidos “exactamente”. Si bien, la extensión del modelo

Figura 4.1: Interpolación mediante splines de la función $\omega'(E)$ a partir de datos experimentales obtenidos de un ensayo uniaxial de tracción-compresión. (a) Distribución discreta de los datos experimentales $\tilde{\sigma}_1(\tilde{E}_1)$. (b) Función continua $\sigma_1(E_1)$ obtenida mediante interpolación de los datos experimentales. (c) Puntos $\bar{\omega}'(\bar{E}_1)$ uniformemente distribuidos que son solución de la Ec. (4.5). (d) Función $\omega'(E_1)$ obtenida mediante interpolación de los puntos uniformemente distribuidos $\bar{\omega}'(\bar{E}_1)$.

basado en splines de Sussman y Bathe a isotropía transversal y ortotropía no es en absoluto evidente. El número de curvas experimentales que se necesitan prescribir es de tres para el modelo transversalmente isótropo y de seis para el ortótropo. Por otro lado, la fórmula de inversión de Kearsley y Zapas [70] resulta invalidada debido a la falta de isotropía en el material por lo que debe ser reformulada de una forma más general [73]. También se debe plantear otra hipótesis de descomposición para la función de energía almacenada del tipo de la de Valanis-Landel. En este apartado se presenta la extensión a ortotropía incompresible del modelo isótropo llevada a cabo por Latorre y Montáns [76], además se invita al lector a consultar la extensión a isotropía transversal llevada a cabo por los mismos autores en [73].

La naturaleza ortótropa de un material está caracterizada por la existencia de tres planos de simetría ortogonales con respecto a los cuales el comportamiento mecánico del material conserva la simetría. Los vectores unitarios normales a estos planos constituyen un triedro a derechas $\mathbf{X}_{pr} = \{\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k\} = \{\mathbf{a}_0, \mathbf{b}_0, \mathbf{c}_0\}$ que define las direcciones preferentes de ortotropía del material en la configuración inicial. Obviamente, se debe incluir esta dependencia con la dirección en la función de energía para ser capaces de reproducir las simetrías correspondientes y cumplir con los principios de invariancia requeridos, tal que $\mathcal{W}(\mathbf{E}, \mathbf{a}_0, \mathbf{b}_0)$, donde $\mathbf{E}$ es el tensor de deformaciones logarítmicas (Hencky) para la deformación desviadora considerada. $\mathcal{W}(\mathbf{E}, \mathbf{a}_0, \mathbf{b}_0)$ se puede enunciar en función de siete invariantes independientes expresados en función de las componentes de $\mathbf{E}$ representadas en las direcciones principales de ortotropía $\mathbf{X}_{pr}$ ([71]), es decir

$$\mathcal{W} = \mathcal{W}(E_{11}, E_{22}, E_{33}, E_{12}^2, E_{23}^2, E_{31}^2, E_{12}E_{23}E_{31}) \quad (4.7)$$

donde $E_{ij} = \mathbf{e}_i \cdot \mathbf{E} \cdot \mathbf{e}_j$ con $i, j = \{1, 2, 3\}$. Debido a la restricción de incompresibilidad de la Ec.(4.2) el número de invariantes independientes se reduce a seis. La función de energía se desacopla entonces en términos de seis de estos siete invariantes independientes del siguiente modo

$$\mathcal{W} = \omega_{11} + \omega_{22} + \omega_{33} + 2\omega_{12}(E_{12}) + 2\omega_{23}(E_{23}) + 2\omega_{31}(E_{31}) \quad (4.8)$$

donde los términos ω_{ij} para $i \neq j$ se requiere que sean funciones simétricas respecto al origen y la dependencia con el invariante $E_{12}E_{23}E_{31}$ no se incluye, no obstante en el artículo [76] se puede comprobar que este modelo predice satisfactoriamente el comportamiento mecánico de materiales blandos. La incorporación de términos adicionales de acoplamiento no aportaría una mejora considerable y sin embargo dificultaría el procedimiento de determinación de la función de energía a partir de los datos experimentales.

Las seis funciones diferentes involucradas en la Ec.(4.8) pueden ser determinadas a partir de un conjunto adecuado de seis curvas experimentales, para una descripción detallada del procedimiento se remite al lector a la Referencia [76],

donde se explican dos formas distintas de obtener $\omega'_{11}(E_{11})$, $\omega'_{22}(E_{22})$ y $\omega'_{33}(E_{33})$ y las funciones $\omega'_{12}(E_{12})$, $\omega'_{23}(E_{23})$ y $\omega'_{31}(E_{31})$ se determinan a partir de los respectivos ensayos de cortante puro. Nótese que el número de funciones independientes coincide con el número de parámetros del material independientes que definen el comportamiento totalmente desacoplado de los materiales ortótropos dentro del marco de pequeñas deformaciones. Además, en la Referencia [82] se demuestra que las deformaciones logarítmicas representan la extensión natural de las deformaciones infinitesimales al campo de las deformaciones finitas. Para poder determinar las funciones ω' por equilibrio para el caso de anisotropía, como se ha comentado arriba, se tiene que generalizar la fórmula de inversión original de Sussman y Bathe de la Ec.(4.6), como se muestra a continuación —véase [76].

Como se ha visto, la fórmula de Kearsley-Zapas resuelve la ecuación de equilibrio de un ensayo uniaxial tracción-compresión para el caso de materiales isótropos hiperelásticos e incompresibles, donde la ecuación de gobierno es —la tensión en la dirección del ensayo uniaxial se denota por $\sigma_u \equiv \sigma_1$

$$\sigma_u(E_1) = \omega'(E_1) - \omega'(y(E_1)) \quad (4.9)$$

donde el último sumando se debe a la presión hidrostática inicialmente desconocida, que se determina planteando las ecuaciones de equilibrio en las direcciones transversales, en concreto $\sigma_2 = \sigma_3 = 0$. Para resolver la Ec.(4.9) para el caso general de un material anisótropo se deben considerar las siguientes expresiones recursivas

$$\sigma_u(E_1) = \omega'(E_1) - \omega'(y(E_1)) \quad (4.10)$$

$$\sigma_u(y(E_1)) = \omega'(y(E_1)) - \omega'(y^{(2)}(E_1)) \quad (4.11)$$

...

$$\sigma_u(y^{(k)}(E_1)) = \omega'(y^{(k)}(E_1)) - \omega'(y^{(k+1)}(E_1)) \quad (4.12)$$

...

donde se define

$$y^{(k)}(E_1) := \underbrace{y(y(\dots(y(E_1))))}_{k \text{ times}} \quad (4.13)$$

con

$$y^{(0)}(E_1) := E_1 \quad (4.14)$$

Sumando todas las ecuaciones se obtiene la *fórmula de inversión generalizada* para el ensayo uniaxial

$$\omega'(E_1) = \sum_{k=0}^{\infty} \sigma_u(y^{(k)}(E_1)) \quad (4.15)$$

donde se ha usado el hecho de que $|y^{(k)}(E_1)| < |E_1|$ y $\omega'(0) = 0$. Como $\sigma_u(0) = 0$, esta solución converge a la precisión requerida en un número finito de términos. Advuértase que $y(E_1)$ puede ser una composición de funciones no lineales.

4.4. Modelo bi-lineal

El número y tipo de experimentos que se requieren para cada modelo hiperelástico varía en la literatura. En materiales isótropos usualmente se utiliza un único ensayo de tracción para caracterizar el material [83], [84],[85],[86], [87]. Algunos trabajos utilizan curvas de tensión junto con curvas de tensión equibiaxial [88], [89], [90], curvas de un ensayo tracción-compresión [91] y curvas de ensayos biaxiales [89], [92]. Sin embargo, no hay una explicación física que recomiende un conjunto de ensayos salvo la evidencia numérica basada en un modelo particular. Lo mismo ocurre con los materiales anisótropos, especialmente con los tejidos biológicos, pues estos materiales son más complejos y las curvas experimentales son más difíciles de obtener por lo que frecuentemente se utilizan los datos experimentales correspondientes a tracción solamente. Algunas veces se usan también simplemente ensayos equibiaxiales. En definitiva, no parece estar claro en la literatura cuál es el número de ensayos necesarios para determinar adecuadamente el comportamiento del material y cuál es la razón física subyacente.

En los modelos WYPIWYG se necesitan tanto la parte de tracción de las curvas uniaxiales como la de compresión. No se puede obtener la función de energía almacenada en estos modelos sin el conocimiento explícito de los datos experimentales de tracción y compresión. Si uno de los comportamientos no se conociera, habría que hacer una suposición razonable, por ejemplo, hay evidencias experimentales de que algunos materiales presentan simetría entre la curva de tracción y la de compresión. A continuación se va a explicar la razón de por qué se necesitan ambas partes de la curva para definir completamente los modelos WYPIWYG y también por qué esto no es una desventaja que presentan estos modelos, sino que realmente para poder determinar adecuadamente cualquier otro modelo basado en las mismas hipótesis del material son también necesarias para que los parámetros del material representen mejor el comportamiento global del mismo. Los conceptos explicados en este apartado son generales y aplicables a cualquier material, compresible o incompresible, isótropo o anisótropo, y a cualquier función de energía almacenada.

Con el fin de explicar el problema en el contexto simple más sencillo, se considera un material incompresible bilineal en pequeñas deformaciones que presenta un comportamiento lineal bastante diferente a tracción que a compresión. Realizando un ensayo a tracción en la dirección 1 se obtiene

$$\sigma_1 = 2\mu_t \varepsilon_1 + p \quad (4.16)$$

donde μ_t es una constante, p es la presión hidrostática, ε_1 es la deformación infinitesimal en el eje 1 y σ_1 es la tensión la dirección 1. En los otros ejes se tiene

$$0 = 2\mu_c\varepsilon_2 + p \quad (4.17)$$

donde debido a la isotropía del material y a la restricción de incompresibilidad $\varepsilon_2 \equiv \varepsilon_3 = -\frac{1}{2}\varepsilon_1$ son las deformaciones transversales y μ_c es otra constante del material, generalmente distinta a μ_t ya que el material en estas direcciones se encuentra comprimido. Despejando p en la Ec. (4.17) y sustituyendo en la Ec. (4.16) resulta

$$\sigma_1 = (2\mu_t + \mu_c)\varepsilon_1 = Y_t\varepsilon_1 \quad \text{with } \varepsilon_1 > 0 \quad (4.18)$$

donde Y_t es el módulo de Young durante el ensayo de tracción. Con este simple ejemplo se muestra que es imposible determinar tanto μ_t como μ_c de un ensayo de tracción, pues sólo se conoce su combinación Y_t . Por supuesto que en el típico caso lineal, en el que $\mu_t = \mu_c \equiv \mu$ y por tanto $Y \equiv Y_t = 3\mu$, la parte de tracción es suficiente.

Si se considera ahora un ensayo equibiaxial realizado en los ejes 1 y 2 se obtiene

$$\sigma_1 \equiv \sigma_2 = 2\mu_t\varepsilon_1 + p \quad (4.19)$$

y debido a la incompresibilidad $\varepsilon_3 = -2\varepsilon_1$ y la ecuación de equilibrio que falta queda

$$0 = -4\mu_c\varepsilon_1 + p \quad (4.20)$$

despejando p en la Ec. (4.20) y sustituyendo en la Ec. (4.19)

$$\sigma_1 \equiv \sigma_2 = (2\mu_t + 4\mu_c)\varepsilon_1 = B_t\varepsilon_1 \quad (4.21)$$

donde B_t es el módulo durante el ensayo equibiaxial. Es imposible determinar B_t a partir de Y_t solamente, por lo que es obviamente imposible también predecir

el comportamiento durante el ensayo equibiaxial sólo con los datos del ensayo a tracción. Sin embargo, conociendo Y_t y B_t se pueden obtener μ_t y μ_c por lo que el comportamiento del material queda completamente determinado. Además, el módulo de compresión uniaxial puede ser también obtenido como

$$Y_c = 2\mu_c + \mu_t = \frac{1}{2}B_t \quad (4.22)$$

de este modo, con el conocimiento de la curva de compresión, se puede predecir el comportamiento durante el ensayo equibiaxial. Nótese que el módulo de compresión uniaxial y el módulo durante el ensayo equibiaxial están relacionados por un factor de dos, es decir, se puede conocer uno a partir del otro sin necesidad de conocer

4.4. MODELO BI-LINEAL

la curva de tracción uniaxial. El comportamiento del material está completamente determinado a partir de estos dos ensayos: ensayo de tracción uniaxial y ensayo de tensión equibiaxial. En consecuencia, el comportamiento a cortante simple viene dado por

$$\begin{aligned}\sigma_{11} &= (\mu_t - \mu_c) \gamma / 2 \\ \sigma_{22} &= (\mu_t - \mu_c) \gamma / 2 \\ \tau_{12} &= (\mu_t + \mu_c) \gamma / 2\end{aligned}\tag{4.23}$$

Se advierte que desde un punto de vista matemático, se puede utilizar también este ensayo para determinar completamente el comportamiento del material.

En resumen, se necesitan dos curvas (o pendientes) y sólo dos, para caracterizar completamente el material bilineal presentado para cualquier estado de carga. Estas dos curvas determinan completamente la curva uniaxial de tensión-compresión. Ensayos adicionales no aportan información extra y por tanto serían redundantes. No obstante se pueden usar, por ejemplo, para comprobar si las hipótesis constitutivas, como incompresibilidad, isotropía, etc., son correctas. Por el contrario, obviar la rama de compresión en el ensayo uniaxial de un material bilineal es similar a omitir el coeficiente de Poisson en un material compresible lineal: las deformaciones transversales no se capturarían correctamente y el modelo no podría representar el comportamiento del material en una situación general de carga. Evidentemente, estos conceptos se pueden extender a materiales no lineales.

Capítulo 5

Modelado del daño

5.1. Introducción

Como se ha visto en capítulos anteriores, los polímeros y tejidos biológicos usualmente se modelan como materiales hiperelásticos isocóricos ([71], [95], [96], [9]). Sin embargo, las gomas, los elastómeros reforzados con fibras y los tejidos biológicos suelen presentar un comportamiento disipativo conocido como efecto Mullins ([31], [34], [32], [33], [98]). La causa del efecto Mullins, aunque se suele relacionar con la rotura de enlaces de las fibras de refuerzo, no está completamente entendida por lo que es usual tratarla fenomenológicamente ([97], [98], [99], [100], [101]).

5.2. Modelo de daño isótropo WYPIWYG

El efecto Mullins es complejo y exhibe muchos aspectos diferentes, como diferentes curvas de descarga-recarga (este efecto se suele relacionar con viscosidad), distintos patrones de daño para pequeñas y grandes deformaciones, deformaciones permanentes (residuales) y anisotropía inducida. Sin embargo, la aproximación más sencilla es modelar el efecto como un ablandamiento isótropo ([8], [9], [97], [99], [102]). Estos modelos isótropos pueden aplicarse también a materiales reforzados con fibras donde el efecto puede considerarse sólo para la matriz isótropa o también asociado a las fibras usando variables escalares internas adicionales para los constituyentes, véase [101], [103], [104]. En la mecánica del continuo, el efecto Mullins se suele representar mediante modelos de daño ([8], [98], [105], [106]) o mediante la pseudoelasticidad ([99], [107]). El enfoque generalizado ([8], [106], [108]) es realizar una hipótesis en la función de energía almacenada sin dañar, usando por ejemplo los modelos Neo-Hookean o de Ogden, y posteriormente aplicando un factor de reducción $(1 - D)$, donde $D \in [0, 1)$ es la variable de daño de Rabot-

nov [54]. Por lo general, se suele establecer un criterio de daño y una función de evolución de la variable de daño (por ejemplo una función de saturación de daño, véase: [8], [103], [104]), la cual suele incluir más parámetros del material, o una curva uniaxial de daño maestra ([106], [109]).

En este capítulo se plantea un enfoque totalmente diferente. Se extiende la filosofía de hiperelasticidad WYPIWYG a los modelos de daño isótropo. Como se ha comentado en el Capítulo 4, los modelos hiperelásticos por lo general prescriben de antemano la forma de función de energía almacenada. Esta función depende de unos parámetros del material que se obtienen mediante un algoritmo de optimización, de tal modo que las predicciones representen lo mejor posible los datos experimentales. Por el contrario, los modelos basados en splines, también conocidos como modelos WYPIWYG, no utilizan parámetros del material sino simplemente los datos experimentales y además son capaces de capturar exactamente las curvas tensión-deformación. Aunque la formulación de daño propuesta en este capítulo podría emplearse con cualquier modelo hiperelástico, si bien, está basada en la idea fundamental de estos modelos WYPIWYG. Este nuevo enfoque sigue también de alguna manera las ideas introducidas por Gurtin y Francis en [109] y generalizadas para tres dimensiones por de Souza Neto *et al.* en [110]. En estos trabajos, las curvas de descarga y recarga se normalizan y escalan usando una función hipotética de la variable de daño. Sin embargo, en la formulación que se propone en este capítulo, la “normalización” es arbitraria (bajo algunas condiciones) y obtenida directamente de los datos experimentales, característica fundamental de los modelos WYPIWYG. Por tanto, el procedimiento resultante captura “exactamente” tanto la curva de carga inicial como las curvas de descarga-recarga sin emplear ningún parámetro material explícito ni funciones de evolución de daño explícitas.

Como resumen, los puntos más importantes tratados en el siguiente artículo son:

- Se desarrollan las ecuaciones constitutivas para el daño discontinuo en materiales hiperelásticos, isótropos e incompresibles, siguiendo un nuevo enfoque similar al del operador división típico de plasticidad computacional.
- Se introduce el parámetro de daño escalar y la formulación discreta, incluyendo el módulo algorítmico tangente.
- Finalmente se muestran algunos ejemplos demostrativos.

A new approach to modeling isotropic damage for Mullins effect in hyperelastic materials

Mar Miñano · Francisco Javier Montáns

Abstract In this work we present a new approach to damage mechanics in hyperelastic materials and an efficient numerical procedure for modelling the Mullins effect in isochoric, isotropic materials. The formulation is based on the idea that both the virgin loading and the damaged unloading-reloading behavior may be measured, but only the unloading-reloading curve corresponds to hyperelastic behavior. The damaged unloading-reloading curve is the true hyperelastic behavior and may be described by any suitable hyperelastic constitutive model. We employ a spline-based formulation which is known to exactly capture the behavior. The virgin loading curve, which does not correspond to hyperelastic behavior and involves damage evolution is only employed to compute the energy release rate. The procedure does not employ any material parameter (and hence no parameter-fitting procedure) or any explicit damage evolution function. We highlight similarities and differences of the present model with usual damage mechanics models and with pseudo-elasticity. As a result of the detailed computational procedure which simply involves the solution of a nonlinear scalar function, the virgin loading curve and the damaged unloading-reloading curves are exactly captured. The computational algorithm for three-dimensional implicit finite element analysis is also addressed in detail. Examples show that there is no significant increase in computational effort respect to a pure hyperelastic model.

Keywords Damage · Hyperelasticity · Logarithmic strains · Mullins effect · living tissues · Polymers · Biological tissues.

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1 Introduction

Rubber-like materials and biological tissues are usually modelled as hyperelastic isochoric materials [1], [2], [3], [4], [5]. A hyperelastic material does not dissipate energy during closed cycles and the stresses are state functions of the strains [1], [2]. However, rubber, carbon-filled elastomers and biological tissues usually present a dissipative behavior known as Mullins effect [6], [7], [8], [9], [10], [11], [12]. The reason for Mullins effect, although often related to filler-polymer link breakages, is not fully understood and it is usually treated phenomenologically [12], [13], [14], [15], [16]. The general Mullins behavior is complex and has many distinct aspects, as different unloading-reloading curves (an effect which may also be related to viscosity), different patterns of damage at low and large strains, permanent (residual) strains and induced anisotropy. See review in [12] and a recent model for damage-induced anisotropy in [17]. However, the simpler approach is to model the effect as an isotropic softening one [2], [5], [13], [16], [18], [19]. The resulting procedure may be applied also to fiber-reinforced materials where the effect may be considered only for the isotropic matrix or also associated to the fibers using additional scalar internal variables for the additional constituents, see [20], [21], [22], [23], [24], among others.

In continuum mechanics, the Mullins effect is usually accounted for by means of damage models [2], [12], [25], [26] or Pseudo-elasticity [13], [27], [28]. Damage-related models have also been successfully employed in bone-remodelling [29], [30] and other damage-related biological tissue phenomena [20], [21], [23], [24]. The usual approach [2], [18], [26], [31] is to make an hypothesis on the undamaged stored energy function, say for example a Neo-Hookean or an Ogden model [32], and then apply a reduction factor $(1 - D)$, where $D \in [0, 1)$ is the Rabotnov damage variable [33]. However, note that it is not possible to measure the undamaged stored energy function, but only the damaged one, because the virgin loading curve represents itself an evolution of damage. A damage criterion and a constitutive (evolution) function which usually include more material parameters (for example a damage saturation function [2], [20], [23] or an undimensional master damage curve [26], [31], [34]) is typically established for the damage variable. Eventually, a parameter-fitting procedure is employed in order to obtain the final model for hyperelasticity with damage [21], [23], [24].

The approach we propose is different. Usual hyperelastic models prescribe a priori the general shape of stress-strain curve and the material parameters simply adjust that shape to the experimental data. On the contrary, spline-based hyperelastic models do not employ any material parameter but just the experimental data and are capable of exactly capturing the experimental stress-strain curves [35], [36], [37]. These models preserve material-symmetries congruency if properly formulated [38] and the results are insensitive to any material parameter-

fitting procedure, an important issue raised for traditional hyperelastic models [39]. Even though the present proposed formulation could be employed with any hyperelastic model, the idea behind those models have motivated the formulation. It also follows somehow the ideas given by Gurtin and Francis [34] for one dimension and generalized by de Souza-Neto et al. [31] for three dimensions. In these works, the unloading-reloading curves are normalized and scaled using a hypothetical function of the damage variable. However, herein a new formulation is developed in which the “normalization” is arbitrary (under some conditions) and also obtained directly from experimental data. Then, the resulting procedure exactly captures both the initial loading and the unloading-reloading prescribed curves without employing any explicit material parameter or any explicit damage evolution function.

In the following sections we first develop the continuum constitutive equations for isochoric, isotropic discontinuous damage following a novel interpretation parallel to that of the operator split typical of computational plasticity and which we also employed successfully in both continuum and computational visco-hyperelasticity [40]. Then, we introduce the practical damage scalar parameter and the discrete (stress-point) formulation, including the algorithmic tangent. Finally, we show some demonstrative examples.

2 Stress power

In this work we use logarithmic strains as the working strain measures because of their special properties as a natural extension of infinitesimal strains [43], [44], [45]. Let $\mathbf{b}$ be the loads per unit volume V and $\mathbf{t}$ the loads at the boundary S . If $\mathbf{v}$ is the velocity at a given point in the domain, then it can be shown that [46]

$$\mathcal{P} = \int_V \mathbf{b} \cdot \mathbf{v} \, dV + \int_S \mathbf{t} \cdot \mathbf{v} = \int_{{}^0V} \mathbf{T} : \dot{\mathbf{E}} \, d {}^0V \quad (1)$$

where 0V is the reference volume, $\mathbf{E}$ are the logarithmic strains in the reference configuration and $\mathbf{T}$ are the generalized Kirchhoff stresses, work-conjugate of the logarithmic stresses, see [36], [37] [46], [47]. The double-dot operation stands for the usual double-index contraction. In the case of isotropy, $\mathbf{T}$ can be identified with the rotated Kirchhoff stress tensor [48], and in the case of isochoric behavior it can also be identified with the rotated Cauchy stress tensor —i.e. rotated to the material configuration with the rotation tensor given by the polar decomposition of the deformation gradient. Let w_D be an internal variable and $\mathcal{W}(\mathbf{E}, w_D)$ the stored energy (or pseudo-elastic stored energy [13]). The preservation of energy states that

$$\mathbf{T} : \dot{\mathbf{E}} = \dot{\mathcal{W}} = \frac{\partial \mathcal{W}(\mathbf{E}, w_D)}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial \mathcal{W}(\mathbf{E}, w_D)}{\partial w_D} \frac{\partial w_D}{\partial \mathbf{E}} : \dot{\mathbf{E}} \quad (2)$$

where $\mathcal{W}(\mathbf{E}, w_D)$ is the stored energy per unit reference volume. Equation (2) simply states that the mechanical energy is either stored or dissipated. Then obviously

$$\mathbf{T} = \frac{d\mathcal{W}(\mathbf{E})}{d\mathbf{E}} = \left. \frac{\partial \mathcal{W}(\mathbf{E}, w_D)}{\partial \mathbf{E}} \right|_{\dot{w}_D=0} + \left. \frac{\partial \mathcal{W}(\mathbf{E}, w_D)}{\partial w_D} \right|_{\dot{\mathbf{E}}=\mathbf{0}} \frac{\partial w_D}{\partial \mathbf{E}} \quad (3)$$

where we used the notation $d(\cdot)/d\mathbf{E}$ to emphasize that the derivative is taken respect to all arguments. We note that Eqs. (2) and (3) differ from the usual setting –c.f. Eq. (6.277) of Reference [2]– but a similar concept is found in pseudo-elasticity — c.f. Eq.(22) of Ref. [14]. Note that w_D is not a reduction factor, i.e. no hypothesis on how w_D affects $\mathcal{W}$ has still been taken. The differentiation in Eq. (3) corresponds to the usual partial derivative concept and can naturally be interpreted as a trial-hyperelastic stress predictor, damage-stress-corrector operator split. A similar structure for the continuum formulation (either material or corotational) has led to effective computational schemes for anisotropic visco-hyperelasticity valid for large deviations from thermodynamic equilibrium [40]. However note that here, in contrast to viscoelasticity or computational plasticity, the trial and final states correspond to the same strains.

3 Damage mechanics for isotropic, isochoric hyperelasticity

Consider the following uncoupled form of the stored energy function

$$\mathcal{W} = \mathcal{U}(J) + \mathcal{W}^d(\mathbf{E}^d, w_D) \quad (4)$$

We use herein the Valanis-Landel decomposition [41], verified in isotropy both theoretically [1] and experimentally [42] up to moderately large strains. This hypothesis is also used, for example, in Ogden’s model [32]. Since for a fixed value of w_D Eq. (4) constitutes a hyperelastic stored energy, we can extend the Valanis-Landel hypothesis to Eq. (4) as

$$\bar{\mathcal{W}}^d(\lambda_1^d, \lambda_2^d, \lambda_3^d, w_D) = \bar{\omega}(\lambda_1^d, w_D) + \bar{\omega}(\lambda_2^d, w_D) + \bar{\omega}(\lambda_3^d, w_D) \quad (5)$$

with the isochoric stretches λ_i^d being expressed in terms of the stretches λ_i as

$$\lambda_1^d = J^{-1/3} \lambda_1 = (\lambda_1 \lambda_2 \lambda_3)^{-1/3} \lambda_1 \quad (6)$$

The principal logarithmic strains are

$$E_1^d = \ln \lambda_1^d = \ln \lambda_1 - \frac{1}{3} (\ln J) = E_1 - \frac{1}{3} (E_1 + E_2 + E_3)$$

The function $\mathcal{U}(J)$, where J is the (Jacobian) determinant of the deformation gradient, can be considered as a penalty function to numerically enforce incompressibility. Frequently, damage is considered to affect only the isochoric contribution to the stored energy, see for example [12], [20], [23], [24]. We also assume as

a constitutive hypothesis that damage does not affect incompressibility. Then we can write

$$\mathcal{W}^d(\ln \lambda_1^d, \ln \lambda_2^d, \ln \lambda_3^d, w_D) = \omega(E_1^d, w_D) + \omega(E_2^d, w_D) + \omega(E_3^d, w_D) \quad (7)$$

Without much loss of generality, we adopt a physical meaning to give the damage variable as the maximum isochoric energy attained up to time t (note that until now no specific function has been adopted for the dependency of $\mathcal{W}^d$ on w_D , but we simply state that damage is somehow related to deformation energy)

$$w_D = \max_{\tau \in (-\infty, t)} (\mathcal{W}^d(\tau)) \quad (8)$$

The maximum stored energy, or a quantity derived from it has been used by a number of authors as damage variable, see for example [19], [23], [24]. For different levels of damage we can write

$$\mathcal{W}^d(\mathbf{E}^d, w_{D1}), \mathcal{W}^d(\mathbf{E}^d, w_{D2}), \dots \quad (9)$$

or alternatively, during unloading-reloading without further damage

$$\mathcal{W}_{D1}^d(\mathbf{E}^d), \mathcal{W}_{D2}^d(\mathbf{E}^d), \dots \quad (10)$$

These functions for a fixed, given damage are the true hyperelastic functions. Equations (4) and (5) are potential functions which establish the stored energy as a function also of damage (a dissipative variable). Then we note that the existence of such (pseudo-elastic) potential is merely a constitutive hypothesis not equivalent to the existence of a hyperelastic potential. However, as a difference to usual pseudo-elasticity approaches, no specific (i.e. additive) form has been adopted —c.f. Eq. (41) of Ref. [14] or Eq. (3.8) of Ref. [13]. We also require that $\dot{w}_D \geq 0$, i.e. the damage process is irreversible and the material is not self-healing.

Energies (10) can be written using the Valanis-Landel decomposition as

$$\mathcal{W}_{Dn}^d(\mathbf{E}^d) = \omega_{Dn}(E_1^d) + \omega_{Dn}(E_2^d) + \omega_{Dn}(E_3^d) \quad (11)$$

where index n refers to the n damaged function, i.e. for damage w_{Dn} . We assume, based on experimental evidence, that damage decreases the stored energy, i.e. $\partial \mathcal{W}^d(\mathbf{E}^d, w_D) / \partial w_D \leq 0$. The tensor

$$\mathbf{Y} = -\frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \frac{\partial w_D}{\partial \mathbf{E}} = \gamma \mathbf{D} \quad (12)$$

is the energy release rate tensor [50], whereas the scalar $\gamma = -\partial \mathcal{W}^d(\mathbf{E}^d, w_D) / \partial w_D$ is the scalar damage power loss factor (or damage energy release rate multiplier).

The stored energy rate is

$$\dot{\mathcal{W}} = \dot{\mathcal{U}}(J) + \dot{\mathcal{W}}^d(\mathbf{E}^d, w_D) \quad (13)$$

$$= \frac{\partial \mathcal{U}(J)}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial \mathcal{W}(\mathbf{E}, w_D)}{\partial \mathbf{E}} \bigg|_{\dot{w}_D=0} : \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \underbrace{\frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \bigg|_{\dot{\mathbf{E}}=0}}_{\leq 0} \underbrace{\dot{w}_D}_{\geq 0} \quad (14)$$

$$= \frac{\partial \mathcal{U}(J)}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}^d} : \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \underbrace{\frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D}}_{\leq 0} \underbrace{\frac{\partial w_D}{\partial \mathbf{E}} : \dot{\mathbf{E}}}_{\geq 0} \quad (15)$$

$$= \mathbf{T}^v : \dot{\mathbf{E}} + ({}^{tr}\mathbf{T}^d - \mathbf{Y}) : \dot{\mathbf{E}} \quad (16)$$

$$= \mathbf{T}^v : \dot{\mathbf{E}} + \mathbf{T}^d : \dot{\mathbf{E}} \quad (17)$$

where ${}^{tr}\mathbf{T}^d$ is interpreted as the trial isochoric generalized Kirchhoff stress tensor (stored energy tensor) defined as with the damage frozen (i.e. equal to the power input), $\mathbf{Y}$ is the correction due to damage (power loss) and $\mathbf{T}^d$ is the resulting isochoric, traceless, generalized Kirchhoff stress tensor, i.e.

$${}^{tr}\mathbf{T}^d := \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial \mathbf{E}} \bigg|_{\dot{w}_D=0} = \frac{\partial \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}} \quad (18)$$

$\mathbf{Y}$ is given in Equation (12), and

$$\mathbf{T}^d := \frac{d\mathcal{W}^d(\mathbf{E}^d, w_D)}{d\mathbf{E}} \quad (19)$$

where we again used the notation $d(\cdot)/d\mathbf{E}$ to emphasize that the derivative is taken respect to all arguments. This results into

$$\begin{cases} \dot{\mathcal{W}}^d = \frac{\partial \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}} : \dot{\mathbf{E}} & \text{for no damage increase; } \dot{w}_D = 0, \\ \dot{\mathcal{W}}^d = \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial \mathbf{E}} \bigg|_{\dot{w}_D=0} : \dot{\mathbf{E}} + \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \bigg|_{\dot{\mathbf{E}}=0} \frac{\partial w_D}{\partial \mathbf{E}} : \dot{\mathbf{E}} & \text{for } \dot{w}_D > 0 \end{cases} \quad (20)$$

In an equivalent manner

$$\begin{cases} \mathbf{T}^d = {}^{tr}\mathbf{T}^d & \text{for no damage increase; } \dot{w}_D = 0 \\ \mathbf{T}^d = {}^{tr}\mathbf{T}^d - \mathbf{Y} & \text{for damage increase; } \dot{w}_D > 0 \end{cases} \quad (21)$$

A general interpretation of all these quantities is given in Figure 1. Note that up to now the current set-up mimics the typical procedure used in computational

Fig. 1 (a) Virgin loading curve and unloading-reloading hyperelastic curve. (b) Definition of the trial stress state and the released energy rate. (c) Definition of the master hyperelastic curve. (d) Parallelism with the radial return algorithm of Wilkins in the stress space.

plasticity. In line with the physical meaning we chose for the damage variable w_D , the damage criterion we use is the stored energy

$$f_D = \mathcal{W}^d - w_D \leq 0 \iff \mathcal{W}^d \leq w_D \quad (22)$$

This criterion is the Maxwell statement of the well-known von Mises yield criterion [51]. For the case of linear hyperelasticity with μ being the shear modulus

$$\mathcal{W}_{lin}^d = \mu \mathbf{E}^d : \mathbf{E}^d = \frac{1}{\mu} \mathbf{T}^d : \mathbf{T}^d = \frac{1}{\mu} \|\mathbf{T}^d\|^2 \quad (23)$$

and the criterion may be written in terms of the von Mises and Huber statements, of course in this case using logarithmic strain measures and their work-conjugate stresses as done in large strain elastoplasticity [52], [46]; i.e. the plasticity parallelism still holds.

The consistency condition during damage evolution, when $\dot{w}_D > 0$ and $f_D = 0$, is

$$\dot{f}_D = 0 \Rightarrow \frac{\partial \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \bigg|_{\dot{\mathbf{E}}=0} \frac{\partial w_D}{\partial \mathbf{E}} : \dot{\mathbf{E}} - \frac{\partial w_D}{\partial \mathbf{E}} : \dot{\mathbf{E}} = 0 \quad (24)$$

i.e.

$$\dot{f}_D = \left({}^{tr}\mathbf{T}^d - \mathbf{Y} - \frac{\partial w_D}{\partial \mathbf{E}} \right) : \dot{\mathbf{E}} = 0 \quad \text{for } \dot{w}_D > 0 \quad (25)$$

Because damage evolution can only happen with incremental strains $\dot{\mathbf{E}} \neq \mathbf{0}$ (we note that this is a constitutive hypothesis which does not consider, for example ageing)

$$\mathbf{D} := \frac{\partial w_D}{\partial \mathbf{E}} = {}^{tr}\mathbf{T}^d - \mathbf{Y} \quad (26)$$

Since

$$\frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \bigg|_{\dot{\mathbf{E}}=0} \frac{\partial w_D}{\partial \mathbf{E}} = -\gamma(\mathbf{E}) ({}^{tr}\mathbf{T}^d - \mathbf{Y}) = -\mathbf{Y} \Rightarrow \gamma(\mathbf{E}) ({}^{tr}\mathbf{T}^d - \mathbf{Y}) = \mathbf{Y} \quad (27)$$

where the energy release rate multiplier $\gamma(\mathbf{E})$ is a scalar function, we have

$$\mathbf{Y} = \frac{\gamma}{1+\gamma} {}^{tr}\mathbf{T}^d \Rightarrow \mathbf{T}^d = {}^{tr}\mathbf{T}^d - \mathbf{Y} \Rightarrow \mathbf{D} = \mathbf{T}^d = \frac{1}{1+\gamma} {}^{tr}\mathbf{T}^d \quad (28)$$

i.e., the energy release rate is proportional to the trial stresses and then $\mathbf{T}^d$ is also proportional. This is a consequence of considering an isotropic scalar damage variable. We note that $0 < 1/(1+\gamma) \leq 1$. In comparison to computational elastoplasticity, Eq. (28) is in essence the classical radial return algorithm of Wilkins [53].

We note that due to isotropy ${}^{tr}\mathbf{T}^d$, $\mathbf{T}^d$, $\mathbf{Y}$ and $\mathbf{E}$ all have the same eigenvectors and commute. We also note that since during damage evolution $\dot{w}_D > 0$,

$$\dot{f}_D = \left({}^{tr}\mathbf{T}^d - \mathbf{Y} - \frac{\partial w_D}{\partial \mathbf{E}} \right) : \dot{\mathbf{E}} = 0 \implies ({}^{tr}\mathbf{T}^d - \mathbf{Y}) : \dot{\mathbf{E}} > 0 \implies \mathbf{T}^d : \dot{\mathbf{E}} > 0 \quad (29)$$

so

$$\mathbf{N} : \dot{\mathbf{E}} > 0 \quad \text{with} \quad \mathbf{N} = \frac{{}^{tr}\mathbf{T}^d}{\|{}^{tr}\mathbf{T}^d\|} = \frac{\mathbf{Y}}{\|\mathbf{Y}\|} = \frac{\mathbf{T}^d}{\|\mathbf{T}^d\|} = \frac{\mathbf{D}}{\|\mathbf{D}\|} \quad (30)$$

which is a stability condition (i.e. the system gets energy). This condition may also be easily recognized as the normality rule of plasticity [49].

Furthermore, the second derivative of the isochoric energy is

$$\begin{aligned} \frac{d^2 \mathcal{W}^d(\mathbf{E}^d, w_D)}{d\mathbf{E}d\mathbf{E}} &= \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} : \frac{\partial^2 \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}^d \partial \mathbf{E}^d} : \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} \\ &+ \frac{\partial^2 \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D^2} \frac{\partial w_D}{\partial \mathbf{E}} \otimes \frac{\partial w_D}{\partial \mathbf{E}} + \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial w_D} \frac{\partial^2 w_D}{\partial \mathbf{E} \partial \mathbf{E}} \end{aligned} \quad (31)$$

i.e.

$$\frac{\partial \mathbf{T}}{\partial \mathbf{E}} = \frac{\partial \mathbf{T}^v}{\partial \mathbf{E}} + \frac{\partial {}^{tr}\mathbf{T}^d}{\partial \mathbf{E}} - \frac{\partial \gamma}{\partial w_D} \mathbf{D} \otimes \mathbf{D} - \gamma \frac{\partial \mathbf{D}}{\partial \mathbf{E}} \quad (32)$$

where

$$\mathbf{T}^v = \frac{\partial U(J)}{\partial \mathbf{E}} \text{ and } \frac{\partial \mathbf{T}^v}{\partial \mathbf{E}} = \frac{\partial^2 \mathcal{U}(J)}{\partial \mathbf{E} \partial \mathbf{E}} \quad (33)$$

are the volumetric (penalty) contributions to the stresses and the constitutive tangent. Then

$$\mathbb{C} = {}^{tr}\mathbb{C} - \gamma \frac{\partial \mathbf{D}}{\partial \mathbf{E}} - \frac{\partial \gamma}{\partial w_D} \mathbf{D} \otimes \mathbf{D} \quad (34)$$

where

$${}^{tr}\mathbb{C} = \frac{\partial^2 U(J)}{\partial \mathbf{E} \partial \mathbf{E}} + \frac{\partial {}^{tr}\mathbf{T}^d}{\partial \mathbf{E}} \quad (35)$$

and the symbol $\otimes$ stands for the outer (dyadic) product. The reader familiar with computational plasticity will recognize the form of this tangent as the same of the algorithmic (“consistent”) tangent of plasticity —cf. Eq. (3.3.8) and Box 3.2 of Ref. [53]. The comparison of Eq. (34) with the usual damage mechanics theory can also be easily performed —cf. Eq. (6.289) of Reference [2].

However, there are two key differences with the usual procedures employed in plasticity. The present theory is a continuum theory, whereas the comparison has been performed with the usual algorithmic procedure. Furthermore, here the stored energy function $\mathcal{W}_{D_n}^d$ can be readily obtained from experiments. In fact, as mentioned, in isotropic materials for any given set of discrete experimental stress-strain points, it is possible to obtain a stored energy function $\mathcal{W}_{D_n}^d$ whose derivatives $\partial \mathcal{W}_{D_n}^d / \partial \mathbf{E}$ are exactly the experimental stresses for the given experimental strains [35]. The derivatives of these stored energy functions are obtained solving the differential equilibrium equation and using piece-wise cubic splines, see details in the afore-mentioned References. The ideas of the present procedure could be applied to any suitable constitutive model (for example Ogden’s model [32]). However, in the examples below we apply the procedure to spline-based hyperelasticity.

4 Consistency of isotropic behavior

Isotropic behavior and the use of a single isotropic damage variable requires that the energy release rate is proportional to the stresses, i.e. the fulfilment of Equation (28), so $\mathbf{T}^d$, $\mathbf{Y}$ and ${}^{tr}\mathbf{T}^d$ must be proportional. Note that ${}^{tr}\mathbf{T}^d$ is the derivative of a strain energy $\mathcal{W}_{D1}^d$ for a given (frozen) damage w_{D1} at a given strain $\mathbf{E}$, whereas $\mathbf{T}^d$ is the derivative of a new (unloading) stored energy function $\mathcal{W}_{D2}^d$ for a new (arbitrary) damage w_{D2} at the same strain $\mathbf{E}$. However, in principle, given two arbitrary isotropic and isochoric stored energy functions $\mathcal{W}_{D1}^d$ and $\mathcal{W}_{D2}^d$, their derivatives (gradients) are not necessarily proportional at a given strain point.

Consider the following quotient of two stored energy functions corresponding to two different levels of damage

$$\frac{\mathcal{W}_{D1}^d(\mathbf{E}^d)}{\mathcal{W}_{D2}^d(\mathbf{E}^d)} = \zeta(\mathbf{E}^d) \Rightarrow \frac{\partial \mathcal{W}_{D1}^d}{\partial \mathbf{E}^d} = \zeta(\mathbf{E}^d) \frac{\partial \mathcal{W}_{D2}^d}{\partial \mathbf{E}^d} + \mathcal{W}_{D2}^d \frac{\partial \zeta(\mathbf{E}^d)}{\partial \mathbf{E}^d} \quad (36)$$

which means that $\partial \mathcal{W}_{D1}^d / \partial \mathbf{E}^d$ and $\partial \mathcal{W}_{D2}^d / \partial \mathbf{E}^d$ are proportional if the ratio $\zeta(\mathbf{E}^d)$ is constant or if its derivative is also proportional to them, i.e.

$$\frac{\partial \mathcal{W}_{D1}^d}{\partial \mathbf{E}^d} = \zeta(\mathbf{E}^d) \frac{\partial \mathcal{W}_{D2}^d}{\partial \mathbf{E}^d} + \mathcal{W}_{D2}^d(\mathbf{E}^d) \theta(\mathbf{E}^d) \frac{\mathcal{W}_{D2}^d}{\partial \mathbf{E}^d} = \varphi(\mathbf{E}^d) \frac{\mathcal{W}_{D2}^d}{\partial \mathbf{E}^d} \quad (37)$$

where $\varphi(\mathbf{E}^d) := \zeta(\mathbf{E}^d) + \mathcal{W}_{D2}^d(\mathbf{E}^d) \theta(\mathbf{E}^d)$ is a scalar function. However, the Valanis-Landel decomposition we use herein, implies

$$\mathcal{W}_{D1}^d = \omega_{D1}(E_1^d) + \omega_{D1}(E_2^d) + \omega_{D1}(E_3^d) \quad (38)$$

$$\mathcal{W}_{D2}^d = \omega_{D2}(E_1^d) + \omega_{D2}(E_2^d) + \omega_{D2}(E_3^d) \quad (39)$$

where E_i^d are the principal isochoric logarithmic strains. Then their derivatives are

$$\frac{\partial \mathcal{W}_{D1}^d}{\partial \mathbf{E}^d} = \frac{\partial \omega_{D1}}{\partial E_1^d} \frac{\partial E_1^d}{\partial \mathbf{E}^d} + \frac{\partial \omega_{D1}}{\partial E_2^d} \frac{\partial E_2^d}{\partial \mathbf{E}^d} + \frac{\partial \omega_{D1}}{\partial E_3^d} \frac{\partial E_3^d}{\partial \mathbf{E}^d} \quad (40)$$

and

$$\frac{\partial \mathcal{W}_{D2}^d}{\partial \mathbf{E}^d} = \frac{\partial \omega_{D2}}{\partial E_1^d} \frac{\partial E_1^d}{\partial \mathbf{E}^d} + \frac{\partial \omega_{D2}}{\partial E_2^d} \frac{\partial E_2^d}{\partial \mathbf{E}^d} + \frac{\partial \omega_{D2}}{\partial E_3^d} \frac{\partial E_3^d}{\partial \mathbf{E}^d} \quad (41)$$

where $\partial E_i^d / \partial \mathbf{E}^d$ are the principal directions of isochoric strains (and stresses) and $\partial \omega_{Dn} / \partial E_i^d$ are the principal deviatoric stresses given by stored energy $\mathcal{W}_{Dn}^d$. The required proportionality between $\partial \mathcal{W}_{D1}^d / \partial \mathbf{E}^d$ and $\partial \mathcal{W}_{D2}^d / \partial \mathbf{E}^d$ implies that for the same (but arbitrary) strains $\mathbf{E}^d$

$$\frac{\partial \omega_{D1} / \partial E_1^d}{\partial \omega_{D2} / \partial E_1^d} = \frac{\partial \omega_{D1} / \partial E_2^d}{\partial \omega_{D2} / \partial E_2^d} = \frac{\partial \omega_{D1} / \partial E_3^d}{\partial \omega_{D2} / \partial E_3^d} \quad (42)$$

Obviously the components of strain may take arbitrary values, so ω_{D1} and ω_{D2} (and their derivatives) must have the same proportionality at *every* strain level, a condition that $\mathcal{W}_{D1}^d$ and $\mathcal{W}_{D2}^d$ must hence also fulfill; i.e. ζ must be constant for given w_{D1} and w_{D2} , but otherwise may depend on w_D . The immediate consequence is that for isotropic hyperelastic damage the user may only prescribe one single hyperelastic function pattern (shape) to the maximum possible strain level

$$\mathcal{W}_0^d(E_1^d, E_2^d, E_3^d) = \omega_0(E_1^d) + \omega_0(E_2^d) + \omega_0(E_3^d) \quad (43)$$

and then every hyperelastic function must be proportional and determined as

$$\mathcal{W}^d(E_1^d, E_2^d, E_3^d, w_D) = \psi(w_D) \mathcal{W}_0^d(E_1^d, E_2^d, E_3^d) \quad (44)$$

where $\psi \geq 1$ if damage is less than the damage with which the energy $\mathcal{W}_0^d$ has been determined. The factor of proportionality $\psi(w_D)$ is of course different for different levels of damage (note that no explicit physical meaning has been given to ψ). Then

$$\frac{\mathcal{W}_{D1}^d(\mathbf{E}^d)}{\mathcal{W}_{D2}^d(\mathbf{E}^d)} = \zeta = \frac{\psi(w_{D1})}{\psi(w_{D2})} \quad (45)$$

The isochoric energy rate results, in terms of the new variable $\psi(w_D)$

$$\begin{aligned} \dot{\mathcal{W}}^d &= \left. \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial \mathbf{E}} \right|_{\dot{w}_D=0} : \dot{\mathbf{E}} + \underbrace{\frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial \psi}}_{\leq 0} \underbrace{\frac{d\psi}{dw_D} \frac{\partial w_D}{\partial \mathbf{E}}}_{\geq 0} : \dot{\mathbf{E}} \\ &= \left. \frac{\partial \mathcal{W}^d(\mathbf{E}^d, w_D)}{\partial \mathbf{E}} \right|_{\dot{w}_D=0} : \dot{\mathbf{E}} + \underbrace{\mathcal{W}_0^d \frac{d\psi}{dw_D}}_{\leq 0} \underbrace{\frac{\partial w_D}{\partial \mathbf{E}}}_{\geq 0} : \dot{\mathbf{E}} \end{aligned} \quad (46)$$

i.e. we obtain again

$$\mathbf{T}^d = {}^{tr}\mathbf{T}^d - \mathbf{Y} \quad (47)$$

with the resulting energy release rate

$$\mathbf{Y} = -\mathcal{W}_0^d \frac{d\psi}{dw_D} \mathbf{D} \Rightarrow \gamma = -\mathcal{W}_0^d \frac{d\psi}{dw_D} = -\frac{\mathcal{W}_0^d}{dw_D/d\psi} \quad (48)$$

and from Eq. (28)

$$\mathbf{T}^d = \frac{dw_D/d\psi}{dw_D/d\psi - \mathcal{W}_0^d} {}^{tr}\mathbf{T}^d \quad (49)$$

Hence only two scalar functions ($dw_D/d\psi$ and $\mathcal{W}_0^d$) are needed and these functions can be obtained from a tensile loading-unloading test. The energy $\mathcal{W}_0^d(\mathbf{E})$ can be determined from the user-prescribed (experimentally obtained) spline-based

stored energy function (“master” hyperelastic curve) for the possible maximum damage. The second one is determined by the user-prescribed uniaxial virgin test (“master” damage curve) as the quotient between the stress given by the master damage curve T and the one T_0 given by the master hyperelastic curve $\mathcal{W}_0^d$,

$$\tilde{\psi}(E) = \frac{T}{T_0} = \psi(w_D(E)) \quad (50)$$

where $w_D(E) = \tilde{\psi}(E) \mathcal{W}_0^d(E)$. Note that Eq. (50) holds at the instant of the first unloading (no further damage evolution). We perform the change of argument in the ψ function because the stored energy is a valid scalar in the general three-dimensional case, whereas E is valid in the unidimensional test case. It is computationally advantageous to obtain $w_D(\psi(E))$ instead of $\psi(w_D(E))$. The function $w_D(\psi(E))$ may be interpolated in terms of splines, but based on physical grounds we should guarantee that w_D decreases as ψ increases (i.e. damage decreases the stored energy). For the uniaxial case, obviously

$$\mathcal{W}_0^d(E) = \omega_0(E^d) + 2\omega_0(-\tfrac{1}{2}E^d) \quad (51)$$

where E^d is the isochoric uniaxial strain (i.e. the uniaxial strain in the case of incompressibility) and ω_0 is the energy function for the strain components in the Valanis-Landel decomposition of $\mathcal{W}_0^d$.

An important practical issue is to notice that the mandatory proportionality of the hyperelastic unloading-reloading curves is not a very restrictive condition because if for example the material is largely damaged, the first part of the $w_D(\psi(E))$ curve (high values of ψ) is not too relevant respect to the last part of $w_D(\psi(E))$ (low values of ψ). Hence, several unloading-reloading curves at different damage levels may be used, see Figure 2. The used $\mathcal{W}_0^d(\mathbf{E})$ -curve may be obtained from a scaled composition of all damaged curves, each one to the corresponding strain level as shown in Figure 2. To this end, the spline-based procedure is specially interesting. Needless to say that convexity of the resulting function may be checked if needed.

Equation (44) has identical form as the usual ansatz of classical damage formulations, see for example Eq. (6.274) of [2]. However, we note that we have obtained it (not postulated) as a result of isotropy and the Valanis-Landel decomposition. Furthermore, it is important to note that $\mathcal{W}_0^d$ is not a hypothetical (unmeasurable) undamaged stored energy, but a damaged (measurable) one. The crucial point here is that the undamaged energy employed in most works ([2], [19], [31], [23], etc) cannot be determined experimentally (*it simply does not exist* because the material suffers damage during loading), whereas $\mathcal{W}_0^d$ can be easily obtained. The virgin loading curve may not be obtained from a hyperelastic curve because itself implies a damage, irreversible, dissipative procedure. We emphasize that we only use the stress-strain points of the virgin loading curve to obtain the ratio $\tilde{\psi}$. This curve

Fig. 2 Generation of a composite piecewise master damaged hyperelastic curve.

is *not* explicitly employed in the computational simulations, but simply obtained as a consequence of damage evolution. Hence, our formulation clearly differs from that of [34] and [31]. The proportionality between the stored energy functions, obtained as a requirement of the isotropic formulation fulfilling the Valanis-Landel decomposition, is here guaranteed and it is not equivalent to normalizing them or expressing them in terms of an adimensional strain.

We further note here that if D is the usual damage parameter of Rabotnov [33], then $\psi \neq (1 - D)$. It is interesting to relate our formulation to the typical set-up. In the usual formulation

$$\hat{\mathcal{W}}^d(\mathbf{E}^d, D) = (1 - D) \hat{\mathcal{W}}^0(\mathbf{E}^d) \quad (52)$$

where $\hat{\mathcal{W}}^0(\mathbf{E}^d)$ is the undamaged curve, and $D \in [0, 1)$ is the Rabotnov damage parameter. As mentioned, neither $\hat{\mathcal{W}}^0(\mathbf{E}^d)$ (*this is not the virgin loading curve*) nor D (*we do not know the undamaged state corresponding to $D = 0$*) can be measured. However, even though having questionable practical application, conceptually Eq. (52) may be related to the current formulation through the maximum possible ψ , which for the uniaxial case is

$$\psi_{\max} = \psi(0) = \lim_{w_D \rightarrow 0} \frac{\mathcal{W}^d(E, w_D)}{\mathcal{W}_0^d(E)} = \frac{d^2 \mathcal{W}^d(E, 0) / dE^2}{d^2 \mathcal{W}_0^d / dE^2} \quad (53)$$

This value relates the ratio of the slope of the master damage curve (virgin curve) at the origin to the slope of the reference (master) hyperelastic curve (unloading-reloading curve) at the origin. Then, the hypothetical “undamaged” hyperelastic curve is

$$\hat{\mathcal{W}}^0(\mathbf{E}^d) = \psi_{\max} \mathcal{W}_0^d(\mathbf{E}^d) \quad (54)$$

and the damaged curve is

$$\hat{\mathcal{W}}^d(\mathbf{E}^d, D) = (1 - D) \hat{\mathcal{W}}^0(\mathbf{E}^d) = (1 - D) \psi_{\max} \mathcal{W}_0^d(\mathbf{E}^d) = \psi(w_D) \mathcal{W}_0^d(\mathbf{E}^d) \quad (55)$$

so

$$D = 1 - \frac{\psi(w_D)}{\psi_{\max}} \quad (56)$$

The maximum Rabotnov damage that can be computed using the present approach is $D = 1 - 1/\psi_{\max} \in [0, 1)$. Note that $\dot{D} \geq 0$ implies here that $d\psi/dw_D \leq 0$, the aforementioned restriction. Finally, the function ψ may be related to the Kachanov [25] damage variable ψ_K as

$$\psi_K = \frac{\psi(w_D)}{\psi_{\max}} \in [1, 1/\psi_{\max}] \subset [1, 0) \quad (57)$$

which is related to our function ψ as its relative value.

5 Computational procedure

The computational procedure is based on the hyperelastic-predictor, damage-corrector scheme. Because the model is isotropic and damage isochoric, an efficient scalar procedure is possible.

5.1 Local iterative algorithm

During damage progress, the main task of the algorithm is to determine the multiplier ${}^{t+\Delta t}\psi$ at time step $t + \Delta t$. Once the multiplier is determined, the stored energy is given by Eq. (44) and the stresses are determined as in hyperelasticity without damage.

We note that the trial stress is determined by the hyperelastic function for ${}^t\psi$ because by definition damage is frozen

$${}^{tr}\mathbf{T}^d = {}^t\psi \frac{\partial \mathcal{W}_0^d(\mathbf{E}^d)}{\partial \mathbf{E}} = {}^t\psi {}^{t+\Delta t}\mathbf{T}_0^d({}^{t+\Delta t}\mathbf{E}^d) \quad (58)$$

Then if ${}^{t+\Delta t}\psi$ is known, it is obvious that at unloading

$${}^{t+\Delta t}\mathbf{T}^d = \frac{{}^{t+\Delta t}\psi}{{}^t\psi} {}^{tr}\mathbf{T}^d = {}^{t+\Delta t}\psi {}^{t+\Delta t}\mathbf{T}_0^d({}^{t+\Delta t}\mathbf{E}^d) \quad (59)$$

A Newton algorithm may be established in order to obtain ψ from the damage consistency condition $\dot{f}_D = 0$ where f_D is given by Eq. (22):

$${}^{t+\Delta t}f_D^{(k+1)} \simeq {}^{t+\Delta t}f_D^{(k)} + \frac{\partial {}^{t+\Delta t}f_D^{(k)}}{\partial {}^{t+\Delta t}\psi^{(k)}} \Delta\psi^{(k)} \rightarrow 0 \quad (60)$$

so

$$\Delta\psi^{(k)} = - \left(\frac{\partial {}^{t+\Delta t}f_D^{(k)}}{\partial {}^{t+\Delta t}\psi^{(k)}} \right)^{-1} {}^{t+\Delta t}f_D^{(k)} \quad (61)$$

Then, assuming that at a given stress point and instant $t + \Delta t$ the deformation gradient ${}^{t+\Delta t}\mathbf{X}$ and the parameter of the previous step ${}^t\psi$ are known, the computational procedure summarized in Table 1 determines the new ${}^{t+\Delta t}\psi$ and the actual isochoric stresses ${}^{t+\Delta t}\mathbf{T}^d$. Note that this procedure is in essence a procedure to solve the nonlinear Equation (28) in the form Eq. (49)

Table 1: Stress-point local integration algorithm

1. From ${}^{t+\Delta t}\mathbf{X}$ compute logarithmic strains ${}^{t+\Delta t}\mathbf{E} = \frac{1}{2} \ln ({}^{t+\Delta t}\mathbf{X}^T {}^{t+\Delta t}\mathbf{X})$
 2. Compute Jacobian ${}^{t+\Delta t}J = \det ({}^{t+\Delta t}\mathbf{X})$ and ${}^{t+\Delta t}\mathbf{E}^d = {}^{t+\Delta t}\mathbf{E} - \frac{1}{3} \text{tr} ({}^{t+\Delta t}\mathbf{E}) \mathbf{I}$
 3. For ${}^{t+\Delta t}\mathbf{E}^d$ compute ${}^{t+\Delta t}\mathcal{W}_0^d ({}^{t+\Delta t}E_1^d, {}^{t+\Delta t}E_2^d, {}^{t+\Delta t}E_3^d)$
 4. Compute ${}^{tr}f_D = {}^{t+\Delta t}\mathcal{W}_0^d {}^t\psi - {}^tw_D ({}^t\psi)$
 5. if ${}^{tr}f_D \leq 0$ no damage evolution: ${}^{t+\Delta t}\psi = {}^t\psi$; ${}^{t+\Delta t}\mathbf{T}^d = {}^{t+\Delta t}\psi {}^{t+\Delta t}\mathbf{T}_0^d$
 6. if ${}^{tr}f_D > 0$, damage increase:
 - 6.1. ${}^{t+\Delta t}f_D^{(0)} = {}^{tr}f_D$; ${}^{t+\Delta t}\psi^{(0)} = {}^t\psi$
 - 6.2. Do while $\left| {}^{t+\Delta t}f_D^{(k)} \right| > \text{tolerance}$
 - 6.2.1. $\partial {}^{t+\Delta t}f_D^{(k)} / \partial {}^{t+\Delta t}\psi^{(k)} = {}^{t+\Delta t}\mathcal{W}_0^d - \partial {}^{t+\Delta t}w_D / \partial {}^{t+\Delta t}\psi^{(k)}$
 - 6.2.2. ${}^{t+\Delta t}\psi^{(k+1)} = {}^{t+\Delta t}\psi^{(k)} - {}^{t+\Delta t}f_D^{(k)} / \left[\partial {}^{t+\Delta t}f_D^{(k)} / \partial {}^{t+\Delta t}\psi^{(k)} \right]$
 - 6.2.3. ${}^{t+\Delta t}f^{(k+1)} = {}^{t+\Delta t}\mathcal{W}_0^d {}^{t+\Delta t}\psi^{(k+1)} - w_D ({}^{t+\Delta t}\psi^{(k+1)})$
 - 6.3. ${}^{t+\Delta t}\psi = {}^{t+\Delta t}\psi^{(k+1)}$; ${}^{t+\Delta t}\mathbf{T}^d = {}^{t+\Delta t}\psi {}^{t+\Delta t}\mathbf{T}_0^d$
-
-

As mentioned, in the case of isotropy

$$\mathbf{T} = \bar{\boldsymbol{\tau}} = J \bar{\boldsymbol{\sigma}} \quad (62)$$

where $\mathbf{T}$ are the generalized Kirchhoff stresses (work-conjugate of the material logarithmic strains in the most general case), $\bar{\boldsymbol{\tau}}$ are the rotated Kirchhoff stresses (see [48]), $\bar{\boldsymbol{\sigma}}$ are the rotated Cauchy stresses. The volumetric component is

$${}^{t+\Delta t}\mathbf{T}^v = {}^{t+\Delta t}J {}^{t+\Delta t}p \mathbf{I} \quad \text{with } p = \frac{1}{J} \frac{d\mathcal{U}(J)}{d(\ln J)} \quad (63)$$

and

$${}^{t+\Delta t}\mathbf{T} = {}^{t+\Delta t}\mathbf{T}^v + {}^{t+\Delta t}\mathbf{T}^d \quad (64)$$

Obviously, this stress measure may be converted to any other stress measure, for example the second Piola-Kirchhoff stress tensor or the Cauchy stress tensor.

5.2 Consistent tangent moduli

At the structural level, a Newton-Raphson procedure is usually employed in order to establish equilibrium. During these global iterations, the displacements are changed and the new deformation gradients ${}^{t+\Delta t}\mathbf{X}$ are obtained at the integration points. From these deformation gradients, the new logarithmic strains ${}^{t+\Delta t}\mathbf{E}$ may be computed. Hence, in order to preserve quadratic convergence and retain efficiency in the global iterative procedure, the algorithmic tangent which relates the variation of generalized Kirchhoff stresses to the variation of these logarithmic strains must be derived [54]. Since the algorithm relates logarithmic strains with their work-conjugate stresses, the resulting stresses and the constitutive tangent must be then converted to the stress and strain measures employed by the finite element program (frequently Second Piola-Kirchhoff stresses and Green-Lagrange strains). As this is a usual procedure, we do not elaborate on these details. The reader may refer to References [1], [46], [48], [55].

To obtain the algorithmic constitutive tangent we can take advantage of the previous algorithm, Eq. (59):

$$\frac{\partial {}^{t+\Delta t}\mathbf{T}^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi \frac{\partial {}^{t+\Delta t}\mathbf{T}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} + {}^{t+\Delta t}\mathbf{T}_0^d \otimes \frac{\partial {}^{t+\Delta t}\psi}{\partial {}^{t+\Delta t}\mathbf{E}} \quad (65)$$

where

$$\frac{\partial {}^{t+\Delta t}\psi}{\partial {}^{t+\Delta t}\mathbf{E}} = \frac{d {}^{t+\Delta t}\psi}{d {}^{t+\Delta t}w_D} \frac{\partial {}^{t+\Delta t}w_D}{\partial {}^{t+\Delta t}\mathbf{E}^d} : \frac{\partial {}^{t+\Delta t}\mathbf{E}^d}{\partial {}^{t+\Delta t}\mathbf{E}} \quad (66)$$

with the deviatoric projector

$$\frac{\partial {}^{t+\Delta t}\mathbf{E}^d}{\partial {}^{t+\Delta t}\mathbf{E}} = \mathbb{P}^S := \mathbb{I} - \frac{1}{3}\mathbf{I} \otimes \mathbf{I} \quad (67)$$

However since $\partial {}^{t+\Delta t}f_D / \partial {}^{t+\Delta t}\mathbf{E}$ must vanish during damage evolution

$${}^{t+\Delta t}\psi \frac{\partial {}^{t+\Delta t}\mathcal{W}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} + {}^{t+\Delta t}\mathcal{W}_0^d \frac{d {}^{t+\Delta t}\psi}{d {}^{t+\Delta t}w_D} \frac{\partial {}^{t+\Delta t}w_D}{\partial {}^{t+\Delta t}\mathbf{E}} - \frac{\partial {}^{t+\Delta t}w_D}{\partial {}^{t+\Delta t}\mathbf{E}} = \mathbf{0} \quad (68)$$

Thus

$$\frac{\partial {}^{t+\Delta t}w_D}{\partial {}^{t+\Delta t}\mathbf{E}} = \frac{{}^{t+\Delta t}\psi}{1 - {}^{t+\Delta t}\mathcal{W}_0^d \frac{d {}^{t+\Delta t}\psi}{d {}^{t+\Delta t}w_D}} {}^{t+\Delta t}\mathbf{T}_0^d \quad (69)$$

and

$$\frac{\partial {}^{t+\Delta t}\mathbf{T}^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi \frac{\partial {}^{t+\Delta t}\mathbf{T}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} + \frac{{}^{t+\Delta t}\psi}{d {}^{t+\Delta t}w_D / d {}^{t+\Delta t}\psi - {}^{t+\Delta t}\mathcal{W}_0^d} {}^{t+\Delta t}\mathbf{T}_0^d \otimes {}^{t+\Delta t}\mathbf{T}_0^d \quad (70)$$

Finally, we obtain

$${}^{t+\Delta t}\mathbb{C} = \frac{\partial^2 U({}^{t+\Delta t}J)}{\partial (\ln {}^{t+\Delta t}J)^2} \frac{\partial \ln J}{\partial \mathbf{E}} \otimes \frac{\partial \ln J}{\partial \mathbf{E}} + \frac{\partial {}^{t+\Delta t}\mathbf{T}^d}{\partial {}^{t+\Delta t}\mathbf{E}} \quad (71)$$

where

$$\frac{\partial \ln J}{\partial \mathbf{E}} = \frac{\partial ({}^{t+\Delta t}E_1 + {}^{t+\Delta t}E_2 + {}^{t+\Delta t}E_3)}{\partial {}^{t+\Delta t}\mathbf{E}} = \sum_{i=1}^3 {}^{t+\Delta t}\mathbf{N}_i \otimes {}^{t+\Delta t}\mathbf{N}_i = \mathbf{I} \quad (72)$$

and

$$\frac{\partial {}^{t+\Delta t}\mathbf{T}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} = \mathbb{P}^S : \frac{\partial^2 \mathcal{W}_0^d({}^{t+\Delta t}\mathbf{E}^d)}{\partial {}^{t+\Delta t}\mathbf{E}^d \partial {}^{t+\Delta t}\mathbf{E}^d} : \mathbb{P}^S \quad (73)$$

From the Valanis-Landel decomposition, we obtain in general [1]

$$\frac{\partial^2 \mathcal{W}_0^d(\mathbf{E}^d)}{\partial \mathbf{E}^d \partial \mathbf{E}^d} = \sum_{i=1}^3 \frac{\partial^2 \omega_0(E_i^d)}{\partial (E_i^d)^2} \mathbf{N}_i \otimes \mathbf{N}_i \otimes \mathbf{N}_i \otimes \mathbf{N}_i + \sum_{i=1}^3 \sum_{j \neq i} \frac{T_{0j}^d - T_{0i}^d}{E_j^d - E_i^d} \mathbf{N}_i \overset{s}{\otimes} \mathbf{N}_j \otimes \mathbf{N}_i \overset{s}{\otimes} \mathbf{N}_j \quad (74)$$

where $\overset{s}{\otimes}$ stands for the symmetrized outer (dyadic) product. In summary

$${}^{t+\Delta t}\mathbb{C} = \frac{\partial^2 U({}^{t+\Delta t}J)}{\partial (\ln {}^{t+\Delta t}J)^2} \mathbf{I} \otimes \mathbf{I} + {}^{t+\Delta t}\psi \mathbb{P}^S : \frac{\partial^2 \mathcal{W}_0^d({}^{t+\Delta t}\mathbf{E}^d)}{\partial {}^{t+\Delta t}\mathbf{E}^d \partial {}^{t+\Delta t}\mathbf{E}^d} : \mathbb{P}^S - {}^{t+\Delta t}\beta {}^{t+\Delta t}\mathbf{T}_0^d \otimes {}^{t+\Delta t}\mathbf{T}_0^d \quad (75)$$

where

$${}^{t+\Delta t}\beta = \begin{cases} 0 & \text{if no damage evolution takes place} \\ \frac{{}^{t+\Delta t}\psi}{{}^{t+\Delta t}\mathcal{W}_0^d - \partial {}^{t+\Delta t}w_D / \partial {}^{t+\Delta t}\psi} & \text{for damage increase} \end{cases} \quad (76)$$

6 Examples

In this section we show some demonstrative examples using the same uniaxial experimental data. The material data needed for the model is simply an experimental virgin loading curve and a damaged unloading-reloading curve. This damaged (master) unloading-reloading curve must be given up to the maximum strain level to be attained in the simulations. Note that obviously the model cannot predict an experimentally undetermined behavior.

The “experimental” data herein considered corresponds to uniaxial tensile tests of sulfur-vulcanized SBR filled with 50% phr of N220 carbon-black, extracted

from [12]. The experimental data has been adapted to eliminate undesired effects, which cannot be modelled with this simple damage model (they need a further improvement on the model) as permanent residual strains (the damaged curves are moved to start at zero strains) and cyclic hysteresis during unloading-reloading (the same curve is employed during unloading and reloading).

The computational procedure is as follows. Both experimental curves are interpolated using piece-wise splines in order to obtain analytical, continuous functions. Because of the needs of the spline-based procedure, in particular to apply the Kaersley and Zapas inversion formulae to obtain the stored energy [35], identical behavior in compression is prescribed. Furthermore, both curves are slightly extrapolated in order to avoid the well-known border effect of spline interpolation.

In Figure 3a we show the original data employed and the resulting uniform spline interpolation. Note that spline-based hyperelastic models exactly capture the given stress-strain data, but a uniform spline interpolation is employed for computational convenience [35], [36]. Initial spline interpolation and the resulting interpolation from the computed stored energy $\mathcal{W}_0^d$ is also always coincident for the unloading-reloading (hyperelastic) case, see details about this procedure in [35], [36], [37]. The material is considered quasi-incompressible. Hence, we prescribed a penalty volumetric function with a large equivalent bulk modulus (10^3 times the largest value in the constitutive tensor) in order to numerically enforce incompressibility when needed. No further information is needed for the model.

The ratio between the virgin loading curve and the master (unloading-reloading) curve for each strain level E gives the multiplier function $\tilde{\psi}(E)$ as a function of the strain. However, for each strain level the stored energy $\mathcal{W}_0^d$ is easily computed, and hence also $\mathcal{W}^d$. Then it is straightforward to obtain $\psi(w_D)$, or conversely the more practical $w_D(\psi)$, which is the function used in the computational algorithm. The result for this example is shown in Figure 3b. Note that the condition $dw_D/d\psi \leq 0$ is fulfilled for every ψ , a condition which should always be checked.

As a first simulation we have prescribed the uniaxial strain history E_1 shown in Figure 4a, where due to incompressibility $E_2 = E_3 = -0.5E_1$. As it can be seen in Figure 4b, the predicted stress-strain data exactly mimics the prescribed data. We note that we plot $T_1 - T_2$ to eliminate the undetermined pressure. The resulting damage parameter evolution against the strain is shown in Figure 4c. In Figure 4d we show the evolution of the reference isochoric strain during the simulations. Note that during loading-unloading the predictions follow the same path in this plot.

As a second simulation, we impose a simple shear history, i.e. the deformation gradient is

$${}^t_0\mathbf{X} = \begin{bmatrix} 1 & \gamma(t) & \\ & 1 & \\ & & 1 \end{bmatrix} \quad (77)$$

Fig. 3 Experimental data and initial uniform spline interpolation. a) Original stress-strain data and spline fit. b) Computed proportionality function $\psi(w_D)$ against the damage variable w_D .

where $\gamma(t)$ is the shearing parameter. Note that the imposed deformations are isochoric. The time history for the shear parameter is shown in Figure 5a. The strains consequence of the deformation gradient being imposed are shown in Figure 5b. Note that E_{11} and E_{22} are nonvanishing and a maximum is obtained for the shear component E_{12} at $\gamma = 3.018$, see [43]. Depending on the nonlinearity of stresses with strains this maximum is observed in shear stresses at different values of γ . For the specific data employed, that maximum is still not reached for the given strain history, as it can be seen in Figure 5c. However, as seen in Figure 5d,

Fig. 4 Predictions for the uniaxial test. a) Prescribed uniaxial strain. b) Predictions versus uniaxial prescribed data. c) Evolution of the damage parameter during the simulation. d) Evolution of the reference isochoric stored energy during the simulation.

note that even though they are negligible for small strains, at large strains the components T_{11} and T_{22} reach values much larger than the shear stresses [43].

As a final simulation, in order to assess the applicability of the model to more complex situations and to show the efficiency of the numerical tangent, we perform a combined nonproportional axial-torsion load test. In this case the test is stress-driven. We prescribe the stresses given in Figure 6a. The components $T_{22} = T_{33} =$

Fig. 5 Simple shear test prediction. a) Imposed history of the (engineering) shear parameter. b) Resulting strains computed from the deformation gradient. c) Predictions for the T_{12} stress against the shear parameter γ . d) Results of the simulation for the T_{11}^d and T_{22}^d components.

$T_{13} = T_{23} = 0$. The stress path is shown in Figure 6b. The predictions for strains using the model are given in Figure 6c. Note that as a result of the isochoric behavior imposed via a penalty volumetric energy, the components E_{22} and E_{33} are nonvanishing but $E_{22} + E_{33} = -E_{11}$. The strain path prediction in the $E_{11} - E_{12}$ plane is shown in Figure 6d.

The evolution of the reference isochoric energy $\mathcal{W}_0^d$, the damage variable w_D and the energy multiplier ψ are shown in Figure 7.

Fig. 6 Axial-torsion test. a) History of the prescribed axial stress T_{11} and shear stress T_{12} . b) Prescribed stress path. c) Predictions for the strain components E_{11} , E_{22} , E_{33} and E_{12} . d) Predicted $E_{11} - E_{12}$ strain path.

In Figure 8 we show the numerical performance of the algorithm. Plain Newton algorithms (without line searches) have been employed both locally and globally. In Figure 8a we show the number of local iterations employed in the computation of the energy multiplier parameter ψ , i.e. the number of iterations to fulfill the consistency condition, Eq. (60) up to a relative tolerance of 10^{-10} . Only during damage evolution local iterations are necessary. In such case, usually 3 local iterations are employed per global iteration. The number of these global equilibrium iterations employed per step are shown in Figure 8b. Typically, 5-6 global iterations are employed per step to reach a relative tolerance in the norm of the residual of forces of 10^{-10} . However we highlight that there is no relevant penalty in the global iterations because of damage evolution; i.e. the number of global iterations employed are mainly a consequence of the hyperelastic behavior. Note that there is no clear correlation between Figures 8a and 8b. This is not surprising

Fig. 7 Axial-torsion test. a) Evolution of the reference energy. b) Evolution of the damage variable w_D . c) Evolution of the energy scaling parameter.

because the degree of nonlinearity exhibited by both the virgin loading and the unloading-reloading curves is similar as shown in Figure 3.

7 Conclusions

In this paper we introduce a new phenomenological formulation and computational procedure for large strain quasi-incompressible isotropic damage mechanics. The model may be employed to simulate the Mullins effect in hyperelastic, isochoric materials. The approach is based on the idea that stresses of the undamaged material and thus undamaged stored energies are not measurable. Since it is convenient that phenomenological models are built upon experimentally obtainable quantities, then as a reference stored energy we employ a damaged stored energy obtained from damaged unloading-reloading stress-strain data. The stress-strain data from the virgin loading curve is used only to compute the released energy through an intermediate parameter.

Fig. 8 Axial-torsion test. a) Total number of local iterations per step employed in the computation of ψ . b) Number of global (equilibrium) iterations employed per step.

The continuum formulation is based on an operator split based on partial derivatives which naturally can be interpreted as a trial stress predictor, energy-release-rate damage-corrector decomposition. Thanks to isotropy, the local computational procedure consists on solving a nonlinear scalar equation for damage evolution.

The consistent algorithmic tangent is also obtained in order to preserve the asymptotic quadratic convergence rate of Newton algorithms during equilibrium iterations.

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5.3. Modelo de daño ortótropo WYPIWYG

Como ya se ha comentado en los Capítulos 1 y 3, los refuerzos (fibras y partículas de carbono, sílice, etc.) que se añaden a los materiales poliméricos y las fibras de colágeno en los tejidos y otros tipos de materiales biológicos, transfieren a dichos materiales cierto grado de anisotropía. Para representar el comportamiento de materiales anisótropos hay dos tipos de enfoques. El primero, es puramente fenomenológico. Los modelos de Fung [111] y de Itskov y Ehret [112], [113] para tejidos biológicos y el de Itskov y Aksel [114] para polímeros, son algunos ejemplos. El segundo enfoque está basado en la estructura y se ha heredado de la mecánica de los materiales compuestos. Algunos ejemplos de este tipo se encuentran en las siguientes referencias [115], [116], [117]. En todos estos modelos es frecuente usar algoritmos de optimización para obtener los parámetros del material. La falta de unicidad de estos parámetros es un problema bien conocido. Estos modelos pueden también presentar falta de congruencia de las simetrías del material.

Por supuesto estos materiales anisótropos también pueden exhibir efecto Mullins. En el caso de los polímeros reforzados con carbono este efecto se atribuye a la rotura de enlaces entre las cadenas poliméricas ([118], [32]), al deslizamiento ([119]), a la rotura del relleno ([121]) y a enlaces débiles entre la matriz y el relleno ([98], [120]). Para el caso de tejidos biológicos, se atribuye a la rotura de fibrillas de colágeno y de la matriz de proteoglicanos. Mientras que para materiales duros hay muchos enfoques para modelar el daño en general (diversas referencias se pueden encontrar en el siguiente artículo de revisión [122]), para materiales blandos se han propuesto menos enfoques diferentes. La formulación más usada para los materiales blandos es la mecánica del daño continuo (de aquí en adelante se denominará por sus iniciales en inglés *CDM*). La formulación para daño isótropo propuesta por Simó [102] se ha extendido a materiales anisótropos empleando diferentes funciones de la energía de deformación y distintas ecuaciones de evolución para las variables de daño. Otro tipo de formulación que parece tener éxito es la pseudoelasticidad en el marco de Ogden y Roxburg [99]. En este enfoque, se formula un potencial pseudoelástico que incluye la disipación debida al daño y especialmente a cargas cíclicas. Este enfoque ha sido seguido por Dorfmann y Ogden [100] para modelar exactamente el comportamiento histerético de una goma reforzada con carbono. Nótese, que tanto la formulación CDM como la pseudoelasticidad se construyen sobre la idea de la existencia de una energía sin dañar hipotética. Desde un punto de vista práctico, puesto que los parámetros del material son normalmente obtenidos mediante algoritmos de optimización tipo Levenberg-Maquardt o mediante análisis de sensibilidad, su significado físico no tiene real relevancia.

En este apartado se presenta la extensión a ortotropía del modelo isótropo del apartado anterior. Una vez más, la idea de esta formulación es evitar el uso de funciones de energía almacenada analíticas, con todos los problemas mencionados

que conllevan, y en su lugar obtener las energías almacenadas directamente de los datos experimentales usando un enfoque numérico. El modelador consigue mediante simulaciones capturar “exactamente” los datos experimentales prescritos, que para el caso de materiales ortótropos incompresibles que exhiben efecto Mullins son seis curvas experimentales de carga inicial y seis de descarga. No se requieren ecuaciones de evolución explícitas ni parámetros del material explícitos. Simplemente se emplean las curvas tensión-deformación para extraer directamente toda la información necesaria. De este modo, la curva de carga inicial y las curvas de descarga y recarga hiperelásticas se consiguen representar para la precisión numérica deseada. La formulación también puede ser empleada para tejidos biológicos ya que el daño de la matriz isótropa y la desviación anisótropa pueden ser modelados independientemente.

Como resumen, los puntos más importantes del siguiente artículo son:

- Se introduce la teoría continua y se desarrolla el algoritmo de integración numérica.
- Se explica cómo extraer la información necesaria de los experimentos.
- Se muestran diversos ejemplos bajo deformaciones homogéneas y no homogéneas que demuestran la capacidad de predicción del modelo.

WYPIWYG anisotropic damage mechanics for soft materials

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Abstract Polymeric and biological materials present a softening effect known as Mullins effect. This effect is typically modelled within the framework of continuum damage mechanics or within the framework of pseudoelasticity. In both cases, a stored energy function shape and a damage evolution law are proposed and some material parameters that modulate those shapes are best-fitted to experimental data through optimization algorithms. The What-You-Prescribe-Is-What-You-Get (WYPIWYG) approach presents a different approximation to the problem. These formulations are based in WYPIWYG hyperelasticity. WYPIWYG hyperelasticity captures to any desired precision the prescribed experimental data without using material parameters nor optimization algorithms, still preserving similar computational efficiency for finite element analysis than classical hyperelastic models. In this paper a WYPIWYG anisotropic formulation for softening in rubber-like materials and biological tissues is presented. The proposal follows the WYPIWYG ideas so no explicit damage evolution expression is employed and no material parameters or optimization algorithms are needed. Instead, all the needed information is obtained from the presented experimental data.

1 Introduction

The basic ingredient to model the behavior of soft materials like rubber [1], [2], [3] or biological tissues [4], [5], [6] is hyperelasticity. Hyperelastic behavior constitutes the basic nondissipative elastic behavior at large strains [2] and as so, it is equivalent to the elastic behavior at small strains. However, whereas path independence is fulfilled at small strains by the symmetry of the elasticity tensor, at large strains some integrability requirements need to be fulfilled. Nowadays the simplest and standard way to do so is to assume an *analytical* strain energy function density from which the stresses are obtained as a function of the strains. Some material parameters permit the different assumed stored energies to fit available experimental data, and because of the variable success when addressing different materials,

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there are hundreds of strain energy proposals in the literature. For isotropic materials the Neo-Hookean model [7] is the simplest one, and the Ogden model [8] one of the most successful ones. For anisotropic materials there are two approaches. The first one is purely phenomenological. The models of Fung [9] and Itskov and Ehret [11], [10] for biological tissues and Itskov and Aksel [12] for rubber-like materials, are some examples. The other approach is structure-based, inherited from the mechanics of composite materials [15]. The models of Lanir [13], Humphrey and Yin [14], Holzapfel et al [15], and Gasser et al [16] are examples of this kind. In all these models, it is frequent to use optimization algorithms to obtain the material parameters [17], [18], [19]. Non-uniqueness of these parameters is a well known and frequently reported problem. These models may also lack numerical material-symmetries congruency [20]. Furthermore, in the case of structure-based models, it is necessary to properly account for fibers working in tension and (not) working in compression [21], they may present unrealistic transverse strains [22], [23] and are frequently fitted with incomplete material data resulting in arbitrary behavior in other loading situations [24]. Many of these models are not compatible with the full infinitesimal theory for their respective symmetry groups [25], [26].

Rubber-like materials and biological tissues exhibit a softening phenomenon known as Mullins effect [27], [28]. In the case of carbon-filled rubber materials is attributed to bond rupture between polymeric chains [29], [30], slipping [31], disentanglement [32], filler rupture [33] and between them and the filler [34], [35]. A review for rubber-like solids is given by Diani et al [35]. For the case of biological tissues, it is attributed to the permanent orientation of collagen fibres and breakage of collagen fibrils [38], [39] and of proteoglycans [36], [37], [40]. Whereas in hard materials there are many possible approaches to model damage in general (see review in [41]), in soft materials fewer approaches have been followed.

The most used formulation for soft materials is the Continuum Damage Mechanics (CDM) approach. In this approach, a hypothetical undamaged energy is penalized by a damage coefficient $(1 - D)$, where $D \in (0, 1]$ is the damage variable of Rabotnov. For isotropic materials the formulation of Simo [42] is one of the best known references, see also [43] and [44]. This framework has been extended to anisotropic materials employing different strain energy functions and different damage evolution equations. For example in Calvo et al [45], different damage parameters D_m and D_f for matrix and fibers are considered and associated exponential-type expressions are employed in terms of Simo energy strains. The same group has extended the model to capture permanent set [46], viscous effects [47] and additional continuous damage [73]. A comparison of damage functions in soft tissue can be found in Pena [47] and in Balzani and Schmidt [49]. A comparison of continuous and discontinuous damage functions can be found in [73], where they conclude that continuous damage may be used only to model hysteresis and stabilization in the first cycles of the loading path because of the rapid damage saturation.

Damage has also been used to characterize the irreversible stress drop in rectus sheath [50]. Localization of damage (and hence mesh dependency) may happen in these cases [48] as it is well known [51], but the quasi-incompressible nature of soft tissues help to regularize the problem [52]. In this last work, a mixture theory is employed to account for non-affine deformations and they capture the monotonic loading experiments of [50]. This framework has also been used by Saez et al [53] to develop a microsphere-based approach to damage in soft fibred tissue. The microsphere approach had been previously used by Miehe and co-workers [54], [55], [56] for elastomers and by Caner and Carol [57] and Alastrué et al [58] for biological tissues. The continuum damage formulation has also been extended to include smooth muscle cells in arteries [59]. Active damage has also been included in the different damage formulation in [10], which includes damage from evolution functions of the structural tensors in order to guarantee polyconvexity. Polyconvex energy functions with damage have also been used in [60]. Similar conceptual formulations by direct modification of the energy function and more oriented to failure are found in the works of Volokh [61], [62]. Other formulation including a damage evolution function in terms of the fourth invariant may be found in [63]. The continuum damage framework has also been employed at different scales. In [88] a microstructural damage for fibers which links damage with fiber recruiting distribution is formulated and the result compared with CDM and pseudoelasticity. In Schmidt et al [64] statistical distributions of quantities at the collagen fibril level, including proteoglycan orientation are introduced in order to enhance the microstructural understanding of the behavior of the tissue. With the same purpose Blanco et al [65] have developed a model at the mesoscale in which inelastic phenomena in the fibre is assumed to be caused only by degradation processes in the fibrils by means of two failure modes. In a more general setting, truss-like microstructures with damage following the same framework have been formulated via relaxed incremental variational formulations as to avoid loss of convexity and their related problems [66]. This relaxed formulation was subsequently applied to model damage-induced hysteresis in arterial walls [67].

Another type of formulation which seems to be successful is the pseudoelasticity framework of Ogden and Roxburg [68]. In this framework, a pseudo-elastic potential is formulated which includes the “dissipation” due to damage and specially to cyclic loading (a feature not modelled in the discontinuous CDM framework). This approach has been followed by Dorfmann and Ogden [69] to accurately model the cyclic hysteretic behavior of a rubber compound 60phr of Carbon black after preconditioning and then extended to model the permanent set present in these materials [70] and thereafter to model changes in material symmetry in [71]. This same model was also applied to model the muscle of tobacco hornworm caterpillar *Manduca sexta*, including the active muscle effect [72] and also in [73] to simulate anisotropic damage in fibrous biological tissues. The thermodynamics of

Pseudoelasticity is studied in [74], where they find that the usual pseudoelastic materials do not dissipate the energy (for example into heat) but store it. Hence a modification is proposed. On the other hand, a practical comparison between pseudo-elastic and damage models for modelling Mullins effect can be found in Gracia et al [75]. Here we note that both CDM and pseudoelasticity are built on the idea of the existence of a hypothetical undamaged energy. From a practical point of view, since the material parameters of these models are typically obtained through optimization algorithms like the Levenberg-Marquardt algorithm [76] or sensitivity analysis, its physical meaning has no actual relevance. However, it is apparent that the undamaged energy does not exist because any loading from virgin state entails itself a damage process, i.e. the primary loading curve does not proceed from a hyperelastic behavior. Then, that undamaged energy cannot be measured neither directly nor indirectly through stress-strain curves.

Let us summarize the ideas behind the commented approaches in few words. Hyperelasticity is modelled through *assumed* analytical stored energy function shapes. These shapes are *best-fitted* to experimental data through some material parameters. Damage is modelled through different formulations which again *assume* the shape of some undamaged stored energy and also *assume* an evolution equation. This evolution equation is also *best-fitted* to experimental data through some material parameters. Conceptually, this is a global approach similar to the global approach followed by Rayleigh to compute natural frequencies of deflections in plates: a global analytical solution is assumed except from some global parameters that are computed as to obtain a best fit of the corresponding energy of the structure. This global approach has been superseded in practice by the local approach given, for example by finite elements.

In the last years we have been pursuing the different, local approach. The idea behind the approach is to avoid the use of analytical stored energy functions (with all the mentioned problems) but instead to obtain the stored energy directly from experimental data using a numerical approach. We have named it the "What-You-Prescribe-Is-What-You-Get" (WYPIWYG) approach [77] because as the name claims, the modeler will get from simulations "exactly" (i.e. to the desired precision) the prescribed data, and the prescribed data is a complete set of experimental tests; for example 6 curves (including the compression part when applicable) for incompressible orthotropic materials. The models are based on a spline (local) interpolation between terms of the derivative of the stored energy which are obtained from an inversion formula which solves the equilibrium equations of the tests. The first model of this kind is that of Sussman and Bathe [89] for incompressible isotropic materials which use the Kaersley and Zapas formula. We have developed WYPIWYG formulations for transversely isotropic [79], orthotropic [77] and isotropic compressible materials [80]. For example WYPIWYG formulations, which are a natural extension of the infinitesimal theory, are capable

of capturing to any desired precision and in any loading situation the behavior of any isotropic compressible model following the Valanis-Landel decomposition using just their predictions for a uniaxial tension-compression test. Furthermore, the orthotropic incompressible WYPIWYG model captures exactly six experimental, independent stress-strain curves which define the material behavior the same way that six moduli does it in the infinitesimal framework. In fact, WYPIWYG anisotropic formulations are in agreement with the infinitesimal theory [25], [26] and preserve material-symmetries congruency [20]. These models have also been used successfully in modelling very accurately soft biological tissues and have been used also in anisotropic viscoelasticity [81] to model independently equilibrated and nonequilibrated stored energies. These models have been also formulated mimicking the infinitesimal theory.

The purpose of this work is to extend the approach to model Mullins-type damage effects in rubber-like materials and soft biological tissues. The basic ideas are given for isotropic materials in Miñano and Montáns [90]. In this approach we do not make an hypothesis on any undamaged stored energy. We do not use explicit evolution equations and we do not employ material parameters nor optimization algorithms. We just employ stress-strain data directly to extract all the needed information. Then, the primary loading and hyperelastic unloading-reloading curves are captured to any desired numerical precision. In this work we extend the WYPIWYG damage formulation to anisotropic materials. The formulation may be employed also to model biological tissues because damage of the isotropic matrix and the anisotropic deviation may be modelled independently.

The rest of the manuscript is structured as follows. First we introduce the continuum theory and then we develop the numerical integration algorithm. Subsequently we explain how to extract the information from the experiments. The last part of the manuscript is devoted to numerical examples under homogeneous deformations and under nonhomogeneous ones. Both isotropic and anisotropic examples are given.

2 One-dimensional, infinitesimal motivation

2.1 Continuum theory

In this section we introduce a simplest one-dimensional formulation just for motivation. Consider a bar with a constant stress behavior $\sigma(\varepsilon)$ as depicted in Figure 1. In that figure ε is the infinitesimal strain, σ is the stress and the horizontal line at σ_m is the monotonic loading from virgin state. The first slope in the bilinear curve corresponds to the initial elastic behavior which in this simplest case is $E_{\max} \rightarrow \infty$. This modulus is valid until the stress σ_m is reached. The horizontal line at σ_m when ε is increasing until $\varepsilon = \varepsilon_m$ is the damage evolution. During load-

Fig. 1 The simplest uniaxial model. (a) Feasible domain, stored and released energies. (b) Potential W . (c) Evolution of the stored elastic energy. (d) Procedure to search for a solution

ing in that curve the Young modulus E decreases due to damage. Upon damage, the unloading-reloading curve is linear with a slope given by E , and for $\sigma = 0$, we obtain $\epsilon = 0$, i.e. no permanent strain, note that although during initial loading the curve resembles a rigid-plastic one, upon unloading the differences are apparent because (1) there are no permanent strains and (2) each stress-strain pair in the feasible domain can be reached only through a unique inelastic path; i.e. we can say that the stresses are a path-independent function of the strains and an additional variable, say w .

Assume that E_0 is the minimum possible Young modulus (for example because after that, the bar breaks apart) which is attained when the strains reach the value of $\epsilon = \epsilon_m$. The stored energy density is, see Figure 1

$$\mathcal{W}(\epsilon, w) = \frac{1}{2} E(w) \epsilon^2 = \frac{1}{2} \sigma(w) \epsilon \quad (1)$$

where w is a damage variable and $E(w)$ is the Young modulus for that level of damage. The stress is given by Hooke's law $\sigma(w) = E(w) \epsilon$. For the maximum damage given by w_0 , we have the reference strain energy $\mathcal{W}_0$ defined as

$$\mathcal{W}_0(\epsilon) := \mathcal{W}(\epsilon, w_0) = \frac{1}{2} E_0 \epsilon^2 = \frac{1}{2} \sigma_0 \epsilon \quad (2)$$

Fig. 2 Difference between damage and plasticity. Left: in damage procedures the stress is a state function of damage and strain. Right: in plasticity a stress point may be reached through multiple paths, so they are not derived from a potential

and hence we can write for any strain ε

$$\psi(w) = \frac{\mathcal{W}(\varepsilon, w)}{\mathcal{W}(\varepsilon, w_0)} = \frac{\sigma(\varepsilon, w)}{\sigma_0(\varepsilon)} = \frac{E}{E_0} \quad (3)$$

This relation is apparent in the drawing in Figure 1, and is valid even if the virgin loading curve $\sigma(\varepsilon)$ is nonlinear, the case shown in Figure 3. Therefore, if we know the function $\psi(w)$, we readily know the elastic stored energy or the stress:

$$\mathcal{W}(\varepsilon, w) = \psi(w) \mathcal{W}_0(\varepsilon) \quad (4)$$

Note that $\mathcal{W}_0(\varepsilon)$ is the strain energy after a large damage, not the initial one, and that $\psi(w) \geq 1$. The maximum value is $\psi(w(\varepsilon_{\min})) = E_{\max}/E_0$. For the example at hand $\psi_{\max} \rightarrow \infty$. Note also that $\psi(w)$ may be readily obtained from the $\sigma_m(\varepsilon)$

Fig. 3 General nonlinear case: computational procedure

–maximum load– and the $\sigma_0(\varepsilon)$ –reference stress– curves as

$$\tilde{\psi}(\varepsilon) = \frac{\sigma_m}{\sigma_0(\varepsilon)} = \frac{w(\varepsilon)}{\Psi_0(\varepsilon)} = \psi(w(\varepsilon)) \quad (5)$$

The damage variable w has still not been defined. However, whatever is the meaning we want to select for this variable, the evolution is determined by the curve $\sigma_m(\varepsilon)$. Since we desire a damage variable with scalar meaning that may be used in three-dimensional problems, a variable with energy meaning is a good choice. In some problems, the stored energy may decrease during damage evolution. Hence the input energy may be a better choice. We note that in damage we can propose a potential function W which consists on the total elastic energy, both stored $\mathcal{W}$ and released $\mathcal{G}$, i.e.

$$W = \mathcal{W} + \mathcal{G} \quad (6)$$

Note that for the particular case at hand we can write $W = 2\mathcal{W}$. This energy is the area below the curve $\sigma_m(\varepsilon)$. Obviously, if $\mathcal{P}$ is the external power due to the load F acting on a velocity v , we have

$$Fv = \mathcal{P} = \dot{W} = \sigma \dot{\varepsilon} = \dot{\mathcal{W}} + \dot{\mathcal{G}} \quad (7)$$

i.e.

$$\begin{aligned}\frac{dW}{d\varepsilon} &= \frac{d\mathcal{W}}{d\varepsilon} + \frac{d\mathcal{G}}{d\varepsilon} \\ &= \left[\psi \frac{d\mathcal{W}_0}{d\varepsilon} + \mathcal{W}_0 \frac{d\psi}{d\varepsilon} \right] + \frac{d\mathcal{G}}{d\varepsilon}\end{aligned}\quad (8)$$

so the energy release rate is

$$Y := \frac{d\mathcal{G}}{d\varepsilon} = -\mathcal{W}_0 \frac{d\psi}{d\varepsilon} \quad \text{and} \quad \frac{dW}{d\varepsilon} = \psi \frac{d\mathcal{W}_0}{d\varepsilon} \quad (9)$$

During loading at the curve σ_m we have

$$\mathcal{P} = \sigma \dot{\varepsilon} = \frac{dW(\varepsilon, w)}{d\varepsilon} \dot{\varepsilon} = \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} \dot{\varepsilon} + \frac{\partial W(\varepsilon, w)}{\partial w} \dot{w} \quad (10)$$

$$= \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} \dot{\varepsilon} + \frac{\partial W(\varepsilon, w)}{\partial w} \frac{dw}{d\varepsilon} \dot{\varepsilon} \quad (11)$$

i.e.

$$\frac{dW(\varepsilon, w)}{d\varepsilon} = \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} + \frac{\partial W(\varepsilon, w)}{\partial w} \frac{dw}{d\varepsilon} \quad (12)$$

$$= \left[\psi \frac{d\mathcal{W}_0}{d\varepsilon} + \mathcal{W}_0 \frac{d\psi}{d\varepsilon} \right] + \frac{d\mathcal{G}}{d\varepsilon} \quad (13)$$

or

$$\frac{\partial W(\varepsilon, w)}{\partial \varepsilon} \equiv \frac{d\mathcal{W}}{d\varepsilon} = \psi \frac{d\mathcal{W}_0}{d\varepsilon} + \mathcal{W}_0 \frac{d\psi}{d\varepsilon} \quad (14)$$

and

$$\frac{dW}{d\varepsilon} = \psi \frac{d\mathcal{W}_0}{d\varepsilon} = \frac{d\mathcal{W}}{d\varepsilon} - \mathcal{W}_0 \frac{d\psi}{d\varepsilon} \quad (15)$$

Now we can choose as meaning for w

$$w = \max_{\tau \in (-\infty, t]} W(\tau) \quad (16)$$

so during damage evolution

$$W = w \quad \text{and} \quad \dot{W} = \dot{w} \quad (17)$$

and using Eqs. (15) and (14)

$$\sigma = \psi \frac{d\mathcal{W}_0}{d\varepsilon} \equiv \frac{dW(\varepsilon, w)}{d\varepsilon} = \frac{1}{1 + \gamma} \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} = \frac{1}{1 + \gamma} {}^{tr}\sigma \quad (18)$$

where

$$\gamma = -\frac{\partial W(\varepsilon, w)}{\partial w} = \mathcal{W}_0 \frac{d\psi}{dw} > 0 \quad (19)$$

is the energy release ratio and

$$\sigma^{|e} \equiv {}^{tr}\sigma := \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} \geq \sigma = \psi \frac{d\mathcal{W}_0}{d\varepsilon} \quad (20)$$

is the trial stress, a concept similar to the algorithmic trial stress in computational elastoplasticity. Note that for the particular case at hand we can write ${}^{tr}\sigma = 2\sigma$ because half of the input energy will be stored and half released. A convenient alternative is to express w as a function of ψ , or vice-versa, ψ as a function of w , so

$$Y = \frac{d\mathcal{G}}{d\varepsilon} = -\frac{\partial W(\varepsilon, w)}{\partial w} \frac{dw}{d\varepsilon} = -\mathcal{W}_0 \frac{d\psi}{dw} \frac{dw}{d\varepsilon} \quad (21)$$

and using $d\psi/dw \leq 0$

$$\gamma = -\frac{\partial W(\varepsilon, w)}{\partial w} = -\mathcal{W}_0 \frac{d\psi}{dw} \geq 0 \quad (22)$$

and

$$\sigma = \psi \frac{d\mathcal{W}_0}{d\varepsilon} \equiv \frac{dW(\varepsilon, w)}{d\varepsilon} = \frac{1}{1 - \mathcal{W}_0 \frac{d\psi}{dw}} {}^{tr}\sigma \quad (23)$$

During unloading $\dot{\mathcal{G}} = 0$, $\dot{w} = 0$, and

$$\sigma = \frac{dW(\varepsilon, w)}{d\varepsilon} = \frac{\partial W(\varepsilon, w)}{\partial \varepsilon} = \frac{\partial \mathcal{W}(\varepsilon, w)}{\partial \varepsilon} = \psi(w) \frac{d\mathcal{W}_0(\varepsilon)}{d\varepsilon} = \psi(w) \sigma_0 \quad (24)$$

i.e. $\sigma = {}^{tr}\sigma$, which corresponds to the state in which damage is frozen.

The continuum tangent modulus during damage evolution is obtained as

$$E_T = \frac{d\sigma}{d\varepsilon} = \frac{d^2 W(\varepsilon, w)}{d\varepsilon^2} = \psi \frac{d^2 \mathcal{W}_0}{d\varepsilon^2} + \frac{d\psi}{dw} \sigma_0 \frac{dw}{d\varepsilon} \quad (25)$$

Since during damage evolution Eq. (17) holds,

$$E_T = \psi E_0 + \frac{d\psi}{dw} \psi \sigma_0 \sigma_0 \quad (26)$$

During unloading-reloading, the tangent modulus is the elastic one, i.e. the one for $d\psi/dw = 0$

$$E_T = \psi E_0 \quad (27)$$

2.2 Computational procedure

If the stored energy is always increasing during damage, we can use the maximum stored energy as damage variable, i.e.

$$w_D = \max_{\tau \in (-\infty, t]} \mathcal{W}(\tau) \quad (28)$$

and write $\psi(w_D)$ —note the abuse of notation. Then, the damage evolution condition may be alternatively written as

$$f := \mathcal{W} - w_D \leq 0 \quad (29)$$

Note that just adding $\mathcal{G}$ we recover the previous equation:

$$f := W - w \equiv (\mathcal{W} + \mathcal{G}) - (w_D + \mathcal{G}) = \mathcal{W} - w_D \leq 0 \quad (30)$$

Then, to check whether there is damage evolution, we can perform the following check. If

$${}^{tr}f := {}^{tr}\mathcal{W}({}^{t+\Delta t}\varepsilon, {}^tw_D) - {}^tw_D > 0 \quad (31)$$

then damage evolution takes place. The computation of the new w_D is straightforward because the value is such that

$$f = \mathcal{W}(\varepsilon, w_D) - w_D \equiv \psi(w_D) \mathcal{W}_0(\varepsilon) - w_D = 0 \quad (32)$$

This is in general a nonlinear equation which solution is solved by a Newton-Raphson procedure, i.e.

$$f^{(j+1)} = f^{(j)} + \frac{df^{(j)}}{dw_D^{(j)}} \left(w_D^{(j+1)} - w_D^{(j)} \right) \rightarrow 0 \quad (33)$$

where (j) is the iteration index and

$$\frac{df^{(j)}}{dw_D^{(j)}} = \frac{d\psi}{dw_D^{(j)}} \mathcal{W}_0(\varepsilon) - 1 = -(1 + \gamma_D) \quad (34)$$

with $(\cdot)^{(0)} = {}^{tr}(\cdot)$ and

$$\gamma_D := -\frac{d\psi}{dw_D^{(j)}} \mathcal{W}_0(\varepsilon)$$

Remarkably, the derivative respect to strains of ${}^{tr}f$ yields

$$\begin{aligned} \frac{\partial {}^{tr}f}{\partial \varepsilon} &= \frac{\partial {}^{tr}\mathcal{W}({}^{t+\Delta t}\varepsilon, {}^tw_D)}{\partial \varepsilon} - \frac{\partial {}^tw_D}{\partial \varepsilon} \\ &= {}^t\psi \frac{\partial {}^{t+\Delta t}\mathcal{W}_0({}^{t+\Delta t}\varepsilon)}{\partial \varepsilon} - {}^t\sigma = {}^{tr}\sigma - {}^t\sigma = Y \end{aligned}$$

Upon convergence, the stress may be computed as —note that the elastic behavior still holds, but now with the updated modulus

$$\sigma^{(j+1)} = \psi \left(w_D^{(j+1)} \right) \sigma_0 = \psi \left(w_D^{(j+1)} \right) E_0 \varepsilon = E^{(j+1)} \varepsilon \quad (35)$$

During damage evolution

$$0 = \frac{df}{d\varepsilon} = \frac{d\psi}{dw_D} \mathcal{W}_0 \frac{dw_D}{d\varepsilon} + \psi \sigma_0 - \frac{dw_D}{d\varepsilon} = 0 \quad (36)$$

so

$$\frac{dw_D}{d\varepsilon} = \frac{\psi \sigma_0}{1 - \frac{d\psi}{dw_D} \mathcal{W}_0} = \frac{\psi \sigma_0}{1 + \gamma_D} \quad (37)$$

Then, the tangent may be written as

$$\begin{aligned} E_T &= \frac{d\sigma}{d\varepsilon} = \frac{d(\psi \sigma_0)}{d\varepsilon} = \psi E_0 + \frac{d\psi}{dw_D} \frac{dw_D}{d\varepsilon} \sigma_0 \\ &= \psi E_0 + \frac{\frac{d\psi}{dw_D} \psi}{1 - \frac{d\psi}{dw_D} \mathcal{W}_0} \sigma_0 \sigma_0 \end{aligned} \quad (38)$$

But we can write also

$$0 = \frac{df}{d\varepsilon} = \frac{dW}{d\varepsilon} - \frac{dw}{d\varepsilon} = \psi(w) \sigma_0 - \frac{dw}{d\varepsilon}$$

so the effective algorithmic tangent modulus during damage evolution admits the alternative

$$\begin{aligned} E_T &= \frac{d\sigma}{d\varepsilon} = \frac{d(\psi \sigma_0)}{d\varepsilon} = \psi E_0 + \frac{d\psi}{dw} \frac{dw}{d\varepsilon} \sigma_0 \\ &= \psi E_0 + \frac{d\psi}{dw} \psi \sigma_0 \sigma_0 \end{aligned} \quad (39)$$

3 Isotropic linear model motivation

3.1 Continuum theory

The extension of the previous framework to three dimensions is straightforward. In this case, the stored energy density is

$$\Psi(\boldsymbol{\varepsilon}, w) = \mathcal{U}(\varepsilon^v) + \mathcal{W}(\boldsymbol{\varepsilon}^d, w) = \frac{1}{2} K (\varepsilon^v)^2 + \frac{1}{2} 2\mu(w_D) (\boldsymbol{\varepsilon}^d)^2 \quad (40)$$

$$= \frac{1}{2} \boldsymbol{\sigma}(w_D) : \boldsymbol{\varepsilon} = \frac{1}{2} \boldsymbol{\varepsilon}^d : \mathbb{C}(w_D) : \boldsymbol{\varepsilon}^d \quad (41)$$

where $\boldsymbol{\varepsilon}$ is the deformation tensor, $\varepsilon^v = \text{tr}(\boldsymbol{\varepsilon})$ is the volumetric infinitesimal dilatation, $\text{tr}(\cdot)$ is the trace operator, K is the bulk modulus, $\mu_w(w)$ is the shear modulus for the damage level w and

$$\mathbb{C}(w_D) = K\mathbf{I} \otimes \mathbf{I} + 2\mu(w)\mathbb{P}^d \quad (42)$$

with

$$\mathbb{P}^d := \mathbb{I} - \frac{1}{3}\mathbf{I} \otimes \mathbf{I}$$

We consider as a simplifying hypothesis (useful in the hyperelastic case) that damage only affects the deviatoric part. It can be shown [41] that in isotropy, if we assume the Valanis-Landel decomposition (which holds in the infinitesimal case) the stored energies take the form —note the abuse of notation

$$\mathcal{W}(\boldsymbol{\varepsilon}^d, w) = \psi(w)\mathcal{W}_0(\boldsymbol{\varepsilon}^d) = \psi(w_D)\mathcal{W}_0(\boldsymbol{\varepsilon}^d) \quad (43)$$

where $\mathcal{W}_0(\boldsymbol{\varepsilon}^d)$ is a reference stored function, i.e. that for which $\psi(w) = 1$. Note that this expression is usually assumed in damage mechanics, but in usual theories $\mathcal{W}_0(\boldsymbol{\varepsilon}^d)$ is an undamaged stored energy. In our case, $\mathcal{W}_0(\boldsymbol{\varepsilon}^d)$ is a largely damaged one. In the infinitesimal case, both can be determined the same way, but in the nonlinear case the undamaged energy cannot be determined from experiments, whereas a largely damaged one can be obtained from stress-strain data.

The deviatoric power strain energy rate is

$$\boldsymbol{\sigma}^{|d} : \dot{\boldsymbol{\varepsilon}}^d = \mathcal{P}^d = \dot{W}(\boldsymbol{\varepsilon}^d, w) = \left. \frac{\partial W(\boldsymbol{\varepsilon}^d, w)}{\partial \boldsymbol{\varepsilon}^d} \right|_{\dot{w}=0} : \dot{\boldsymbol{\varepsilon}}^d + \left. \frac{\partial W(\boldsymbol{\varepsilon}^d, w)}{\partial w} \right|_{\dot{\boldsymbol{\varepsilon}}=0} \dot{w} \quad (44)$$

where

$$\left. \frac{\partial W(\boldsymbol{\varepsilon}^d, w)}{\partial \boldsymbol{\varepsilon}^d} \right|_{\dot{w}=0} = {}^{tr}\boldsymbol{\sigma}^{|d} \quad (45)$$

and

$$\left. \frac{\partial W(\boldsymbol{\varepsilon}^d, w)}{\partial w} \right|_{\dot{\boldsymbol{\varepsilon}}=0} = \frac{d\psi}{dw}\mathcal{W}_0(\boldsymbol{\varepsilon}^d) = -\gamma \quad (46)$$

During damage evolution $\dot{w} = \dot{W}$ so

$$\dot{f} := \dot{W} - \dot{w} = {}^{tr}\boldsymbol{\sigma}^{|d} : \dot{\boldsymbol{\varepsilon}}^d - \gamma \frac{dw}{d\varepsilon^d} : \dot{\boldsymbol{\varepsilon}}^d - \frac{dw}{d\varepsilon^d} : \dot{\boldsymbol{\varepsilon}}^d = 0 \quad (47)$$

i.e.

$$\boldsymbol{\sigma}^{|d} = \frac{dw}{d\varepsilon^d} = \frac{1}{1+\gamma} {}^{tr}\boldsymbol{\sigma}^{|d} \quad (48)$$

From this tensor, the complete stress tensor can be rebuilt

$$\boldsymbol{\sigma} = p\mathbf{I} + \boldsymbol{\sigma}^{|d} : \mathbb{P}^d \quad \text{with} \quad p = \frac{d\mathcal{U}}{d\varepsilon^v} \quad (49)$$

3.2 Numerical algorithm

The purpose of the numerical algorithm is to simply compute the value of ${}^{t+\Delta t}\psi$ such that

$$f = \mathcal{W} - w_D = 0 \quad (50)$$

The trial function is

$${}^{tr}f = {}^t\psi \mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\varepsilon}^d) - {}^tw_D({}^t\psi) \quad (51)$$

If ${}^{tr}f > 0$, there is damage evolution. With $f^{(0)} = {}^{tr}f$ the iterations are started with the objective of reaching ${}^{t+\Delta t}f = 0$. Then

$$f^{(i+1)} = f^{(i)} + \frac{\partial f^{(i)}}{\partial \psi^{(i)}} (\psi^{(i+1)} - \psi^{(i)}) \rightarrow 0 \quad (52)$$

gives

$$\psi^{(i+1)} = \psi^{(i)} - \frac{f^{(i)}}{df^{(i)}/d\psi^{(i)}} \quad (53)$$

where

$$\frac{\partial f^{(i)}}{\partial \psi^{(i)}} = \mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\varepsilon}^d) - \frac{dw_D^{(i)}}{d\psi^{(i)}} \quad (54)$$

Once convergence has been obtained and ${}^{t+\Delta t}\psi$ has been determined, we have

$${}^{t+\Delta t}\boldsymbol{\sigma}^{|d} = {}^{t+\Delta t}\psi \frac{d\mathcal{W}_0(\boldsymbol{\varepsilon}^d)}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} = {}^{t+\Delta t}\psi {}^{t+\Delta t}\boldsymbol{\sigma}_0^{|d} \quad (55)$$

and

$${}^{t+\Delta t}\boldsymbol{\sigma} = {}^{t+\Delta t}p \mathbf{I} + {}^{t+\Delta t}\boldsymbol{\sigma}^{|d} : \mathbb{P}^d \quad \text{with} \quad {}^{t+\Delta t}p = \frac{d{}^{t+\Delta t}\mathcal{U}}{d{}^{t+\Delta t}\varepsilon^v} \quad (56)$$

The tangent modulus is obtained from the derivative of the stresses. From the derivative of ${}^{t+\Delta t}\boldsymbol{\sigma}^{|d}$

$$\frac{d{}^{t+\Delta t}\boldsymbol{\sigma}^{|d}}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} = {}^{t+\Delta t}\psi \frac{d^2\mathcal{W}_0(\boldsymbol{\varepsilon}^d)}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} + {}^{t+\Delta t}\boldsymbol{\sigma}_0^{|d} \otimes \frac{d{}^{t+\Delta t}\psi}{d{}^{t+\Delta t}w_D} \frac{d{}^{t+\Delta t}w_D}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} \quad (57)$$

and from the consistency condition

$$\frac{d{}^{t+\Delta t}f}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} = 0 = {}^{t+\Delta t}\psi \frac{d\mathcal{W}_0(\boldsymbol{\varepsilon}^d)}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} + \mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\varepsilon}^d) \frac{d{}^{t+\Delta t}\psi}{d{}^{t+\Delta t}w_D} \frac{d{}^{t+\Delta t}w_D}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} - \frac{d{}^{t+\Delta t}w_D}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} \quad (58)$$

we can factor-out

$$\frac{d{}^{t+\Delta t}w_D}{d{}^{t+\Delta t}\boldsymbol{\varepsilon}^d} = \frac{{}^{t+\Delta t}\psi}{1 - \mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\varepsilon}^d) \frac{d{}^{t+\Delta t}\psi}{d{}^{t+\Delta t}w_D}} {}^{t+\Delta t}\boldsymbol{\sigma}_0^{|d} \quad (59)$$

which does not differ from the continuum set-up. Then —c.f. Eq. (38)

$$\mathbb{C}^{|d} = \frac{d^{t+\Delta t} \boldsymbol{\sigma}^{|d}}{d^{t+\Delta t} \boldsymbol{\epsilon}^d} = {}^{t+\Delta t}\psi \mathbb{C}_0^{|d} + \frac{\mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\epsilon}^d) {}^{t+\Delta t}\psi \frac{d^{t+\Delta t}\psi}{d^{t+\Delta t} w_D}}{1 - \mathcal{W}_0({}^{t+\Delta t}\boldsymbol{\epsilon}^d) \frac{d^{t+\Delta t}\psi}{d^{t+\Delta t} w_D}} {}^{t+\Delta t}\boldsymbol{\sigma}_0^{|d} \otimes {}^{t+\Delta t}\boldsymbol{\sigma}_0^{|d} \quad (60)$$

The full tangent is recovered as

$$\mathbb{C} = K \mathbf{I} \otimes \mathbf{I} + \mathbb{P}^d : \mathbb{C}^{|d} : \mathbb{P}^d \quad (61)$$

4 Anisotropic WYPIWYG damage mechanics

Orthotropic damage may be described by six independent damage variables. We restrict our formulation to the case in which the symmetry planes remain fixed during all the deformation. This is of course a simplifying hypothesis because damage is known to usually develop fully anisotropic behaviour. However, making this hypothesis will allow us to develop a tractable formulation and a procure to determine the behaviour of a damaged material. Then we will consider that the stored energy function may be written as

$$\mathcal{W} = \mathcal{U}(J) + \mathcal{W}^d(\mathbf{E}^d, \mathbf{w}_D) \quad (62)$$

where $\mathcal{U}(J)$ is a volumetric stored energy component which we consider merely as a penalty function because our formulation is for incompressible materials. For the isochoric component we consider a decomposition similar to the Valanis-Landel decomposition. This decomposition has been already used successfully in orthotropic hyperelasticity, see [77] and only neglects one anisotropic invariant

$$\begin{aligned} \mathcal{W}^{or}(\mathbf{E}^d, \mathbf{w}_D) = & \omega_1(E_{11}^d, w_{1D}) + \omega_2(E_{22}^d, w_{2D}) + \omega_3(E_{33}^d, w_{3D}) \\ & + \omega_4(E_{12}^d, w_{4D}) + \omega_5(E_{13}^d, w_{5D}) + \omega_6(E_{23}^d, w_{6D}) \end{aligned} \quad (63)$$

where $\mathbf{w}_D$ is the array of damage variables and

$$E_{ij}^d = \mathbf{a}_i \cdot \mathbf{E}^d \cdot \mathbf{a}_j \quad (64)$$

are the components of the isochoric logarithmic strains in the principal material directions of orthotropy $\mathbf{a}_i$. In order to preserve the material-symmetry consistency [20], we add an isotropic contribution

$$\mathcal{W}^d(\mathbf{E}^d, \mathbf{w}_D) = \mathcal{W}^{is}(\mathbf{E}^d, w_{0D}) + \mathcal{W}^{or}(\mathbf{E}^d, \mathbf{w}_D) \quad (65)$$

such that

$$\mathcal{W}^{is}(\mathbf{E}^d, w_{0D}) = \omega_0(E_1^d, w_{0D}) + \omega_0(E_2^d, w_{0D}) + \omega_0(E_3^d, w_{0D}) \quad (66)$$

where E_i^d are the principal isochoric strains.

The energy rate is

$$\dot{\mathcal{W}}^d = \dot{\mathcal{W}}^{is} + \dot{\mathcal{W}}^{or} = \left(\frac{\partial \mathcal{W}^{is}}{\partial \mathbf{E}^d} \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} + \sum_{i=1}^6 \frac{\partial \mathcal{W}^{or}}{\partial \mathbf{E}^d} \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} + \frac{\partial \mathcal{W}^{is}}{\partial w_{0D}} \frac{\partial w_{0D}}{\partial \mathbf{E}} + \sum_{i=1}^6 \frac{\partial \mathcal{W}^{or}}{\partial w_{iD}} \frac{\partial w_{iD}}{\partial \mathbf{E}} \right) : \dot{\mathbf{E}} \quad (67)$$

We note now that we can work either with $\mathcal{W}$ and w_D or with W and w (speaking generically, not of a particular component).

Then, the deviatoric stress tensor may be split into two parts, the trial one and the energy release rate

$$\mathbf{T}^d = {}^{tr}\mathbf{T}^d - \mathbf{Y} \quad (68)$$

where the trial stress is defined as the energy variation with the damage frozen

$${}^{tr}\mathbf{T}^d = \sum_{i=0}^6 {}^{tr}\mathbf{T}_i^d \quad (69)$$

and the energy release rate is defined as the energy decrease due to damage evolution

$$\mathbf{Y} = -\frac{\partial \mathcal{W}^{is}}{\partial w_{0D}} \frac{\partial w_{0D}}{\partial \mathbf{E}} - \sum_{i=1}^6 \frac{\partial \mathcal{W}^{or}}{\partial w_{iD}} \frac{\partial w_{iD}}{\partial \mathbf{E}} = -\sum_{i=0}^6 \frac{\partial \mathcal{W}^d}{\partial w_{iD}} \frac{\partial w_{iD}}{\partial \mathbf{E}} \quad (70)$$

$$= \mathbf{Y}^{is} + \sum_{i=1}^6 \mathbf{Y}_i^{or} = \sum_{i=0}^6 \mathbf{Y}_i = \sum_{i=0}^6 \gamma_i \mathbf{D}_i \quad (71)$$

where the energy loss factors are

$$\gamma_i = -\frac{\partial \mathcal{W}^d}{\partial w_{iD}} \quad (72)$$

i.e.

$$\gamma_0 = -\frac{\partial \mathcal{W}^{iso}}{\partial w_{0D}} \text{ and } \gamma_i = -\frac{\partial \omega_i}{\partial w_{iD}} \text{ with } i = 1, \dots, 6 \quad (73)$$

Then, we assume that different damage criteria may be established

$$\begin{cases} f_0 = \mathcal{W}^{iso}(\mathbf{E}^d, w_{0D}) - w_{0D} \leq 0 \\ f_i = \omega_i(E_{kl}^d, w_{iD}) - w_{iD} \leq 0 \text{ with } i = 1, \dots, 6 \end{cases} \quad (74)$$

where (k, l) are the indices corresponding to the Voigt indices i , i.e. $i = 1, \dots, 6$ correspond to $(k, l) = (1, 1), (2, 2), \dots, (2, 3)$. The damage variables are

$$\begin{cases} w_{0D}(t) = \max_{\tau \in (-\infty, t]} [\mathcal{W}^{iso}(\mathbf{E}^d(\tau), w_{0D}(\tau))] \\ w_{iD}(t) = \max_{\tau \in (-\infty, t]} [\omega_i(E_{kl}^d(\tau), w_{iD}(\tau))] \text{ with } i = 1, \dots, 6 \end{cases} \quad (75)$$

Then, during damage evolution $\dot{w}_{iD} > 0$ with $\dot{\mathbf{E}} \neq 0$ and $f_i = 0$ we must have $\dot{f}_i = 0$, so

$$\frac{\partial \omega_i(E_{kl}^d, w_{iD})}{\partial \mathbf{E}} + \frac{\partial \omega_i(E_{kl}^d, w_{iD})}{\partial w_{iD}} \frac{\partial w_{iD}}{\partial \mathbf{E}} - \frac{\partial w_{iD}}{\partial \mathbf{E}} = \mathbf{0} \quad (76)$$

i.e.

$$\mathbf{D}_i = \frac{\partial w_{iD}}{\partial \mathbf{E}} = {}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i \quad (77)$$

and in a similar way

$$\mathbf{D}_0 = \frac{\partial \mathcal{W}^{iso}}{\partial \mathbf{E}} = {}^{tr}\mathbf{T}_0^d - \mathbf{Y}_0$$

Since for example

$$\frac{\partial \omega_i(E_{kl}^d, w_{iD})}{\partial w_{iD}} \frac{\partial w_{iD}}{\partial \mathbf{E}} = -\gamma_i(\mathbf{E}) ({}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i) = -\mathbf{Y}_i \Rightarrow \gamma_i(\mathbf{E}) ({}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i) = \mathbf{Y}_i \quad (78)$$

where $\gamma_i(\mathbf{E})$ is a scalar function, we have for $i = 0, \dots, 6$

$$\mathbf{Y}_i = \frac{\gamma_i}{1 + \gamma_i} {}^{tr}\mathbf{T}_i^d \Rightarrow \mathbf{T}_i^d = {}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i \Rightarrow \mathbf{D}_i = \mathbf{T}_i^d = \frac{1}{1 + \gamma_i} {}^{tr}\mathbf{T}_i^d \quad (79)$$

We recall that the damage variables are increasing functions, so $\dot{w}_{iD} \geq 0$. During damage evolution, the derivative of the damage criterion then gives

$$\dot{f}_i = \left({}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i - \frac{\partial w_{iD}}{\partial \mathbf{E}} \right) : \dot{\mathbf{E}} = 0 \Rightarrow ({}^{tr}\mathbf{T}_i^d - \mathbf{Y}_i) : \dot{\mathbf{E}} > 0 \Rightarrow \mathbf{T}_i^d : \dot{\mathbf{E}} > 0 \quad (80)$$

so

$$\mathbf{N}_i : \dot{\mathbf{E}} > 0 \text{ with } \mathbf{N}_i = \frac{{}^{tr}\mathbf{T}_i^d}{\|{}^{tr}\mathbf{T}_i^d\|} = \frac{\mathbf{Y}_i}{\|\mathbf{Y}_i\|} = \frac{\mathbf{T}_i^d}{\|\mathbf{T}_i^d\|} = \frac{\mathbf{D}_i}{\|\mathbf{D}_i\|} \quad (81)$$

which is a stability condition (i.e. the system gets energy). This condition may also be easily recognized as the normality rule of plasticity and implies that the damage evolution variable i is active only if $\mathbf{T}_i^d : \dot{\mathbf{E}} > 0$. The formulation is similar to that of multisurface plasticity.

5 Practical implementation

5.1 Computation of stresses

For the case of isotropic damage, we have seen that damaged stored energy functions (and hence their strain derivatives, the stresses) must be proportional [Miñano & Montáns]. Hence, for the isotropic component we must have

$$\mathcal{W}^{is}(\mathbf{E}^d, w_{0D}) = \psi_0(w_{0D}) \hat{\mathcal{W}}^{is}(\mathbf{E}^d) \quad (82)$$

which results into

$$\omega_0(\mathbf{E}^d, w_{0D}) \equiv \omega_{0D}(\mathbf{E}^d) = \psi_0(w_{0D}) \hat{\omega}_0(\mathbf{E}^d) \quad (83)$$

where $\hat{\omega}_0(\mathbf{E}^d)$ is a reference hyperelastic function for a given damage level and ψ_0 is the scaling function which is $\psi_0 = 1$ for the reference damage state and ω_{0D} is the hyperelastic function for a given (fixed) damage w_{0D} .

In this formulation, we proceed in a similar way with the orthotropic functions

$$\omega_i(\mathbf{E}^d, w_{iD}) \equiv \omega_{iD}(\mathbf{E}^d) = \psi_i(w_{iD}) \hat{\omega}_i(\mathbf{E}^d) \quad (84)$$

which obviously brakes the proportionality of the global stored energy for the general case of orthotropy. In Equation (84) the functions $\hat{\omega}_i(\mathbf{E}^d)$ are the hyperelastic functions of the Valanis-Landel-type decomposition for a reference damage, whereas the functions $\psi_i(w_{iD})$ are the corresponding scaling functions.

The main task of the local iterative algorithm is to determine the scaling factors ψ_i , because once determined, the stresses are computed as in non-damaged hyperelasticity, simply by derivation of the strain energy $\mathcal{W}^d(\mathbf{E}^d, \mathbf{w}_D) = \mathcal{W}_D^d(\mathbf{E}^d)$

$$\mathbf{T}^d = \frac{\partial \mathcal{W}_D^d(\mathbf{E}^d)}{\partial \mathbf{E}} = \psi_0(w_{0D}) \frac{\partial \hat{\mathcal{W}}^{is}(\mathbf{E}^d)}{\partial \mathbf{E}} + \sum_{i=1}^6 \psi_i(w_{iD}) \frac{\partial \hat{\omega}_i(\mathbf{E}^d)}{\partial \mathbf{E}} \quad (85)$$

where

$$\mathbf{T}^{is} \equiv \mathbf{T}_0^d = \frac{\partial \mathcal{W}_D^{is}(\mathbf{E}^d)}{\partial \mathbf{E}^d} = \sum_{j=1}^3 \psi_0(w_{0D}) \frac{\partial \hat{\omega}_0}{\partial E_j^d} \frac{\partial E_j^d}{\partial \mathbf{E}} \quad (86)$$

and

$$\frac{\partial \hat{\omega}_i(\mathbf{E}^d)}{\partial \mathbf{E}} = \frac{\partial \hat{\omega}_i}{\partial E_{kl}^d} \frac{\partial E_{kl}^d}{\partial \mathbf{E}^d} : \frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} \quad (\text{no sum}) \quad (87)$$

where E_{kl}^d are the strain components corresponding to the strain energy components $\hat{\omega}_i$. We note that taking into account symmetries

$$E_{kl}^d = \frac{1}{2} (\mathbf{a}_k \cdot \mathbf{E}^d \cdot \mathbf{a}_l + \mathbf{a}_k \cdot \mathbf{E}^d \cdot \mathbf{a}_l) = \frac{1}{2} (\mathbf{a}_k \otimes \mathbf{a}_l + \mathbf{a}_l \otimes \mathbf{a}_k) : \mathbf{E}^d \quad (88)$$

so

$$\frac{\partial E_{kl}^d}{\partial \mathbf{E}^d} = \frac{1}{2} (\mathbf{a}_k \otimes \mathbf{a}_l + \mathbf{a}_l \otimes \mathbf{a}_k) \quad (89)$$

and

$$\frac{\partial \mathbf{E}^d}{\partial \mathbf{E}} = \mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} =: \mathbb{P}^d \quad (90)$$

is the deviatoric projector tensor, with $\mathbb{I}$ and $\mathbf{I}$ being the fourth-order and second order identity tensors.

Assume that we know the function $\psi_i(w_{iD})$, or conversely $w_{iD}(\psi_i)$. The strains at $t + \Delta t$, namely ${}^{t+\Delta t}\mathbf{E}$ and the values of the multiplier functions ${}^t\psi_i$ allow for the computation of the components of the trial stresses

$${}^{tr}\mathbf{T}_0^d = {}^t\psi_0(w_{0D}) \frac{\partial \hat{\mathcal{W}}^{is}({}^{t+\Delta t}\mathbf{E}^d)}{\partial \mathbf{E}} = {}^t\psi_0(w_{0D}) \hat{\mathbf{T}}_0^d \quad (91)$$

and

$${}^{tr}\mathbf{T}_i^d = {}^t\psi_i(w_{iD}) \frac{\partial \hat{\omega}_i({}^{t+\Delta t}\mathbf{E}^d)}{\partial \mathbf{E}} = {}^t\psi_i(w_{iD}) \hat{\mathbf{T}}_i^d \quad (92)$$

so

$${}^{tr}\mathbf{T}^d = \sum_{i=0}^6 {}^{tr}\mathbf{T}_i^d = {}^{tr}\mathbf{T}_0^d + \sum_{i=1}^6 {}^{tr}\mathbf{T}_i^d = \sum_{i=0}^6 {}^t\psi_i \hat{\mathbf{T}}_i^d = {}^t\psi_0 \hat{\mathbf{T}}_0^d + \sum_{i=1}^6 {}^t\psi_i \hat{\mathbf{T}}_i^d \quad (93)$$

In case of no damage progress, these stresses are the actual stresses, i.e. ${}^{t+\Delta t}\mathbf{T}^d = {}^{tr}\mathbf{T}^d$. However, damage progress will happen if any of the damage criteria is not satisfied, i.e. ${}^{tr}f_i > 0$. These damage criteria may be written as

$${}^{tr}f_0 := {}^t\psi_0 \hat{\mathcal{W}}^{is}({}^{t+\Delta t}\mathbf{E}^d) - w_{0D} \quad (94)$$

and for $i > 0$

$${}^{tr}f_i := {}^t\psi_i \hat{\omega}_i({}^{t+\Delta t}\mathbf{E}^d) - w_{iD} \quad (95)$$

If any of ${}^{tr}f_i > 0$, the computation of the new ${}^{t+\Delta t}\psi_i$ must be performed, otherwise ${}^{t+\Delta t}\psi = {}^t\psi$. For the computation of the new multiplier, a Newton-Raphson algorithm is used:

$${}^{t+\Delta t}f_i = {}^t f_i + \frac{\partial {}^t f_i}{\partial {}^t\psi_i} ({}^{t+\Delta t}\psi_i - {}^t\psi_i) \longrightarrow 0 \quad (96)$$

so

$${}^{t+\Delta t}\psi_i = {}^t\psi_i - \left(\frac{\partial {}^t f_i}{\partial {}^t\psi_i} \right)^{-1} {}^t f_i \quad (97)$$

where

$$\frac{\partial {}^t f_i}{\partial {}^t\psi_i} = \hat{\omega}_i({}^{t+\Delta t}\mathbf{E}^d) - \frac{\partial w_{iD}}{\partial {}^t\psi_i} \quad (98)$$

Once the solution for the ${}^{t+\Delta t}\psi_i$ has been attained, the corresponding stresses are readily obtained as

$${}^{t+\Delta t}\mathbf{T}^d = {}^{t+\Delta t}\mathbf{T}^v + \sum_{i=0}^6 {}^{t+\Delta t}\psi_i \hat{\mathbf{T}}_i^d \quad (99)$$

where ${}^{t+\Delta t}\mathbf{T}^v = \partial \mathcal{U}(J) / \partial {}^{t+\Delta t}\mathbf{E}$ is the volumetric component obtained from the penalty function (or more precisely from a separate interpolation in a finite element mixed formulation).

5.2 Computation of the algorithmic tangent moduli

The algorithmic tangent moduli for the global Newton procedure may be easily obtained from Eq. (99)

$$\frac{\partial^{t+\Delta t}\mathbf{T}^d}{\partial^{t+\Delta t}\mathbf{E}} = \sum_{i=0}^6 \left({}^{t+\Delta t}\psi_i \frac{\partial^{t+\Delta t}\hat{\mathbf{T}}_i^d}{\partial^{t+\Delta t}\mathbf{E}} + {}^{t+\Delta t}\hat{\mathbf{T}}_i^d \otimes \frac{\partial {}^{t+\Delta t}\psi_i}{\partial^{t+\Delta t}w_{iD}} \frac{\partial^{t+\Delta t}w_{iD}}{\partial^{t+\Delta t}\mathbf{E}} \right) \quad (100)$$

In order to compute $\partial^{t+\Delta t}w_{iD}/\partial^{t+\Delta t}\mathbf{E}$ we use the fact that the damage criterion f_i and its rate $\dot{f}_i$ must vanish if there is damage evolution $\dot{w}_{iD} > 0$. Then, for $i > 0$

$$\dot{f}_i = \frac{\partial f_i}{\partial \mathbf{E}} : \dot{\mathbf{E}} = 0 \Rightarrow \frac{\partial^{t+\Delta t}f_i}{\partial^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi_i {}^{t+\Delta t}\hat{\mathbf{T}}_i^d + {}^{t+\Delta t}\hat{\omega}_i \frac{\partial {}^{t+\Delta t}\psi_i}{\partial^{t+\Delta t}w_{iD}} \frac{\partial^{t+\Delta t}w_{iD}}{\partial^{t+\Delta t}\mathbf{E}} - \frac{\partial^{t+\Delta t}w_{iD}}{\partial^{t+\Delta t}\mathbf{E}} = \mathbf{0} \quad (101)$$

so

$$\frac{\partial^{t+\Delta t}w_{iD}}{\partial^{t+\Delta t}\mathbf{E}} = \frac{{}^{t+\Delta t}\psi_i \frac{\partial^{t+\Delta t}w_{iD}}{\partial {}^{t+\Delta t}\psi_i}}{\frac{\partial^{t+\Delta t}w_{iD}}{\partial {}^{t+\Delta t}\psi_i} - {}^{t+\Delta t}\hat{\omega}_i} {}^{t+\Delta t}\hat{\mathbf{T}}_i^d \quad (102)$$

Therefore, taking a similar expression for $i = 0$, Eq. (100) yields

$$\begin{aligned} \frac{\partial^{t+\Delta t}\mathbf{T}^d}{\partial^{t+\Delta t}\mathbf{E}} &= \sum_{i=0}^6 \frac{\partial^{t+\Delta t}\mathbf{T}_i^d}{\partial^{t+\Delta t}\mathbf{E}} \\ &= {}^{t+\Delta t}\psi_0 \frac{\partial^{t+\Delta t}\hat{\mathbf{T}}_0^d}{\partial^{t+\Delta t}\mathbf{E}} + \frac{{}^{t+\Delta t}\psi_0}{\frac{\partial^{t+\Delta t}w_{0D}}{\partial {}^{t+\Delta t}\psi_0} - {}^{t+\Delta t}\hat{\omega}_0^{is}} {}^{t+\Delta t}\hat{\mathbf{T}}_0^d \otimes {}^{t+\Delta t}\hat{\mathbf{T}}_0^d \\ &\quad + \sum_{i=1}^6 \left({}^{t+\Delta t}\psi_i \frac{\partial^{t+\Delta t}\hat{\mathbf{T}}_i^d}{\partial^{t+\Delta t}\mathbf{E}} + \frac{{}^{t+\Delta t}\psi_i}{\frac{\partial^{t+\Delta t}w_{iD}}{\partial {}^{t+\Delta t}\psi_i} - {}^{t+\Delta t}\hat{\omega}_i} {}^{t+\Delta t}\hat{\mathbf{T}}_i^d \otimes {}^{t+\Delta t}\hat{\mathbf{T}}_i^d \right) \end{aligned} \quad (103)$$

(104)

i.e.

$$\begin{aligned} \mathbb{C} &= \mathbb{C}^v + \mathbb{C}^d = \mathbb{C}^v + \mathbb{C}^{is} + \mathbb{C}^{or} \\ &= \frac{\partial^2 \mathcal{U}}{\partial \mathbf{E} \partial \mathbf{E}} + \frac{\partial^{t+\Delta t}\mathbf{T}^d}{\partial^{t+\Delta t}\mathbf{E}} \end{aligned} \quad (105)$$

5.3 Algorithm

Then the following computational procedure may be established:

1. For ${}^{t+\Delta t}\mathbf{E}^d$ compute ${}^{t+\Delta t}\hat{\mathcal{W}}^{is} \left({}^{t+\Delta t}E_1^{iso}, {}^{t+\Delta t}E_2^{iso}, {}^{t+\Delta t}E_3^{iso} \right)$ and ${}^{t+\Delta t}\hat{\omega}_i \left({}^{t+\Delta t}\mathbf{E}^d \right)$, $i = 1, \dots, 6$
2. Compute ${}^{tr}f_0 = {}^{t+\Delta t}\hat{\mathcal{W}}^{is} {}^t\psi_0 - {}^tw_{0D} ({}^t\psi_0)$
3. If ${}^{tr}f_0 \leq 0$, no further isotropic damage:
 - (a) ${}^{t+\Delta t}\psi_0 = {}^t\psi_0$; ${}^{t+\Delta t}\mathbf{T}_0^d = {}^{t+\Delta t}\psi_0 {}^{t+\Delta t}\hat{\mathbf{T}}_0^d$
 - (b) $\frac{\partial {}^{t+\Delta t}\mathbf{T}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi_0 \frac{\partial {}^{t+\Delta t}\hat{\mathbf{T}}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}}$
4. If ${}^{tr}f_0 > 0$, there is isotropic damage evolution:
 - (a) ${}^{t+\Delta t}f_0^{(0)} = {}^{tr}f_0$; ${}^{t+\Delta t}\psi_0^{(0)} = {}^t\psi_0$
 - (b) Do while $\left| {}^{t+\Delta t}f_0^{(k)} \right| > \text{tolerance}$
 - i. $\partial {}^{t+\Delta t}f_0^{(k)} / \partial {}^{t+\Delta t}\psi_0^{(k)} = {}^{t+\Delta t}\hat{\mathcal{W}}^{is} - \partial w_{0D} / \partial {}^{t+\Delta t}\psi_0^{(k)}$
 - ii. ${}^{t+\Delta t}\psi_0^{(k+1)} = {}^{t+\Delta t}\psi_0^{(k)} - {}^{t+\Delta t}f_0^{(k)} / \left[\partial {}^{t+\Delta t}f_0^{(k)} / \partial {}^{t+\Delta t}\psi_0^{(k)} \right]$
 - iii. ${}^{t+\Delta t}f_0^{(k+1)} = {}^{t+\Delta t}\hat{\mathcal{W}}^{is} {}^{t+\Delta t}\psi_0^{(k+1)} - w_{0D} \left({}^{t+\Delta t}\psi_0^{(k+1)} \right)$
 - iv. $k \leftarrow k + 1$
 - (c) $\frac{\partial {}^{t+\Delta t}\mathbf{T}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi_0 \frac{\partial {}^{t+\Delta t}\hat{\mathbf{T}}_0^d}{\partial {}^{t+\Delta t}\mathbf{E}} + \frac{{}^{t+\Delta t}\psi_0}{\frac{\partial {}^{t+\Delta t}w_{0D}}{\partial {}^{t+\Delta t}\psi_0} - {}^{t+\Delta t}\hat{\mathcal{W}}^{is}} {}^{t+\Delta t}\hat{\mathbf{T}}_0^d \otimes {}^{t+\Delta t}\hat{\mathbf{T}}_0^d$
5. ${}^{tr}f_i = {}^{t+\Delta t}\hat{\omega}_i {}^t\psi_i - {}^tw_{iD} ({}^t\psi_i)$, $i = 1, \dots, 6$
6. For $i = 1, \dots, 6$
 - (a) if ${}^{tr}f_i \leq 0$ no damage progress on i^{th} -component:
 - i. ${}^{t+\Delta t}\psi_i = {}^t\psi_i$; ${}^{t+\Delta t}\mathbf{T}_i^d = {}^{t+\Delta t}\psi_i {}^{t+\Delta t}\hat{\mathbf{T}}_i^d$
 - ii. $\frac{\partial {}^{t+\Delta t}\mathbf{T}_i^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi_i \frac{\partial {}^{t+\Delta t}\hat{\mathbf{T}}_i^d}{\partial {}^{t+\Delta t}\mathbf{E}}$
 - (b) if ${}^{tr}f_i > 0$, damage progress on i^{th} -component
 - i. ${}^{t+\Delta t}f_i^{(0)} = {}^{tr}f_i$; ${}^{t+\Delta t}\psi_i^{(0)} = {}^t\psi_i$
 - ii. Do while $\left| {}^{t+\Delta t}f_i^{(k)} \right| > \text{tolerance}$
 - A. if $i > 0$ then $\partial {}^{t+\Delta t}f_i^{(k)} / \partial {}^{t+\Delta t}\psi_i^{(k)} = {}^{t+\Delta t}\hat{\omega}_i - \partial w_{iD} / \partial {}^{t+\Delta t}\psi_i^{(k)}$
 - B. ${}^{t+\Delta t}\psi_i^{(k+1)} = {}^{t+\Delta t}\psi_i^{(k)} - {}^{t+\Delta t}f_i^{(k)} / \left[\partial {}^{t+\Delta t}f_i^{(k)} / \partial {}^{t+\Delta t}\psi_i^{(k)} \right]$
 - C. ${}^{t+\Delta t}f_i^{(k+1)} = {}^{t+\Delta t}\hat{\omega}_i {}^{t+\Delta t}\psi_i^{(k+1)} - w_{iD} \left({}^{t+\Delta t}\psi_i^{(k+1)} \right)$
 - D. $k \leftarrow k + 1$
 - iii. ${}^{t+\Delta t}\psi_i = {}^{t+\Delta t}\psi_i^{(k+1)}$; ${}^{t+\Delta t}\mathbf{T}_i^d = {}^{t+\Delta t}\psi_i {}^{t+\Delta t}\hat{\mathbf{T}}_i^d$
 - iv. $\frac{\partial {}^{t+\Delta t}\mathbf{T}_i^d}{\partial {}^{t+\Delta t}\mathbf{E}} = {}^{t+\Delta t}\psi_i \frac{\partial {}^{t+\Delta t}\hat{\mathbf{T}}_i^d}{\partial {}^{t+\Delta t}\mathbf{E}} + \frac{{}^{t+\Delta t}\psi_i}{\frac{\partial {}^{t+\Delta t}w_{iD}}{\partial {}^{t+\Delta t}\psi_i} - {}^{t+\Delta t}\hat{\omega}_i} {}^{t+\Delta t}\hat{\mathbf{T}}_i^d \otimes {}^{t+\Delta t}\hat{\mathbf{T}}_i^d$
7. ${}^{t+\Delta t}\mathbf{T}^d = \sum_{i=0}^6 {}^{t+\Delta t}\mathbf{T}_i^d$.

$$8. \mathbb{C} = \frac{\partial^2 \mathcal{U}}{\partial \mathbf{E} \partial \mathbf{E}} + \sum_{i=0}^6 \frac{\partial^{t+\Delta t} \mathbf{T}^d}{\partial^{t+\Delta t} \mathbf{E}}$$

5.4 Extraction of the information from experiments

The experimental data we need to get the functions corresponding to the Master damage curves and the Master hyperelastic curves are three uniaxial loading tests up to the maximum strain level to be attained in the simulations, performed in the three preferred directions of the material on three identical material samples. With these experimental data we can already obtain the energy functions corresponding to the Master damage curve in each preferred material direction, cf. [86]. On the other hand in order to obtain the energy functions corresponding to the Master hyperelastic curves, we need to load a simple sample to the maximum deformation expected in the simulations, for which the damage is maximum $\psi_i = 1$, in each of the three directions successively (one after another). Thereafter we have to reload uniaxially the same specimen, damaged to the maximum value under study, in each of the preferred material directions to the same maximum value of deformation and unload. That is, the damaged sample will be subjected to a load test and subsequent unloading in each direction successively. With these experimental data we are already able to obtain the functions corresponding to the Master hyperelastic curves, again see Ref. [86].

In the above-described procedure, the main information needed from experiments are the curves $w_{iD}(\psi_i)$, $\hat{w}_i(E_{kl}^d)$ and $^{iso}(\mathbf{E}^d)$. Unless there is some physical insight in the material being tested, it is difficult if not impossible to distinguish from uniaxial tests which part corresponds to the isotropic part and which one is the orthotropic contribution. If the nature of the material being tested is known, it could be the case that the isotropic contribution may be devised or determined (for example performing tests on the isolated matrix component or assuming that the behavior in one direction is mainly due to that component). We note that in any case, the hyperelastic orthotropic damaged curve should be below the isotropic counterpart so isotropic damage w_{0D} affects equally all directions whereas orthotropic damage w_{iD} affects only the corresponding direction. In fact, because the proposed isochoric orthotropic model is fully determined with six experimental curves, only six of the damage variables w_{iD} ($i = 0, \dots, 6$) are independent.

Now assume that we have determined the part that corresponds to isotropic behavior. To do so, we simply determine the unloading-reloading curve for isotropy (for example the lowest one among all directions) and the corresponding master damage curve. Following the procedure detailed in [90] we obtain the functions $\hat{\mathcal{W}}^{is}(\mathbf{E})$ (see [89], [86]) and $w_{0D}(\psi_0)$. With these data, we can determine the isochoric, isotropic contribution in the principal orthotropy directions, i.e. E_{kl} and

Fig. 4 Generation of a composite piecewise master damage hyperelastic curve.

perform the additive decomposition of Eq. (65):

$$\mathcal{W}^d = \mathcal{W}^{is} + \mathcal{W}^{or} \Rightarrow \mathcal{W}^{or} = \mathcal{W}^d - \mathcal{W}^{is} \quad (106)$$

which in terms of stresses is

$$\mathbf{T}^{or}(\mathbf{E}) = \frac{\partial \mathcal{W}}{\partial \mathbf{E}} - \frac{\partial \mathcal{W}^{is}}{\partial \mathbf{E}} = \mathbf{T}^d(\mathbf{E}) - \mathbf{T}^{is}(\mathbf{E}) \quad (107)$$

Since for the six needed experiments $\mathbf{T}^d(\mathbf{E})$ is known and $\mathbf{T}^{is}(\mathbf{E})$ can be determined, then six curves corresponding to $\mathbf{T}^{or}(\mathbf{E})$ may be obtained. Furthermore, from Eqs. (106) and (85)

$$\mathbf{T}^{or}(\mathbf{E}) = \sum_{i=1}^6 \psi_i(w_{iD}) \frac{\partial \hat{\omega}_i(\mathbf{E}^d)}{\partial \mathbf{E}} = \sum_{i=1}^6 \psi_i(w_{iD}) \hat{\mathbf{T}}_i^d(\mathbf{E}) \quad (108)$$

The functions $\hat{\omega}_i$ are then determined directly from the hyperelastic curve $\hat{\mathbf{T}}^d(\mathbf{E}) - \hat{\mathbf{T}}^{is}(\mathbf{E})$ assuming that both prescribed $\hat{\mathbf{T}}^d(\mathbf{E})$ and $\hat{\mathbf{T}}^{is}(\mathbf{E})$ curves correspond to the same level of damage. Then, the values of the multipliers ψ_i are obtained from the already known multipliers ψ_0 and the master damage curve for each direction

$$\psi_i = \frac{T^d - \psi_0 \hat{T}^{iso}}{\hat{T}_i^d} \quad (109)$$

where the unbold symbols imply that we are using the uniaxial values.

Fig. 5 (a) Virgin loading curve and unloading-reloading hyperelastic curve. (b) Definition of the trial stress state and the released energy rate. (c) Definition of the master hyperelastic curve. (d) Parallelism with the radial return algorithm of Wilkins in the stress space.

5.5 Examples

5.5.1 Isotropic material

The aim of this example is merely to show the capabilities of the spline-based damage model for isotropic hyperelastic materials presented in Ref. [90]. The material data needed is an experimental virgin loading curve and a damaged unloading-reloading curve which must be given up to the maximum value of strain that will be attained during the simulations. We evaluate our model using tensile test data on intraluminal venous thrombus extracted from Ref. [88]. Due to the absence of experimental data for the compression behavior, we have assumed the antisymmetric stress distribution $\tilde{\sigma}_i(-\tilde{E}_i) = -\tilde{\sigma}_i(\tilde{E}_i)$, as can be seen in Fig. 7.

with respect to N_i and N_j) are shown in Fig. 8a. The deformation imposed is depicted in Fig. 8b. The projection of the corresponding Hencky strain tensor $\mathbf{E}$ into the basis of the material preferred directions $\mathbf{X}_{pr} = \{e_i, e_j, e_k\}$ furnishes the

Fig. 6 Schematic representation of the discontinuum formulation with the definition of the trial state and the energy release rate.

pure shear state below

$$[\mathbf{E}]_{\mathbf{X}_{pr}} = \begin{bmatrix} 0 & E_i & 0 \\ E_i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (110)$$

The Generalized Kirchhoff stress tensor $\mathbf{T}$ can be derived from

$$\mathbf{T} = \frac{\partial \mathcal{W}}{\partial \mathbf{E}} + p \mathbf{I} \quad (111)$$

where the hydrostatic pressure p becomes zero due to the plane stress condition $\sigma_k = T_k = 0$, namely

$$0 = T_k = \omega'_{kk}(E_k) + p = \omega'_{kk}(0) + p = p \quad (112)$$

Therefore, the tensor $\mathbf{T}$ is simply

$$[\mathbf{T}]_{\mathbf{X}_{pr}} = \begin{bmatrix} 0 & \omega'_{ij}(E_i) & 0 \\ \omega'_{ij}(E_i) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Fig. 7 Experimental data from the virgin loading test and from the unloading-reloading test and initial uniform spline interpolation.

Fig. 8 Pure shear test in the plane $ij = 12$. **a** Representation of the reference configuration in principal strain basis $\{N_i, N_j, N_k\}$ with $(i \neq j \neq k)$ and e_i and e_j define the orientation of the material preferred directions. **b** Kinematics of deformation in the biaxial test and its associated principal stretches.

resulting a state of pure shear also in stresses, which implies that for this particular test, principal directions of stresses and strains are coincident and thus $\mathbf{E}$ and $\mathbf{T}$ commute as well as $\mathbf{T}$ is completely coincident with $\boldsymbol{\sigma}$, see [86] so the Cauchy

Fig. 9 Pure shear test prediction.

stress tensor expressed in the basis of principal stretches is

$$[\sigma]_{\mathbf{N}} = [\mathbf{T}]_{\mathbf{N}} = \begin{bmatrix} \omega'_{ij}(E_i) & 0 & 0 \\ 0 & -\omega'_{ij}(E_i) & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The results are shown in Fig. 9, once again it can be seen as the model accurately reproduces the experimental data for the shear stress T_{12} .

In order to illustrate the simulation capabilities of the presented orthotropic damage model, several numerical examples performed over a bidimensional plate with a concentric circular hole (similar to that of the isotropic example, see Fig. 10) made of a nearly incompressible orthotropic hyperelastic material in which the preferred material axes are not aligned with the test axes the plate is loaded about the x -axis. A value of $k = 30 \text{ MPa}$ has been selected to numerically enforce incompressibility. We have used fully integrated (3 x 3 Gauss integration) 9/3 u/p mixed finite elements. For the incremental (global) analysis, a Newton-Rapshon scheme, without line searches, is employed.

The function of the displacements imposed with the time and the instants selected to study are shown in Fig. 11.

Fig. 10 Rectangular plate with a concentric hole: reference configuration, initial orientation α of the preferred material directions and finite element mesh. Dimensions of the plate: $l_0 \times h_0 = 32 \times 16 \text{ mm}^2$. Radius of the hole: $r_0 = 4 \text{ mm}$.

Fig. 11 Prescribed uniaxial strain for the uniaxial test performed on the rectangular plate where are indicated the instants under study.

The results for principal direction orientation of $\alpha = 30^\circ$ are shown in Fig. 12 where α is the angle represented in Fig. 10 between the x -axis and the preferred material direction e_1 . We have selected an orientation for the preferred material of 30° as representative example, nevertheless the model works identically whatever the preferred orientation. In Fig. , the deformed configuration of the plate and the distribution of the computed deviatoric Cauchy stress norm for the different instants are depicted. For comparison purposes, the same computations have been performed using the orthotropic hyperelastic model, see Reference [86], the results are shown in Fig. 13. It can be observed as the results for both models are the same for the first two steps of loading and different for the steps of unloading and reloading. In the case of the orthotropic damage model, the unloading and the

reloading coincide for the same deformation, below the maximum reached before unloading. For the simply orthotropic hyperelastic model coincide the loading, the unloading and the reloading, because there is only one path.

The distributions of the damage variable ψ_1 (damage variable associated with the preferred material direction e_1) for the different times are shown in Fig. 14, where we can see that the most damaged areas are those that sustain more stress and that once a value of damage is reached, it can not heal even we unload completely.

6 Conclusions

In this work we have developed a WYPIWYG model for damage mechanics in anisotropic materials. The model uses the WYPIWYG approach in which no apriori analytical functions are given, no material parameters are employed in the formulation and the experimental data are exactly captured. The model is built upon the isotropic model which may be thought of as the isotropic matrix in composite materials as, for example, biological tissues. The model is capable of capturing the behavior in six experiments showing the Mullins effect. The model is amenable for modelling damage-induced anisotropy.

We have also developed a very efficient computational algorithm. The local algorithm entails mainly scalar iterations which are easily solved with a Newton-Raphson algorithm. The algorithm has been linearized in order to preserve the second order convergence of Newton algorithms. The number of iterations employed are similar to those employed for a hyperelastic model.

The present model does not include a permanent set, typically found in materials exhibiting the Mullins effect. This extension is currently under progress.

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Fig. 12 Uniaxial tension of a rectangular plate with a concentric circular hole under a plain strain condition using the orthotropic hyperelastic damage model: Deformed configuration (length = 45mm) and distributions of $\|\sigma^d\|$ (MPa) at instants, from top to bottom, $t = 10\text{ s}$, $t = 20\text{ s}$, $t = 30\text{ s}$ and $t = 50\text{ s}$.

Fig. 13 Uniaxial tension of a rectangular plate with a concentric circular hole under a plain strain condition using the orthotropic hyperelastic model: Deformed configuration (length = 45 mm) and distributions of $\|\sigma^d\|$ (MPa) at instants, from top to bottom, $t = 10\text{ s}$, $t = 20\text{ s}$, $t = 30\text{ s}$ and $t = 50\text{ s}$.

Fig. 14 Distributions of the damage variable ψ_1 associated with the preferred direction e_1 for the instants, from top to bottom, $t = 10\text{ s}$, $t = 20\text{ s}$, $t = 30\text{ s}$ and $t = 50\text{ s}$.

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Capítulo 6

Conclusiones

Para poder plantear un nuevo enfoque en la mecánica del daño continuo, primero se ha llevado a cabo una revisión exhaustiva de los modelos y formulaciones existentes en la literatura relativa a la mecánica del daño. Para hacer la revisión un poco más breve, se ha centrado en la mecánica del daño continuo, puesto que es el enfoque más empleado en la mecánica computacional.

Al haber encontrado bastantes similitudes con los clásicos algoritmos de plasticidad, se ha realizado un análisis comparativo de distintos algoritmos para elastoplasticidad anisótropa en pequeñas deformaciones, a fin de tener una idea sobre cuál es la mejor implementación numérica. Los algoritmos en pequeñas deformaciones se usan con frecuencia como el único ingrediente iterativo de algoritmos en grandes deformaciones basados en deformaciones logarítmicas. Las deformaciones logarítmicas han sido las empleadas en esta tesis debido a sus propiedades especiales, tales como la ausencia de cambio de métrica en operaciones de empuje y tiro. Esta propiedad es especialmente relevante en las formulaciones para materiales anisótropos desarrolladas en esta tesis doctoral.

Los algoritmos de plasticidad actualmente más usados están basados en la idea del retorno al punto más cercano, denominado en inglés Closest Point Projection. La formulación más general es la del General Closest Point Projection, que es una implementación vectorial en el que todas las ecuaciones se reducen de forma residual. No obstante existen implementaciones que pueden ser más eficientes conservando las características óptimas del algoritmo general.

Se ha comparado un nuevo algoritmo propuesto implícito desarrollado usando sólo dos ecuaciones escalares contra la implementación general (vectorial) del Closest Point Projection y contra el Governing Parameter Method desarrollado por Kojić *et al.* [39]. Se ha demostrado que distintas implementaciones de la idea del algoritmo CPP resultan en distintos caminos de iteraciones y por tanto en diferentes tasas de convergencia cuando no se está en la zona de atracción se la solución. Se ha demostrado que aunque todos ellos tienen convergencia cuadrática

asintótica, el número de iteraciones empleado hasta llegar a la zona de atracción es manifiestamente distinto y, por lo tanto, la eficiencia computacional de las tres implementaciones difiere sustancialmente. Al contrario que el algoritmo GCPP, el algoritmo propuesto es válido para el caso de plasticidad perfecta, por el caso de endurecimiento cinemático puro, para el caso de endurecimiento isótropo y para el de endurecimiento mixto sin necesidad de ninguna modificación. Esto conduce a un algoritmo claramente más robusto. Por supuesto en los tres algoritmos estudiados la solución final es la misma, puesto que se pueden entender como diferentes implementaciones del método de integración de backward-Euler. Cabe destacar que a diferencia del método GCPP y del GPM, el número de iteraciones empeladas para el caso especial de plasticidad de von Mises con endurecimiento lineal y para otros casos particulares de carga en plasticidad de Hill es sólo una, tal y como ocurre con los clásicos algoritmos de Wilkins y Kreig y Key.

Por otro lado, como trabajo principal de esta tesis, se ha introducido una nueva formulación fenomenológica del daño para modelar algunos aspectos del efecto Mullins en materiales blandos. Obviamente la formulación es igual de válida para materiales cuyas deformaciones sean pequeñas. Asimismo se ha desarrollado un procedimiento computacional para grandes deformaciones casi-incompresibles tanto isótropas como ortótropas basado en la filosofía WYPIWYG. En el enfoque WYPIWYG no se prescriben funciones analíticas de antemano, no se emplean parámetros del material y los datos experimentales se capturan "exactamente" (para la precisión numérica deseada). Esta nueva aproximación al modelado del daño en materiales hipereelásticos está basada en la idea de que las tensiones del material sin dañar y por tanto sus energías almacenadas sin dañar, no se pueden medir. Como es conveniente que los modelos fenomenológicos estén contruidos sobre cantidades experimentalmente obtenibles, entonces como energía almacenada de referencia se emplea una energía almacenada dañada obtenida de los datos experimentales correspondientes a la curva de daño de descarga y recarga. Los datos de tensión-deformación correspondientes a la curva virgen se usan sólo para calcular la energía liberada a través de un parámetro intermedio. La formulación continua está basada en un operador división basado a su vez en derivadas parciales las cuales pueden ser interpretadas naturalmente como una predicción de la tensión de prueba y un corrector de daño debido a la tasa de energía liberada. El algoritmo local es altamente eficiente ya que conlleva principalmente iteraciones escalares que son fácilmente resueltas mediante un algoritmo tipo Newton-Raphson. El módulo tangente algorítmico coincide con el continuo al ser el problema función de estado. Este módulo tangente se obtiene también con el fin de conservar la convergencia cuadrática de los algoritmos tipo Newton, durante las iteraciones de equilibrio.

El modelo es puramente fenomenológico y general. Por lo tanto es aplicable tanto a materiales poliméricos, por ejemplo con refuerzos, como a materiales biológi-

cos. El modelo además recupera el modelo infinitesimal en el límite, lo cual no ocurre con la mayor parte de los modelos utilizados para materiales biológicos. Para conservar la propiedad de congruencia de simetrías del material, se puede realizar la separación de la energía en la proveniente de una parte isótropa, que cumple la descomposición de Valanis-Landel, más una parte anisótropa, que constituye la desviación de la primera y que está motivada en una descomposición idéntica a la utilizada en deformaciones infinitesimales, pero usando deformaciones logarítmicas en lugar de infinitesimales. Es posible interpretar la parte isótropa como la matriz (elastina y proteoglicanos) y la desviación anisótropa como la contribución de las fibras de colágeno. No obstante estas consideraciones son irrelevantes a la hora de determinar el modelo. Sin embargo permiten, por ejemplo, separar los efectos de daño de la matriz de la del colágeno.

Puesto que la contribución isótropa y la anisótropa son tratadas por separado, es posible modelar efectos de anisotropía inducida por el daño. Tal y como se ha demostrado en un ejemplo, el efecto del daño en una dirección afecta al comportamiento en las otras, generando por lo tanto dicha anisotropía. No obstante, no se ha abordado un estudio detallado de estos efectos y de como realizar el modelado de forma específica.

Entre las limitaciones del modelo están la imposibilidad de modelar deformaciones permanentes, que provienen de un efecto disipativo, modelar ciclos histéricos frecuentemente presentes tanto en materiales poliméricos como en materiales biológicos, o modelar daño continuo (relajación del punto de descarga). No obstante, estas extensiones constituyen trabajos futuros dentro de esta línea de investigación.

6.1. Trabajo futuro

Como en la realización de cualquier tesis doctoral, siempre quedan temas abiertos, detalles mejorables, cuestiones no resueltas y proyectos por abordar. Algunos de los temas más interesantes se describen muy brevemente a continuación.

- Estudiar el modelado de la anisotropía inducida en un material isótropo debida al proceso de deterioro del mismo al deformar en una dirección preferente.
- Mejorar la implementación basada en splines por la aparición a veces, de efectos no deseados por los conocidos efectos de borde por ejemplo. Una mejora al respecto se está llevando actualmente a cabo. Dichas mejoras incluyen también el control de propiedades a veces deseables en las funciones de energía como la policonvexidad, elipticidad, entre otras.
- Los modelos desarrollados pueden ser extendidos y acoplados con otros modelos para simular efectos no contemplados en esta tesis. Se tiene previsto

modelar conjuntamente el daño y las deformaciones plásticas que suelen aparecer en los materiales blandos cuando se retira la carga. Otros efectos son la adición de un daño continuo que se refleja experimentalmente en la relajación del punto de descarga, y disipación cíclica. Al respecto de la disipación cíclica, parte se debe en realidad a efectos viscosos. Por tanto, otra tarea pendiente es el acoplamiento de estos modelos de daño con los modelos viscoelásticos desarrollados en el grupo.

- Por otro lado, también se pretende llevar a cabo la aplicación de los modelos al campo de la biomecánica tisular y de materiales compuestos.

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