XXIII CONVEGNO GRUPPO ITALIANO DI MECCANICA COMPUTAZIONALE

X CONVEGNO GRUPPO MECCANICA DEI MATERIALI

II CONVEGNO GRUPPO BIOMECCANICA

GIMC GMA GBMA 2023

BOOK OF ABSTRACTS

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Paolo Fuschi
Aurora Angela Pisano
Editors

INDICE

166. **Boiardi A.S., Noselli G.**
Swimming of active filaments emerging from mechanical instabilities

167. **Lenarda P., Preve D., Bianchi D., Gizzi A.**
Phase field modeling and FEM simulation of bone fracture occurring in human vertebra after screws fixation procedure

168. **Bernard C., Carotenuto R.A., Argenziano M., Zingales M., Fraldi M., Deseri L.**
Investigating the influence of chemo-mechanical coupling in the remodelling of lipid membranes

169. **Valoroso N.**
Graded damage VS phase-field for modeling quasi-brittle fracture

170. **Panteghini A.**
A simple method to compute a closed-form spectral decomposition of a symmetric second order tensor

171. **Chianese C., Marmo F., Rosati F.**
Form Finding of Membrane Shells with Isogeometric Analysis

173. **Leonetti L.**
Material point method and isogeometric analysis

175. **Ongaro G., Pingaro M., Trovalusci P., Bertani R.**
Multiscale strategy for identification of elastic and fracture properties of polymer-based nanocomposites

177. **Gatta C., Pingaro M., Addessi D., Trovalisci P.**
Modeling of polycrystalline composites coupling virtual elements and nonlinear interface finite elements

179. **Ruocco E., Musone V., Iannuzzo A.**
Artificial Neural Networks for evaluation of cracks in masonry arches

181. **Parrinello F.**
Analysis of fracture propagation by the Hybrid Equilibrium Element formulation

182. **Ricci M., Carrara P., Flaschel M., Kumar S., Marfia S., De Lorenzis L.**
Validating the EUCLID Approach for Unsupervised Discovery of Hyperelastic Constitutive Laws Using Experimental Data

184. **Palladino S., Esposito L., Zona R., Minutolo V., Sacco E.**
Crack propagation procedure for designing hollowed structures

188. **Farhadi S., Corrado M., Ventura G.**
Pre-stressed wire breakage detection using Back Propagation Neural Networks with experimental and numerical datasets

190. **Zona R., Esposito L., Palladino S., Minutolo V.**
Limit Analysis through Residual dislocation based Finite Elements and nonlinear compatibility domain secant approximation with penalty factor

Solids from structures

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Keywords: Flutter instability; Non-Hermitian mechanics; Homogenization

Proper design of architected materials made up with elastic structures is believed to yield unchallenged mechanical properties in terms of stiffness, anisotropy, dynamic characteristics, and toughness. When the structure is elastic and periodic, homogenization becomes the formal procedure to obtain the response of an equivalent elastic solid. Homogenization of periodic grids of elastic rods, prestressed with axial forces and deformed incrementally under bending lead to prestressed elastic solids, which may show the emergence of material instabilities such as shear band formation [1]. A design paradigm is established for artificial materials where follower micro-forces, so far ignored in homogenization schemes, are introduced as loads prestressing an elastic two-dimensional grid made up of linear elastic rods (reacting to elongation, flexure and shear). A rigorous application of Floquet-Bloch wave asymptotics yields an unsymmetric acoustic tensor governing the incremental dynamics of the effective material [2]. The latter is therefore the incremental response of a hypo-elastic solid, which does not follow from a strain potential and thus does not belong to hyper-elasticity. The solid is shown to display flutter, a material instability corresponding to a Hopf bifurcation, which was advocated as possible in plastic solids, but never experimentally found and so far believed to be impossible in elasticity [2]. In elastic structures flutter can be originated from different loading systems [3], which can be used to architect new discrete materials. The discovery of elastic materials capable of sucking up or delivering energy in closed strain cycles through interaction with the environment paves the way to realizations involving micro and nano technologies and finds definite applications in the field of energy harvesting.

Acknowledgements Financial support from ERC-ADG-2021-101052956-BEYOND is gratefully acknowledged.

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Microfluidic systems for single-cell biophysical characterization

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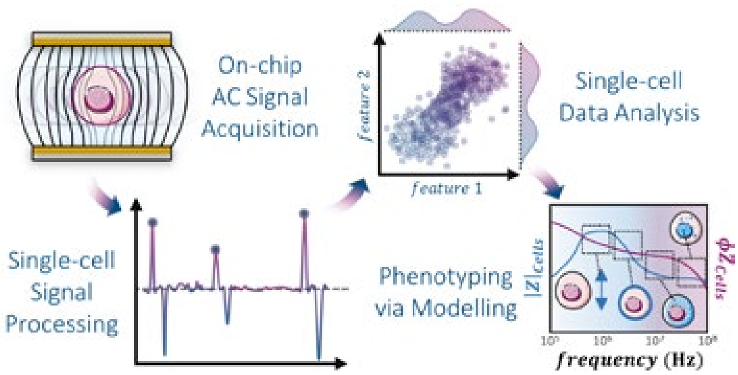
Keywords: single-cell analysis, impedance cytometry, microfluidics.

The cell is the fundamental unit of life. Understanding cell function in health and disease is critical to diagnosis and treatment. Modern approaches towards personalized and precision medicine highlight the potential of single-cell analysis and manipulation for the development of novel therapeutic solutions. This raises the need to develop suitable, advanced technological tools.

Microfluidic impedance cytometry is a label-free, high-throughput technique that uses electric fields to stratify the heterogeneity of cellular systems, based on their biophysical properties, such as cell size, shape, and deformability. Emerging applications range from fundamental life-science and drug-assessment research to point-of-care diagnostics and precision medicine. Novel chip designs and data analytic strategies are laying the foundation for multiparametric cell characterization and subpopulation distinction, which are essential to understand biological function and follow disease progression.

We present recent approaches to elucidate cellular and subcellular features from impedance cytometry data, covering the related subjects of device design and data analytics (i.e., signal processing, dielectric modelling, population clustering). We give special emphasis to the exciting recent developments of the technique and provide our perspective on future challenges and directions. Its synergistic application with microfluidic separation, sensor science and machine learning can form an essential toolkit for label-free quantification and isolation of subpopulations to stratify heterogeneous biosystems.



On Phase-Field Modeling of Ductile Fracture

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Keywords: Ductile Fracture, Phase Field, Variational Formulation.

The computational modeling of ductile fracture is a complex problem due to the co-existence of different competing dissipation mechanisms at the microscale resulting in evolving displacement discontinuities at the macroscale. Phase-field modeling of brittle fracture has emerged as one of the more computationally effective smeared approaches to the simulation of crack propagation in solids. After the publication of the first papers about a decade ago, its extension to ductile fracture has attracted growing attention, with the appearance of a rapidly increasing number of contributions proposing different approaches and applications.

Starting from established variational statements of finite-step elastoplasticity for generalized standard materials, a mixed variational statement for the phase-field modeling of ductile fracture is presented, incorporating in a rigorous way a variational finite-step update for both the elastoplastic and the phase-field dissipation. The complex interaction between ductile and brittle dissipation mechanisms is modeled by assuming a plasticity driven crack propagation model, with the addition of a non-variational function of the effective plastic strain that modulates the current value of the critical fracture energy.

Several modeling and computational aspects are discussed and an application to the simulation of ductile fracture of 2D paperboard laminates is presented.

Mechanics of cohesive interface: damage, contact, interlocking, dilatancy

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Interface mechanics refers to the study of the behavior of the link between materials or structures that are held together by cohesive forces. In other words, interface mechanics is concerned with the behavior of the connection between two materials or structures that are bonded together by adhesion forces. Interface mechanics plays an important role in a wide range of engineering applications, including adhesive bonding, composite materials, and fracture mechanics. In these applications, the performance of the structure is often strongly determined by the behavior of the interface between the materials or structural elements. Understanding the mechanics of cohesive interfaces is important for designing and analyzing structures that rely on adhesive bonding or other forms of cohesive forces. This involves studying the deformation, fracture, and failure of the interface under different loading conditions, as well as the influence of factors such as temperature, moisture, and chemical exposure on the behavior of the interface. Overall, interface mechanics is an important area of study that helps engineers and scientists design and optimize structures that rely on adhesion forces for their strength and durability.

The literature on the modeling of cohesive interfaces and of their use in the different fields of the application is absolutely huge. The models relating the relative displacement $\mathbf{s}$ with the traction $\boldsymbol{\tau}$ describe the degradation of the link between the two surfaces constituting the interface by accounting for the coupling of the normal and tangential effects, i.e. considering the mixity of the crack opening.

The interface modeling starts from the pioneering works concerning the fracture mechanics developed by Dugdale [11], who presented a theoretical model for analyzing the behavior of slits in steel sheets assuming a perfectly plastic response at the edges of a slit in a steel sheet, with a limited value of the maximum strain. Barenblatt [4] presented a theoretical framework for analyzing the behavior of cracks in brittle materials, introducing a relationship between the cohesive force and the opening of the crack lips increasing up to a maximum value of the tension and, subsequently, decreasing until it is zero. Hillerborg et al. [13] proposed a cohesive fracture mechanics approach for studying the crack growth in concrete structures in the framework of the finite element method accounting for a degradation law relating the traction to the crack opening. In figures 1(a) and 1(b), two possible interface opening responses considered by Hillerborg et al. are illustrated. The first one corresponds to the Dugdale [11] model, while the second illustrates a degrading response of the crack opening, as suggested by Barenblatt [4]. Figure 1(c), illustrates the schematic profile of the traction at the crack lips, for a softening behavior defining the so-called process zone.

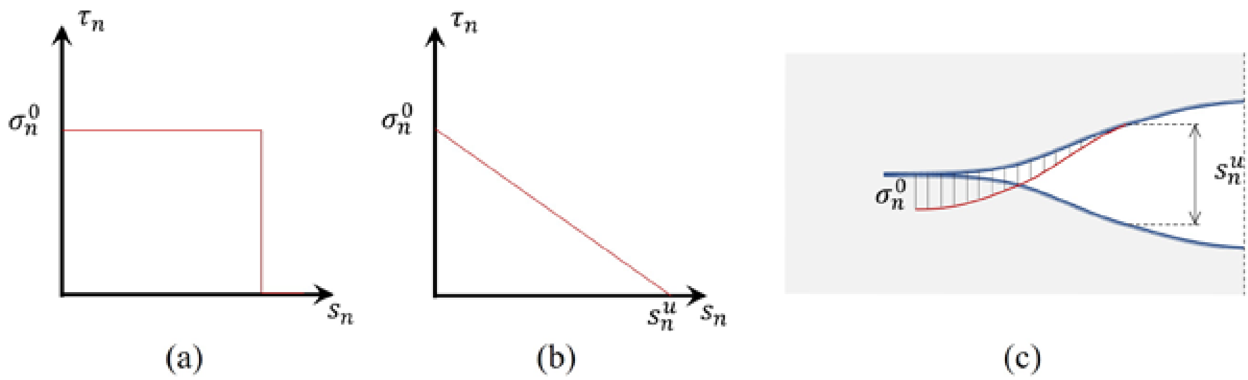

Figure 1: Traction vs crack opening for (a) ductile and (b) cohesive material; (c) schematic of the traction profile on the crack lips for a softening crack opening response.

Among the most adopted interface models, Needleman [17] studied the void nucleation process from the initial detachment through the complete decohesion of rigid spherical inclusions in a composite material, proposing a nonlinear elastic interface model characterized by a maximum cohesion strength and a smooth softening branch for mixed mode decohesion. Tvergaard [25] developed an interface model able to account for different effects arising at the interface: mixity mode of decohesion, elastic unloading after degradation, frictional effect of the surface in contact. A very interesting aspect of the Tvergaard interface model is the possibility to consider the friction arising at the interface when decohesion is lost and shear and compressive normal stresses are present. Indeed, the proposed model is almost simple as it consider a Coulomb friction only after that the complete decohesion of the interface occurred, leading to a sharp discontinuity in the interface response. Chaboche et al. [8] proposed an improvement of the Tvergaard model introducing additional terms that force a continuity and monotonicity in the tangential stiffness degradation between the decohesion and the Coulomb frictional response occurring after complete separation. Ortiz and Pandolfi [18] proposed a three-dimensional interface damage model in the framework of finite strain assumption. The initial interface model has been then improved introducing also the effect of the unilateral contact and friction [20].

Mechanics of interface received great attention by Italian researches. Far to be exhaustive, among the others, Corigliano and Allix [10] adopted the interface model for investigating the interlaminar degradation of composite materials. Lenci [14] developed an interface model to study the crack growth between two elastic half-planes, showing that the derivative of the solution is logarithmically unbounded and that logarithmic stress singularities may exist. Giambanco et al. [12] formulated elasto-plastic non-standard interface model for reproducing the softening response occurring during the decohesion process in masonry, accounting for the dilatancy related to the roughness of contact surfaces after joint decohesion. Bertoldi et al. [5] presented a rigorous analytical derivation of a nonlocal interface model from the microstructure properties by considering the gradient approximation of the interface constitutive law. Carpinteri et al. [7] investigated the interface decohesion in double cantilever laminated beams. Paggi and Wriggers [19] developed a nonlocal cohesive zone model for finite thickness interfaces. Marulli et al. [16] combined a phase-field approach with the cohesive zone model for studying the crack propagation in layered structures. Bonetti et al. [6] derived a damaging interface model from asymptotic analysis of a micro-cracked layer. Parrinello and Borino [21] proposed an interface constitutive model based on the non-associative damage mechanics and frictional plasticity in a thermodynamically consistent framework. Confalonieri e Perego [9] formulated and validated an interface cohesive model for mixed mode I-mode II fracture proposing a bilinear traction-separation law.

A suitable way for introducing the coupling between damage and friction has been proposed by Alfano and Sacco [2] by developing a micromechanical analysis of the interface response. The proposed model has been successfully adopted in a wide range of engineering applications, such as hydraulic fracture mechanics [1], masonry structures [22].

The initial Alfano-Sacco interface model has been successively improved for accounting of the effects of the dilatancy and interlocking [24, 23]. As for the original model, the mechanical response of the interface has been derived developing a micromechanical analysis in the framework of 2D and 3D rough surfaces in contact and adhesion.

Recently, the Alfano-Sacco interface model has been implemented in a Virtual Element Method code to study the nucleation and evolution of the fracture in a cohesive solid [3, 15]. In figure 2, a numerical result concerning a L shape structural element is schematically illustrated.

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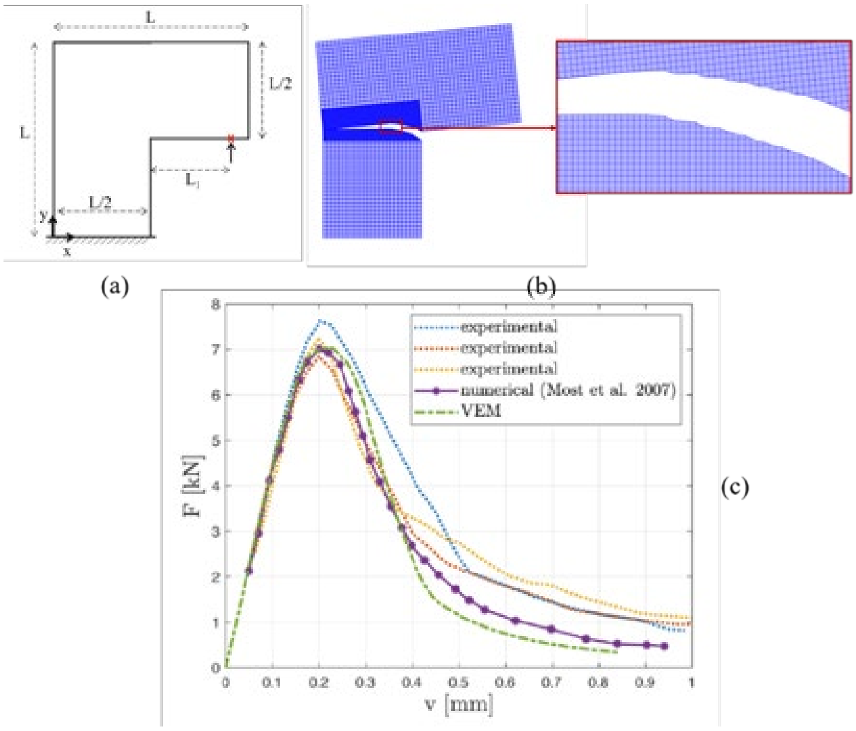

Figure 2: (a) L shape structural element; (b) deformed element with the crack opening; (c) mechanical response.

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Multiscale modeling of vascular adaptation

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Keywords: Agent-based model (ABM), Atherosclerosis, Restenosis.

Atherosclerosis and restenosis are complex vascular adaptation processes, influenced by different systemic, biological and biomechanical factors and characterized by a network of interconnected, heterogeneous mechanobiological events occurring at different spatiotemporal scales. A thorough understanding of the causes and underlying mechanisms of these adverse processes is lacking. From the biomechanical perspective, both the hemodynamic and structural forces play a role in the pathogenesis of atherosclerosis and restenosis, by influencing cellular activity [1,2]. Recently, computational multiscale agent-based modeling frameworks, integrating both continuous- and agent-based methods and inspired by the systems biology principles, have emerged as promising tools to decipher the mechanobiological processes underlying vascular adaptation. By enabling the identification of patient's pathological pathways, these frameworks have the potential to contribute to the improvement of disease diagnosis and treatments, in the optic of personalized medicine [3].

In this context, a multiscale agent-based modeling framework of vascular adaptation was developed, integrating continuum and agent-based methods, in order to analyze the interactions, cause-effect relationships, feedback mechanisms and cascade signaling pathways across different spatial and temporal scales [3]. The multiscale framework integrated: (i) a biomechanics module at the tissue-scale, simulating the hemodynamics (with low-density lipoprotein transport in case of atherosclerosis) and/or the solid mechanics with a continuum approach (computational fluid dynamics (CFD) and finite element (FE) analyses) and (ii) a tissue remodeling module at cell-scale, replicating cellular activities and subsequent arterial wall remodeling in response to hemodynamic, mechanical, gene expression-based inflammatory stimuli, through an agent-based model (ABM) of cellular dynamics (Fig. 1). The multiscale framework was applied to investigate the mechanobiological mechanisms governing arterial wall remodeling in atherosclerosis [4], restenosis following percutaneous transluminal angioplasty [5] and in-stent restenosis, in patient-specific superficial femoral arteries (SFAs) [6,7].

The multiscale framework captured relevant mechanobiological mechanisms underlying atherosclerosis and the arterial wall response to endovascular procedures. In particular, the validated patient-specific framework of in-stent restenosis was able to predict the short- and long-term arterial response to the endovascular intervention in patient-specific stented SFAs, by considering post-operative hemodynamic and inflammatory-related monocyte gene expression effects on cellular dynamics [6,7]. The proposed approach lays the foundations towards predictive in-silico models in the context of personalized medicine, promising to (i) provide further insights into the disease mechanisms, and (ii) identify patient's pathological pathways, enabling patient stratification and personalized diagnosis and therapy.

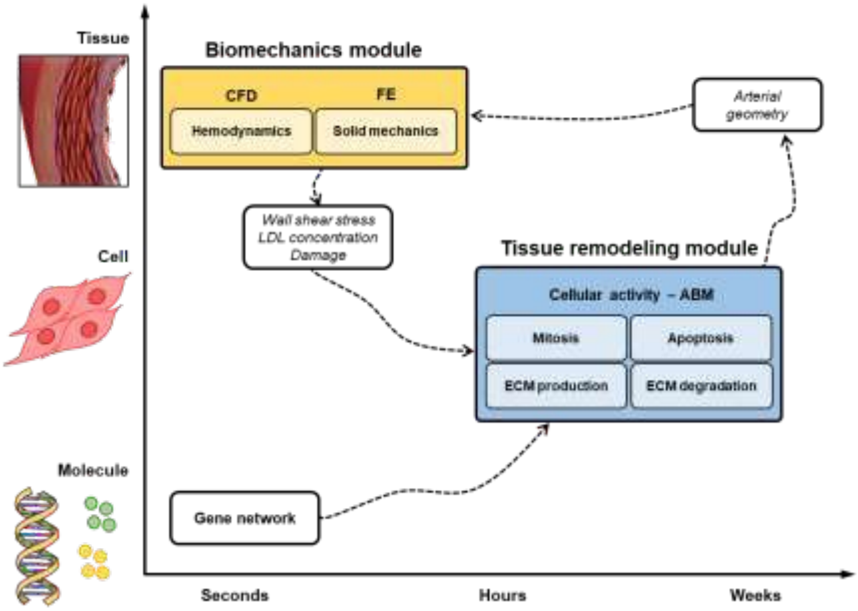

Figure 1: Multiscale agent-based modeling framework of vascular adaptation.

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Model order reduction of nonlinear vibratory systems through direct parametrisation of invariant manifolds

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Keywords: Periodic orbits, invariant manifold, nonlinear dynamics, model order reduction, MEMS.

Micro-electro-mechanical systems (MEMS) represent a fundamental piece of our economy and life. Indeed, their small size combined with high sensitivity to external stimuli allows adopting them as sensors and actuators in most technological components as cell-phones, earphones, and smart glasses. Nevertheless, the high demand of MEMS devices makes this industrial field competitive and it forces companies to achieve constant improvements of their products to thrive in the market. As a result, precise and accurate mathematical methods to predict the response of MEMS devices are essential since traditional "trial and error" approaches are not sustainable considering the high costs of the fabrication process. Among the different classes of mathematical methods adopted in industry, full order solution schemes are usually adopted since they are reliable and accurate when it comes to elaborated geometries that cannot be modelled by analytical approaches. They are however not adequate when modelling devices that need to operate at resonance since steady state periodic solutions are computational demanding for large scale systems of differential equations. Therefore, resonating devices i.e., devices that operate at resonance as MEMS gyroscopes and micromirrors, are challenging to design and optimise using full order methods. As a result, model order reduction strategies i.e., techniques aimed at reducing the computational complexity of numerical models, are essential. Among the different methods available in literature the parametrisation method for invariant manifolds (PIM) represents one of the most appealing techniques for dimensionality reduction of nonlinear systems since it provides a mean to derive reduced models by parametrising the system motion along a low dimensional invariant set of the phase space. This approach has several benefits compared to other model order reduction strategies since it exactly addresses non-resonant coupling, that leads to failure of energy-based approaches as the proper orthogonal decomposition followed by hyper-reduction. In the present work, a direct formulation of the PIM (DPIM) is proposed for geometrically nonlinear structures discretised with the finite element method [**?**, **?**, **?**]. The governing equations of the discretised problem are given as:

$$\mathbf{M}\ddot{\mathbf{U}} + \mathbf{C}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} + \boldsymbol{G}(\mathbf{U},\mathbf{U}) + \boldsymbol{H}(\mathbf{U},\mathbf{U},\mathbf{U}) = \mathbf{F}, \tag{1}$$

with $\mathbf{M}$ mass matrix, $\mathbf{C}$ damping matrix, $\mathbf{K}$ stiffness matrix, $\mathbf{U}$ displacement vector, $\boldsymbol{G}$ quadratic nonlinear operator, $\boldsymbol{H}$ cubic nonlinear operator, and $\mathbf{F}$ external force vector. Dimensionality reduction is obtained by introducing nonlinear lifting operators between nodal displacement $\mathbf{U}$, velocity $\mathbf{V} = \dot{\mathbf{U}}$, and normal coordinates i.e., the coordinates defined over the parametrised set. Explicit relations and computational aspects of the method are detailed for both autonomous [**?**] and non-autonomous [**?**] systems, together with extension of the method to nonlinear piezoelectric structures. The method is applied to structures of academic and industrial relevance as the MEMS arch resonator subjected to a 1:2 internal resonance reported in Fig. **??**. The resulting algorithm shows accuracy and performance that make it one of the most efficient dimensionality reduction methods for nonlinear vibrating structures.

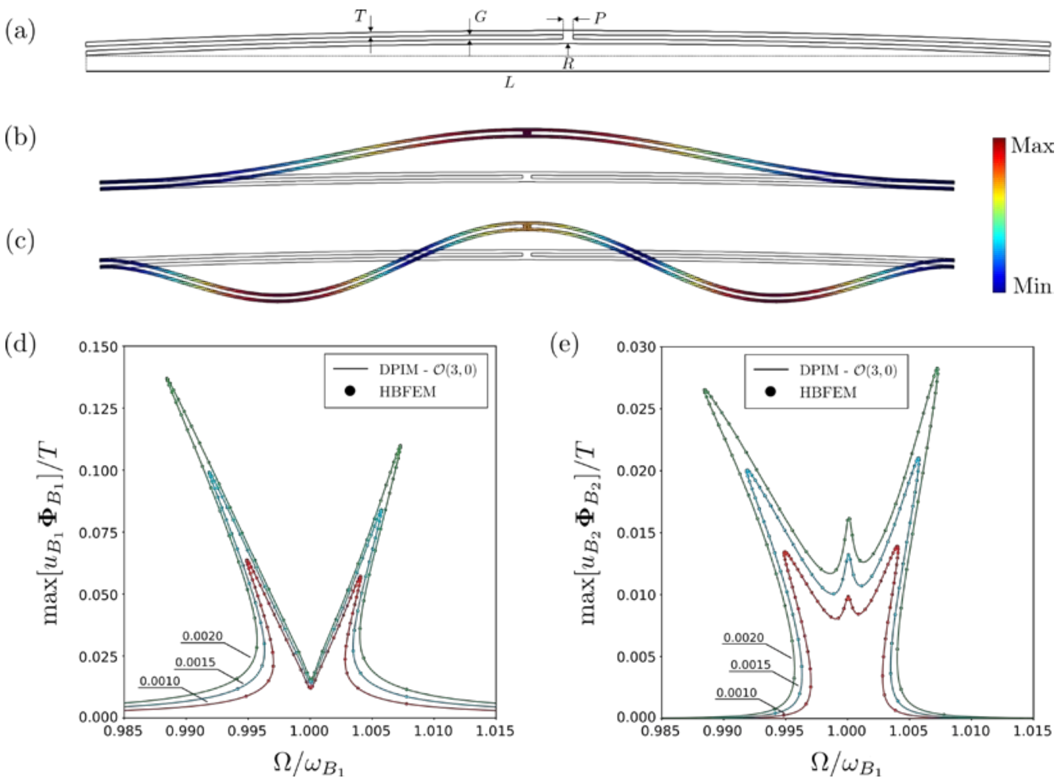

Figure 1: Example application of the DPIM to a MEMS resonator subjected to transversal loading. (a) geometry of the structure: L = 649.5 μm, R = 6.675 μm, P = 6.5 μm, T = 2.5 μm, and G = 2.5 μm. (b-c) coupled eigenmodes in 1:2 internal resonance. (d-e) comparison between frequency response curves computed with the proposed method (DPIM) and full order harmonic balance solutions of the finite element system (HBFEM). Solutions are computed for multiple harmonic forcing amplitude values and they are reported as tags in (d-e).

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Coupling mechanics with species diffusion in engineering modelling

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Keywords: Ionic polymer metal composites, bioelectricity, corrosion, lithium-ion batteries.

We present recent advances in the coupling of mechanics with species diffusion in the mathematical modelling of a range of engineering problems. First, we devote our attention to ionic polymer metal composites, a class of electroactive smart materials used as actuators and sensors. We account for the cross-diffusion of solvent and ions and for the Maxwell stress in the multi-physics formulation, and discuss their role in qualitatively explaining peculiar experimental observations [1]. Second, we propose a model able to capture the coupling between electrical and mechanical signalling in a cluster of biological cells and their extracellular environment [2]. The model describes the evolution in space and time of cluster deformation and membrane voltage due to the diffusion of water and ions through aquaporins and ion channels, respectively. Suitably complemented with the description of growth, this model may serve as a useful platform for the study of developmental bioelectricity. Third, we study the delamination of an adhesive sandwich layer driven by the diffusion of a corrosive species [3]. As a critical amount of this species reacts with the adhesive-substrate interface, the delamination tip advances. This study is of importance to quantify the life expectancy of adhesively-bonded joints employed in shipbuilding. The fourth case study is motivated by the short-circuiting of solid-state lithium-ion batteries due to the growth of thin lithium filaments through-the-thickness of the solid electrolyte, as lithium diffuses and is plated on the cathode surface during the charging process [4]. We employ strain gradient plasticity to explain the high compressive strength characterising these constrained lithium filaments, as compared to bulk lithium.

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Variational Methods to Fracture- Phase Field Approach

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Keywords: Phase-field, Fracture, Thin Structures, Size effect.

The Phase Field Method (PFM) has emerged as a crucial tool in fracture mechanics research, offering the capability to incorporate complex material models and efficiently study intricate fracture phenomena. This study focuses on two key areas where the PFM demonstrates its capabilities.

Firstly, a thermodynamically consistent framework for the coupled thermo-mechanical phase-field model in thin-walled structures using fully-integrated finite elements is examined. This framework enables the utilization of three-dimensional constitutive thermo-mechanical models, leading to locking-free elements through Enhanced Assumed Strain (EAS) and Assumed Natural Strain (ANS) techniques. The proposed model considers the same degradation function for both displacement and thermal fields. Efficient numerical solution schemes are employed for solving the coupled equations, and numerical examples are provided to demonstrate the practicality and reliability of the proposed framework, including cases with [1] and without [2] the phase-field approach. As an example, phase field and temperature distribution for a plate with notch and hole along with the reaction forces is presented in Fig. 1. Furthermore, the model is extended to incorporate Functionally Graded Ma-

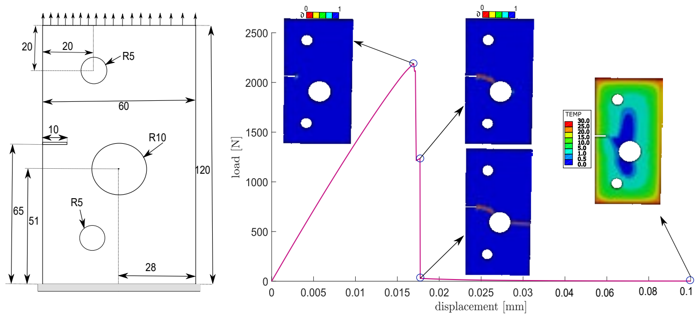

Figure 1: Phase-field and temperature distribution for a plate with notch and hole along with reactions.

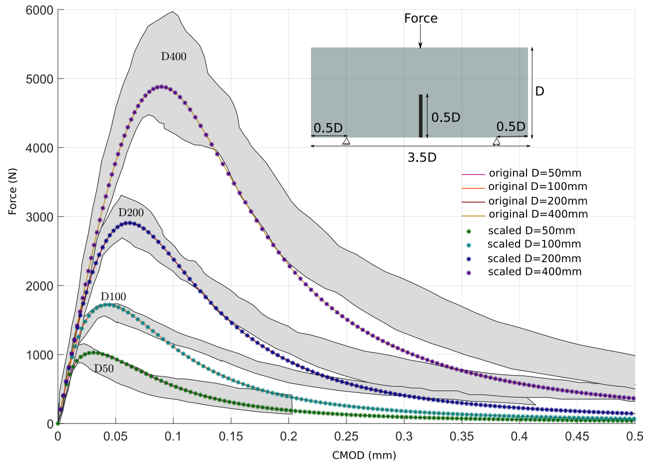

Figure 2: Comparison of Force Vs. Crack mouth opening displacement of concrete with experimental results.

terials [3] (FGM), showcasing its applicability in capturing material heterogeneity in thin-walled structures.

Secondly, the study explores the efficient simulation of the size scale effect using the PFM. A novel geometric scaling framework is introduced, allowing for an accurate representation of the geometric transformation relationship between material models and scaling. The framework utilizes a scaling matrix to seamlessly transform between the original and scaled domains while preserving the variational formulation. It successfully handles various scaling scenarios, such as lateral expansion, horizontal expansion, and symmetric scaling. The framework is applied to different models and demonstrates the ability to mimic the behavior of original and scaled models without additional model development or computational resources. Furthermore, the framework recovers size scale laws and identifies structural bifurcations within a reasonable computational time. Additionally, mesh issues related to the phase field are addressed, enhancing the robustness of the modeling framework. As an example, a comparison with the experimental results on concrete for a three-point bending specimen is shown in Fig 2.

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Development of a multi-GPU solver for atmospheric entry flows with gas-surface interactions

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Keywords: hypersonics, non-equilibrium, multitemperature, Park, State-to-State, shock wave/boundary layer interaction, gas-surface interaction, catalysis, ablation, immersed boundary, CUDA, GPU.

The understanding of atmospheric re-entry is fundamental in the aerospace engineering field. The heat load experienced by a space vehicle while entering in the atmosphere is extreme and its correct prediction is necessary in the view of an appropriate design of the thermal shield. Technology progression allows to exploit sophisticated facilities able to reproduce the macroscopic features of entry flows. However, high fidelity experimental reproduction is still hard due to two main reasons, namely the cost of an experiment and the difficulty in reproducing each aspect of the flight conditions [1]. This led many companies to invest more and more in numerical tools, representing a valid alternative to provide accurate predictions of interesting information, such as heat flux, pressure distribution or shock stand-off distance for bluff bodies. Of course, the development of an efficient numerical tool is not trivial and requires particular attention. Indeed, dealing with hypersonic flows, one must account for 'real gas' effects, known as *thermochemical non-equilibrium* phenomena [2].

By the years, many researchers have been devoting efforts to the development of physical models able to describe the correct evolution of the challenging conditions encountered during the re-entry. The high velocities of a space vehicle induce the formation of strong shock waves in front of it, across which the temperature reaches values of the order of 10000 K. It is immediate to understand that these extreme conditions implicate the conversion of the kinetic energy into internal energy, whose total content involves translational, rotational, vibrational and electronic modes. Also, molecular dissociation occurs due to the particle collisions in the shock layer and, if the temperature is large enough, ionization takes place. The latter is a relevant aspect of re-entry flows as the presence of electrons in the mixture is responsible for the well-known *blackout*. For the purpose of heat mitigation, several strategies are adopted. The employment of ablative material for the Thermal Protection System (TPS) has become very common. Thanks to material degradation, the heat flux on the surface of the vehicle is reduced, even if this introduces further complexity in the numerical modeling. The material directly interacts with the species in the mixture, leading to the occurrence of gas-surface interactions (GSI) such as catalysis and ablation.

From the thermophysical modeling point of view, two main approaches are adopted in this work. The first one is the multitemperature model proposed by Park [3], very common in the scientific community due to its simplicity; however, in some critical case its basic assumptions are not suitable, and the more sophisticated State-to-State approach must be adopted [4]. It can provide much more accurate results, but the computational cost is order of magnitude higher that the first thermochemical model.

Concerning the numerical approach, classical commercial solvers exploit finite-volume methods applied in a body-fitted multi-block grids, very common in Computational Fluid Dynamics (CFD). Nevertheless, when dealing with complex and/or moving geometries, the employment of body-conformal domains can be complicated due to the need of run time remeshing procedures. In this context, Immersed Boundary Methods (IBM) are suitable for a more versatile numerical solver [5]. Such an approach allows for a unique Cartesian grid generation, that can be refined in the most critical region to increase the accuracy of the numerical solution.

Taking into account all the above mentioned phenomena is a complex task as the numerical model employed must be accurate and cheap at the same time. Indeed, given the huge computational cost required by these kinds of numerical simulations, an affordable strategy must be thought in order to speed-up the calculations. Graphics Processing Units (GPUs) provide high performances for general purposes in the scientific field. NVIDIA Corporation is still actively working in the development of efficient interfaces between hardware and software. The most famous one is Compute Unified Device Architecture (CUDA) that allows a very easy interface with basic programming languages such as C/C++ or Fortran [6]. Thanks to GPU programming, very fast simulations are possible even in the most demanding configurations.

All the aforementioned aspects are addressed in this work, which aims at illustrating the main challenges in modeling hypersonic flows. A comparison of the current tools is presented for interesting aerospace applications, such as shock wave/boundary layer interaction and bluff body flows, in the presence of gas-surface interactions and thermochemical non-equilibrium, with the hope it can inspire further developments for technology progression.

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FE and IGA techniques for the analysis of the axial-symmetric masonry domes

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Keywords: Finite element, Isogeometric analysis, Masonry dome.

The majority of the masonry existing buildings in Europe and in Italy are characterized by curved members. In particular, they could be reckoned in the most significant architectural heritage, historically meaningful through the centuries. Moreover, to date, many of these ancient masonry structures have been largely used. For this reason, their structural assessment has been even more considering as both a national and an international priority to guarantee their historical and artistic preservation over time. Therefore, the mechanical behaviour prediction of the curved masonry elements as vaults and domes is necessary. Indeed, there has been evidence in the close dependence among their response, their geometry and the intrinsic characteristics of the masonry material, not reacting in tension.
Recently, the computational analysis has received a great attention thanks to the large amount of scientific studies, providing different procedures [1-3]. In particular, the Limit Analysis has appeared as a reliable and suitable approach for the prediction of the load-carrying capacity of masonry curved members. Likewise, the development of Finite Element modelling (FE) and Discrete Macro-Element Methods (DMEM) have revealed their efficiency in the simulation of the complex structural response of masonry [4-5].

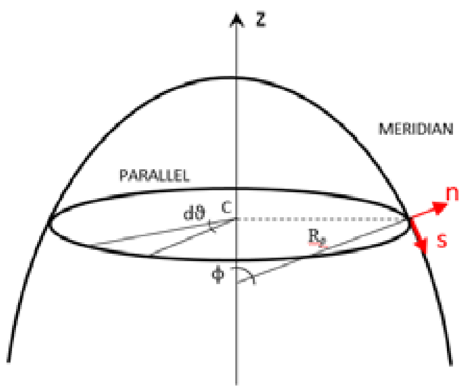

Figure 1: sketch of the structural model.

The purpose of this research is to present a numerical approach, based on the first-order shear deformation shell theory, able at assessing the mechanical response of masonry domes, modelled as shells of revolution. Indeed, as schematically displayed in Fig. 1, the dome geometry can be dissected by vertical planes, identifying the meridians, and horizontal planes which define the parallels. A curvilinear abscissa s is introduced on the typical meridian, as represented in Fig. 1. Two consecutive meridians define an arch characterized by the radius R_m, which is invariable when the abscissa s remains constant. The parallel is shaped by the radius R_p, as depicted in Fig. 1. The stresses that develop inside the dome are transmitted along the meridians and parallels under the axial-symmetric load conditions and find their own balance. Organizing the local displacement parameters and the strains in the vectors $\boldsymbol{d} = \{u\ v\ \varphi_s\}^T$ and $\boldsymbol{\varepsilon} = \{\varepsilon_s\ \varepsilon_\vartheta\ \gamma_s\ \chi_s\ \chi_\vartheta\}^T$, respectively, the following strain-displacement relationships (1) can be introduced [6]:

$$\varepsilon_s = \frac{du}{ds} + \frac{1}{R_m} v \qquad \varepsilon_\vartheta = \frac{\cot\Phi}{R_p} u + \frac{v}{R_p} \qquad \gamma_s = -\frac{u}{R_m} + \frac{dv}{ds} - \varphi_s \tag{1}$$

$$\chi_s = \frac{d\varphi_s}{ds} \qquad \chi_\vartheta = \frac{\cot\Phi}{R_p}\varphi_s$$

where, ε_s and ε_ϑ are the membrane axial strains, γ_s is the meridian out-of-plane shear strain, χ_s and χ_ϑ represent the curvatures.

Masonry is characterized by a poor strength in tension. In this approach, the masonry is modelled as a no-tension material, resulting in the admissibility condition for normal stress $\sigma \leq 0$, with σ the maximum principal stress.

The equilibrium equations are recovered via the static-kinematic duality for which the kinematic matrix operator is the adjoint of static matrix operator and viceversa [7]. Introducing the stress resultants as N_s and N_ϑ the axial forces, T_s the shear force and M_s and M_ϑ the bending moments, and the distributed loads as the tangential load p_s, the normal load q and the distributed bending moment m_s, the equilibrium equations are written (2):

$$\frac{dN_s}{ds} + \frac{\cot\Phi}{R_p}\cdot N_s - \frac{\cot\Phi}{R_p}\cdot N_\vartheta + \frac{T_s}{R_m} + p_s = 0 \qquad -\frac{N_s}{R_m} - \frac{N_\vartheta}{R_p} + \frac{dT_s}{ds} + \frac{\cot\Phi}{R_p}\cdot T_s + q = 0$$

$$T_s + \frac{dM_s}{ds} + \frac{\cot\Phi}{R_p}\cdot M_s - \frac{\cot\Phi}{R_p}\cdot M_\vartheta + m_s = 0 \tag{2}$$

Finally, taking into account the constitutive equations, the stress resultants and the kinematic parameters $\boldsymbol{\varepsilon}$ relationships are determined.

The theoretical model is implemented via two numerical procedures based on *i)* finite element (FE) formulation and *ii)* iso-geometrical analysis (IGA) [8-11]. The FE procedure is defined by a classical formulation based on the introduction of Lagrangian shape functions and a curved element is modelled able to reproduce also non-constant curvatures. Likewise, the IGA procedure is employed in order to suggest a powerful approach for reproducing the response of masonry domes of complex geometry with low computational cost.

The theoretical model and the adopted numerical procedures are illustrated and then discussed, along with the outcomes display, sensitivity analyses and comparisons between the two numerical suggested approaches.

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An efficient isogeometric formulation for geometrically exact viscoelastic beams

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Keywords: Isogeometric Collocation, Viscoelasticity, 3D curved beams.

In this contribution we propose a novel isogeometric collocation (IGA-C) formulation for the solution of the linear viscoelastic problem of shear-deformable geometrically exact beams [1]. IGA-C methods have already been successfully applied to geometrically exact beams [2],[3],[4]. However, most of the existing geometrically exact formulations, including those based on the classical finite element method, are restricted to linear elastic materials. An isogeometric formulation for geometrically exact elasto-visco-plastic beams has been recently proposed in [5], where a mixed formulation is preferred for computational efficiency.

In the present contribution we demonstrate that an efficient displacement-based formulation can be developed without any significant additional computational cost. Indeed, using a second-order accurate trapezoidal time-integration scheme for the evolution equations, our formulation allows to compute the internal variables exploiting the same kinematic unknowns used in the primal formulation. The linear viscoelastic material response is modeled adopting the Generalized Maxwell Model for 1D solids.

Overall, very high efficiency is achieved with the present method thanks to the combination of a series of desirable features that can be summarized as follows: i) the formulation is displacement-based, meaning that only incremental displacements and rotations are the primary unknowns; ii) the governing equations are discretized in space using the isogeometric collocation scheme, meaning that, in contrast to Galerkin-based formulations, no loops for element integration are needed; iii) finite rotations are updated using the (incremental, material) rotation vector, leading to two main benefits: minimum number of rotation unknowns (namely the three components of the incremental rotation vector) and no singularity problems; iv) the same SO(3)-consistent linearization of the governing equations and update procedures as for static linear elastic material can be used, meaning that no additional computational effort is required due to the viscoelastic material; v) a standard second-order accurate time integrator scheme turns out to be consistent with the underlying geometric structure of the kinematic problem.

Moreover, exploiting the isogeometric analysis features, which are all preserved, the formulation here proposed permits accurately managing beams and beam structures with highly complex initial shape and topology [6], paving the way to many potential applications in the field of architectured materials, meta-materials, morphing devices, etc. for which efficiency is a fundamental requirement.

A series of numerical applications will be also presented in order to demonstrate the above attributes. Fig.1 shows an example of a 1m-long cantilever viscoelastic beam with square cross section with side 0.1 m. A concentrate couple is applied at the free end with magnitude equal to $0.5M_{roll}$, where M_{roll} is the moment which would force the beam to deform instantaneously into a full circle. The time-history of the load is shown in the upper plot of the figure. The material considered has an infinity Young modulus of 40 MPa, while the viscoelastic behavior is described by a single Maxwell

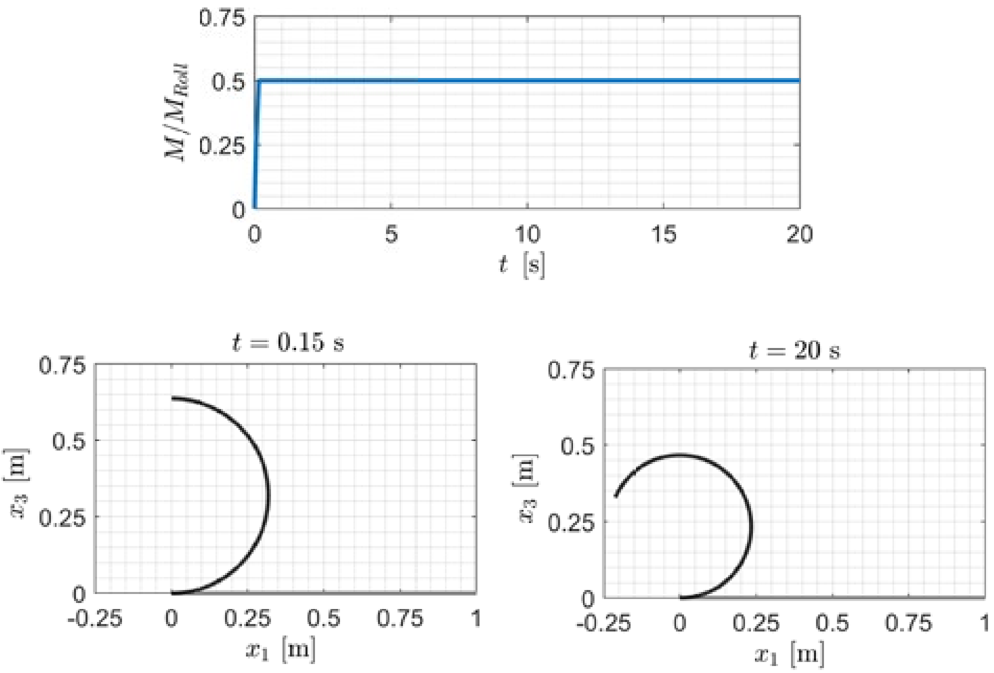

Figure 1: Top figure: Time history of the load. Bottom left: instantaneous response at 0.15 s. Bottom right: long term response at $t = 20$ s.

element with Young modulus equal to 530 MPa and relaxation time of 50 s. The total simulation time is 20 s, with a time step of 0.05 s. As can be observed, the instantaneous elastic response, as expected, is a half circle (see Fig.1 bottom-left), whereas the deformation keeps increasing under constant moment due to the viscous effects (see Fig.1 bottom-right).

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Mixed isogeometric collocation methods with application to cardiac electromechanics

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Keywords: Isogeometric collocation, incompressible elasticity, cardiac electromechanics

We investigate primal and mixed u-p isogeometric collocation methods for application to nearly-incompressible isotropic elasticity [1] with a special focus on cardiac electromechanics. As benchmarks for what might be considered acceptable accuracy, we employ constant-pressure Abaqus finite elements that are widely used in engineering applications. As a basis of comparisons, we present results for compressible elasticity. The performance of the proposed methods will be evaluated on benchmark problems. Small deformations will be initially considered, but also an extension to large deformations will be introduced. A final example of a coupled electromechanical problem in large deformations will be shown [2].

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Crack patterns in masonry panels coupled with the soil

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Keywords: No-tension material, fundamental solution, integral equation, half-plane elasticity.

One of the main sources of damage in masonry structures is related to differential settlements, which can be caused by different phenomena, such as. tunnelling operations, subway construction, underground car parks, soil weakening due to pipe breakage, etc. The corresponding structural effects need to be computed correctly. Furthermore, such settlements are sometimes unknown and need to be located in order to either correct the underground interventions (for instance in the case of car shelter, tube or gallery construction) or to directly remove their causes (for instance pipe breakage). The influence of the soil on the structural behaviour of the overhead structure is therefore evident.

Most of the work on the topic has been developed by uncoupling the soil from the structure, thus, without taking directly into account the soil behaviour's influence on the building. The soil settlement is usually included as boundary condition, i.e. as constant or variable displacement applied on a restricted foundation line. Furthermore, the real no-tension feature is rarely considered in the masonry model.

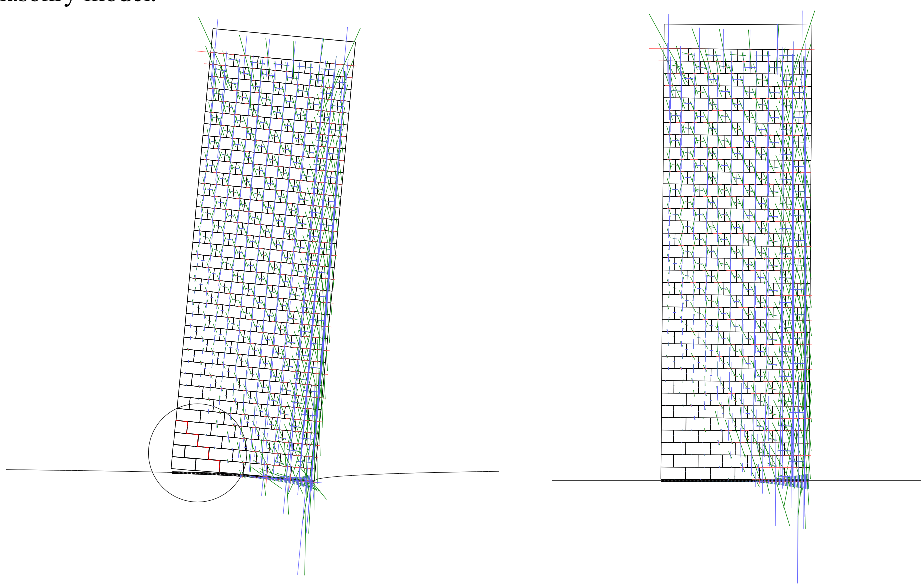

Figure 1: Masonry panel under vertical and horizontal load on the top. Left: with the soil. Right: fixed foundation line.

Based on some experiences of the authors [1-3], the present contribution proposes an approach to investigate the effects of differential settlements on masonry structures by explicitly coupling the soil with the structure while still considering as composed of no-tension material. The soil behaviour is included through a boundary integral approach, which avoids mesh discretisation issues.

Initial numerical examples have demonstrated that the results are affected by the presence of the soil. Indeed, Fig. 1 shows that the mechanical behaviour of the soil influences the crack pattern (in red on the left). With the present approach, voids and inclusions in the soil can be modelled in order to properly describe the source of settlement.

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A new invariant conforming finite element formulation based on the Kirchhoff-Love beam model

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Keywords: Invariant formulation, Geodesic interpolation, Mixed formulation, Conforming finite element, Kirchhoff-Love rod.

In this contribute a new non linear invariant formulation for beam Finite Element (FE) based on the Kirchhoff-Love rod model is presented. Following the idea of Crisfield [1] a re-formulation of the smallest rotation map suitable to account at the element formulation the orthogonality and inextensibility constraints analogously to [2, 3]. On this way, a new geodetic interpolation suitable for the Kirchhoff-Love rod model is obtained then a new family of conforming FEs is designed. Since the configuration space of the beam model is given by the cartesian product $\mathbb{R}^3 \times \mathbf{S}^2 \times \mathbf{S}^1$ the FE formulation designed is prone to locking (membrane and flexural locking), then a mixed approach is preferred in order to improve the efficiency of the numerical methodology. The Hessian of the FE is symmetric since the second variation is performed accounting the Levi-Civita connection of the manifold. Furthermore, these beam FEs can be coupled easily with the shell and plate FEs proposed in [4]. In conclusion the proposed FEs presents high accuracy end robustness as shown by the several numerical investigation proposed.

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Static response bounds of steel frames with uncertain semi-rigid connections

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Keywords: Semi-rigid connections, Interval Analysis, Lower Bound and Upper Bound.

To simplify the analysis and design of frame structures, connections are commonly idealized as perfectly rigid or ideally hinged. However, the actual behavior ranges between these extreme cases, so that semi-rigid or partially restrained (PR) connections are more realistic idealizations (see e.g., [1]). The effects of connection flexibility are commonly incorporated into structural analysis by means of rotational springs at the end nodes of beams. In the context of a simplified linear-elastic analysis, such springs are characterized by their initial rotational stiffness which is expressed in terms of the so-called *fixity factor* (see e.g., [2]). Experimental tests have shown a large scatter of connection stiffness and capacity, even when the same kind of connection is considered. This implies that a deterministic model of the connections may lead to misleading estimates of the actual behavior. Some studies in the literature investigated the influence of uncertain properties of semi-rigid connections on the overall behavior of frames using the classical probabilistic model (see e.g., [3]-[5]). In practical engineering, especially at the early stages of the design, available information is often insufficient to obtain a full probabilistic characterization of the uncertain properties of connections. To cope with this issue, some studies addressed the analysis of frame structures with uncertain semi-rigid connections by using non-probabilistic approaches such as the interval model (see e.g., [6]) and fuzzy sets (see e.g., [7]).

The present study addresses the static analysis of steel frames with semi-rigid connections modelled as rotational springs with uncertain initial stiffness (or *fixity factor*) described as an interval variable [8] with assigned Lower Bound (LB) and Upper Bound (UB). To reduce overestimation due to the so-called *dependency phenomenon*, interval uncertainties are handled by means of the *Improved Interval Analysis via Extra Unitary Interval* [9]. Assuming a linear-elastic behaviour of the rotational springs, the uncertain stiffness of the PR connections is incorporated into the classical matrix stiffness method by interval extension. Due to uncertainty affecting the semi-rigid connections, all response quantities turn out to be described by intervals which define a range of structural behaviour. The bounds of the interval displacements and nodal forces are here evaluated by applying a sensitivity-based procedure which provides accurate results as long as monotonic problems are dealt with. This procedure involves the following main steps: *i*) to evaluate sensitivities of the response quantity of interest to the uncertain parameters; *ii*) to predict the monotonic increasing or decreasing behaviour of the response with respect to each uncertain parameter by studying the sign of sensitivities; *iii*) to identify the combinations of the endpoints of the interval parameters which provide accurate estimates of the LB and UB of the response.

Numerical results concerning a single-bay three-story steel frame with PR beam-to-columns connections (see Fig. 1a) subjected to deterministic static loads are reported for validation purposes. The fluctuations of the *fixity factors* around their nominal values are modelled as dimensionless interval variables with deviation amplitude $\Delta\alpha$, so that $r = 6$ interval parameters are involved. Figure 1b displays the LB and UB of the normalized horizontal displacement of the third floor versus the deviation amplitude of the uncertain parameters $\Delta\alpha$. The accuracy of the presented procedure is assessed by comparison with a time-consuming combinatorial procedure, known as *vertex method* [10] which provides the exact bounds of the response for monotonic problems. In the present case, the *vertex method* involves 2^6 deterministic analyses, as many as are all possible combinations of the endpoints of the interval parameters. An excellent agreement between the sensitivity-based procedure and the *vertex method* can be observed. As expected, the region enclosed by the bounds becomes wider as the degree of uncertainty increases. For comparison purposes, the solutions pertaining to the extreme cases of perfectly rigid and ideally hinged beam-to-column connections are also plotted.

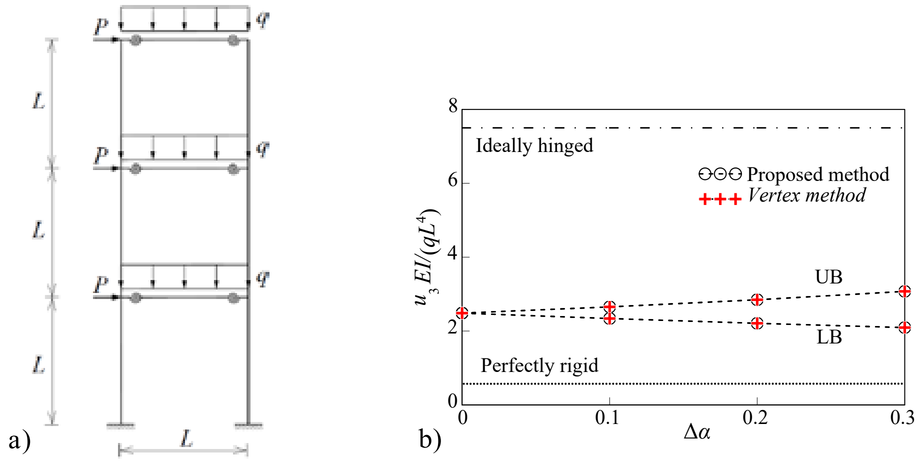

Figure 1: a) frame with partially restrained beam-to-column connections; b) bounds of the normalized horizontal displacement of the top floor versus the deviation amplitude of the uncertain parameters.

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Study of a bi-mass chain with a band gap, and an engineering implementation based on tensegrity prisms

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Keywords: Metamaterial, Band gap, Tensegrity.

In this communication a Maxwell-Rayleigh model is outlined, describing a unidimensional elastic system with hosting and resonant masses [1]. Despite its simplicity this discrete model allows one to deduce, through Piola heuristic homogenization and a variational approach based on Hamilton least action principle, a dispersion relation, revealing the existence of a band gap, in which the propagation of harmonic perturbations is inhibited. Figure 1 illustrates the harmonic perturbations admissible for this system, in terms of nondimensional angular frequency and wavenumber, specified by the so-called acoustic and optical branches, which constitute lower and upper bounds for the band gap. The band frequency range can be tuned controlling the features (mass, stiffness, characteristic length) of the original system. As a meaningful engineering application, reference is made to tensegrity prisms, including compressed bars and tensioned cables, for which it is possible to tune the overall tangent stiffness by governing the cable pre-tensioning, see e.g. [2] and [3]. The preliminary design of a unidimensional chain with hosting and resonant masses, whose mutual elastic connections are constituted indeed of tensegrity prisms, is hence proposed, inhibiting harmonic perturbations in the frequency range of 1-10 Hz, typical of surface seismic waves, see also [4] and [5].

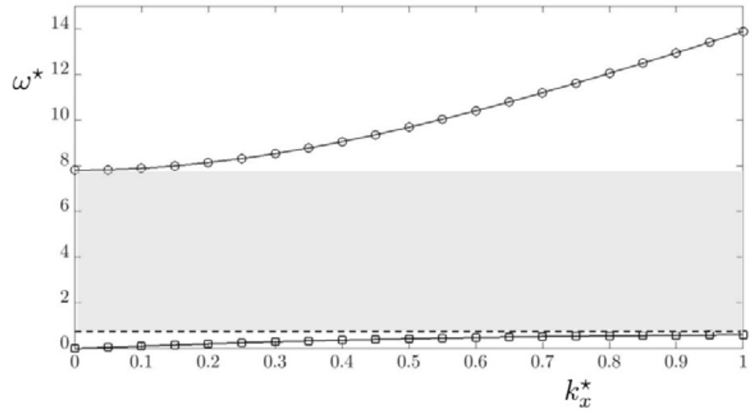

Figure 1: Plane of nondimensional angular frequency ω^* and wavenumber k_x^*. Acoustic and optical branches, marked by squares and circles respectively, delimiting the band gap, grey coloured.

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Instabilities at different scales in an innovative metamaterial

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Keywords: Elastic stability, Periodic lattice, Floquet-Bloch wave analysis.

An important topic in the study of metamaterials and periodic lattices is the stability, because it is possible to tune the mechanical properties of these architected materials, by obtaining extreme features. Here, we analyze a 2D periodic lattice made up of a square grid of elastic beams with rigid finite-size joints and derive a closed form solution of the stability domain of the periodic structure subjected to a macro-stress, as depicted in Figure 1 for diamond-shaped nodes.

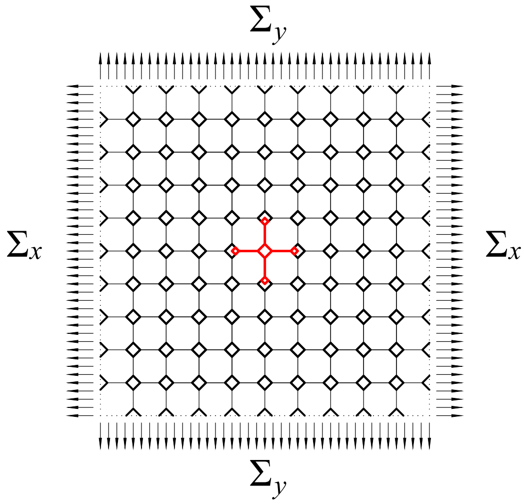

Figure 1: Periodic lattice scheme.

Inspired by works dealing with simpler cases (e.g. [1-3]), we choose a suitable representative volume element (RVE, shown in red in Figure 1) and we assume that the rods are inextensible. By means of this assumption, we derive the critical modes wavelengths by using the Floquet-Bloch theorem (as done [3]). Indeed, it is possible to describe the displacement field in the following form

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{0})\, e^{\frac{i}{L}\boldsymbol{k}\cdot\boldsymbol{x}}\,, \tag{1}$$

where $\boldsymbol{x}$ is the joint coordinate vector

$$\boldsymbol{x} = n_1 L\boldsymbol{i} + n_2 L\boldsymbol{j}\,, \quad (n_1, n_2) \in \mathbb{Z}^2\,, \tag{2}$$

$\boldsymbol{k}$ is the dimensionless wave vector and L is the total length of the cell.

Then, a parametric analysis of the stability domain has been performed by varying the size of the joints. It has been shown that for particular values of the joints size it is possible to obtain critical modes at the microscopic scale (blue line in Figure 2) rather than at the macroscopic scale (orange line in Figure 2).

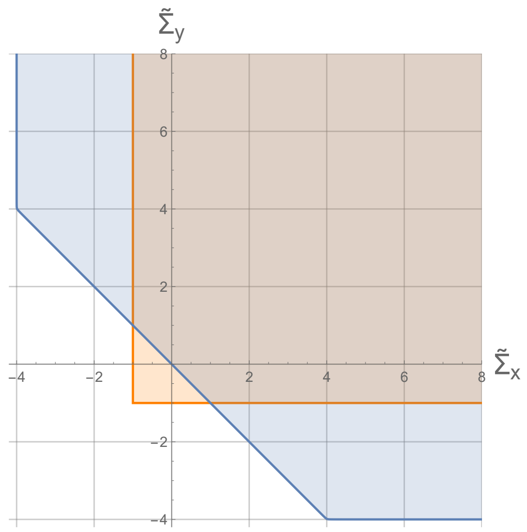

Figure 2: Stability domain plotted in a dimensionless stresses plane.

Finally, the analytical approach has been validated with finite element analyses, by considering both a periodic medium and a finite number of cells.

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Advances in frequency up-conversion of vibration energy harvesters

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Keywords: Piezoelectric energy harvesting, Nonlinear dynamics, Magnetic plucking

Vibration energy harvesting received growing interest in recent decades due to the progress of low-power electronics which makes the development of autonomous sensors an alternative to the consumption of lithium batteries [1]. Among various transduction mechanisms, the use of piezoelectric materials for the creation of resonators has proved successful due to their excellent power density over a large range of voltages. The biggest disadvantage of the linear systems is the mismatch between their natural frequencies (hundreds or thousands of Hz) and the environmental ones (1-100 Hz), which leads to low amounts of energy harvested. This problem can be addressed by widening the operating band with nonlinear techniques [2] such as magnetic plucking, impact-based mechanisms, and snap-through buckling. Magnetic interaction is advantageous as it is contactless and avoids damage to the piezoelectric crystals to achieve the frequency up-conversion. However, its effectiveness strongly depends on the relative velocity between the electromechanical system and the low-frequency system equipped with magnets [3]. There are operational contexts in which the velocity of the harvester is very low (e.g. less than 0.5 m/s) as in the case of human motion, and the frequency up-conversion does not occur.

In this work, we present advances in the field of magnetic force manipulation to improve the magnetic plucking at low velocity [4]. It is possible to manipulate the magnetic force-distance curve between the magnets with the addition of magnetic material (shielding) and a suitable arrangement of the magnetizations to create impulsive phenomena even at low operational velocities. Computational models based on the magnetic nodes approach have been developed which require a low computational cost and are in excellent agreement with magnetic finite element simulations. The experiments confirm what has been supposed on the conceptual side and the influence of various aspects (distance between the magnets, shielding thickness, magnetic configuration) is studied in the case of hard ferromagnetic magnets (NdFeB) through parametric analyses. A computational study on a mesoscale energy harvester is also proposed which demonstrates the performance benefit of the technique in terms of phase portrait response. The result of the work demonstrates that with the proposed technique it is possible to have an activation of the structural mode of interest when in the case of traditional magnetic interaction (i.e. without shielding) it would not occur. The originality of the work extends the application to the sensing and actuation fields.

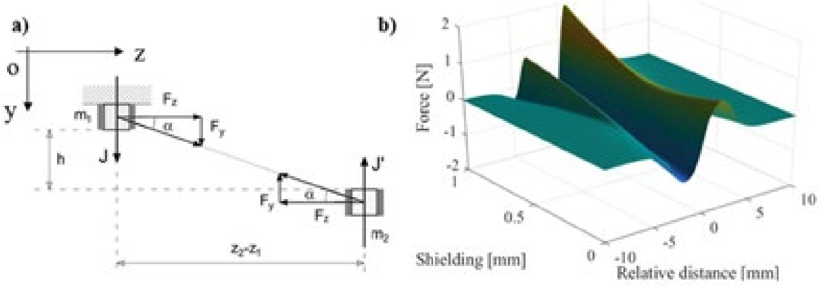

Figure 1: a) schematic of the interacting magnets with shielding, b) parametric analyses of the F_z component of the magnetic force for gap h=0.5 mm, J=1.32 T, and varying shielding thickness

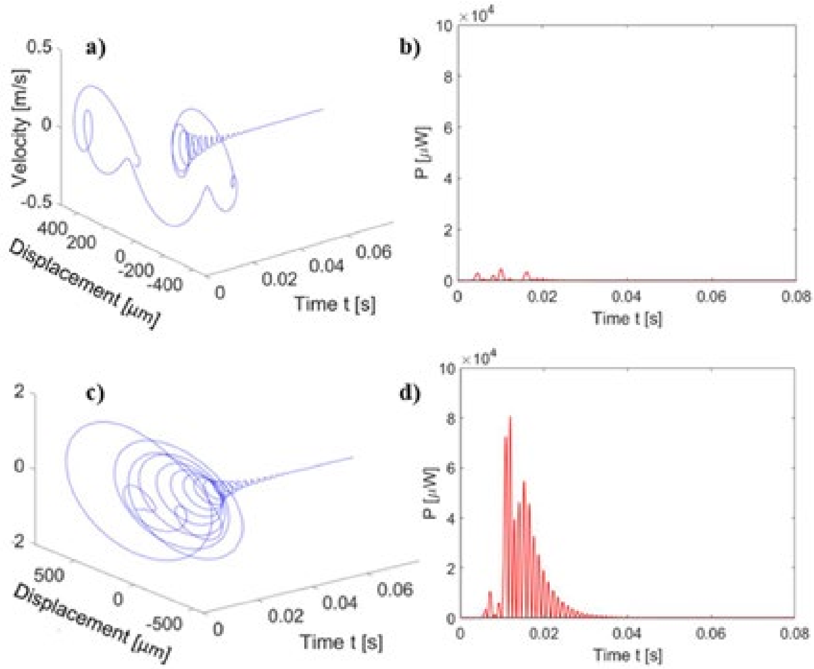

Figure 2: simulated results for h=0.5, R=100 kΩ, velocity of interaction 0.9 m/s, for a typical piezoelectric harvester. Phase portrait and istantaneous power for the magnetic plucking without shielding a), b), and with the proposed technique c) and d).

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A multi-physic predictive model for corrosion in concrete

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Keywords: Reinforced concrete, corrosion, cracking, phase field.

Environmental effects on reinforced concrete elements represent the most common and threatening form of degradation. In fact, due to exposure to the outer environment, the structural integrity of reinforced concrete structures reduces as corrosion related phenomena evolve [1]. To investigate the environmental deterioration mechanisms affecting reinforced concrete elements, the present work presents a numerical model analysing the carbonation corrosion deterioration phenomena [2, 3]. The description of the concrete carbonation process is performed using a transport-diffusion-reaction coupled system of equations, describing the diffusion and reaction of the carbon dioxide through the concrete pores while also accounting for the effects of moisture content on the carbonation process [4, 5]. Due to carbonation, a change in the concrete material properties is observed. Additionally, the pH value of the concrete pore water drops to neutral levels causing the progressive depassivation of the steel reabar. As the passive layer protecting the rebar dissolves, the corrosion process begins leading to the formation of rusts deposits on the rebar surface. Using the electrochemical kinetics equations, the change in volume associated with the formation of rust is numerically evaluated over the depassivated portion of the rebar [3]. Lastly, cracking and eventually spalling of the concrete cover is observed due to the increase in pressures on the concrete cover surrounding the steel rebar as more rust accumulates. Using the phase field model for fracture, the rupture of the concrete cover is described [6].

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Self-contractile biopolymer gels: a continuum mechanics perspective

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Keywords: self-contractile, elastic gels, continuum mechanics.

Self-contractile active gels are usually generated by polymerizing actin in the presence of cross-linkers and clusters of myosin as molecular motors [1]. Mechanics of active gels present interesting characteristics: self-contractions generate internal stresses and stiffen the material, so driving the network into a highly nonlinear, stiffened regime; and morphing from flat to curved geometries can be expected when thin discs of active gels are considered [2].

We explore some of those mechanisms from the point of view of continuum mechanics of remodeling bodies[3, 4]. Self-contractions are viewed as the effects of network remodeling. It drives the change in the mechanical stiffness of the polymer and the chain shortening, which are two of the main mechanisms evidenced in the experiments [2, 5].

It is evidenced the competitive roles of contraction and liquid transport in driving the mechanics of active gels. With reference to a specific problem whose analysis has been inspired by the work presented in [2], where the contraction dynamics of an active gel disc, whose geometry is defined by radius and thickness, has been followed and described with great details, we'll show how gel dynamics inherits length scales which are typical of the liquid transport processes and the gel dimensions' aspect ratio (radius to thickness) impact on the gel dynamics.

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Digital twin models for high-fidelity contact mechanics simulations

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Keywords: Contact Mechanics, Digital twin models, Roughness, Finite Element Analysis.

The solution of contact problems between bodies is an important topic in physics and engineering [1,2]. Surface-surface interactions play a key role in stress transfer, friction, wear, and also for heat and electric conduction. In this regard, the miniaturization trend observed nowadays in technology requires the development of high-fidelity contact mechanics simulations accounting for surface textures and microscopic roughness, which are observable over multiple length scales [3].

In this field, the application of the Boundary Element Method (BEM) has been widely exploited [4] since it benefits from the sole discretization of the boundary and not of the bulk. However, the methodology is intrinsically limited to problems where the Green functions relating the displacements of the points belonging to the boundary to the applied contact tractions are available, and to linear problems where the principle of superposition can be invoked. Therefore, although some significant efforts have been made to extend and apply BEM to adhesion [5-7] and viscoelasticity [8], the underlying model assumptions preclude its straightforward generalization to nonlinear interface and bulk constitutive relations, and also to multi-field coupled problems. Notable examples regard, for instance, contact-induced fracture, or fully coupled nonlinear thermo-mechanical problems, to cite a few.

To overcome the above limitations, the Finite Element Method (FEM) would be the natural remedy. However, due to the higher computational cost associated to the discretization of the bulk and the complexity in meshing nonplanar interfaces, its application to contact problems with roughness has been largely confined to few instances [9,10]. Moreover, the convergence of contact search algorithms in the presence of multi-scale roughness –that cannot be smoothed out by regularization techniques since one wants to preserve the original high-resolution topological features– can be extremely problematic.

In this work, the advantages of a novel finite element discretization technique relying on the eMbedded Profile for Joint Roughness (MPJR) interface finite element [11], and the associated contact solution scheme, are discussed in relation to challenging engineering problems.

The method is based on a direct embedding of the deviation from planarity into the interface finite element, to be used as a correction to the normal gap function. The method, applicable to both rigid-deformable and to deformable-deformable solids in contact, is particularly efficient from the computational point of view for the following main reasons: (*i*) the interface is globally discretized as nominally flat; (*ii*) any height field perturbing the planarity can be incorporated, either given by a continuous analytical function when available, or directly provided by discrete profilometric/AFM measured data; (*iii*) no smoothing or regularization of the height field is required; (*iv*) contact search algorithms can be fully avoided by considering a fixed pairing of nodes at the interface.

To allow the use of the MPJR interface finite element in most of the commercial FEA software and minimize the access to external files, the profile/surface data field is stored into a history variable as a set of elevations for the corresponding spatial coordinates, operation done only once at the initialization of the FE simulation. During the contact problem, the normal gap is computed based on the kinematic relations of the interface finite element and then it is corrected by considering the actual embedded elevations at the nodal level as a perturbation from the initially assumed planarity.

The methodology has been applied to frictional contacts in partial slip [12] and also in a full sliding regime [13] for viscoelastic solids. Moreover, the method has been extended to 3D with friction and adhesion [14].

Further advanced applications shown in this work regard the exploitation of the proposed methodology to complex nonlinear contact problems involving coatings, thermo-mechanical loads, fracture in the bulk, and also wear. In all of those problems, the methodology will benefit from the major advancements in FEA research, with the aim of addressing tribological problems of high industrial relevance.

Acknowledgements

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A coupled approach to predict cone-cracks in spherical indentation tests with smooth or rough indenters

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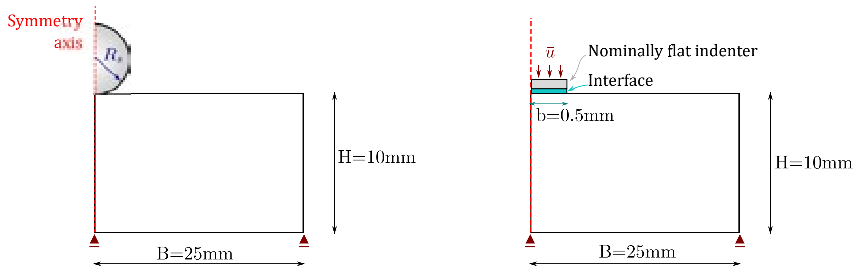
Keywords: spherical indentation, fracture mechanics, contact mechanics, roughness.

Indentation tests are largely exploited in non-destructive experiments to characterize the mechanical properties of the materials from the resulting crack patterns, which can be directly related to hardness and fracture properties of the material. The phase-field approach has been proved to be an efficient tool for failure simulations of brittle and ductile materials under different loading conditions, and it has been successfully applied in [1, 2] to simulate flat punch indentation tests. The consistent computational cost related to the indenter discretization and the nonconformal contact problem limits the simulation of more complex indenting geometries. In order to overcome this issue, this work proposes an efficient theoretical and numerical framework for simulating cracking phenomena due to nonconformal contacts with indenter profiles of arbitrary shapes.

The formulation relies on a coupled approach involving the phase-field variational framework to model the cracking process of the indented material, and the MPJR (eMbedded Profile for Joint Roughness) interface finite elements [3, 4] to solve the nonconformal contact problem between the indenter and the substrate.

The MPJR interface finite elements embed the indenter geometry so that the model consists of a nominally flat indenter without the need for an explicit discretization of its profile, see Fig. 1. Their formulation, in fact, considers the actual indenter profile as a correction to the normal gap at the interface between the indenter and the substrate, and solves the contact problem between the two solids. In the proposed work, the MPJR formulation has been specialized for 2D axisymmetric case to simulate the case of spherical indentation efficiently.



(a) Real geometry. (b) Model geometry.

Figure 1: Real geometry (left) and model geometry obtained using the MPJR interface finite elements (right).

The novel framework is applied to predict cone-crack formation in the case of indentation tests with smooth spherical indenters shown in Fig.2, with validation against experimental data.

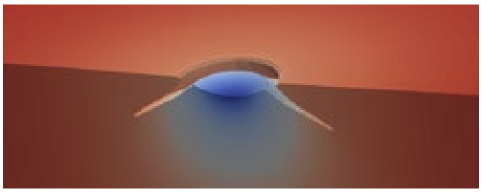


Figure 2: 3D view of the crack pattern due to a smooth spherical indenter.

Moreover, the coupled approach permits the evaluation of the micro-scale effect of the presence of roughness on the indenter and on the sampled surfaces, usually neglected in the standard simulations: the rough profile can be directly introduced in the simulation through the interface finite elements, see Fig.3.

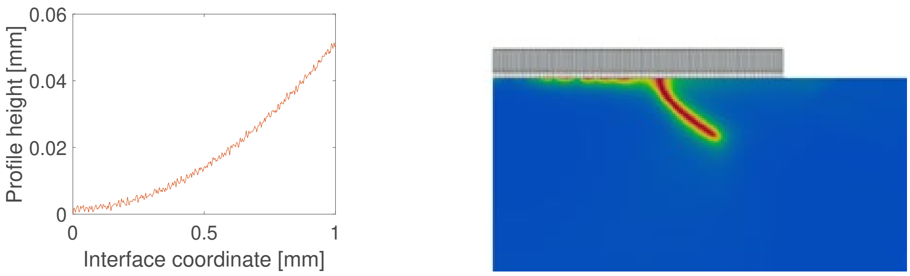


Figure 3: Axisymmetric simulation of a cone-crack (right) caused by the rough profile of spherical indenter embedded in the interface (left).

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Energetically orthogonal fracture mode partitioning of the J-integral for cohesive interfaces

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Keywords: Cohesive zone model, mixed-mode fracture, J-integral.

The cohesive zone model (CZM) was developed in the '60s of the last century, independently, by Dugdale [1] to investigate plastic fracture and Barenblatt [2] to account for the finite strength of brittle materials. More recently, numerical implementations of the CZM have gained increasing popularity, in particular for the analysis of delamination in composite laminates [3].

According to the CZM, the damage phenomena occurring in the fracture process zone (FPZ) ahead of the crack tip are described by cohesive laws, which relate the stresses acting on the fracture surface with the corresponding relative displacements. In a plane problem, the cohesive laws express the normal and tangential interfacial stresses, σ_n and σ_t, as functions of the normal and tangential relative displacements, δ_n and δ_t. Cohesive laws can be classified in different ways. A first, fundamental distinction is between cohesive laws that can be derived from a cohesive potential function, $\Phi\left(\delta_t, \delta_n\right)$, and those that cannot. Another distinction is between uncoupled cohesive laws, for which σ_t is a function of only δ_t and σ_n is a function of only δ_n, and coupled cohesive laws, for which the interfacial stresses depend on both the relative displacements [4].

A powerful tool for the theoretical and experimental investigation of cohesive laws [5] is offered by the path-independent J-integral introduced by Rice [6]. For a general cohesive interface,

$$J = \int_{(0,0)}^{(\Delta_t,\Delta_n)} \sigma_t\left(\delta_t, \delta_n\right) \mathrm{d}\delta_t + \sigma_n\left(\delta_t, \delta_n\right) \mathrm{d}\delta_n, \tag{1}$$

where Δ_t and Δ_n are the tangential and normal relative displacement at the crack tip, respectively.

If the cohesive laws are potential-based, then the interfacial stresses can be obtained as follows:

$$\sigma_t = \frac{\partial \Phi}{\partial \delta_t} \qquad \text{and} \qquad \sigma_n = \frac{\partial \Phi}{\partial \delta_n}. \tag{2}$$

By substituting Eqs. (2) into (1),

$$J = \int_{(0,0)}^{(\Delta_t,\Delta_n)} \frac{\partial \Phi}{\partial \delta_t} \mathrm{d}\delta_t + \frac{\partial \Phi}{\partial \delta_n} \mathrm{d}\delta_n = \int_{(0,0)}^{(\Delta_t,\Delta_n)} \mathrm{d}\Phi = \Phi\left(\Delta_t, \Delta_n\right), \tag{3}$$

where the final result is independent of the integration path in the plane of δ_t and δ_n because $\mathrm{d}\Phi$ is an exact differential.

If the cohesive laws are uncoupled, then the cohesive potential function can be decomposed as

$$\Phi\left(\delta_t, \delta_n\right) = \Phi_{\mathrm{I}}\left(\delta_n\right) + \Phi_{\mathrm{II}}\left(\delta_t\right), \tag{4}$$

where $\Phi_{\mathrm{I}}\left(\delta_n\right)$ and $\Phi_{\mathrm{II}}\left(\delta_t\right)$ are the mode I and mode II cohesive potential functions, respectively. As a consequence, the J-integral, Eq. (1), can be split into the sum of a mode I contribution,

$$J_{\mathrm{I}} = \int_{(0,0)}^{(\Delta_t,\Delta_n)} \sigma_n\left(\delta_n\right) \mathrm{d}\delta_n = \int_{0}^{\Delta_n} \sigma_n\left(\delta_n\right) \mathrm{d}\delta_n = \Phi_{\mathrm{I}}\left(\Delta_n\right), \tag{5}$$

and a mode II contribution,

$$J_{\mathrm{II}} = \int_{(0,0)}^{(\Delta_t,\Delta_n)} \sigma_t(\delta_t)\,\mathrm{d}\delta_t = \int_0^{\Delta_t} \sigma_t(\delta_t)\,\mathrm{d}\delta_t = \Phi_{\mathrm{II}}(\Delta_t)\,. \tag{6}$$

However, if the cohesive laws are coupled, then the fracture mode partitioning is not trivial as $\sigma_t(\delta_t, \delta_n)\,\mathrm{d}\delta_t$ and $\sigma_n(\delta_t, \delta_n)\,\mathrm{d}\delta_n$ are not exact differentials. As a consequence, the line integrals in Eqs. (5) and (6) depend on the integration paths [7]. Moreover, it can be shown by examples that even physically inconsistent, negative values of J_{I} and J_{II} can be obtained from the above equations.

This work explains how the J-integral can be split into the sum of two physically consistent, positive definite, mode I and mode II contributions. To this aim, the concept of energetic orthogonality between fracture modes is exploited. More in detail, it is assumed that mode I is related to a null tangential relative displacement at the crack tip, $\Delta_t = 0$, and that the forces related to mode II are energetically orthogonal to those related to mode I. The same concept has already been applied to partition fracture modes in finite element models by the virtual crack closure technique (VCCT) [8, 9] and in beam-theory models of laminated beams [10]. Here, the method will be first illustrated with respect to linear, coupled cohesive laws and then extended to nonlinear, coupled cohesive laws.

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Spontaneous nonreciprocal oscillations in polyelectrolyte gel filaments

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Keywords: flutter and divergence instability, polyelectrolyte gels, artificial cilia.

Soft actuators typically require time-varying or spatially modulated control to be operationally effective. The scope of the present paper is to show, theoretically and experimentally, that a natural way to overcome this limitation is to exploit mechanical instabilities.

We report experiments on active filaments of polyelectrolyte gels subject to a steady and uniform electric field. A large enough intensity of the field initiates the motion of the active filaments, leading to periodic oscillations. We develop a mathematical model based on morphoelastic rod's theory for polyelectrolyte gel filaments beating in a viscous fluid and carry out the stability analysis of the governing equations to show the emergence of flutter and divergence instabilities for suitable values of the system's parameters [1].

We confirm the results of the stability analysis with numerical simulations for the nonlinear equations of motion to show that such instabilities may lead to periodic self-sustained oscillations, in agreement with experiments. The key mechanism that underlies such behavior is the capability of the filament to undergo active shape changes depending on its local orientation relative to the external electric field, in striking similarity with gravitropism, the mechanism that drives shape changes in plants via differential growth induced by gravity [2, 3, 4]. Interestingly, the resulting oscillations are nonreciprocal in nature, and hence able to generate thrust and directed flow at low Reynolds number.

The exploitation of mechanical instabilities in soft actuators represents a new avenue for the advancement in engineering design in fields such as micro-robotics and micro-fluidics.

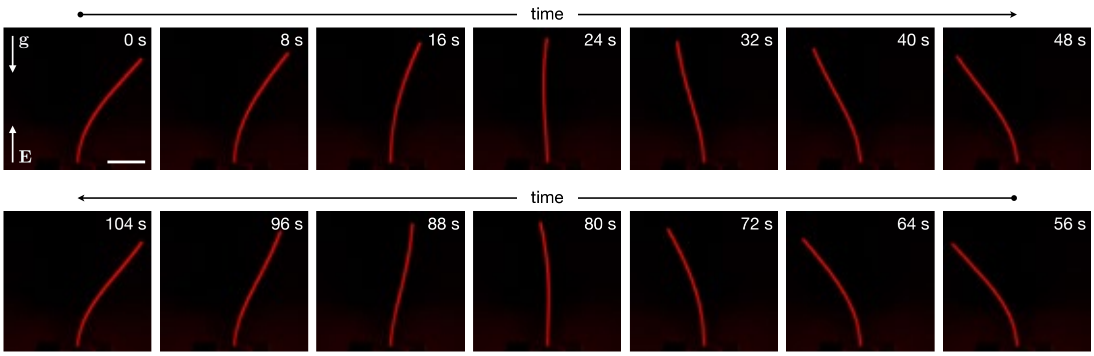

Figure 1: A polyelectrolyte gel filament in a solution of sodium chloride in water is clamped at its base and exhibits periodic oscillations when subject to a static and uniform electric field **E** directed along the vertical line. The snapshots are taken 8 seconds apart while the scale bar indicates 10 mm.

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A coupled Lattice-Boltzmann and Langevin-dynamics method for simulating transport of nanoscale vesicles in microchannels

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Keywords: Nanovesicles transport, Lattice-Boltzmann, Langevin dynamics

Modelling all the constituents of biological fluids is challenging because of the different length scales between cells (8÷120 µm) and vesicles (30÷150 nm) and their complex dynamics. Understanding such dynamics is crucial to exploit the presence of nanoscale vesicles (NVs), such as exosomes, for disease detection and treatment, as well as the development of personalized therapeutic strategies involving microfluidic devices [1]. In this context, a coupled Lattice-Boltzmann (LB) and Langevin dynamics (LD) method [2-3] has proven to be a suitable three-dimensional multiscale approach to perform *in silico* parametric studies.
Here, a two-way coupled LB-LD method is adopted to investigate the transport of NVs in microchannels. The flow evolution is modeled on a three-dimensional computational lattice (D3Q19). 19 distribution functions $f_i(\boldsymbol{r},\ t)$ (i = 0, ..., 18) representing particles at position $\boldsymbol{r}$, time t, and flowing with velocity $\boldsymbol{e}_i$ are transported using the Boltzmann equation

$$f_i(\boldsymbol{r} + \Delta t\boldsymbol{e}_i,\ t + \Delta t) = f_i(\boldsymbol{r},\ t) - \frac{\Delta t}{\tau}\,[f_i(\boldsymbol{r},\ t) - f_i^{eq}(\boldsymbol{r},\ t)] + f_i^{S}(\boldsymbol{r},\ t) \qquad (1)$$

where the equilibrium state $f_i^{eq}(\boldsymbol{r},\ t)$ is reached over the unique relaxation time τ, and $f_i^{S}(\boldsymbol{r},\ t)$ is a forcing term accounting for the presence of NVs, treated as sub-lattice point particles (Fig. 1). The dynamics of the *i*-th NV is described via the Langevin equation:

$$m_v{}^i\frac{d\boldsymbol{u}_v{}^i}{dt} = \boldsymbol{F}_v{}^i + \boldsymbol{S}_v{}^i + \boldsymbol{C}_v{}^i \qquad (2)$$

where the friction force exerted by the fluid, $\boldsymbol{F}_v$, follows the Stokes' law; each component of the stochastic force, $\boldsymbol{S}_v$, exhibits a Gaussian distribution with zero mean; and the conservative forces, $\boldsymbol{C}_v$, describing the vesicle-vesicle and vesicle-wall interactions are defined starting from the standard Lennard–Jones potential.
First, by setting the stochastic forces to zero, a single NV (diameter 100 nm) with initial nonzero velocity is released into quiescent water to only observe the deterministic vesicle-fluid interaction. A fluid lattice domain of 100^3 nodes with periodic boundary conditions in all directions is chosen to limit the confinement effect on the NV velocity relaxation. Fig. 2(a) shows that for inertial NVs the velocity decays exponentially in the short term and as a power law in the long term. Interestingly, the velocity of NVs with negligible inertia, e.g., exosomes, follows only the power law. The contribution of additional stochastic forces is then evaluated. The stochastic relaxation curve obtained averaging ten independent simulations qualitatively agrees with the deterministic curve under the same flow conditions, see Fig. 2(b).
Then, a dilute concentration of 100 NVs with three diameter sizes (10, 50, 100, 500 nm) was simulated in a 100^3 fluid lattice domain at room temperature to evaluate Brownian diffusivity. Fig. 3 shows that the long-term diffusivity follows the Stokes–Einstein theory and the mean squared displacement (MSD) decreases as the diameter of NVs increases.

All results show that the complex dynamics of NVs is correctly described, including long-range many-body hydrodynamics interactions, thermal fluctuation, and vesicle-vesicle interactions. The method is promising for further investigation of diffusivity of NVs in several blood flows.

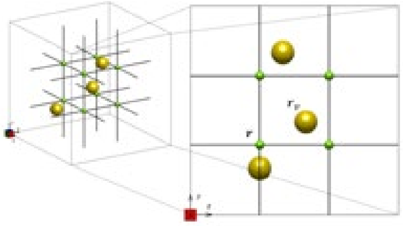
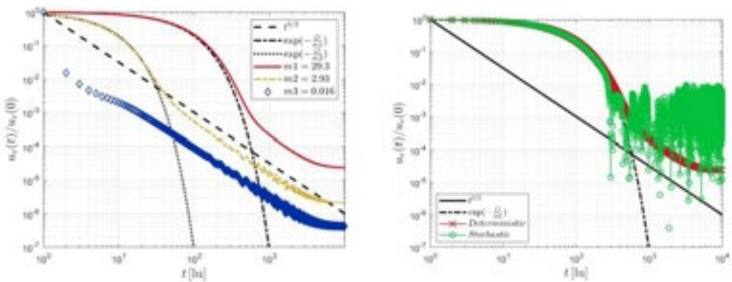


Figure 1: Lattice nodes (green) defined at site $\boldsymbol{r}$; sub-lattice NVs (yellow) at position $\boldsymbol{r_v}$.



(a) (b)

Figure 2: NV velocity relaxation under (a) deterministic and (b) stochastic condition.

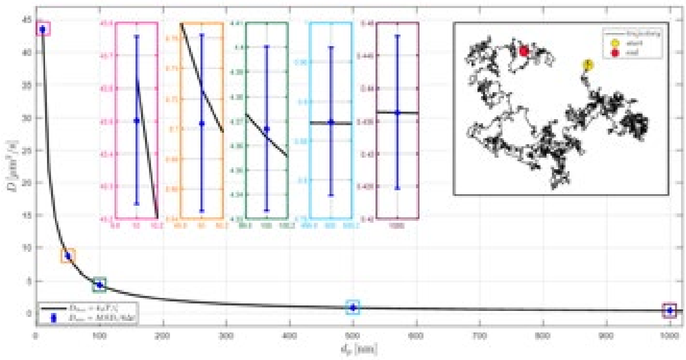


Figure 3: Self-diffusivity of dilute concentration of 100 NVs as a function of NVs size.

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Analysis of the distribution and orientation of oxygenated and non-oxygenated blood in a Double Outlet Right Ventricle.

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Keywords: Double Outlet Right Ventricle, Cardiac Flow, Direct Numerical Simulation.

Double Outlet Right Ventricle (DORV) is a malformation of the fetal heart in the uterus that affects the ventricular chambers following the shift to the right of the aorta, it presents the right ventricle (RV) with both the aorta and the pulmonary outflow tracts originating from it, and the left ventricle that communicates to the right through a ventricular septal defect (VSD). DORV is rare and the causes are unclear, in some cases it happens to babies who have defects within their chromosomes [1]. Symptoms of DORV usually appear during the first days or weeks after birth, although sometimes the defect can be identified before birth using fetal echocardiography. DORV is always associated with a VSD, an opening in the interventricular septum that puts the two ventricles in communication and allows blood to drain from the left ventricle (LV) into the RV.

Due to this malformation, the direct communication between pulmonary and aortic arteries leads to an increase of pressure in the pulmonary circulation that can damage the lungs. However, the principal criticality is due to the oxygenated and non-oxygenated blood that mix inside the RV, which can eject part of the oxygenated blood in the lungs and, importantly, a significant amount of non-oxygenated blood in the systemic circulation that may be insufficient for vital function. This incorrect division of the flow can damage lungs, tissues and various organs and, in some cases, endanger life support. In fact, most children with DORV require heart surgery within the first year of life. The degree of severity to which the pathology reflects in the immediate cardiovascular function depends crucially on the relative oxygen distribution between the pulmonary and systemic circulations. An outcome that depends on the details of the vortical flow pattern that develops inside the two-ventricles domain.

This study analyzes one complete case through the use of numerical simulations which allows to identify the concentrations of oxygenated and non-oxygenated blood transiting though the RV. The time-varying geometry of the two ventricular chambers was extracted from 3D-transesophageal echocardiography (TEE); the moving boundaries of the ventricular cavities are obtained by a semi-automatic procedure through dedicated software (4D LV-Analysis, 4D RV-Function; Tomtec Imaging Systems GmbH, Unterschleissheim, Germany) that also identifies the size and location of the valves. The numerical method, described in [2], solved the incompressible Navier-Stokes and continuity equations using the fractional step technique in the immersed boundary method; it is implemented in in a bi-periodic Cartesian domain to optimize the solution of the elliptic equation. Although the overall geometry is imposed from data extracted from subject's imaging, the dynamics of the valvular leaflets withing such geometry follows from fluid-structure-interaction; this is is implemented here using a simplified approach where the valvular moving geometry is extracted from images and parameterized with few degrees of freedom (e.g. the number of independent leaflets) and their dynamics is dictated by the integral kinematic condition that the motion of the leaflet surface matches with the velocity of the fluid at the same position. This procedure is described in details in

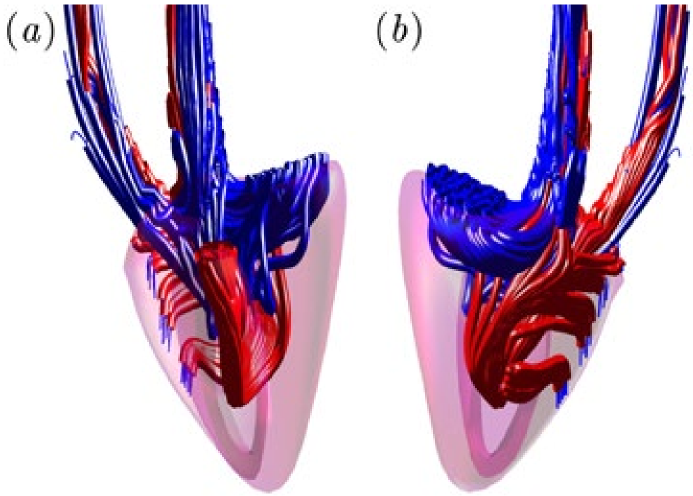

Figure 1: Streamlines of the steady-streaming (systolic phase-average) - (*a*) front view - (*b*) back view

[2], the result is a system of linear equations whose *i*th term reads

$$\left[\int_{A_v}\left(\frac{\partial \mathbf{X}_v}{\partial \varphi_i}\cdot \boldsymbol{n}\right)\left(\frac{\partial \mathbf{X}_v}{\partial \varphi_j}\cdot \boldsymbol{n}\right)dA\right]\frac{d\varphi_j}{dt}=\int_{A_v}(\boldsymbol{v}\cdot\boldsymbol{n})\left(\frac{\partial \mathbf{X}_v}{\partial \varphi_i}\cdot \boldsymbol{n}\right)dA; \tag{1}$$

where $\boldsymbol{n}$ is the normal to the valvular surface and the subscript $_v$ stands for either the mitral or the tricuspid valve (summation over j is implicit and extends to 2 or 3 for the mitral and tricuspid valve, respectively).

The resulting fluid dynamics shows substantial differences from that of the ventricles taken individually [3], because the communications between them through the VSD creates both a short circuit between the pulmonary and primary circulation that are not more in series, and the oxygenated blood from the left side mixes with the non-oxygenated on the right. The analysis of blood concentration permitted to quantify the relative percentage of oxygenated blood ejected into the pulmonary artery and of non-oxygenated blood into the aortic artery (see figure 1). The analysis of this specific case aims to demonstrate how the fluid dynamics analysis of this rare malformation, properly coupled with imaging technology, can provide information that could not be obtained otherwise and that are relevant for a careful clinical management including timely therapeutic intervention.

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Modeling and experimental analysis of the relationship between mechanical response and microstructure in arterial tissues

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Keywords: Soft tissues, Constitutive models, Imaging-based mechanical tests.

Analysis of microstructural properties of biological soft tissue plays an important role in understanding its mechanical response and remodeling. Soft tissues, such as aorta walls, can be regarded as fibrous materials assembled form ground matrix.

Alterations occurring to the embedded families of collagen fibers have been shown to play a significant role in the pathogenesis of aortic degeneration. By combing digital image correlation (DIC), small-angle light scattering (SALS) and multiscale computational modeling, the still not well know relationship between mechanical response and microstructure in healthy and pathological arterial tissues was investigated.

The study was conducted on pathological tissue samples, specifically affected by aneurysm. An aortic aneurysm is a localized bulging of the aorta characterized by partial weakening of the blood vessel. Irregular hemodynamics have been shown to accelerate the progression of such pathology with common basis provided by diabetes, male sex, smoking, and hypertension. In addition, imbalance of tissue biochemical pathways results in the onset of pathological remodeling and thus histological changes that affect vascular mechanics [1].

Experimental tests and computational analyses were performed. The experimental mechanical characterization is made through biaxial force-controlled tensile tests at different tensile ratios, both along the circumferential and the axial direction. Using DIC, first displacement and then the strain field could be accurately identified to reconstruct the internal strain field in the specimen at each loading condition. From these data, stress-strain curves were reconstructed, accounting at each value of load (i.e., stress via specimen thickness) also for the variability of the deformation within specimen. A second imaging, technique, namely SALS, is used to analyze the microstructure. By performing SALS and tensile tests simultaneously, we can provide information on the preferential orientation and distribution of collagen fibers during mechanical loading.

To perform the modeling analysis, the arterial tissue was described as a non linear hyperelastic material, using a micro-macro description for the mechanics of crimped collagen fibers. In fact, the straightening of crimped fibers in biological soft tissues is responsible for their non linear macroscopic mechanical response. Therefore, the stress-strain curve takes the characteristic J-shaped curve, reproduced un the model by explicitly depending on a set of clearly observable microstructural parameters [2].

A finite element implementation of such multiscale modelling technique is considered to reproduce then non homogeneous strain field as obtained from DIC images. For the finite element discretization, quadrilateral elements have been introduced, generated in Wolfram Mathematica. In each material point of the domain the presence of crimped fibers in their undeformed configuration was considered, with different orientations as read from SALS measures. Other microstructural parameters, e.g., radius and amplitude were calibrated through a process of parametric identification and numerical optimization for the fixed tension ratio 1:1.

A comparison of experimental and modeling results validated the proposed model and showed an existing relationship between arterial tissue microstructure and mechanics. The results obtained are not only representative of the mean mechanical response, but also of the dispersion of strains in the tissue as obtained from DIC. This correspondence, albeit with different degrees, is maintained even moving away from the calibration condition of the model, that is the tension ratio 1:1, towards different tension ratios.

Another important result is that the model is representative of the tissue behavior in terms of collagen fiber realignment as obtained from SALS measures during mechanical loading.

The present work has shown how a multiscale modelling technique is predictive of the mechanical response but also of the microstructure in terms of fiber thickness, amplitude, and orientation of collagen fibers during loading. The strong interconnection between mechanics and microstructure is hence highlighted, developing a predictive tool that can serve in future studies of tissue remodeling.

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A predictive model of epi-off UVA-riboflavin crosslinking treatment on porcine corneas

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Keywords: epi-off crosslinking, cornea stiffening, in-depth stromal stiffening, analytical formulae

A set of pressure inflation experiments, performed on untreated porcine corneas and on the same corneas after epi-off crosslink (CLX, a stiffening procedure, based on UV-A irradiation on tissue soaked in riboflavin, used in ophthalmology to strengthen weak corneas), was published in [2]. The experimental work, involving 90 pig corneas, aimed at understanding the relevance of the irradiation duration on the corneal stiffening. Corneas were divided in 5 groups, each group receiving the same riboflavin imbibition, while the duration of the irradiation was different for each group, i. e., 2.5, 5, 10, 15 and 20 minutes. Results demonstrated that the irradiation duration has a marked effect on the stromal stiffening with respect to the pre-CXL condition, and a positive correlation between irradiation duration and stiffening was found. The increment of stiffness in terms of equivalent elastic modulus E was obtained by interpreting the inflation results through a classic linear model of spherical shells. The model provided a unique number for the elastic modulus, E_b, before the treatment, and E_a, after the treatment, and their difference measures somehow the effect of the CXL, but clearly the simplifying assumptions (homogeneity, uniform thickness, spherical shaper, isotropy) necessary to apply the linear shell model do not find correspondence to real cases.

In a parallel study, we tried to provide a more satisfactory interpretation of the experimental results reported in [2] by using finite element simulations, with the goal to understand the in-depth modification of the collagen stiffness [3]. For each test we had the images of the pressurized cornea as a function of the increasing IOP, but we did not have information on the internal microstructure of the stroma. We used a very simple one-dimensional model of the through thickness stiffening of the stroma, by assuming that the stiffening reached an uniform value $E_c = cE_b$ from the anterior surface to a specific depth $(1-d)t$, with t the central corneal thickness. The coefficients d and c were obtained by fitting the results of the inflation tests on post-CXL corneas. The piecewise-constant stiffening profile was suitably converted in stiffness coefficients in a more sophisticated model of the human cornea, that accounts for the presence of distributed collagen fibrils to confer anisotropy and in-homogeneity to the material [1]. Regrettably, but unsurprisingly, the approximation was not satisfying. The reason was to be ascribed to the fact that the stiffening profile was way too far from the actual distribution of stiffness which also in pre-CXL conditions is characterized by a through thickness variability [3].

Aim of this work is to improve in a more realistic way the one-dimensional CXL stiffening profile model proposed in [3], by considering not only the irradiation duration, but also the presence of a gradient in the stromal stiffness before CXL. We observe that an accurate evaluation of the stiffness profile can provide an excellent prediction of the post-CLX stiffening of the cornea.

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Silicone oil tamponade flow dynamics following everyday movements

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Keywords: ocular fluid dynamics, silicone oil tamponade, wall shear stresses

Pars plana vitrectomy is a surgical procedure performed following retinal detachment and consists in the replacement of the vitreous with a fluid substitute. Understanding how the presence of tamponade affects the forces acting on the endothelium and the near-wall transport is a main concern in assessing the effectiveness of the surgical technique and its outcome. While gas tamponade is characterized by large sloshing movements, silicone oil is less prone to such displacements of the interface, for short time scales. Nevertheless, much larger forces developing at the surface, compared to the gas tamponade case, are observed following saccadic movements. After the surgical procedure, the patient is instructed to maintain a prescribed posture; however, some everyday movements, leading to abnormal wall shear stresses, are unavoidable. Therefore, their effect is worth a detailed investigation since abnormal wall shear stresses may promote the re-detachment of the tear edges and eventually of the retina.

We numerically investigate the multiphase flow of silicone oil tamponade with aqueous at different filling ratios in human eye models (Figure 1(a,b)), in steady and unsteady conditions. The two fluid phases are simulated through the VOF method embedded in OpenFoam.
In contrast to the gas tamponade case [1], the static interface shape is dominated by surface tension, and large surface wetting of the silicone oil is obtained only with very large filling ratios (Figure 1(c)).

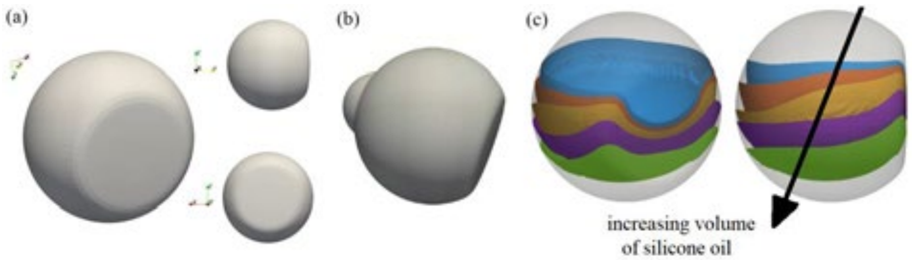

Figure 1: (a,b) Two models of human eye: emmetropic eye (a) and posterior staphyloma (b). (c) Initial conditions for the transient simulations with varying filling ratios.

The unsteady equations are solved in the non-inertial reference frame by including the apparent forces induced by accelerations in the momentum equations. We study: *i*) a transient saccadic movement (see Figure 2(a)), *ii*) a sudden car braking, *iii*) a head rotation, and *iv*) a stand-up movement [1]. We describe the large-scale flow features (Figure 2(b)) and then focus on the topology of the wall shear stresses. In the latter framework, we identify stable and unstable manifolds and critical points, and discuss the link to the forces acting on the retinal surface and the near-wall transport. The same approach has been successfully applied to cardiovascular flows [2].

We also compare the results against a model of an eye with staphyloma in its posterior part, a pathology frequently associated with the retinal detachment.

For the saccadic motion, larger filling ratios are associated to higher and more uniform stresses over the whole surface wetted by the silicone oil (Figure 2(c)). After the transient, persistent attracting wall shear stress manifolds appear at the surface wetted by aqueous below and aligned with the interface (Figure 2(d)). Similar persistent patterns are observed in the silicone oil phase (above the interface): in the posterior eye, for the rotating head and car braking movements. Movements such as a stand-up from a supine condition induce more intense velocities and intricate manifold patterns also in the silicone oil phase, although the interface and contact line barely move. The analysis is concluded with the large-time dynamics of the silicone oil-aqueous interface by simulating a transient from a supine to a standing position and subsequently analyzing the picture of the shear stresses induced by the sloshing.

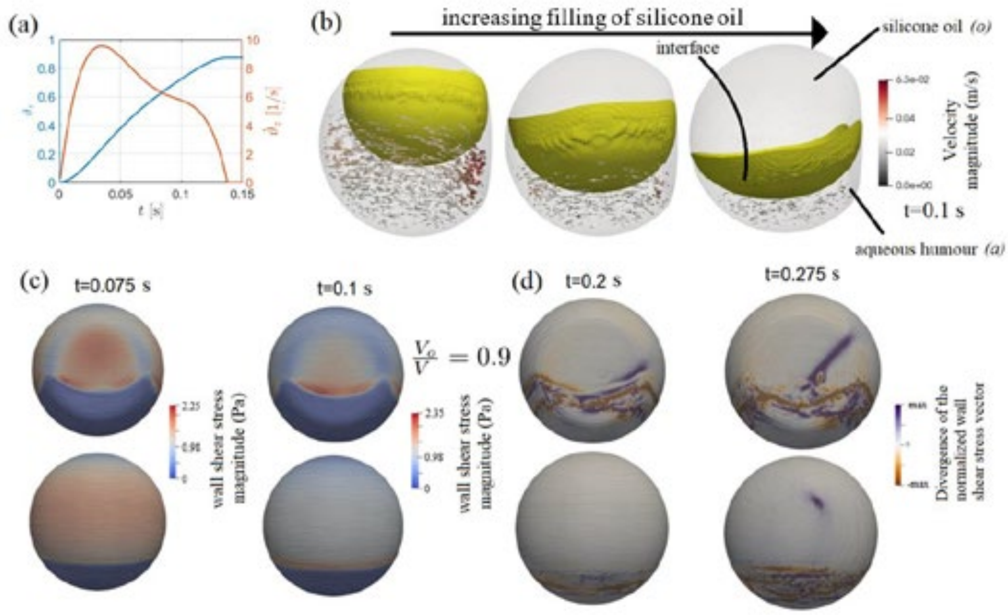

Figure 2: (a) Rotation angle and angular velocity as functions of time (in seconds) for the saccadic movement. (b) Interface position (yellow) and flow field (arrows) during the saccadic movement, for three different filling ratios. (c) Colormaps of the wall shear stress magnitude, superimposed to Line Contour Integral (LIC) lines of the same vector, for two instants during saccade. (d) Colormaps of the divergence of the wall shear stress vector normalized with its magnitude, superimposed to LIC lines of the wall shear stress vector, for two different instants following the saccadic movement.

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Advanced computational modeling of the failure behaviour of FRCM composites

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Keywords: FRCM, Fiber/matrix bond, Interfaces.

Among the large use of composite materials for strengthening interventions of masonry and concrete structures, Fiber Reinforced Cementitious Matrix (FRCM) systems have increased their interests among materialists and scientists due to their numerous advantages compared to traditional Fiber Reinforced polymer (FRP) materials, primarily the high resistance to high temperature and transpirability. For such inorganic-matrix composites, different types of fiber (glass, carbon, aramid, basalt) can be applied together with cement-based, lime-based or geopolymer-based matrixes, allowing for a better compatibility with substrates due to the high vapor permeability of mortar. At the same time, such systems are sustainable and reversible, and can be easy applicable also on irregular substrates, on wet support providing better performances at elevated temperature. In such a context, a large attention of the scientific community has been increasingly devoted to the bond behavior of FRCM externally applied to different kinds of structures from an experimental, theoretical and computational standpoint, as provided by direct single-lap or double-lap tests.

According to the National guidelines, single lap shear bond tests performed on FRCM systems can have as final result different failure modes [1], depending on the matrix thickness, but also on the mechanical properties of the composite and substrate, and treatment of the substrate: a) debonding of the fiber at the matrix-fiber interface; b) interlaminar (delamination) failure of the matrix; c) detachment of the entire composite strip without damage of the substrate; d) debonding of the composite strip within the substrate; e) debonding of the fiber at the matrix-fiber interface followed by spalling of the matrix that covers the textile; and f) rupture of the fibers.

In the present study, such nonlinear cracking phenomena are studied computationally, accounting for the complex interaction between matrix and fibers, applying the main basics of a concrete damaged plasticity modeling [2], cohesive crack modeling [3] and eXtended Finite Element Method (XFEM) [4] for a single-lap shear test as represented in Figure 1.

The properties of the matrix follow two different analytical approximations, namely, an exponential law from the existing literature, and a polynomial approximation calibrated to yield a better response in the softening branch (Figure 1). A validation of the proposed model is performed in a systematic way for different fibers stiffness, fiber-matrix interfacial strength or specimen geometry, in order to predict the cause and location of damage in the selected specimen, together with its global mechanical response (Figure 2). This would give the ability to design FRCM reinforcements according to some fixed requests, in an inexpensive way, possibly reducing the experimental time and cost.

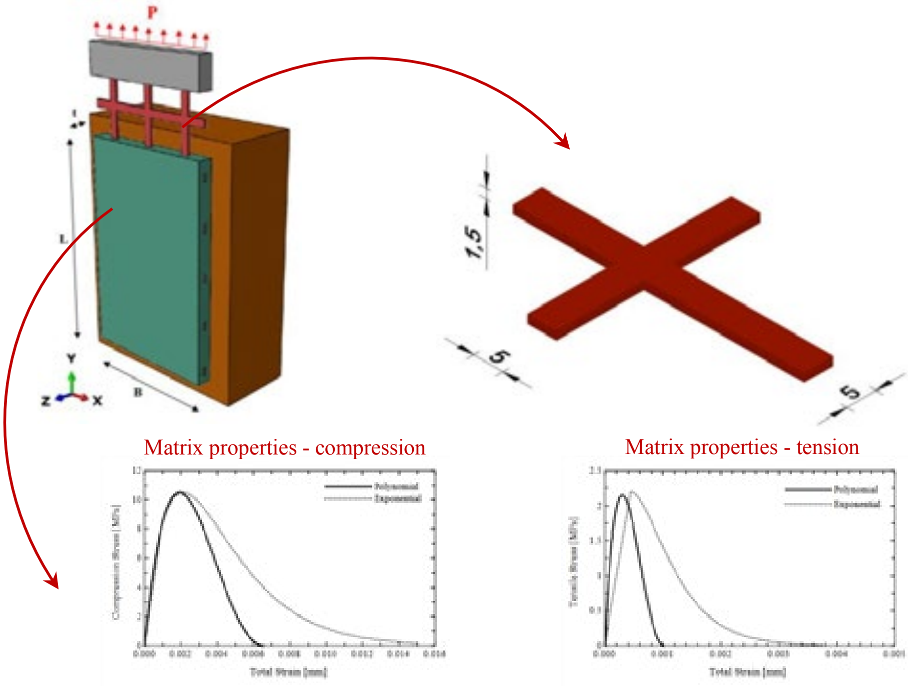

Figure 1: Numerical model of the FRCM single-lap shear test.

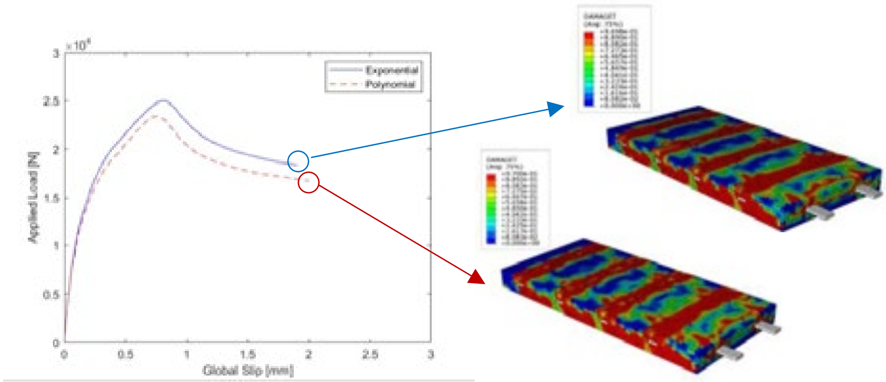

Figure 2: Some numerical results from the systematic investigation.

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Formulation of inelastic laws in hemivariational and thermodynamic frameworks

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Keywords: inelastic phenomena, hemivariational approach, thermodynamics.

Modeling of inelastic phenomena is a challenge from a mechanical and engineering points of view. The reason is that dissipation makes the system to be dependent upon the history of the deformation. In the first part of the talk we will present the theoretical framework for modeling a dissipative spring from two points of view: the thermodynamic [1] and the hemivariational ones [2]. In particular, we will propose how to derive kinematic, see the Fig. 1, and isotropic hardening hysteretic behavior with and without the related flow rules assumption [5,6]. In the second part of the talk we will show how it is possible to adjust the hysteretic shape of the force-displacement diagram by changing the functional shape of the dissipation energy. Thus, we will show how the coupling, in the dissipation energy, between damage and plasticity induces fatigue and therefore the change of the hysteretic cycle along the time evolution. Thus, we will show the derivation of the S-N curve (or Whöler diagram). Finally, we will show how the use of granular micromechanics (in the same form Navier [3] and Cauchy [4] used almost two hundred years ago to derive linear elasticity constitutive equations) yields an immediate generalization of the spring's behavior to that of a 3D continuum.

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Multifield hierarchical metadevices with filtering functionalities

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Keywords: Multiscale acoustic metamaterial, Variational-asymptotic homogenization, Complex frequency spectrum.

This work presents multifield multiscale tunable devices serving as acoustic metafilters [1].

At the mesoscale, the metadevice is constituted by a stack of two different periodically alternating layers: a homogeneous polymeric stratum treated as viscoelastic and a microstructured layer.

This last is characterized by a periodic microscale cell made by a stiff linear elastic external coating, a viscoelastic phase, and an internal piezoelectric disk shunted by an external electrical circuit with a controllable impedance/admittance.

By means of a two-scale variational-asymptotic homogenization technique [2], the frequency-dependent overall constitutive properties of the microstructured layer have been determined.

Subsequently, the free in-plane propagation of waves inside the metadevice has been investigated exploiting Floquet-Bloch theory [3].

It turns out that triggering the shunting effect leads to a stiffening of the piezoelectric phase [4] which ultimately reflects itself into the opening of low-frequency band gap in the metadevice frequency spectrum.

The filtering capabilities are tested against geometrical features and tuning parameter values.

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Linear mechanics of rectangular box-girder bridges

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Keywords: Box-girders**,** Linear mechanics, Generalized Beam Theory.

Mechanics of box-girder bridges cannot be properly predicted by the classical beam theory. The inadequacy of the classical beam theory depends on several phenomena occurring in real box girders, namely: (i) warping, (ii) shear flange deformation (shear-lag), (iii) shear web deformation, as well as (iv) distortion of the cross-section in its own plane. The Euler-Bernoulli and Timoshenko models, as well as the Vlasov theory for Thin Walled Beams (TWB), assume that the cross-section is undeformable in its own plane and this is enough to make them inapplicable for the study of box-girder bridges behaviour whose cross-section is deformable, in general.

In this work, the flexural and torsional behaviour of rectangular box-girder bridges are discussed separately. The methodology adopted involves the following steps: (i) first, the flexural and torsional behaviour of a box girder with undeformable but warpable cross-section is approached, (ii) than the hypothesis of undeformable cross-section is removed and the most comprehensive case of the flexural and torsional behaviour of a box girder with a deformable cross-section is dealt with. Thanks to this study strategy, the role of distortion, both in bending and in torsion, is investigated for assessing the extent.

The important topic of shear-lag in bending is discussed. Under the hypothesis of undeformable cross-section, a new method, based on the reduced geometric characteristics of the cross-section, is proposed to study the combined effect of shear-lag of the flanges and shear deformation of the web in classic unwarpable beam models of Euler-Bernoulli and Timoshenko. In particular, this method relies on the effective flange width and the effective shear area. The analytical expression here suggested for the effective flange width is compared with others from literature and different formulas for the effective shear area are offered and compared to each other.

For each of the cases before mentioned, namely flexural and torsional behaviour of a box girder with undeformable and deformable cross-section, a minimal model based on the Generalized Beam Theory is formulated. There, use is made of Generalized Beam Theory (GBT) in conjunction with Fourier expansions of the modulating functions, i.e. an approach tailored for simply supported box-girder bridges.

A large literature has been recently developed concerning the Generalized Beam Theory (GBT), which is an implementation of the classical semi-variational method by Kantorovich [1, 2, 3]. The theory, initially proposed by Schardt [4], consists in an extension of the classical beam theories, and is able to account both for distortion and warping of the cross-section. Namely, the displacement field is expressed as a linear combination of known trial functions, defined on the cross-section, and unknown modulating amplitudes, defined on the beam axis. Via a variational approach, ordinary differential equations for the amplitudes are obtained.

When these latter are discretized via a 1D Finite Element approach, the problem is reduced to algebraic, usually with a smaller number of degrees of freedom, compared with pure 2D Finite

Element discretization. Schardt and Heinz [5] used GBT for the local and global vibration analysis of load-free isotropic thin-walled members. Also Silvestre and Camotim [6, 7] adopted GBT but dealing exclusively with members subject to uniform axial force and bending moment. Later, Bebiano et al. [8] provided an application of GBT for the analysis of the dynamic behaviour of open thin-walled members subject to axial force and uniform or non-uniform bending.

All models proposed here are applied to case studies taken from literature and validated by comparisons with finite element analyses. In particular, both dynamics, via the assessment of the natural frequencies, and statics, by the evaluation of displacements and stresses under different load conditions, are approached.

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Multi-objective optimisation of variable angle tow composite bridge structures using a multimodal Koiter algorithm

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Keywords: Variable angle tow composites, bridge structures, optimization, mixed finite elements, linear and buckling analysis.

All over the world, there has been growing interest in using fibre reinforce plastic (FRP) materials to realise new bridges and maintain the existing ones. Composite materials allow faster installation times and superior performance compared to concrete and steel, which have largely been used to construct bridges in the last century. In particular, they have high stiffness- and strength-to-weight ratios, excellent fatigue and corrosion resistance, and reduced maintenance costs, making them appealing lightweight and sustainable materials for various structural applications [1]. Since the end of the last century, scientists have investigated the viability of using FRP with traditional materials (i.e. steel and concrete) to reinforce single structural components to maintain existing bridges. Then, research focused on realising bridge structural components entirely made of FRP materials. In this regard, Davids et al. [2] recently developed and implemented a lightweight, quickly erected, hybrid glass-carbon FRP girder for short- and medium-span bridges with composite concrete decks.

This work aims to investigate the use of the variable angle tow (VAT) technique, which has been successfully employed to enhance the response of structural aerospace applications [3, 4], to improve the response of a glass FRP bridge girder under different loading conditions [1]. In VAT composite laminates, the fibre orientation changes pointwise over the structure, enhancing stiffness tailoring capabilities with respect to traditional laminates where fibre angles are constant [5].

A multi-objective optimization technique is proposed to tailor the bridge stiffness appropriately. The starting point is a FE model of the bridge girder using MISS-4c, an accurate assumed stress shell element designed using a hybrid-Trefftz technique to be accurate at coarse meshes [6]. The optimization problem gives the Pareto points that minimize the linear deflection, maximises the buckling load and the postbuckling response by changing the VAT layup. The geometrically nonlinear behaviour is evaluated efficiently using a multimodal Koiter algorithm [6, 4]. For all loading conditions, the optimised girders with VAT layups performed better than those optimised with unidirectional fibres. Furthermore, the work confirms the viability of Koiter algorithm also in efficient multi-objective optimization problems.

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Onde armoniche piane in miscele sature di terreni

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Keywords: Miscele sature, equazioni di bilancio, propagazione delle onde.

In questo articolo consideriamo il comportamento di una miscela satura di terreni formata da un mezzo granulare dilatante con grani rigidi rotanti immerso in un fluido entrambi incomprimibili e con microstruttura nell'ipotesi che la massa di scambio tra le fasi della miscela sia diversa da zero pertanto costituisce una generalizzazione di Giovine [1].

Per il costituente granulare, introduciamo due campi microstrutturali: il vettore di micro-spin e la frazione di volume; il primo descrive la rotazione dei grani rigidi, mentre lo scalare modella le fluttuazioni dovute alla dilatanza del materiale granulare. Per il costituente fluido, la microstruttura è solo scalare, rappresentata dalla sua frazione di volume.

Successivamente in due esempi si studiano le onde armoniche piane nella miscela satura granulare–fluido come soluzioni non banali del sistema differenziale lineare di ordine uno delle onde, ottenendo così nel primo esempio in assenza dell'onda microstrutturale di volume, due macro–onde longitudinali di velocità accoppiate dei componenti della miscela e due macro–onde di velocità e una micro–rotazionale trasversali tutte indipendenti e di ampiezza arbitraria.

Nel secondo esempio supponendo che l'onda microstrutturale di volume si propaghi nella miscela, otteniamo nove onde longitudinali: otto sono miste e una pura microscopica.

In questo esempio abbiamo considerato anche una soluzione particolare nel caso in cui la velocità di fase dell'onda risulta uguale alla componente normale delle due velocità nello stato imperturbato della miscela granulare–fluido ed inoltre la propagazione avviene con scambio di massa all'equilibrio nulla.

In questo caso si hanno: due macro–onde longitudinali di velocità una dipendente dall'altra dei componenti granulare–fluido e un'onda longitudinale pura microscopica, mentre per le trasversali due macro–onde di velocità e una micro–rotazionale tutte indipendenti e di ampiezza arbitraria.

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Shape morphing in constrained swelling of hydrogels

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Keywords: hydrogels, constrained swelling, shape morphing.

Hydrogels are constituted by an elastomeric network capable of absorbing a solvent; the amount of fluid up taken per unit dry volume of the polymer can be quite significant, leading a significant volume increase [1],[2] (Fig. 1). This class of materials is characterized by outstanding properties, such as high-water content, softness, high compliance, biocompatibility, temperature responsiveness, and permeability to gases, etc., making them suitable for several fields such as in bio-related applications and soft responsive structures. The deformation response is of particular interest if the amount absorbed fluid is spontaneously controlled by environmental stimuli, such as temperature, pH, light radiation, ions or molecules, enzymes, electrical and/or magnetic field, etc. [3]. In particular, the volume change can be controlled in order to obtain shape morphing at will, as has been demonstrated in temperature-sensitive hydrogels [4],[5].

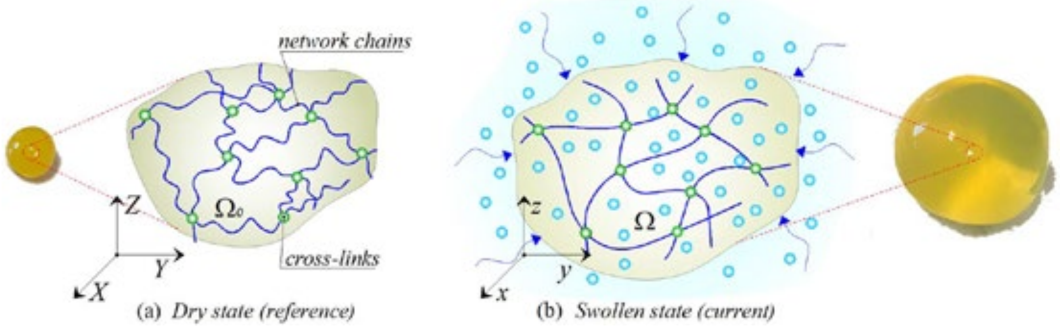

Figure 1: schematic of swelling in gels.

However, designing the material microstructure in order to get the desired responsiveness is not always feasible, and so harnessing a properly designed interaction of hydrogels with other compliant materials, can represent an easy way to obtain precise responsiveness [6].

In the present study, we consider the problem of coupling the hydrogel swelling mechanism with properly designed soft structures, in order to obtain a desired shape morphing driven by the arising constrained swelling. The mechanics of swelling and that of the coupled elastomeric can be described through the stationarity of the respective energy densities defined as (the subscripts g and t refer to the gel and to the tube, respectively):

$$\Psi_{gel} = \left[\Psi_{g,net}\left(\boldsymbol{F}_g\right) + \Psi_{mix}(C_s)\right] + \pi_g\left[(1 + v_s C_s) - J_g\right], \quad \Psi_t = \Psi_{t,net}(\boldsymbol{F}_t) + \pi_t[1 - J_t] \tag{1}$$

where $\Psi_{..,net}$ is the elastic energy density related to the network deformation, Ψ_{mix} is the energy density of solid-fluid mixing, and π_g, π_t are the hydrostatic pressure ensuring the proper volume change of the gel and of the elastomer, i.e. $J_g = \det\left(\boldsymbol{F}_g\right) = 1 + v_s C_s$, $J_t = \det(\boldsymbol{F}_t) = 1$, while $\boldsymbol{F}$ is the deformation gradient, and v_s, C_s the molar volume and the fluid concentration respectively.

In particular, the polymer-fluid mixing energy is provided by [2]:

$$\Psi_{mix} = \frac{k_B' T}{v_s} \cdot \left[\left(J_g - 1\right) \ln\left(\frac{v_s C_s}{J_g}\right) + v_s C_s \frac{\chi}{J_g}\right] \tag{2}$$

where $k'_B = k_B\, A_n$ (k_B, A_n being the Boltzmann constant and the Avogadro number), T is the absolute temperature, and χ is the Flory-Huggins (FH) polymer-fluid interaction parameter [1].

In order to control the deformation arising because of the fluid entering the gel, we consider the swelling to be limited by the presence of a soft tube and/or by the presence of constraints confining the hydrogel domain which is supposed to have an initial spherical shape. Designing the stiffness distribution of the outer soft tube and/or properly positioning the constraints, enables obtaining a controlled final deformed shape of the system at equilibrium (Fig. 2).

By assuming a Neo-Hookean behavior for the involved materials, the stress state in the gel and in the soft tube are expressed as:

$$\boldsymbol{\sigma}_g = \underbrace{\frac{\mu_g}{J_g}\, \boldsymbol{F}_g \boldsymbol{F}_g^T}_{\boldsymbol{\sigma}_{net}} - \underbrace{\pi_g \mathbf{1}}_{\boldsymbol{\sigma}_{mix}}, \qquad \boldsymbol{\sigma}_t = \mu_t\, \boldsymbol{F}_t \boldsymbol{F}_t^T - \pi_t \mathbf{1} \tag{3}$$

where μ_g is the shear modulus of the dry gel, μ_t that of the tube, while the mixing stress in the gel is obtained as: $\boldsymbol{\sigma}_{mix} = -J_g^{-1} \frac{\partial \Psi_{mix}}{\partial \boldsymbol{F}} \boldsymbol{F}^T = \frac{k'_B\, T}{v_s}\left[\frac{1}{J_g} + \frac{\chi}{J_g^2} + \ln\left(\frac{v_s C_s}{J_g}\right)\right] \mathbf{1}$.

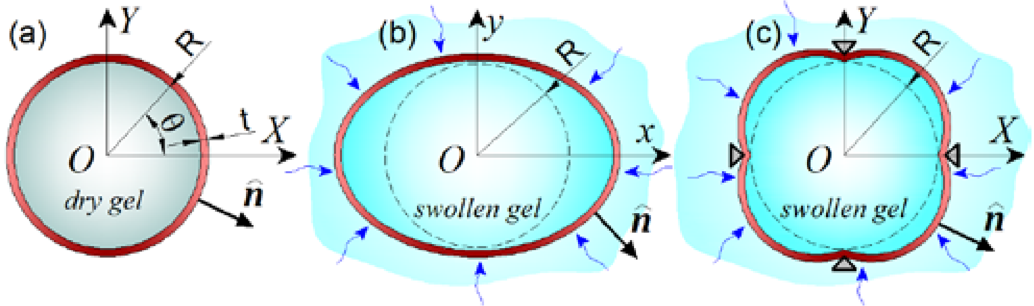

Figure 2: confined swelling of a spherical hydrogel element. The stiffness distribution of the outer surrounding tube (b) or the presence of constraints (c) enables controlling the final equilibrium deformed shape of the system.

The multi-physics model accounting for the fluid diffusion, swelling mechanics and materials coupling, is developed and implemented in a computational framework to predict the final deformed shape of the system under different constraint conditions. It is shown how the swelling mechanism can be exploited to powerlessly generate forces on an elastic structure leading to a reversible controlled morphing.

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A phase-field model for fibrous materials exhibiting an emerging anisotropy with plastic memory effects

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Keywords: Fibrous materials, collagen, tethers, phase-field, anisotropy, plasticity

Fibrous materials may undergo a plastic internal reorganization, which turns out in the emergence of preferential directions. This is a peculiar behavior of many biological tissues, which drive reorientation by external stimuli at chemo-mechanical levels. In particular, it is detected that contractile cells can reorganize fibrous extracellular matrices and form dense tracts of aligned fibers (tethers), that guide the development of tubular tissue structures and may provide paths for the invasion of cancer cells [1]. Tether formation is caused by buckling instability of network fibers under cell-induced compression. These severe localizations can be brought about by mechanical forces, such as the ones due to cell contraction, without involvement of biochemical factors [2].

Due to the complete randomness of the fiber network, the virgin material can be considered homogeneous. When loaded, since some fibers buckle, a transversal anisotropy emerges; if forces are removed, the strength of those fibers can be partially recovered, but memory of the past history is retained. Starting from the results in [3], we propose to describe this process by resorting to a phase-field model, with two gross descriptors for: (i) the emergence of the anisotropy, by means of a macroscopic measure of the stiffness of fibers in the direction of the transverse anisotropy; (ii) the occurrence of the buckling, marking the material in a plastic way.

We show that localization of the phase-fields may occur, which mimics the onset of tethers detected in experiments [2].

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Electrochemo-poromechanics of ionic polymer metal composites: Theory and Numerics

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Keywords: Ionic polymer metal composite, generalized finite element method, actuation.

Ionic polymer metal composites IPMCs consist of an electroactive polymeric membrane plated with metal electrodes and including a fluid phase, constituted by ions dispersed in a solvent, whose motion allows for actuation and sensing applications [1, 2].

In this work [3], the IPMC behaviour is studied through a large deformation electrochemo-poromechanical theory extending a recent proposal of our group [4]. The theory couples the linear momentum balance, the mass balances of solvent and mobile ions, and the Gauss law, thus providing the capability to model peculiar IPMC features, such as the back-relaxation in actuation [1, 5] and the discharge under a sustained mechanical stimulus in short-circuit sensing, both phenomena being aided by the cross-diffusion of solvent and ions. The present extension abandons the assumption that the fluid phase is a *dilute* solution, leading to significant benefits on both the modelling and the computation.

A reliable finite element (FE) implementation of theories suitable to capture the IPMC multi-physics is particularly challenging because the IPMC behaviour turns out to be governed by boundary layers (BLs) occurring in very thin membrane regions adjacent to the electrodes, where steep gradients of ion and solvent concentrations occur, thus leading to a large electric field therein and, in turn, to a high polarisation stress triggering complex electrochemomechanics [6, 7, 8, 9].

We address this issue by adopting the generalized FE method [10] to discretise the BLs. This allows unprecedented analyses of the IPMC behaviour since it becomes possible to explore it under external actions consistent with applications (e.g., up to 3 V drop across the electrodes in actuation), beside obtaining accurate predictions with a reasonable computational cost. Hence, we provide novel results concerning the influence of the membrane permittivity on the species profiles at the BLs, thus shedding a new light on a recent and controversial debate in the literature [11]. Additionally, by leveraging on the mobility matrix, we establish that the initial peak deflection in actuation strongly depends on the constitutive equations for the species transport and discuss the predictions of some experimental results from the literature [12].

Overall, we demonstrate the potential of the proposed model to be an effective tool for the thorough analysis and design of IPMCs.

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Rate-Independent Elastoplastic Ferroelectric Solids

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Motivated by our interest in modelling nonlinear electromechanical coupling for applications in ultra-precise actuation and sensing at finite deformations, we developed a rate-independent model for materials that can undergo ferroelectric hysteresis and elastoplastic deformations. The elastoplasticity framework is based on Kröner's [3, 5] multiplicative decomposition $\boldsymbol{F} = \boldsymbol{F}_{\rm e}\,\boldsymbol{F}_{\rm p}$ of the deformation gradient $\boldsymbol{F}$ into the plastic part $\boldsymbol{F}_{\rm p}$ and the elastic part $\boldsymbol{F}_{\rm e}$. The ferroelecticity framework is based on the additive decomposition $\boldsymbol{\Pi} = \boldsymbol{\Pi}_{\rm r} + \boldsymbol{\Pi}_{\rm i}$ of the material polarisation $\boldsymbol{\Pi}$ into the reversible part $\boldsymbol{\Pi}_{\rm r}$ and the irreversible part $\boldsymbol{\Pi}_{\rm i}$, as proposed by Bassiouny et al. [2]. The plastic deformation $\boldsymbol{C}_{\rm p} = \boldsymbol{F}_{\rm p}^T.\boldsymbol{F}_{\rm p}$, along with the mechanical isotropic hardening $r_{\rm m}$ and kinematic hardening $\mathcal{A}_{\rm m}$, and the irreversible polarisation $\boldsymbol{\Pi}_{\rm i}$, along with the electrical isotropic hardening $r_{\rm e}$ and kinematic hardening $\mathcal{A}_{\rm e}$, are considered as internal variables [4, 5, 2, 1] and assigned appropriate evolution equations.

The independent constitutive variables are the right Cauchy-Green deformation $\boldsymbol{C} = \boldsymbol{F}^T.\boldsymbol{F}$ (in place of $\boldsymbol{F}$, to satisfy frame-indifference), the material polarisation $\boldsymbol{\Pi}$, the absolute temperature Θ and the temperature gradient $\mathcal{G}$, while, $\boldsymbol{C}_{\rm p}$, $\boldsymbol{\Pi}_{\rm i}$, $r_{\rm e}$, $\mathcal{A}_{\rm e}$, $r_{\rm m}$ and $\mathcal{A}_{\rm m}$ are treated as internal variables. The dependent constitutive variables are the Helmholtz free energy per unit referential volume W, the entropy per unit referential volume $\mathcal{S}$, the material electric field $\boldsymbol{E}$, the second Piola Kirchhoff stress $\boldsymbol{S}$ and the material heat flux $\boldsymbol{Q}$:

$$W = \hat{W} \circ (\boldsymbol{C}, \boldsymbol{\Pi}, \Theta; \boldsymbol{C}_{\rm p}, \boldsymbol{\Pi}_{\rm i}, r_{\rm e}, \mathcal{A}_{\rm e}, r_{\rm m}, \mathcal{A}_{\rm m}) = \hat{W}_{\rm m} \circ (\boldsymbol{C}; \boldsymbol{C}_{\rm p}) + \hat{W}_{\rm e} \circ (\boldsymbol{\Pi}; \boldsymbol{\Pi}_{\rm i}) + \hat{W}_{\rm h} \circ (\Theta; r_{\rm e}, \mathcal{A}_{\rm e}, r_{\rm m}, \mathcal{A}_{\rm m}), \tag{1a}$$

$$\mathcal{S} = \hat{\mathcal{S}} \circ (\Theta; r_{\rm e}, \mathcal{A}_{\rm e}, r_{\rm m}, \mathcal{A}_{\rm m}) = -\left(\partial \hat{W}_{\rm h}/\partial \Theta\right) \circ (\Theta; r_{\rm e}, \mathcal{A}_{\rm e}, r_{\rm m}, \mathcal{A}_{\rm m}), \tag{1b}$$

$$\boldsymbol{E} = \hat{\boldsymbol{E}} \circ (\boldsymbol{\Pi}; \boldsymbol{\Pi}_{\rm i}) = \left(\partial \hat{W}_{\rm e}/\partial \boldsymbol{\Pi}\right) \circ (\boldsymbol{\Pi}; \boldsymbol{\Pi}_{\rm i}), \tag{1c}$$

$$\boldsymbol{S} = \hat{\boldsymbol{S}} \circ (\boldsymbol{C}; \boldsymbol{C}_{\rm p}) = 2\left(\partial \hat{W}_{\rm m}/\partial \boldsymbol{C}\right) \circ (\boldsymbol{C}; \boldsymbol{C}_{\rm p}), \tag{1d}$$

$$\boldsymbol{Q} = \hat{\boldsymbol{Q}} \circ (\boldsymbol{C}, \boldsymbol{\Pi}, \Theta, \mathcal{G}; \boldsymbol{C}_{\rm p}, \boldsymbol{\Pi}_{\rm i}, r_{\rm e}, \mathcal{A}_{\rm e}, r_{\rm m}, \mathcal{A}_{\rm m}). \tag{1e}$$

Note the assumed additive decomposition $W = W_{\rm m} + W_{\rm e} + W_{\rm h}$ of the material Helmholtz free energy W into mechanical part $W_{\rm m}$, electrical part $W_{\rm e}$ and thermo-hardening part $W_{\rm h}$.

In order to define the admissible states of the material, we postulate the existence of an electrical switching function $\Phi_{\rm e}$ and of a mechanical yielding function $\Phi_{\rm m}$, defining the electrical switching surface and mechanical yielding surface

$$\Phi_{\rm e} = \tilde{\Phi}_{\rm e} \circ (\boldsymbol{C}, \boldsymbol{\Pi}, \Theta; \boldsymbol{C}_{\rm p}, \boldsymbol{\Pi}_{\rm i}, r_{\rm e}, \mathcal{A}_{\rm e}) = 0, \qquad \Phi_{\rm m} = \tilde{\Phi}_{\rm m} \circ (\boldsymbol{C}, \boldsymbol{\Pi}, \Theta; \boldsymbol{C}_{\rm p}, \boldsymbol{\Pi}_{\rm i}, r_{\rm m}, \mathcal{A}_{\rm m}) = 0. \tag{2}$$

Following Green and Naghdi [4], we use the switching and yielding functions (2) to establish rate-independent evolution laws for the internal variables $\boldsymbol{\Pi}_{\rm i}$, $r_{\rm e}$, $\mathcal{A}_e$, $\boldsymbol{C}_{\rm p}$, $r_{\rm m}$ and $\mathcal{A}_{\rm m}$, i.e., evolution laws that are linear in the rates $\dot{\boldsymbol{E}}$, $\dot{\boldsymbol{C}}$ and $\dot{\Theta}$ of electric field $\boldsymbol{E}$, deformation $\boldsymbol{C}$ and temperature Θ:

$$\dot{\boldsymbol{\Pi}}_{\rm i} = \mathsf{P}_{\rm e} : \dot{\boldsymbol{C}} + \boldsymbol{M}_{\rm e}\,\dot{\boldsymbol{E}} + \dot{\Theta}\,\boldsymbol{R}_{\rm e}, \qquad \dot{\boldsymbol{C}}_{\rm p} = \mathbb{P}_{\rm m} : \dot{\boldsymbol{C}} + \mathsf{M}_{\rm m}\,\dot{\boldsymbol{E}} + \dot{\Theta}\,\boldsymbol{R}_{\rm m}, \tag{3a}$$

$$\dot{r}_{\rm e} = \langle \boldsymbol{U}_{\rm e} \,|\, \dot{\boldsymbol{\Pi}}_{\rm i} \rangle, \qquad \dot{r}_{\rm m} = \boldsymbol{U}_{\rm m} : \dot{\boldsymbol{C}}_{\rm p}, \tag{3b}$$

$$\dot{\mathcal{A}}_{\rm e} = \boldsymbol{T}_{\rm e}\,\dot{\boldsymbol{\Pi}}_{\rm i}, \qquad \dot{\mathcal{A}}_{m} = \mathbb{T}_{\rm m} : \dot{\boldsymbol{C}}_{\rm p}. \tag{3c}$$

In (3), $\mathbb{P}_{\rm m}$ and $\mathbb{T}_{\rm m}$ are fourth-order tensors, $\mathsf{P}_{\rm e}$ and $\mathsf{M}_{\rm m}$ are third-order tensors, $\boldsymbol{R}_{\rm m}$, $\boldsymbol{U}_{\rm m}$ and $\boldsymbol{T}_{\rm e}$ are second-order tensors, $\boldsymbol{R}_{\rm e}$ is a vector and $\boldsymbol{U}_{\rm e}$ is a covector. All these are functions of the independent constitutive variables and of the internal variables.

For illustrative purposes, we consider a one-dimensional benchmark problem with the constitutive variables of Eqs. (1), $W = W_{\mathrm{m}} + W_{\mathrm{e}} + W_{\mathrm{h}}$, $\mathcal{S}$, S, E and Q, given by

$$W_{\mathrm{m}} = \frac{\mu}{2}\left(\mathrm{tr}(\lambda_{\mathrm{p}}^{-2}\,\lambda^2) - 3\right) - \mu\,\ln(J) + \frac{\ell}{2}(\ln(J))^2, \qquad W_{\mathrm{e}} = \frac{1}{2}\chi^{-1}(\Pi - \Pi_{\mathrm{i}})^2,$$

$$W_{\mathrm{h}} = \beta_1\,r_e + \beta_2\,|\mathcal{A}_e| + \beta_3\,r_{\mathrm{m}} + \beta_4\,|\mathcal{A}_{\mathrm{m}}| - \mathcal{C}\,\Theta\big(\ln(\Theta/\Theta_0) - 1\big), \tag{4a}$$

$$\mathcal{S} = \mathcal{C}\,\ln(\Theta/\Theta_0), \qquad S = \mu\,(\lambda_{\mathrm{p}}^{-2} - \lambda^{-2}) + \ell\,\ln(J)\,\lambda^{-2}, \tag{4b}$$

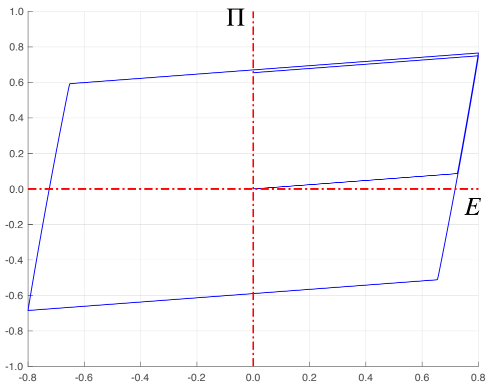
$$E = \frac{1}{\chi}\,(\Pi - \Pi_{\mathrm{i}}), \qquad Q = -k\,\mathcal{G}, \tag{4c}$$

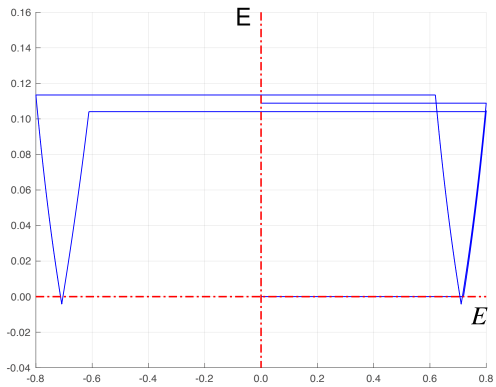
where λ is the axial stretch (λ^2 is the axial eigenvalue of $\boldsymbol{C}$), λ_{p} is the axial plastic stretch (λ_{p}^2 is the axial eigenvalue of $\boldsymbol{C}_{\mathrm{p}}$), $J = \det \boldsymbol{F}$, $\chi > 0$ is a (linear and isotropic) electric susceptivity, $\mathcal{C} > 0$ is a constant specific heat, μ, ℓ, β_1, β_2, β_3, and β_4 are positive material constants, Θ_0 is a reference value of the absolute temperature Θ, and $k > 0$ is a constant thermal conductivity. The electric switching surface Φ_{e} and mechanical yielding surface Φ_{m} are given by

$$\Phi_{\mathrm{e}} = |\chi\,E - d_2\,\mathcal{A}_e|^2 + \alpha\,S\,(\chi\,E - d_2\,\mathcal{A}_e)^2 - (\Pi_{\mathrm{y}0} + d_1\,r_e)^2 = 0, \tag{5a}$$

$$\Phi_{\mathrm{m}} = |S - d_4\,\mathcal{A}_{\mathrm{m}}|^2 + \beta\,(S - d_4\,\mathcal{A}_{\mathrm{m}})E^2 - (S_{\mathrm{y}0} + d_3\,r_{\mathrm{m}})^2 = 0, \tag{5b}$$

where α, β, d_1, d_2, d_3 and d_4 are positive material constants, and $\Pi_{\mathrm{y}0} > 0$ and $S_{\mathrm{y}0} > 0$ take the meaning of first yielding polarisation and first yielding stress, respectively. The figures below show the relationship between the material polarisation Π versus the material electric field E (hysteresis loop, left) and the (axial) Green-Lagrange strain $\mathsf{E} = \frac{1}{2}(\lambda^2 - 1)$ versus the material electric field E (butterfly loop, right), for one sinusoidal loading cycle. These are obtained numerically by solving the differential equations given by the evolutions laws (3) of the internal variables, coupled with Eqs. (4) and (5). The material constants are constrained by the dissipation inequality.





In summary, we developed a non-linear thermo-electromechanical framework that captures electrical hysteresis and butterfly loops in elastoplastic ferroelectric materials. The model is rate-independent in the sense that the rate $\dot{\boldsymbol{\Pi}}_{\mathrm{i}}$ of irreversible polarisation and the rate $\dot{\boldsymbol{C}}_{\mathrm{p}}$ of the plastic deformation $\boldsymbol{C}_{\mathrm{p}}$ are linear in the rate $\dot{\boldsymbol{C}}$ of deformation and the rate $\dot{\boldsymbol{E}}$ of electric field.

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Electro-thermo-chemo-mechanical model and numerical investigations of solid state lithium-ion batteries: theoretical framework

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Keywords: electro-thermo-chemo-mechanics, solid state lithium-ion batteries.

Reliable and readily available energy storage systems are highly recommended by the internationally advocated actions against climate change. The state of art of lithium-ion batteries (LiB) shows unsolved safety concerns, such as flammability after leakages of toxic organic solvents. There is therefore the need of novel electrolytes with excellent transport properties, low interfacial resistance, good mechanical strength and increased safety. All solid state batteries (SSBs) are claimed to be the next-generation battery system, since they combine superior thermal and electrochemical stability and avoid hazardous liquid electrolyte leakage [1].

In this communication, we aim at presenting a new thermodynamically consistent model for a solid-state battery consisting of: a current collector, onto which the positive electrode (e.g. made of LiCoO2) is deposited, a negative electrode (e.g. made of graphite), and a solid state electrolyte comprised of Lithium phosphorus oxynitride (LiPON). Specifically, LiPON has an amorphous structure and it shows two types of nitrogen bonds, either triply- or doubly-coordinated. To describe the electro-chemical behavior of LiPON two-mechanisms model of ionic conduction, recently formulated in [2], has been used. Particularly, movements of charged particles towards the interstitial space and by means of particle hopping representing the main ionic conductivity mechanisms in LiPON. Our multi-physic model attempts at explicitly accounting for the dynamic filling between these two transport mechanisms by means of two paired chemical reactions [2].

The formulation is grounded in the thermo-mechanics of continua and is multi-scale compatible [3; 4; 5; 6]. Conservation principles lead to balance equations for mass, charge, linear and angular momentum, energy, entropy, together with Maxwell's equations under quasi-electrostatic conditions [7]. Constitutive relations between thermodynamics fluxes and forces [4; 6] have been provided after devising the most appropriate form of the Helmholtz free energy and applying the Coleman-Noll procedure to the Clausius-Duhem inequality. Interface conditions on fluxes (current and lithium), at the left and right boundaries of the electrolyte, has been adopted in the form of Butler-Volmer equations [2]. Eventually, the response of the battery has been numerically evaluated via finite element implementation of the governing equations, analyzing the limiting factors as well as the most relevant constitutive parameters according to a sensitivity analysis of the model. Outcomes of numerical simulations will be shown in a companion communication [8] by the same authors.

The present work extends to a battery half-cell a previous model for solid electrolytes [2]. Furthermore, mechanical interactions have been accounted for within a multi-physics model, which stems from a thermodynamically-consistent theory for SSBs capable to couple electro-thermal-chemical-transport phenomena with mechanics. The theory introduces a multiplicative decomposition of the deformation gradient tensor $\mathbf{F}$, which accounts for: the volume expansion/contraction within the positive and negative electrodes due to the interactions of their lattice with lithium species; the thermal deformation inside the whole battery; the competition between the swelling mechanisms due to heat and to volumetric changes during the electrochemical cycling [9]. Our multi-physics theory could open new prospective in the study of the response of lithium-ion batteries.

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Solid state lithium battery, thermo–electro–chemo–mechanical numerical modeling

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Keywords: Solid state lithium battery, thermo–electro–chemo–mechanical, numerical simulations.

In the present presentation, a thermo–electro–chemo–mechanical model has been applied to describe the response of a all-solid-state battery [1]. All solid state batteries are considered the most promising alternatives to current lithium-ion batteries, as safer, even if some drawbacks still need to be solved. Numerical description of the model will be fully developed to highlight the influence of the components of the cell, in particular, focusing on the cathode design, since it results essential for the electro-chemical response of the whole cell [2]. The model is general, and it can be applied to different types of cell, the solid-state battery described consists of: two porous electrodes and a solid state electrolyte, see Fig.1, governed by a two-mechanism of ion conduction to better describe the ionic motility in the electrolyte. The theoretical formulation is grounded in the thermo-mechanics of continua, resulting thermodynamically-consistent [3]. The electro-thermal-chemical response of the cell has been coupled with the mechanical one, giving a comprehensive description of the behaviour of a solid state lithium battery. Conservation principles, which lead to balance equations, and constitutive relations that form the basis of this contribution, are fully presented in a twin presentation [4]. The computational simulations will show how to guide in the selection of the constituents and in the tailoring of the architectures, providing meaningful insights on the electro-chemical response of the cell during operation and predicting limiting factors during charge/discharge cycles.

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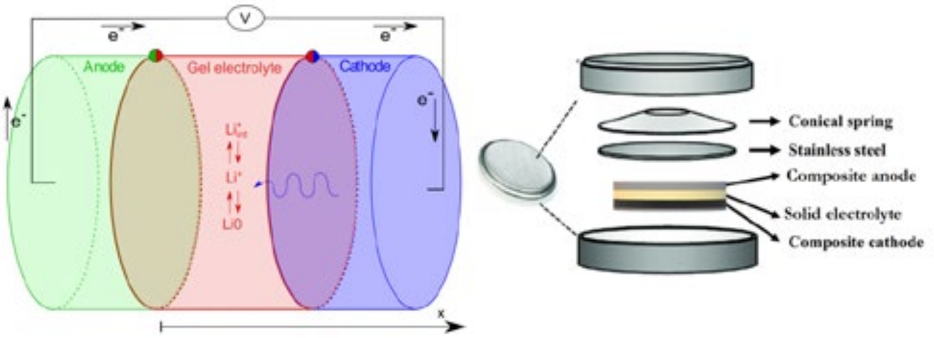

Figure 1: A pictorial view of the all-solid-state electrochemical cell .

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Modelling of extrusion-based bioprinting via Floating Isogeometric Analysis (FLIGA)

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Keywords: Isogeometric analysis, viscoelasticity, extrusion, 3D printing.

Additive manufacturing (AM) enables accurate deposition of materials and cells, allowing for on-demand production of specific biomaterials. In this framework, Ink Engineering is an area of research that designs next-generation biomaterials tailored for additive processes [1]. Among them, polymer-nanoparticle hydrogels are particularly promising since they are suitable for incorporating cells to form scaffolds for tissue engineering or as drug carriers. In any case, the extrusion process triggers high shear stress and extensional flow, potentially harmful for embedded entities. In particular, shear stress mainly arises as the bioink is forced to flow through the needle tip, whereas extensional stress is generated because of the abrupt shrinkage in the region of the needle. During the design of new inks, specific requirements must be considered, in order to provide tailored rheology for extrusion-based AM and facilitate the formulation of biofunctional inks.

In this framework, the aim of the present work is to numerically investigate the extrusion process of a bioink by means of floating isogeometric analysis (FLIGA) originally proposed in [2]. FLIGA is a Lagrangian method that adopts meshless concepts to generalize mesh-based isogeometric analysis (IGA) and is able to handle mechanics problems characterized by extreme deformations along one so-called characteristic direction. For the extrusion process, such a direction of predominant deformation is easily identified (see Figure 1). Then the classical tensor-product structure of B-Spline basis functions is modified, such that multiple B-Spline chains in the characteristic direction are

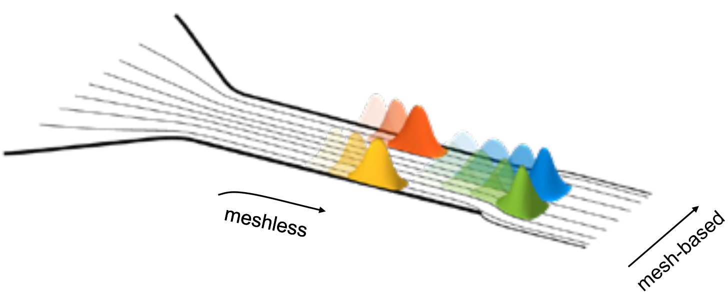

Figure 1: Schematic representation of basis functions evolution (from lightest to darkest for each colour) for FLIGA along the needle.

able to independently float against each other in the parametric domain. Through the *floating* procedure, the basis functions are prevented from undergoing mesh distortion avoiding the drawbacks of remeshing. Moreover, the contact between needle and the printed material is treated robustly due to the smoothness of the isogeometric basis functions. Free surfaces that form behind the needle exit are handled without additional efforts to track boundaries.

In order to demonstrate the capability of the procedure to describe the extrusion process of a bioink, reference is made to a specific application realized in laboratory. The bioink herein considered is a polymer-nanoparticle hydrogel composed of hydroxypropyl methylcellulose (HPMC) and Polyethylene Glycol-block-Polylactide (PEG-b-PLA) nanoparticles. The rheological behavior of the ink is characterized with small amplitude oscillatory shear tests and shear-ramp-rate tests. Experimental results are provided by the group of Prof. Mark Tibbitt at ETH Zürich [3]. The viscoelastic fluid is modelled with the Giesekus differential constitutive model [4] reformulated with the log-conformation approach, in order to preserve the positive-definiteness of the conformation tensor, and to tackle the numerical instabilities occurring with high elastic stress [5]. The parameters that describe the fluid rheology are calibrated on the basis of the experimental data. Finally, the procedure is applied to the simulation of the extrudate swell problem, comparing the results with the available experimental data.

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3D printed PEEK cristallinity prediction: a finite element based numerical workflow

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Keywords: PEEK, Additive Manufacturing, process simulation.

1 Introduction

Additive manufacturing (AM), also known as 3D printing, is a rapidly growing technology that is changing the manufacturing industry. AM enables the production of three-dimensional objects through a layer by layer material deposition. Moreover, with AM it is possible to produce complex geometries and customized designs that are unfeasible with traditional manufacturing techniques. One of the most challenging AM applications is the use of poly-ether-ether-ketone (PEEK), a high-performance thermoplastic that has excellent mechanical, thermal, and chemical properties. When used in AM, PEEK can be optimized to obtain semi-crystalline properties, making it an ideal material for a wide range of applications. The optimization of PEEK for AM involves several factors that affect the final properties of the material [1]. The first factor is the processing temperature that must be set to achieve good adhesion between layers without degrading the material. The second factor is the cooling rate that must be controlled to increase the degree of crystallinity that, in turn, controls PEEK mechanical behavior.
In the present work we propose a numerical workflow to predict the degree of cristallinity of PEEK components printed by Fused Deposition Modeling (FDM). In particular, a non linear transient thermal simulation with evolving boundary condititions coupled with an Avrami's law-based numerical algorithm, is used [2].

2 Methods

Starting from the G-Code file used to print the component, we retrieve the 3D printed geometry and create a volumetric mesh, in which groups of elements are defined and sequentially activated in the thermal simulation run through Ansys® DED Process module. At each thermal step, the elements' temperatures are used to predict the crystallinity degree according to Avrami's Law [2]:

$$X_{vc} = X_{vc\infty}(w_1 F_{vc1} + w_2 F_{vc2}) \tag{1}$$

$$\text{with} \quad w_1 + w_2 = 1$$

$$\text{and} \quad F_{vc,i} = 1 - exp[-C_{i1} \int_0^t T exp[\frac{-C_{i2}}{T - T_g + T_{add,i}} - \frac{C_{i3}}{t(T_{m,i} - T)^2}] n_i t^{n_i - 1} dt]$$

Where X_{vc} is the evaluated volume fraction crystallinity, $X_{vc\infty}$ is the equilibrium volume crystallinity fraction, w_1 and w_1 are the weight factors, n_i is the Avrami coefficient, T is the current

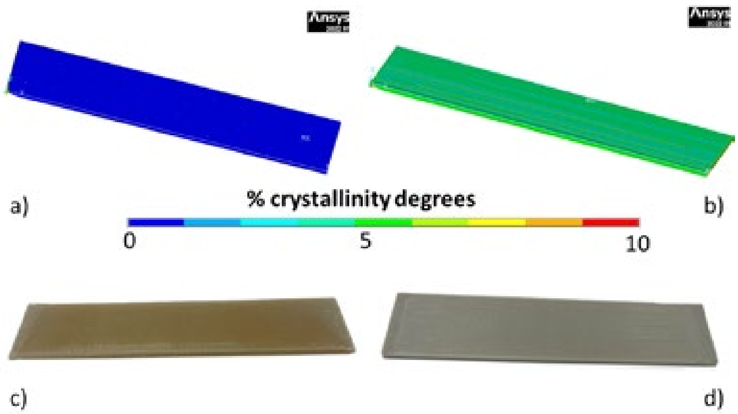

Figure 1: Comparison between the prediction for a) amorph case and b) semicristalline case and the respective printed part c) and d).

temperature, T_g is the glass transition temperature, T_m is the melting temperature $T_{add,i}$, an additional model temperature defined by the Avrami's law and C_{i1},C_{i2},C_{i3} are physical properties of PEEK.

3 Results

To prove the efficiency of the developed framework, we have conducted two simulations in order to represent an amorph and a semicrystalline case, using machine reference temperatures to set bed temperature T_b, chamber temperature T_c and extrusion temperature T_{ext} in the thermal analysis. The results are shown in Figure 1: there is a qualitative match between the crystallinity predictions and the respective real printed components.

4 Discussion

The cristallinity numerical prediction of PEEK printed parts could be a very effective way to produce components with the desired mechanical properties, since it allows to optimize the process parameters directly through the simulations. Further improvements would be required to refine the proposed framework: firstly, optimizing PEEK thermal parameters in order to properly characterize the material, both in thermal simulations and in Avrami's law numerical algorithm; secondly, mesuring the process temperatures with a thermal image camera to reproduce a more accurate FDM process in the numerical simulations.
Finally, the proposed workflow must be validated by identifying the real degrees of crystallinity in the printed part with Differential Scanning Calorimetry (DSC).

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A Particle Finite Element Method for the Simulation of 3D Concrete Printing

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Keywords: 3D printing, PFEM, non-Newtonian fluid.

In the last decades, the development of 3D concrete printing (3DCP), a fast expanding technology with promising applications in building design and construction, has paved the way for creative and environmentally friendly building techniques. The basic goal of 3DCP is to create arbitrary shaped items and structural elements using a robotic arm that is digitally controlled to deposit filaments of cementitious mortar. Numerous benefits would result from the use of this technology, including the ability to quickly construct free-form topologically optimum designs without the use of formwork and a reduction in the amount of human labor, building expenses, and construction times.

However, before 3DCP will be widely adopted, various challenges must yet be resolved on both a practical and numerical level. In particular, the creation of an efficient and accurate computational tools would advance knowledge of the printing process and make it possible to foresee its results in terms of material, structural, and process performances.

In our contribution, the printing process of cementitious materials is simulated through a single-phase fluid model. The motion of the fluid is governed by Lagrangian Navier-Stokes equations with a non-Newtonian rheological law. The Particle Finite Element Method (PFEM) [1] is employed to deal with the large displacements and nonlinearities. Moreover, the intrinsic features of the PFEM has been used to address and resolve several numerical problems, including the precise treatment of inter-layer contact and the imposition of the time-dependent moving boundary condition at the nozzle outlet.

The experimental data for several printing circumstances were used to validate the model [2,3]. The results offered insightful information on the printing process and were in good accord with the experimental ones. The proposed model can be used to evaluate the extrudability of cementitious mixes given the rheological parameters, making it suitable to support experimental campaigns for the development of new cementitious inks, carry out printing parameter optimization, and predict the emergence of plastic and buckling failure during the printing of arbitrarily shaped objects.

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Optimizing structure of 3D printed flexible Insoles through homogenization and finite element analysis

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Keywords: Topological optimization, Additive manufacturing, FEA, orthopaedical devices.

In recent times, novel materials have been developed to imitate the strong and lightweight characteristics observed in natural systems such as bones, honeycombs, sponges, and wood. These materials can have a porous microstructure that alternates between void and solid. Additionally, the advent of innovative manufacturing techniques, such as 3D printing, has enabled the production of cellular materials in different domains, particularly in healthcare [1,2]. However, 3D printing production can be time-consuming based on factors like material (e.g., flexible or rigid), infill pattern, and printing parameters. This study developed a computational tool that integrates numerical homogenization and topological optimization using ANSYS Mechanical to analyze the mechanical performance of 3D printed flexible insoles. Computational homogenization was implemented to simulate the mechanical properties of the infill pattern in terms of their mechanical properties and printing performance (e.g., accuracy and speed). The computed constitutive properties were assigned to the insole geometries, and various loading scenarios were examined concerning therapeutic and usage frameworks. Based on the results of these structural simulations, multiple topology optimization analyses were carried out. In figure 1 the rational of the study is represented for a loading condition replicating the insertion of the insole in the shoes.

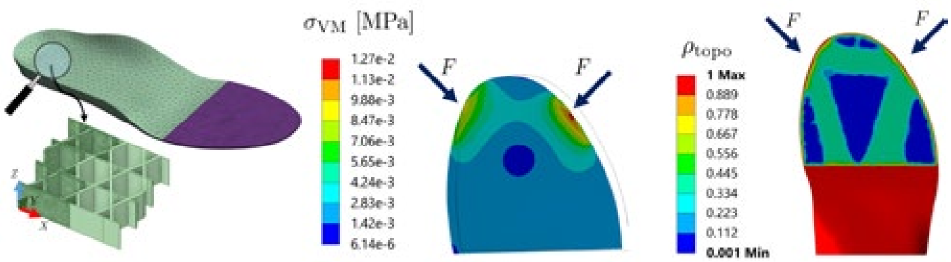

Figure 1: Optimal material distributions for a loading condition investigating the insertion of the insole in the shoes.

The aim of this study was to identify a possible mass distribution that could minimize material usage and printing time, while still ensuring an acceptable structural response during the insertion phase of the insole into the shoe. Additionally, the computational approach employed in this study can optimize material distribution in insoles, reducing printing time and making 3D printing production more effective for various orthopedic devices.

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Mechanical modelling of polymers for tissue bioprinting applications

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Keywords: **Polymer modelling, Multiphysics models, FEM analysis**.

The general aim of bioprinting is to recreate a selected tissue by extruding a bioink, which is a mixture of stem cells encapsulated in an external gel, into a suitable pattern. The immersion of the printed material in a culture medium triggers cell differentiation and their subsequent growth. However, prior to activating these processes, the gel must first be converted into a polymer construct to provide support and preferential pathways to the cells. Photo-polymerisation is one of the most widely adopted techniques to accomplish this. Light interacts with the monomers in the construct, initiating and sustaining growth and cross-linking processes within the medium. To control this process is of pivotal importance, since cellular motility and nutrient diffusion are greatly affected by the disposition and orientation of the polymer network. This 3D printing process is well known, but in many cases it dwells on empirical, application-specific approaches. One of such instances is the production of cultivated meat, which is the background context of the present work. In this framework, the intensity and direction of the UV light has no standard protocol yet, so the definition of an optimal disposition of the light sources can prove essential in minimising the polymerisation times, hence tissue formation times as a whole. This work intends to ground the choice of selected polymerisation parameters to a rational basis. To achieve this, the relevant Physics of what happens after the melted bio-ink is deposited has been represented through multi-physics Finite Element simulations, where the kinetics of polymer cross-linking has been coupled with finite deformation formulations. To deal with the highly non-linear differential equations representing the problem, a parametrised custom Finite Element variational formulation has been implemented.

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Electrically-tunable active metamaterials for damped elastic wave propagation control

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Keywords: tunable metamaterials, active control, dissipative shunted circuits.

An electrically-tunable metamaterial is herein designed for the active control of damped elastic waves. The periodic device is conceived including both elastic phases and a piezoelectric phase, shunted by a dissipative electric circuit whose impedance/admittance can be adjusted on demand. As a consequence, the frequency band structure of the metamaterial can be modified to meet design requirements, possibly changing over time [1].

A significant issue is that in the presence of a dissipative circuit, the frequency spectra are obtained by solving eigen-problems with rational terms.

This circumstance makes the problem particularly difficult to treat, either resorting to analytical or numerical techniques. In this context, a new derationalization strategy is proposed to overcome some limitations of standard approaches. The starting point is an infinite-dimensional rational eigen-problem, obtained by expanding in their Fourier series the periodic terms involved in the governing dynamic equations. A special derationalization is then applied to the truncated eigen-problem. The key idea is exploiting a LU factorization of the matrix collecting the rational terms. The method allows to considerably reduce the size of the problem to solve with respect to available techniques in literature.

This strategy is successfully applied to the case of a three-phase metamaterial shunted by a series RLC circuit with rational admittance [2].

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A metamaterial made of a lattice shell of two orthogonal logarithmic spiral families of fibers

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Keywords: Second gradient surfaces, Homogenized nets, metamaterials.

The objective is to explore the mechanical potential of a material consisting of an orthogonal network of fibers arranged in logarithmic spirals. Therefore, we consider an annular plate described with a second gradient model to evaluate the behavior of such a material in a nonlinear elastic regime when large displacements and deformations occur. Some mechanical tests are performed numerically using the finite element method, directly with a weak formulation based on the elastic energy postulated for this type of fiber network system. Numerical results are analyzed and compared with a much more detailed 3D model. Graphs showing the mechanical properties in all the tests considered are provided to illustrate the overall mechanical behavior of the evaluated system.

The proposed formulation is reasonably comprehensive since it can treat several mechanisms of deformations, including the bending and twisting of the fibers. Moreover, it has been proven in many experimental tests that the model is accurate and predictive.

Numerical tests reveal the nonlinear character of the system in the elastic regime, making it suitable for many technical applications, such as separation septum with shielding capability, reinforcement for valve diaphragms, and flexible couplings.

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Micromechanical analysis of soft lattice metamaterials accounting for randomly distributed imperfections

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Keywords: Metamaterials, Buckling, Imperfections.

Metamaterials, nowadays widely employed in many engineering fields [1], are materials artificially designed to obtain high mechanical, chemical and electromagnetic performances. These are often obtained by tessellation of unit cells (UCs) with truss- or beam-like microstructure made of hyperelastic or rubbery materials. Such soft lattice structures typically absorb energy and mitigate vibrations, show auxetic behavior, have shape-memory and shape-morphing properties and can achieve large elastic deformations and equilibrium instabilities. Hence, their mechanical modeling requires the inclusion of the nonlinear geometric effects [2].

This study focuses on the micromechanical modeling of soft beam-metamaterials analyzing both the pre- and post-buckling behavior. The considered UCs are composed by the assembly of shear-deformable beams accounting for large displacements and finite strains. Firstly, the linear buckling modes are evaluated (Figure 1) and, then, are used to construct the imperfect lattice structures. In fact, the effects of randomly distributed imperfections, typically deriving from the manufacturing processes, are analyzed in terms of both load-displacement global curves and failure modes of the UC (Figure 2).

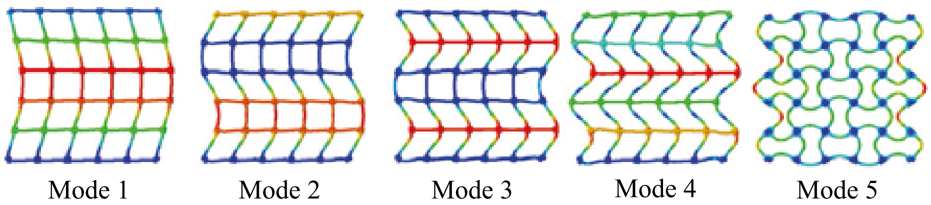

Figure 1: Buckling mode shapes of an example 5×5 square unit cell.

Moreover, the influence of the variation of boundary conditions and geometric patterns considered is analyzed with a view to developing a multiscale strategy tailored to the study of such periodic cellular materials. Attention is paid to both 2D and 3D structures and the obtained results are also compared with experimental outcomes [2] with the aim of validating the numerical investigations.

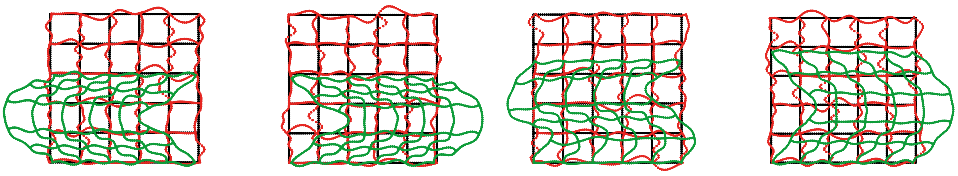

Figure 2: Effect of randomly distributed imperfections (red configurations) on the failure mode (green configurations) of a 5×5 square unit cell.

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Discrete homogenization in large deformations for plane beams lattices

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Keywords: Lattices, Homogenization, Large deformations.

With the increasing use of composite materials in various fields of engineering, the prediction of the macroscopic properties of these materials from their microscopic mechanical behaviour is becoming increasingly important.

This study concerns periodic planar lattices composed of thin rigidly connected elements, considered as micro-beams, with extensional and flexural stiffness. Assuming a significant scale separation between the period and the global deformation, a continuous model was identified based on the asymptotic homogenisation method for discrete media [1]. This homogenisation method was initially developed for static linear cases and for dynamic cases in the context of small deformations [2][3][4].

In this paper, the main innovation is the extension of the discrete homogenisation to the situation of large deformations [5] [6]. Our approach assumes that each beam is only slightly deformed according to a corotational model while the lattice undergoes large deformations (Fig.1). Under these conditions, the forces and moments at the origin/end nodes of the deformed microbeam can be expressed explicitly as a function of the kinematic variables at these ends. The problem is therefore expressed in discrete variational form in Lagrangian parameter space and the equilibrium of the reference cell is studied in its deformed configuration. For single-node unit cells, the self-equilibrium equation (i.e. the microscopic scale equilibrium) is used to relate the local kinematic variables to the global variables. The global equilibrium then provides the equivalent continuous model that accounts for the geometric non-linearity at the macroscopic scale.

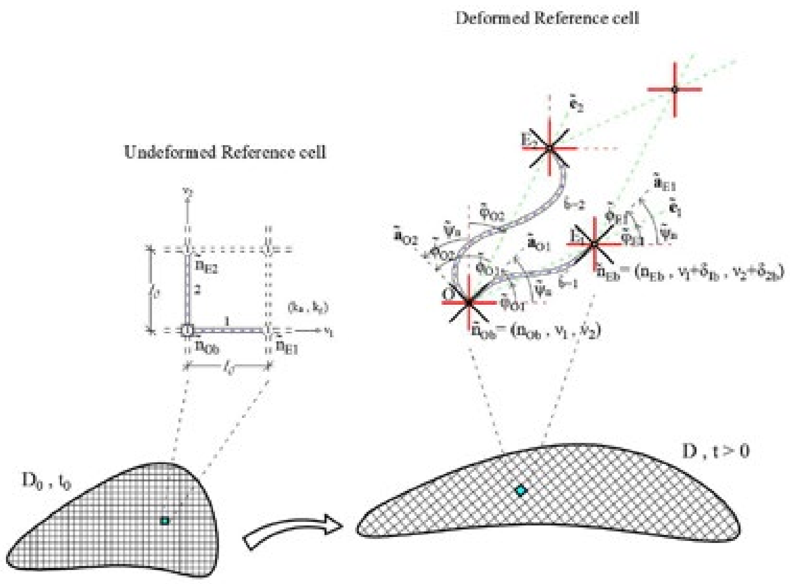

Figure 1: Undeformed lattice and lattice deformed with large deformations according to corotational model of microbeams.

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Corotational force-based beam finite element with rigid joint offsets for the analysis of geometrically nonlinear lattice systems

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Keywords: Lattice structure, geometric nonlinearity, force-based formulation.

The numerical analysis of framed structures is a relevant task in several engineering applications, such as the design of civil constructions and mechanical systems. However, this is also of some importance in more innovative fields, such as the mechanical response study of lattice metamaterials [1]. Hence, in the last decades, several efforts have been made to develop beam-column models capable of describing the behavior of framed structures under nonlinear material and geometric effects. Among them, force-based and mixed finite element (FE) formulations have proven to be a very efficient tool, computationally less expensive but enough accurate as two-dimensional plates/shells and three-dimensional FEs.

This work presents a geometrically nonlinear three-dimensional (3D) beam FE formulation based on the combination of a corotational approach and a higher-order force-based formulation including moderately large deformations. The corotational approach permits decoupling the element rigid-body motions from the deformation displacements and accounts for nodal large rotations and displacements. The approach follows the proposal in [2] where the nonlinear coupling between the axial and torsional stress/strain components is also included to describe the Wagner effect.

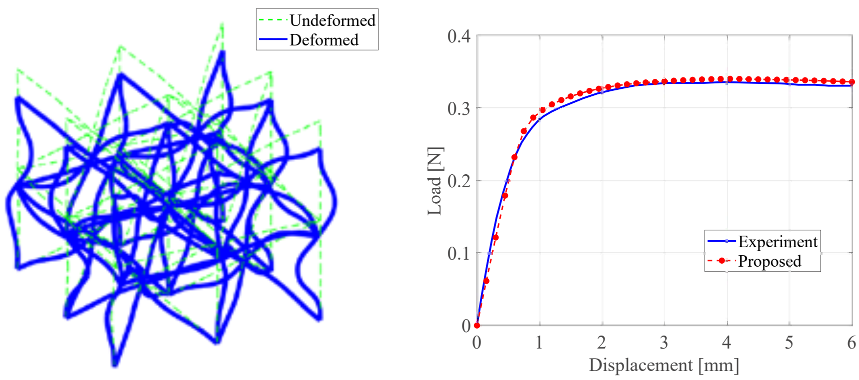

Figure 1: Lattice material sample under compressive load [1]: deformed configuration (left) and load-displacement response curve (right).

The beam formulation is inspired to that proposed by Rezaiee-Pajand and Gharaei-Moghaddam [3]. Based on previous proposals, they developed a force-based formulation for a straight 3D beam undergoing moderately large deformations, i.e., including the von Kármán nonlinear terms in an approximate way. The model imposes the element equilibrium in the deformed configuration, i.e., by accounting for the transverse cross-section displacements, and derives the governing equations on the basis of the Hellinger-Reissner variational principle.

In this work, the corotational approach and the beam formulation are extended to account for the introduction of rigid offsets located at the ends of the elements, which is required in many applications to properly model the connection between different structural elements. To this end, two different methods are proposed. The first method is based on the definition of proper operators that describe the kinematic and static behavior of the rigid offsets under large displacements and rotations [4]. On the contrary, the second method is based on a proper integration of the basic displacements and flexibility matrix that govern the element response.

Numerical simulations of paradigmatic case studies are performed to validate the proposed model, comparing the results with existing solutions from the literature. In addition, the behavior of experimentally tested lattice specimens is numerically reproduced.

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An optimal-transport finite-particle method for mass diffusion

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Keywords: Optimal Transport Theory, diffusion, blob functions.

In contrast to the Optimal Transport Meshfree method, two-field representation of diffusion, so-called *blob methods*, work solely with the mass density field, which is discretized into smoothed mass particles, or *blobs*, of a certain finite width [2, 3]. For diffusion problems, these finite-particle methods have the appeal of setting forth single-field numerical schemes, at great gain in simplification. However, they also raise a number of numerical analysis questions, such as the consistent variational foundation of the schemes, the enforcement of boundary conditions, the optimal selection of particle thickness and the overall accuracy and convergence of the schemes.

In the present work, we resort to a time-discretized variational formulation of mass diffusion, as in [1], but discretize the mass density by means of finite particles, or blobs, as in [2, 3], in order to formulate a class of velocity-free finite-particle methods. The immediate benefit of using finite-width particles, as opposed to Dirac deltas, is that their entropy can be computed directly from the relative entropy, or Kullback-Leibler, functional. This is in contrast to mass discretization based on point masses, such as used in [1], for which the entropy functional needs to be carefully rephrased in a weak form. The motion of the finite particles then follows as the result of a competition between entropy, as given by the Kullback-Leibler functional, and mobility, as represented by the Wasserstein distance between consecutive configurations. Thus, entropy works to disperse the particles uniformly over the domain, whereas mobility works to hinder their motion.

We illustrate the scope and properties of the method by means of a test problem concerned with the injection of mass into a sphere. The ability to inject finite particles into the domain and follow the diffusion-driven trajectories in time, including convergence to a steady uniform density after the injection ends, is quite remarkable. The weak convergence of the scheme is monitored through the time evolution of the moment of inertia of the particles. The test is indicative of robust convergence with respect to time step and number of particles.

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Variational and Topological Methods for Nonlocal Problems

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Keywords: nonlocal elasticity; fractional Laplacian operator; nonlocal dynamics

A very interesting area of nonlinear analysis lies in the study of elliptic equations involving fractional operators. Recently, a great attention has been focused on these problems, both for the pure mathematical research and in view of concrete real-world applications. Indeed, this type of operators arises in a quite natural way in different contexts, such as the description of several physical phenomena. The current literature on these abstract tools and on their applications is, therefore, very interesting and, up to now, quite large; see [4] and the references therein. Moreover, rich mathematical concepts allow in general several approaches, and this is the case for the fractional Laplacian, which can be defined using Fourier analysis, functional calculus, singular integrals or Lévy processes. Its inverse is closely related to the famous potentials introduced by Marcel Riesz in the late 1930s. In contrast to the Laplacian, which is a local operator, the fractional Laplacian is a paradigm of the family of nonlocal linear operators, and this has immediate consequences in the formulation of fundamental theoretical questions related to relativistic periodic problems; see [3]. Motivated by this wide interest in the literature, the leading purpose of this talk is to present some recent results on fractional nonlocal operators and some of its applications to the Eringeen model; see, among others, the recent papers [1] and [2] as well as the references therein.

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Virtual element method for the analysis of cohesive crack propagation

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Keywords: *Virtual Element Method, Cohesive fracture, Crack nucleation and propagation.*

Abstract

The Virtual Element Method (VEM) has attracted a lot of interest from the scientific community and numerous results have been achieved in different research fields, comprising linear elasticity problems, inelastic problems, fluid-flow problems and contact problems [1]. In particular, VEMs can be conveniently applied within the context of computational fracture mechanics.

In this field, the numerical approaches proposed in literature are mainly based on the finite element method (FEM) or on modified forms of this latter such as the extended FEM and the augmented FEM.

The VEM formulation is characterized by the possibility to define polygonal meshes with elements characterized by any number of edges and by the flexibility in mesh generation that allow to introduce a crack just redefining the element in two different elements joined by a crack modelled with an interface element. The features of the VEM appear particularly suitable for the development of a procedure able to follow the crack propagation in a solid, requiring a minimal remeshing [2].

The present work proposes an algorithm of nucleation and growth for fracture evolution in 2D cohesive media. The procedure is based on virtual element method specifically referred to a 4-side 12-node virtual element with piece-wise linear approximation of the displacement field on the edges. The large number of nodes and, consequently of degrees of freedom, is exploited to enrich the strain and stress field evaluation. It is derived by means of the minimization of the complementary energy within the single element. This procedure allows to avoid the stabilization of the element stiffness matrix.

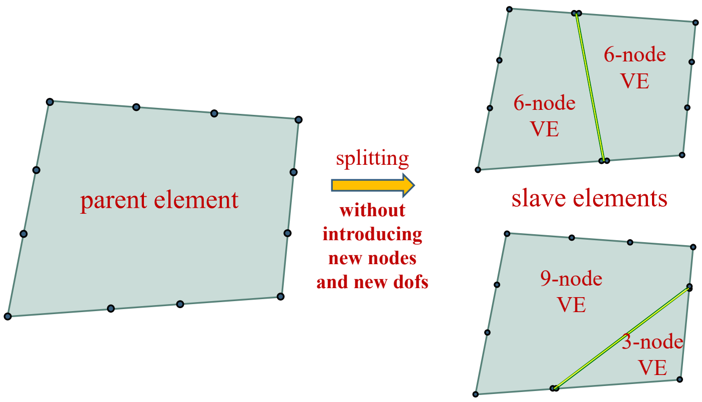

Figure 1: Splitting of the virtual element to simulate the crack.

The fracture is introduced in the solid domain by splitting the virtual element, called parent element, into two slave elements, joined by a cohesive interface (Figure 1). The presence of the two nodes inside any edge of the parent element has been proposed for avoiding the generation of new nodes during the crack evolution. The obtained slave elements are characterized by a different number of nodes depending whether the straight crack within the parent element crosses two opposite or adjacent sides. At the interface, a cohesive law governed by a damage variable in mode I, in mode

II and in mixed mode, and that takes into account for the unilateral effect due to the reclosure of the crack in compression, is adopted [3].

Moreover, different approaches based on stress or damage evaluation have been proposed and compared to evaluate the fracture direction.

Numerical simulations of experimental tests (figure 2) are developed in order to assess the ability of the proposed procedure to satisfactorily reproduce the crack nucleation and growth. The simplicity of the procedure with respect to other more complicated approaches is remarked highlighting the reduced computational effort and storage memory required.

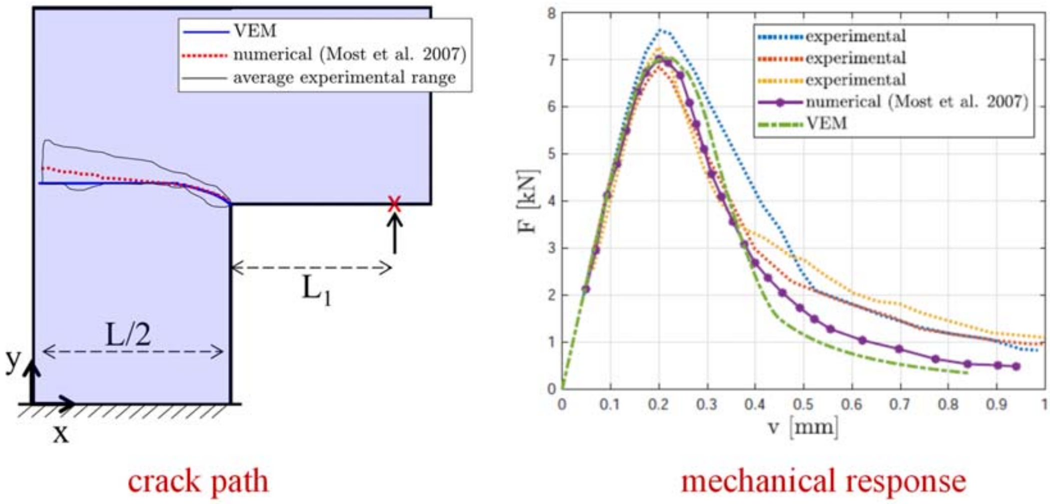

Figure 2: Fracture growth in a L-shaped structural element.

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A continuum approach inspired by a block-based model for the analysis of masonry structures

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Keywords: Masonry, continuum model, block-based model, homogenization.

Due to the inherent nonlinearity and complex interactions between its constituents, the analysis of masonry structures is generally performed using numerical models. Following this approach, block-based models and continuum models are generally adopted. Block-based models allow to explicitly account for the masonry texture, which is essential for the accurate representation of masonry structural behavior. However, due to their high computational demands, they are usually unsuitable for the analysis of large-scale structures.

In this contribution, a novel continuum model for the analysis of masonry structures characterized by a regular periodic texture is proposed. The adopted constitutive law is derived basing on the analysis of a block-based model characterized by finite strength blocks and frictional-cohesive zero-thickness interfaces. The strength domain is obtained as the intersection of different failure surfaces each of them representing a different failure mechanism of the block-based model. Accordingly, the possibility to employ a strain decomposition to explicitly distinguish the onset of each failure mechanism is discussed. Non-associated behavior of interfaces is also considered.

The proposed model is numerically validated on some benchmark examples, also comparing the results with those obtained through a finite element block-based model.

Enhanced Virtual Element formulation for large displacement analysis

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Keywords: Corotational approach, Virtual Element, Self-stabilized elements.

Corotational approach is nowadays recognized as an effective strategy to account for geometric nonlinear effects in the presence of large displacements and rotations and small deformations [1]. Such an approach has been largely adopted in Finite Element codes for geometric nonlinearity, but this has not yet been explored within the framework of the Virtual Element Method (VEM). The latter is a modern numerical procedure recently developed [2] for solving boundary value problems governed by systems of partial differential equations and allows to overcome some limits of the Finite Element Method.

In the present contribution, an enhanced virtual element formulation [3, 4] is introduced within the corotational framework. In this spirit, the kinematics of the virtual element is decomposed in its rigid and deformable parts. In addition to the global coordinate system, (X, Y), a local/corotational system, (x, y), which translates and rotates with the element during its motion, is introduced (Figure 1). Hence, the deformable behavior is evaluated computing the small strain contribution in the corotational system, whereas the large displacement-induced nonlinearity is accounted for through the transformation matrices relating the local and global quantities.

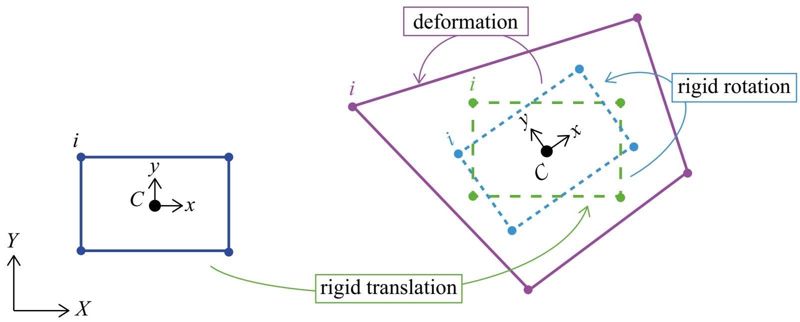

Figure 1: Kinematics of the Virtual Element.

At the local level, the assumed virtual element formulation adopts an enhanced strain description based on the divergence-free polynomial representation [4], while assuming the same approximation functions for the displacements at the element boundary characterizing the standard VEM. This assumption allows to bypass the need of stabilization terms in many practical cases.

Effectiveness and robustness of the proposed virtual element-corotational approach is proved by several benchmark tests. The numerical results, in terms of global response curves and deformed configurations of the analyzed structural members (Figure 2), are validated by comparison with analytical and numerical reference solutions. Finally, some perspectives on the use of the proposed modeling strategy are discussed.

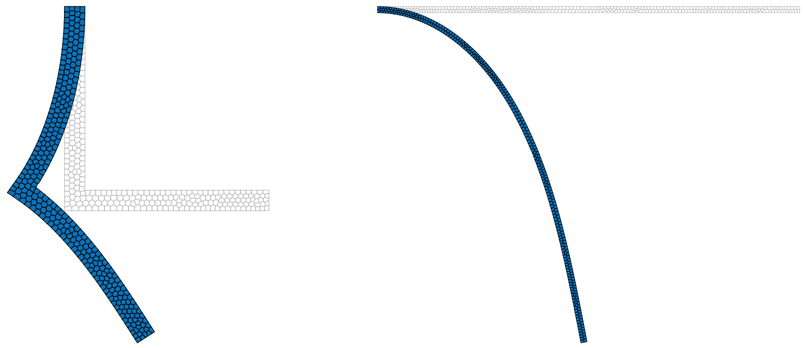

Figure 2: Examples of benchmark test.

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A new advanced fully mechanical tool for manual mini-invasive surgery

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Keywords: mini-invasive surgery, laparoscopic tools, dextrous gripper

ABSTRACT

The paper presents a new tool for minimally invasive surgery that has high dexterity and ease of use by the surgeon who, without special training, can use it even in complex surgical operations. The tool is designed with the master-slave logic of telemanipulators. The results obtained with a prototype of the tool confirm its efficiency.

Introduction

The advantages of minimally invasive surgery (especially laparoscopic surgery) over open-field surgery are well known [1,2]. Minimally invasive surgery tools are inserted into the human body through small holes, and allow the surgeon to perform operations on internal organs by controlling the movement of the tool from the outside. The surgical field is viewed on screen through a camera inserted inside the patient's body.

The tool, consisting of a cannula with a diameter of about 5-10 mm, is inserted into the patient's cavity via a trocar. At the end of the cannula, at the inner part there is the operating head (forceps or scissors, for example) while at the outer end there are the elements of control of the movements of the head by the surgeon. The trocar allows the tool 4 degrees of freedom (dofs), that are defined as “free” dofs, precisely three rotations around the patient entry point and a translation along the axis of the tool itself (Fig. 1a). The head dofs characterize the dexterity of the tool and can vary from 1 (gripper opening-closing) to 4 when they also include the three rotations of the head around a fixed point (spherical motion).

The tools on the market are essentially of two types: manual (with more or less dofs) and robotic, that is, assisted by a robotic system, (with many dofs). The former are generally less dextrous than the latter ones, which are however extremely more expensive (than the former).

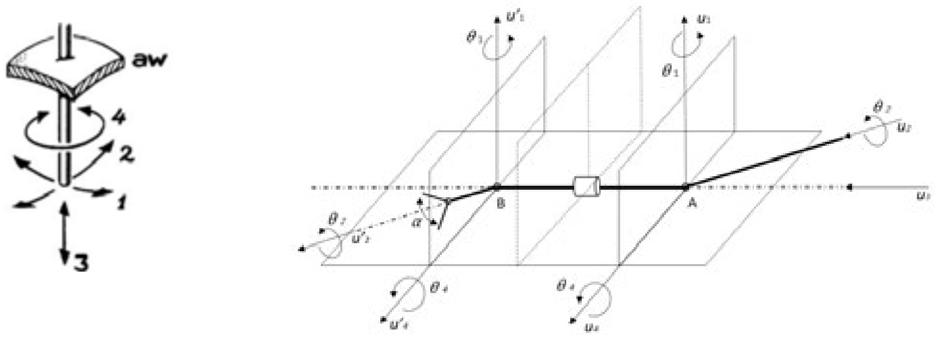
This paper presents a new highly dextrous, inexpensive and disposable hand tool. A prototype is then presented to test and show its characteristics.

The proposed advanced tool

With reference to Fig. 1b, which represents the functional scheme of the tool, and Fig. 2, which represents the prototype built, whose details are shown in [3], the tool consists of three incident segments at point A, external to the patient, and at point B, inside the patient. In particular, the proposed tool has the following characteristics:

- with the same logic of telemanipulators, therefore in an extremely intuitive way, the surgeon outside moves a knob making the same movements of the head inside;
- in any configuration of the tool it is possible to realize rotations around the incident axes at point B of unit vector u_1, (yaw) [+ 45°,-45°], and of unit vector u_2 (e.g., for suture) of [0°, 360°] respectively, and opening-closing of the gripper of an angle α in the field [0°,90°];
- by a simple manoeuvre, it is possible to reconfigure the instrument to perform the rotation about the axis of unit vector u_4 (pitch) [+ 45°,-45°].

Therefore, the tool is highly dextrous, possessing 4 additional free dofs. The tests carried out with the prototype gave very positive results.



a) b)

Figure 1: a) trocar with four free dofs; b) schematic of the tool

Figure 2: The tool prototype inserted in the trocar

Conclusions

This paper presents an instrument for minimally invasive surgery and a prototype that has highlighted its operational dexterity. The prototype satisfied the desired characteristics, and it is now in the stage of its engineering design.

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Durotaxis of tensegrity cell units incorporating asymmetry

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Keywords: Cell mechanobiology, Durotaxis, Cellular tensegrity, Nonlinear elasticity.

The present contribution focuses on some recent results obtained by the authors concerning durotaxis of cell units anchored to the substrate through focal adhesion plaques, a phenomenon which is relevant to cell locomotion [1]. A mechanical pre-strained tensegrity model obeying a Neo-Hookean stress-strain law recently devised by the authors [2, 3, 4] is exploited to investigate how substrate stiffness gradients and asymmetric geometry affect the cell contractility and the growth of the focal adhesion plaque. The cytoskeleton is purposely reduced to its main components, that is actin filaments and microtubules forming a contractile mechanical system obeying the so-called tensegrity self-equilibrium principle [5]. The system contraction is triggered by means of inelastic pre-strains, that simulate pre-contraction and polymerization. In the adopted tensegrity, an element representative of the actomyosin complex is taken in parallel with another element corresponding to the microtubule [2, 3]. The former can only elastically elongate or inelastically contract without bending, while the latter is a compression-bearing buckling-prone element that can also polymerize.

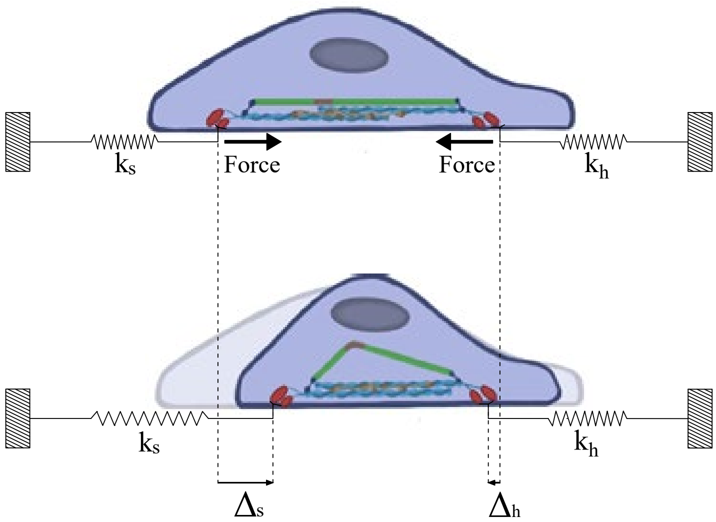

Figure 1: A contractile cell where the cytoskeleton is replaced by the adopted tensegrity and the cell contractility induces two equal forces at the leading and trailing edges of the cell where the plaques of the focal adhesions are located.

A scheme of the adopted mechanical framework is shown in Figure 1. The cell contractile activity produces two equal forces at the leading and trailing edges of the cell where the plaques of the focal adhesions are considered to be located. These forces, in turn, induce a thermodynamically consistent polymerization/depolymerization process of the focal adhesion plaques. As an effect of the mechanosensitivity of the devised structural system, the displacement Δ_s at the edge lying upon the softer substrate will be generally different from Δ_h detected at the edge placed on the hard part of the substrate. The cell net displacement Δ_N can be hence computed as [1] $\Delta_N = \Delta_s - \Delta_h$. The contractile system illustrated in Figure 1 exemplifies the positive durotaxis concept with the cell advancing towards the stiffer side. However, recently, it has been observed that some cells may migrate towards softer substrates [6], thus suggesting the existence of a negative durotaxis, or mollitaxis, effect.

The present contribution shows that both ”classical” positive durotaxis and more recently unveiled mollitaxis can be retraced by means of the proposed essential model, the switching from one mechanism to the other depending on the combination of geometrical asymmetry, stiffness gradients, and inelastic pre-strains. Advantageously, the present model allows us to parametrically investigate the effect of a wide range of asymmetric configurations and stiffness gradients on the cell kinematics and how these affect the process of assembly and disassembly of the focal adhesion plaques subjected to the force exerted by the system.

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Actin based motility unveiled: how chemical energy is converted into motion

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Keywords: Mechanobiology; actin-based motility; cell motility; multiphysics models; thermomechanics of continua.

The chemo-mechanical motor of several biological systems is a polymerization process that converts chemical energy into mechanical work. The chief component in this activity is actin, a multifunctional protein forming filament in the cell cytoskeleton that is capable of generating protrusive forces when polymerization occurs in close proximity to a barrier or to a load [1]. External impulses of a chemical or mechanical nature trigger a chemical reaction, which converts the monomeric form of actin, G-actin, into a polymerized branched-filamentous form, F-actin [2, 3]. Upon polymerization, the cross-linked network acts against the plasma membrane, a pathogenic bacterium or an endosome, pushing them forward and promoting directional motility [4]. In a recent publication [5], we have suggested that the *volumetric expansion* exerted after the phase change from monomeric to a cross-linked network of actin filament ultimately converts chemical energy into motion.

At the leading edge of cells, in fact, actin is organized in a bidimensional dendritic array of branched filaments [6]. Branched actin filaments are generated beneath the plasma membrane by external signal responsive WASP-Arp2/3 machinery and kept functioning by a set of regulatory proteins. Those binding proteins control actin turnover and filament elongation, mediate the initiation of new filaments as branches on pre-existing filaments and promote (de)branching and (de)polymerization, thus regulating the mechanical response of moving cells [7]. Upon mechanical loading, actin networks change density, power, and efficiency, showing load adaptation and reorganization during motility. Microscopically, this is reflected by a change of filament number and an altered geometry. Macroscopically, it leads to a variation of network volume, stiffness, and resistance to mechanical failure.

In this note, a thermodynamically consistent continuum-mechanics formulation will be proposed, stemming from continuity equations that account for actin chemical kinetics - see fig. 1. The model manifests itself in macroscopic descriptors of biochemical and biological details of the relevant processes, thereby resulting in sufficient generality to be appropriate for several biological systems.

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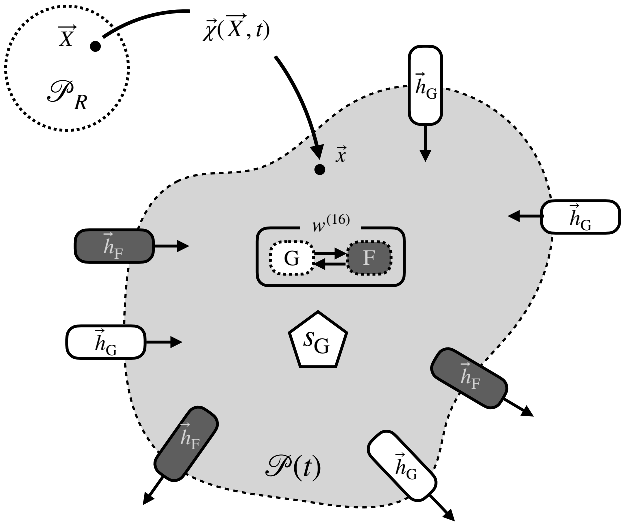

Figure 1: Schematic representation of the mass balance on an advecting cytosol $\mathcal{P}(t)$.

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A computational model of cell motility in biodegradable hydrogel scaffolds for tissue engineering applications

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Keywords: Tissue growth, Culture protocols optimization, Cell motility, Phase-field modeling.

Tissue engineering is a rapidly developing field that has the potential to revolutionize many areas, such as medicine, by recreating functional tissues that replace the lost/damaged ones *in vivo*, or the food sector, by producing meat in the laboratory without the need to breed animals [1]. Tissue growth is facilitated if cells are encapsulated in hydrogel scaffolds that provide them a mechanically supportive environment, while guaranteeing cells viability. Neo-tissue formation in bioprinted scaffolds is the result of a multifactorial process involving cell differentiation, proliferation, extracellular matrix (ECM) production, and assembly of cells in a functional way. In particular, successful tissue production is closely linked to cell motility, which in turn depends on many factors, such as spatio-temporal changes of cellular microenvironment, chemical stimuli triggered by neighbouring cells, and proper transport of growth factors, oxygen, nutrients and waste through the constructs. In this process, all the relevant variables must be fine-tuned in order to maximize the quality and quantity of the final product. However, such optimization is unfeasible through trial-and-error approaches, since the nature and the number of tests would lead to long times and prohibitive costs. Numerical models can therefore be employed to successfully and effectively simulate *in vitro* experiments, as they constitute a valid, fast and low-cost alternative to extensive experimental campaigns.

With this background, a novel computational model has been developed to describe cell motility in bioprinted hydrogels up to the formation of clusters. Cell migration is treated as a diffusive/advective process modeled via a phase-field (PF) approach. The PF governing equations are coupled with transport equations describing the main chemo-mechano-biological mechanisms involved in the process and confirmed by the experimental evidence, such as scaffold degradation, nutrient diffusion into/out of the construct, chemoattractant expression and diffusion through the hydrogel. The model accounts for the twofold nature of cell motility, which consists in the superposition of random advances and rotations (Brownian-like motion), and a directed motion driven by chemical (chemotaxis) and mechanical (durotaxis) cues [2]. Numerical results highlight the role of the nutrient and chemoattractant availability in the construct, as well as of the interplay between cell motion and chemo-mechanical properties of the extracellular environment. The developed computational framework represents then a first step towards an *in silico* predictive tool for the optimization of both scaffold properties and culture protocols for the formation of neo-tissue.

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An *in-silico* approach for process design in extrusion-based bioprinting

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Keywords: Bioprinting, reduced-order model, process design tools.

Extrusion-based bioprinting is an additive manufacturing technique for the fabrication of biological constructs through layer-by-layer deposition of a bio-ink (viable cells suspended in a biomaterial solution) [1]. The planning of a bioprinting procedure demands the definition of several process variables and their optimal setting highly varies case-by-case. In extrusion-based bioprinting typical process variables are, for instance, the dispensing pressure, the nozzle diameter, the target extrusion velocity and/or mass flow rate. Moreover, the need to ensure high cell viability at the end of the process is a major critical concern in the bioprinting planning. In fact, printing mechanisms expose cells to shear and extensional stresses that can lead to the disruption of the outer cell membrane or the onset of apoptotic signals [2].

In order to fulfill technological demands and to maintain stresses below a threshold value that ensures an acceptable level of cell damage, all the afore-mentioned process variables must be properly chosen. Unfortunately, these are closely interconnected each other through the physical response of bio-ink. Shear-thinning behaviour of bio-inks, as well as non-simple geometries of the extruding system, generally introduce a strong non-linear coupling among process variables. High mass flow rate is desirable, for instance, to speed-up printing operations, but at the same time leads to higher stresses that affect cell viabilty. Small nozzle diameters are employed for higher resolutions but these are associated with higher dispensing pressures and eventually lower cell viability. As a consequence, bioprinting planning in laboratory practice is generally made through expensive and time-consuming trial-and-error attempts.

The aim of this work is to contribute to the devolpment of a novel *in-silico* approach that allows for more rational and quick definition of suitable target conditions enabling for effective bioprinting planning. The non-linear coupling among dominant process variables is described via a semi-analytical reduced-order model, calibrated through high-fidelity numerical solutions. A cell damage law depending on bioprinting conditions is also introduced, generalizing state-of-the-art approaches on the basis of available experimental evidence. The proposed approach allows to build up operative nomograms that provide laboratories with process design tools for the planning of bioprinting via fast graphical calculations (see Fig.1). Applications address the prediction of extrusion velocity, mass flow rate and cell viability when both the dispensing pressure and nozzle diameter vary.

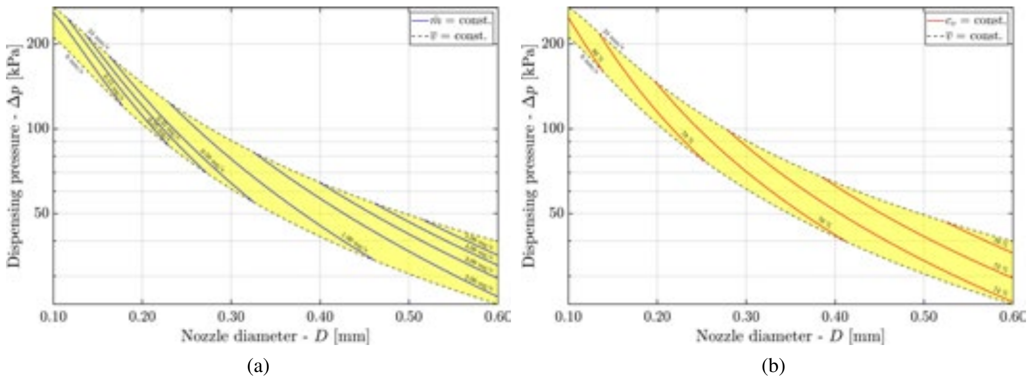

Figure 1: Nomograms built from reduced-order model. (a) Isopleths of mass flow rate $\dot{m}$ and limit extrusion velocities $\overline{v}$. (b) Isopleths of cell viability c_v.

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Extension of the novel Line Element-less Method for plates shaped with re-entrant angles

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Keywords: Plate bending, Line Element-less Method, Re-entrant angles.

Several engineering problems, comprising civil, aeronautical, chemical and mechanical engineering applications [1], often require estimating the response of elastic thin plates of arbitrary or complex shape. Clearly, plate deflection strongly depends on both the geometrical shape and given boundary conditions, and thus approximate numerical methods are usually employed for their analysis. In this context, Finite Element Method (FEM), Boundary Element Method (BEM) and Rayleigh-Ritz approaches are among the most widely used. Very recently, an innovative meshfree method, the so-called Line Element-less Method (LEM), has been proposed to determine the response of plates under uniformly distributed edge moments [2]. Note that, this method is based on the evaluation of line integrals only. Therefore, it does not require any discretization neither in the domain nor in the boundary, and then it appears to be quite convenient when studying plates of complex shapes or boundary conditions. However, using the previous formulation, it was not possible to handle plates in bending, shaped with re-entrant angles; then this contribution aims to extend the aforementioned LEM to this latter case.

Analyses are carried out for several plate shapes, showing the elegance and simplicity of the proposed procedure, which allows the computational cost to be kept at minimum. Further, comparisons of LEM based deflection functions vis-à-vis pertinent Finite Element method will assess the accuracy and reliability of the considered approach.

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A generalized fiber model for the elastoplastic analysis of steel beams including normal stress-shear stresses interaction

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Keywords: 3D beams, plasticity, fiber model, shear and torsion, finite element method.

The fiber model [1] of the cross-section is a very popular approach for the elastoplastic analysis of beams and frames. It consists in evaluating the material response in terms of normal stress at a discrete number of integration points (fibers) over the section for a given increment of the strain field according to the rigid section assumption. The stress field is then integrated numerically for obtaining axial force and bending moments. The interaction with tangential stresses is usually neglected at the fiber level, due to the inaccurate representation of the shear strain over the section based on the rigid section model. In this work, we propose a full coupling of normal stress-shear stresses in a series of control points or generalized fiber, over steel cross section by exploiting the accurate strain field coming from the De Saint Venant problem [2]. A closest point projection provides then the full stress state at each generalized fiber (see Fig.1) and, then, all the stress resultants and moments with a full interaction among all of them. This model of the cross-section is implemented in an accurate mixed finite element of 3D beam with equilibrated stress field, with the possibility of including also non-uniform warping. Numerical tests confirm an excellent accuracy compared with a solid reference solution and the efficiency of the proposal, very similar to the standard fiber beam model.

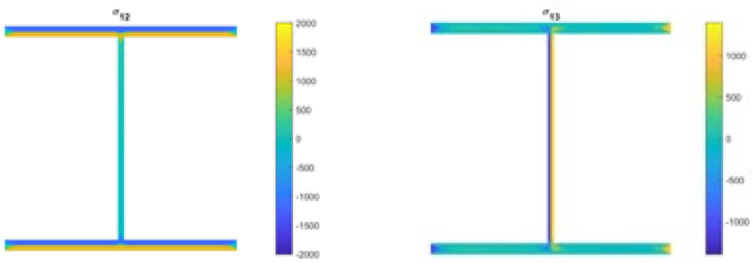

Figure 1: Stress field at collapse for a HEA section under uniform torsion.

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Higher order theories for the structural analysis of anisotropic shells of arbitrary shape with general boundary conditions

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Keywords: Anisotropic elasticity, Doubly-curved shells, Generalized Differential Quadrature.

Recent advances in many engineering applications adopt structural elements of very complex shape and advanced material properties, which are very often characterized by a three-dimensional behaviour. For this reason, the structural response can be well predicted by theoretical formulations if the geometry of the structure [1], as well as the constitutive relationship, is described accurately (Figure 1). On the other hand, refined models significantly increase the computational demand for the derivation of the solution. In this perspective, a generalized two-dimensional formulation [2] based on Higher Order Shear Deformation Theories (HSDTs) lead to accurate results with a reduced number of Degrees of Freedom (DOFs), as can be seen in Figure 1. They are based on the description of the unknown field variable vector $\mathbf{U}^{(k)}$ with the so-called generalized thickness functions, which are collected in the matrix $\mathbf{F}^{(k\tau)}$:

$$\mathbf{U}^{(k)}\left(\alpha_1,\alpha_2,\zeta,t\right)=\sum_{\tau=0}^{N+1}\mathbf{F}^{(k\tau)}\left(\zeta\right)\mathbf{u}^{(\tau)}\left(\alpha_1,\alpha_2,t\right) \tag{1}$$

being $k=1,...,l$ the layer of a stacking sequence of l laminae. As can be seen, the so-called generalized displacement field vector $\mathbf{u}^{(\tau)}$ is introduced for each τ -th kinematic expansion order.

A general lamination scheme with anisotropic constitutive behaviour and general orientation is considered for the elastic constitutive relationship. Starting from the well-known Hooke's law, the constitutive relationship is written for the HSDT formulation as follows:

$$\mathbf{S}^{(\tau)\alpha_i}=\sum_{\eta=0}^{N+1}\sum_{j=1}^{3}\mathbf{A}^{(\tau\eta)\alpha_i\alpha_j}\boldsymbol{\varepsilon}^{(\eta)\alpha_j} \quad \text{for} \;\; \tau=0,...,N+1, \;\; i=1,2,3 \tag{2}$$

where $\mathbf{S}^{(\tau)\alpha_i}, \boldsymbol{\varepsilon}^{(\tau)\alpha_i}$ denote the generalized stress and strain vector, respectively, whereas $\mathbf{A}^{(\tau\eta)\alpha_i\alpha_j}$ is the generalized constitutive matrix. The fundamental dynamic equilibrium equations are derived from the Hamiltonian principle, taking into account the effects of external distributed and concentrated loads applied at the top and bottom surfaces and at the lateral surfaces of the three-dimensional doubly-curved solid [3]. Furthermore, general boundary conditions are enforced to the model with a general distribution of linear elastic spring. The Generalized Differential Quadrature (GDQ) method is adopted for the discretization of the fundamental equations directly in the strong form [4], as well as the boundary conditions. After the derivation of the two-dimensional solution, the prediction of the three-dimensional response can be made with an efficient post-processing technique.

A series of examples are presented, where the solution of both the static and the dynamic structural response of several laminated shell structures is derived. A high level of accuracy is seen with respect to the outcomes of three-dimensional Finite-Element-based models. Some investigations are then performed regarding curved and layered structures made of Functionally Graded Materials (FGMs), Carbon Nanotubes (CNTs), honeycomb and lattice cells, as well as classic composite laminates. Finally, the sensitivity of the geometry and the materials is shown in some systematic parametric investigations.

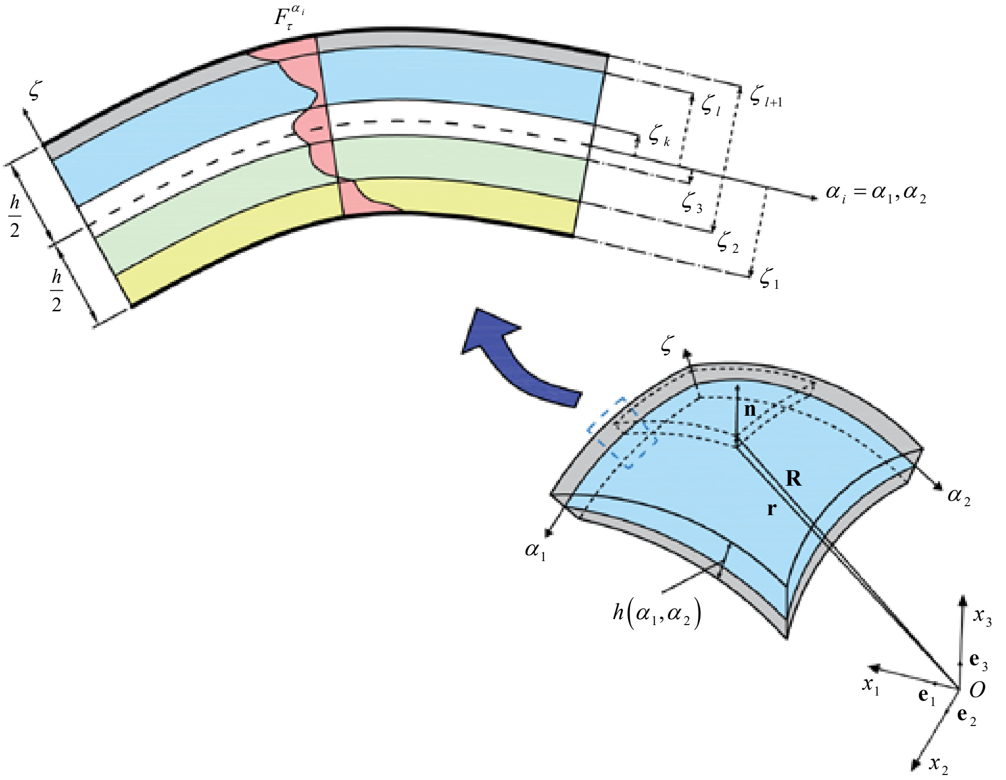

Figure 1: Doubly-curved shell geometry and representation of the HSDT model.

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A self-equilibrated assumed stress solid-shell finite element for large deformations problems

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Keywords: solid shell, corotational formulation, mixed finite element.

The use of mixed Finite Elements (FE) ensures better performance than more traditional displacement based formulations in different contexts. Some of the most significant advantages provided by the mixed FE technique are the elimination of many locking phenomena, the accuracy increasing and the robustness improvement of geometrically nonlinear analyses. The family of mixed shell FE denoted with the acronym MISS (Mixed, Isostatic, Self-equilibrated Stress) [1] has shown successful performance in linear analyses as well as in presence of material and geometrical nonlinearities and for both isotropic and composite laminate materials [2]. MISS FE are based on a Mindlin-Reissner shell model and on assumed stresses that a-priori satisfy equilibrium equations and, in some variants, compatibility equations [3]. This aspect guarantees good accuracy for coarse meshes and high convergence rates.

However, in some cases, solid-shell FEs are preferred on shell models [4]. In fact, they can better describe the connections between panels, allow to employ 3D-based constitutive laws and can exploit simpler strain measures in the geometrically nonlinear context.

Inspired by the good results obtained by MISS FE, in this work we propose a solid-shell FE. It is based on assumed stresses a-priori satisfying equilibrium equations. The FE has eight nodes, each of them with three translational degrees of freedom. The displacement interpolation is assumed only along the element contour. No rank defectiveness and spurious energy modes are detected. The element, formulated in the linear elastic case, is employed for the solution of the geometrically nonlinear problem through a corotational formulation. In particular, we show how, using the corotational technique, it is possible to recover the Green-Lagrange strain measure. Additionally, it is possible to use a simplified Green-Largrange strain measure which is coherent with the solid-shell assumption.

Results obtained with the proposed solid-shell FE are compared with existing mixed solid-shells, obtaining improved performance [4].

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Shear deformable plate with substructuring approach in the SGBEM: displacement method.

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***Keywords**:* Mindlin plate, SGBEM, substructuring approach, displacement method.

Abstract. In the context of SGBEM [1], the deformable shear plate analysis (Mindlin's model [2]) is carried out through a subdivision into macro-elements called e-bem. This subdivision is necessary to take into account zones having different physical and mechanical characteristics or particular conditions for internal constraints. After discretizing the e-bem's boundaries, the analysis is performed through a particular methodology based on a coefficient's matrix called the "progenitor matrix", that allows determining the constitutive relationship that characterizes the behaviour of the e-bem within the displacement method. Suitable conditions, strong compatibility between the assembled system's displacements and those of interface, and weak equilibrium between weighted interface tractions, allow obtaining the solving system of displacement method.

1. Progenitor matrix.

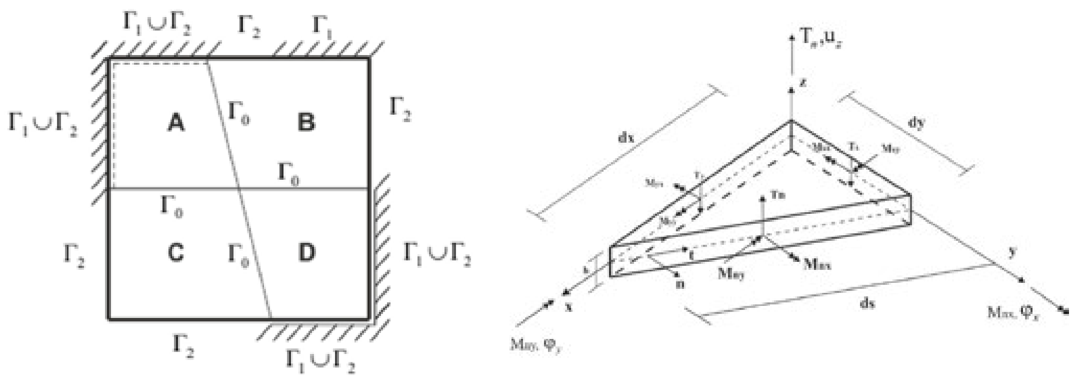

Fig. 1. a) Plate substructuring, b) Boundary quantities of e-bem plate.

Let us consider the plate in Fig. (1.a) subdivided into e-bem (A…D) whose boundary quantities are those in Fig. (1.b); the plate can be subjected to different domain and boundary loading conditions. The boundary of the $i-th$ e-bem of Ω domain, imbedded in the unlimited domain Ω / Ω_∞, can be thought of as boundary $\Gamma = \Gamma^-$ belonging to the actual domain Ω and boundary Γ^+ belonging to the domain Ω_∞ / Ω; the latter must remain unstressed and undeformed when the solution is obtained. Following the steps described in [3, 4], it is possible to obtain for the $i-th$ e-bem the matrix relation:

$$\begin{bmatrix} \mathbf{W}^+ \\ \mathbf{P}^+ \end{bmatrix} = \begin{bmatrix} \mathbf{B}_{uu} & \mathbf{B}_{ut} \\ \mathbf{B}_{tu} & \mathbf{B}_{tt} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{F} \\ \mathbf{V} \end{bmatrix} + \begin{bmatrix} \mathbf{W}_\Omega^+ \\ \mathbf{P}_\Omega^+ \end{bmatrix} \mathbf{F}_\Omega = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{1}$$

In Eq. (1) $\mathbf{B}$ is the "progenitor matrix", which is the starting point for obtaining the constitutive equation of the single e-bem for the displacements method into the substructuring approach; $\mathbf{W}^+$ and $\mathbf{P}^+$ are the weighted displacement and traction vectors on the boundary Γ^+ null by definition; $\mathbf{F} = \left[\mathbf{M}_{nx}, \mathbf{M}_{nx}, \mathbf{T}_n\right]^T$, $\mathbf{V} = \left[-\mathbf{\Phi}_x, -\mathbf{\Phi}_y, -\mathbf{U}_z\right]$ and $\mathbf{F}_\Omega = \left[m_{nx}, m_{nx}, f_z\right]^T$ are the generalized boundary and domain quantities vectors, respectively.

2. Displacement method: solving system.

The boundary of the $i-th$ e-bem is composed of constrained, free and interface parts, that is to say $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_0$. The real boundary conditions imply a reordering and partitioning of the "progenitor matrix" $\mathbf{B}$ [4], making it possible to generate the elasticity relation of the $i-th$ e-bem:

$$\mathbf{P}_0^i = \mathbf{D}_0^i\,\mathbf{U}_0^i + \hat{\mathbf{P}}_0^i + \hat{\mathbf{P}}_{0\Omega}^i \quad \text{on } \Gamma_0 = \Gamma_0^- \tag{2}$$

where $\mathbf{P}_0^i$ is the weighted traction, $\mathbf{D}_0^i$ the symmetric and defined stiffness matrix, $\mathbf{U}_0^i$ the vector of rotations and vertical displacements, $\hat{\mathbf{P}}_0^i$ and $\hat{\mathbf{P}}_{0\Omega}^i$ the vectors of the weighted boundary and domain load terms.

Let us write:

- the compatibility relationship between the interface displacements $\mathbf{U}_0$ of the $i-th$ e-bem and the displacements of the assembled structural system:

$$\mathbf{U}_0 = \mathbf{H}\,\mathbf{X}_0 \tag{3}$$

- the constitutive relation (2) for the set of n e-bems:

$$\mathbf{P}_0 = \mathbf{D}_0\,\mathbf{U}_0 + \hat{\mathbf{P}}_0 + \hat{\mathbf{P}}_{0\Omega} \tag{4}$$

- the equilibrium equation of the weighed tractions in the form:

$$\mathbf{H}^{\mathbf{T}}\mathbf{P}_0 = \mathbf{0} \tag{5}$$

The system of Eqns (3-5) allows determining the solving system of the displacement method:

$$\mathbf{K}_{00}\,\mathbf{X}_0 + \hat{\mathbf{L}}_{0b} + \hat{\mathbf{L}}_{0\Omega} = \mathbf{0} \tag{6}$$

where $\mathbf{K}_{00}$ is the symmetric and positive defined stiffness matrix of the assembled system, $\mathbf{X}_0$ the vector of the unknown interface displacements and $\hat{\mathbf{L}}_{0b}$, $\hat{\mathbf{L}}_{0\Omega}$ the equivalent nodal traction vectors of boundary and domain respectively.

Conclusions.

The proposed approach employs macro-elements in wich equilibrium and compatibility are satisfied point by point by using the fundamental solutions. After a condensation process, through the elimination of the unknowns defined on the free and constrained boundaries, for each e-bem, a relationship is written on the interfaces with other e-bems; the latter relates the weighed tractions to the node displacements and to the external actions.

The regularity equations on the interface sides among e-bems lead to a solving system in terms of interface displacements only.

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A large deformation Kirchhoff-Love shell model hierarchically enhanced with zigzag effects and its spline-based discretization

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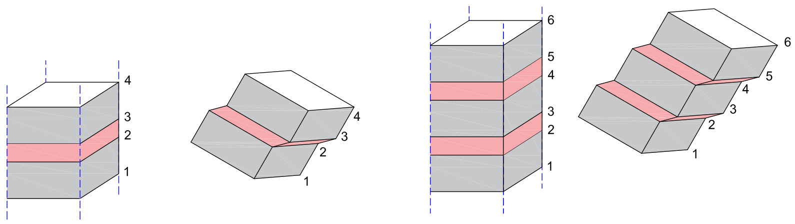
Keywords: Shell, large deformation, zigzag, laminated glass, NURBS.

Many structural applications, e.g. laminated glass, involve composite shells made of stiff plies coupled by soft interlayers and undergoing large deflections and buckling. The large difference in the material properties induces a sectional warping with transverse shear strains concentrated in the soft layers. Theories based on the plane-section hypothesis become unreliable. A large deformation Kirchhoff-Love shell model hierarchically [1] enhanced with warping functions over the thickness is presented for facing such a problem (see Fig.1). The first proposal assumes that all stiff layers maintain the same director orthogonal to the deformed reference surface, with two additional fields for each soft layer, representing the amplitudes of its slip along two directions tangent to the shell surface. The second model enhances the Kirchhoff-Love model with a single zigzag profile for the laminate and its two amplitudes, i.e. one per direction. Cubic C^2 NURBS are used as shape functions in the weak form, with locking avoided by a patch-wise reduced integration. Numerical tests show the model reliability compared to the solid solution and the coarse-mesh accuracy.



3 layers 5 layers

Figure 1: Kinematics of laminates with alternating stiff/soft layers.

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A computed tomography-based limit analysis approach to investigate the mechanical behavior of the human femur prone to fracture

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Keywords: Femur Mechanics, Limit Analysis, Peak Load.

The growth of the prevalence of skeletal diseases has led to increased bone fracture risk. Osteoporosis represents one of the major causes of femur fracture. An osteoporotic femur is characterized by a significant loss of mechanical integrity that makes the bone more prone to fracture. As such, the fracture risk assessment is crucial in clinical practice to prevent the fracture events. However, the current standard of care used clinically (areal bone mineral density (aBMD) measured by Dual X–ray Absorptiometry) is not always effective for identifying cases at high risk of fracture, as it does not take into account many mechanical phenomena affecting the bone structure strength that concur to bone fracture. Improvements in the assessment of bone fracture risk is then an important research area with clear clinical relevance. In this context, an impressive number of patient–specific finite element (FE) models of femur from Computed Tomography (CT) images have been developed [1]. These models can better model the personalized mechanical determinants of fracture and may be able to overcome aBMD limitations in identifying cases at high risk of fracture [2]. However, looking at the different modelling strategies proposed in the literature, the main differences among them are principally in terms of the constitutive modelling which has a great influence in the way of detecting fracture. Although a similar level of accuracy (albeit not optimal) has been obtained from the different techniques, in the Authors' opinion, mechanics-based approaches, not dependent on an accurate post-elastic modelling, oriented to predict just the peak load of the bone at a state of incipient collapse may add a significant improvement in the prediction of bone fracture risk.

The present work aims to propose a refined CT-based FE modelling strategy that implements the theory of limit analysis [3]. This theory allows to determine the peak load of a structural element, without following the evolutive load history that has determined it. A significant simplification provided by the limit analysis numerical procedure applied in this work is that it is based only on sequences of linear elastic analyses. In particular, a numerical procedure, known as Elastic Compensation Method (ECM), able to define a lower bound to the collapse load has been used [4, 5]. The developed strategy has been applied to a fresh-frozen human cadaveric femur, for which the experimental value of fracture load was available, to give a first attempt at the validation of the approach. The femur geometry has been reconstructed from CT images through a semi-automatic segmentation process (ITK-Snap software). Heterogeneous material properties, deriving the local values of bone density from the CT images and then converting into local values of the required material parameters, have been considered. A yield criterion of Tsai–Hu-type, expressed in principal stress space has been used to model the bone tissues. In terms of loading and constraints, the conditions used in the mechanical testing have been simulated. In detail, the distal portion of the femoral shaft was fully constrained and the load was applied on a circular surface of 10 mm at the top of the femoral head with an orientation of 15°. The FE analysis has been performed by employing home-made Matlab codes (Matlab, MathWorks, MA, USA) integrated within the FE software Comsol Multiphysics (Comsol with Matlab, v.5.2 COMSOL, Stockholm, Sweden). The developed CT-based numerical technique showed the ability to accurately predict, at least for the examined femur, the experimental detected fracture load. Thus, the proposed approach seems a promising and effective tool that could be adopted into clinical practice to predict the fracture risk of human femur.

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Numerical simulation of crack propagation using interphases and a FEM-VEM environment.

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Keywords: Embedded interphases, Strain localization, Quasi-brittle materials, VEM, FEM.

During their softening stage, quasi-brittle materials exhibit strain localization in relatively narrow zones. Narrow zones are characterized by the formation of micro-cracks and micro-voids whose evolution represents the macroscopic crack.
The evolution of the localization band can be modeled using the discrete or the continuum approach. Among the computational strategies able to simulate crack propagation in quasi-brittle materials, discrete crack models introduce a strong or weak discontinuity along the inter-element boundaries or inside the elements. The Generalized-Finite Element Method (G-FEM), the Extended- Finite Element Method (X-FEM), the Phantom Node Method (PNM), the Augmented Finite Element Method (A-FEM), are examples of models simulating the intra-element crack propagation.
The Augmented-FEM strategy (A-FEM) separates an element in two standard finite elements and a nonlinear interface where discontinuities localize [1]. An advancement of A-FEM was proposed in [2] and consisted in the use of a zero-thickness interphase model (IPH) in place of the interface (ZTI), adding internal stresses and strains to the contact ones. Unlike ZTI models, IPH does not require a specific traction-displacement jump constitutive law and the constitutive laws adopted for IPH can correspond to those of bulk material.

In this work a new crack tracking algorithm is proposed, in a continuous FEM – discontinuous VEM description. The basic idea consists in separating not localized elements from localized elements, the last forming substructures (that are portions of the structure crossed by a unique crack). While not localized elements are modeled through classic finite elements, localized elements are

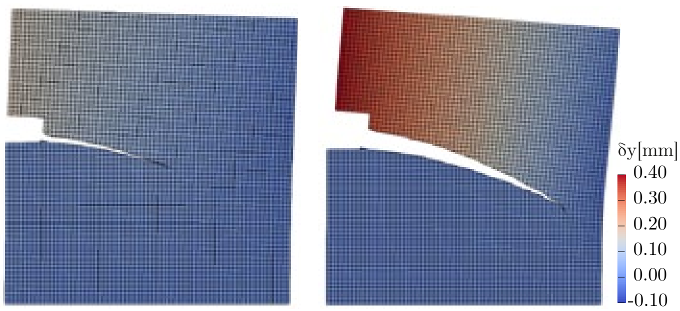

Figure 1: Example of propagation of a fracture in a quasi-brittle material.

substituted by two virtual elements and an interphase. VEM [3] is more flexible than standard FEM, since the element can be a polygon characterized by any number of edges, without constraints, and the original element could be divided into very distorted sub-elements or non-standard elements.
The analysis begins with a discretization of the whole domain using standard FEM. Localization criteria and the spectral analysis of the fracture tensor built at the element level identify finite elements where strains localize. In these elements the orientation of the localization band is calculated. Localized elements are then grouped and localization bands are aligned into unique cracks, based on simple heuristic criteria. Substructures are therefore created, composed of virtual elements and IPHs representing discontinuities. Each substructure is separately solved from the rest of the structure by imposing, as essential boundary conditions, the displacements of its on the side nodes. At the global level, equilibrium is iteratively achieved by considering internal forces coming from substructures.
The main features of the adopted strategy are illustrated through benchmark examples.

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Fatigue life prediction of Ni-Ti peripheral stents using a fracture mechanics approach: a proof of concept

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Keywords: Shape memory alloy, Cyclic behavior, Crack propagation.

Nickel-Titanium (Ni-Ti) stents are the gold standard in the mini-invasive treatment of atherosclerotic diseases affecting peripheral vessels. The fatigue fracture of these devices under in vivo cyclic loads constitutes an open issue of major concern given the severe associated drawbacks such as re-occlusion of the artery [1]. However, the non-linear material response and the reduced dimensions of stent struts increase the complexity of their fatigue assessment, requiring ad hoc and well-defined methods [2,3]. Despite many phenomenological approaches have been proposed, open questions remains and more efforts are still required to find the best way to study and predict Ni-Ti thin struts failure under fatigue loads. This work aims at investigating the possibility of applying fracture mechanics principles for stents life prediction accounting for the propagation of pre-existing manufacturing defects. Accordingly, crack propagation tests were performed on ad hoc samples, characterized by a microstructure comparable to that of stents, to gain the material crack growth rate. An experimental campaign was then performed on multi-wire specimens having the same dimension and material properties of stents. Fracture surfaces were successively inspected through a scanning electron microscope highlighting defects size at the initiation site of fracture. A crack propagation algorithm was calibrated, introducing the non-linear fracture mechanics energetic parameter cyclic J-integral and integrating the crack growth law from the initial defect sizes observed on the fracture surfaces. Finally, the same approach was used to predict the results of another experimental campaign performed on commercially-resembling stents subjected to multi-axial fatigue tests with different load magnitudes (Fig. 1). Finite element simulations were carried out to assess the local cyclic stress-strain response in the failure regions. In both the studied cases, promising life predictions were obtained, demonstrating the role of fracture mechanics in explaining Ni-Ti struts fatigue failures.

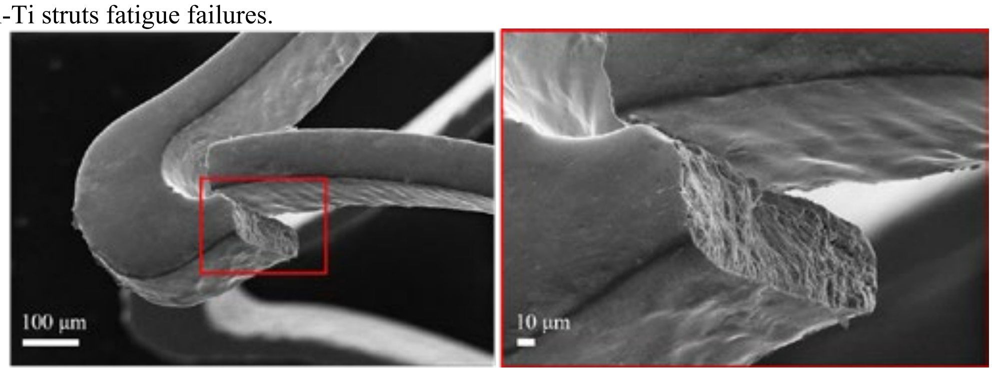

Figure 1: SEM acquisitions of a failed Ni-Ti stent strut with inspection of the fracture surface.

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Experiments and fracture mechanics-based modeling on the puncturing of soft bulk solids and membranes

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Keywords: Puncturing, Soft material, Needle sharpness, Fracture mechanics, Biological tissues.

The integrity of soft materials and biological tissues against puncturing is of great relevance for their performance because of the high sensitivity to local rupture caused by rigid sharp objects [1, 2]. In this work, the mechanics of puncturing is studied with respect to a sharp-tipped rigid needle with a circular cross section, penetrating a target elastomeric material. The failure mode associated with puncturing is identified as a mode-I crack propagation, which is analytically described by a two-dimensional model of the target bulk solid, taking place in a plane normal to the penetration axis [3]. It is shown that the force required for the onset of needle penetration is dependent on two energy contributions, that are, the strain energy stored in the target solid and the energy consumed in crack propagation. More specifically, the force is found to be dependent on the fracture toughness of the material, its stiffness and the sharpness of the penetrating tool. Interplay with possible failure mechanisms due to hole expansion is also discussed. Finally, when the target material is in the form of a thin membrane, additional energy contributions due to the true stresses in the deformed state of the membrane come into play [4]. Supporting the proposed theoretical modeling, a series of puncturing experiments on two commercial silicones is presented [5]. The combined experimental-theoretical findings suggest a simple, yet reliable tool to easily handle and assess safety against puncturing of soft materials, Fig.1.

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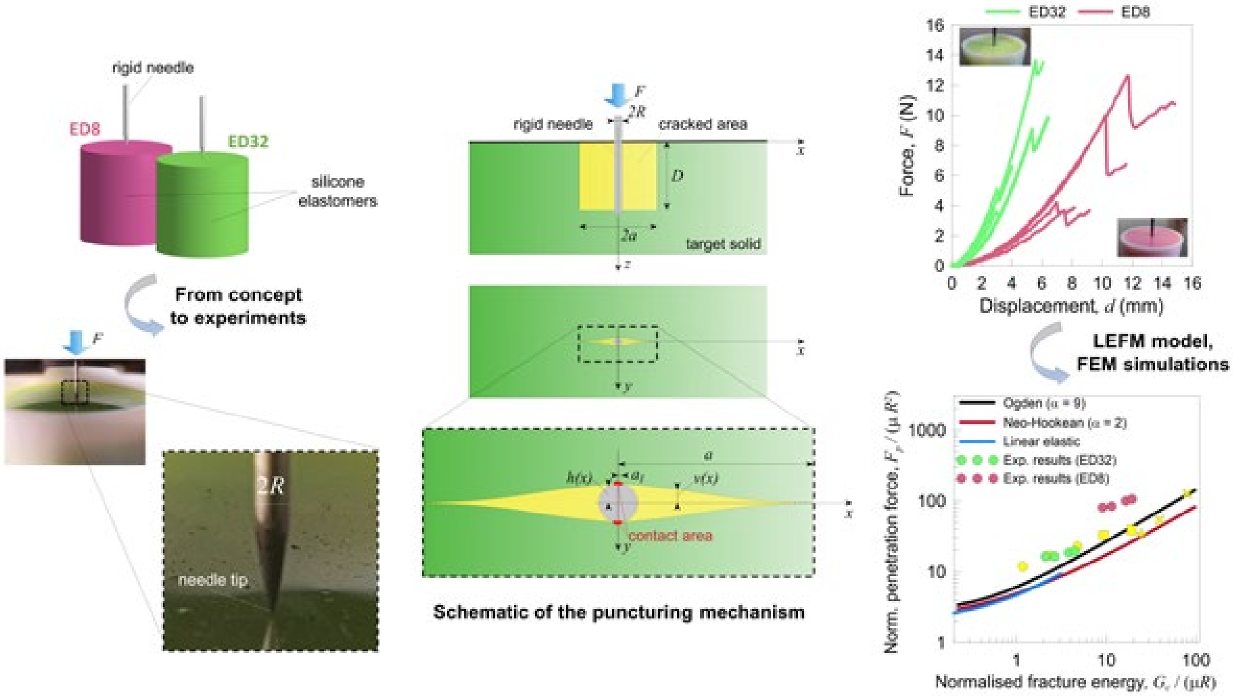

Figure 1: Experiments and modeling on the pucturing of soft elastomers.

Geometric control by active mechanics of epithelial gap closure dynamics

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Keywords: wound healing, phase field, Cahn-Hilliard-Brinkman.

Epithelial wound healing is one of the most important biological processes occurring during the lifetime of an organism. It is a self-repair mechanism closing wounds or gaps within tissues to restore their functional integrity. In this work we derive a new phase-field model for the gap closure by means of a variational principle in the framework of nonequilibrium thermodynamics. We account for the interplay between the crawling with lamellipodia protrusions and the supracellular purse-string tension, acting as Korteweg forces into the chemical potential.

From a perturbative analysis [1] we find that these two mechanisms impose a pressure jump across the gap edge in the sharp interface limit. Moreover, the chemical potential diffuses as a Mullins-Sekerka system, and its interfacial value is given by a Gibbs-Thompson relation for its local potential. The finite element simulations show an excellent quantitative agreement between the closing dynamics and the morphology of the edge with respect to existing biological experiments [2], see Fig. 1. The results shed light on the geometrical control of the gap closure dynamics resulting from the active forces that are chemically activated around the gap edge.

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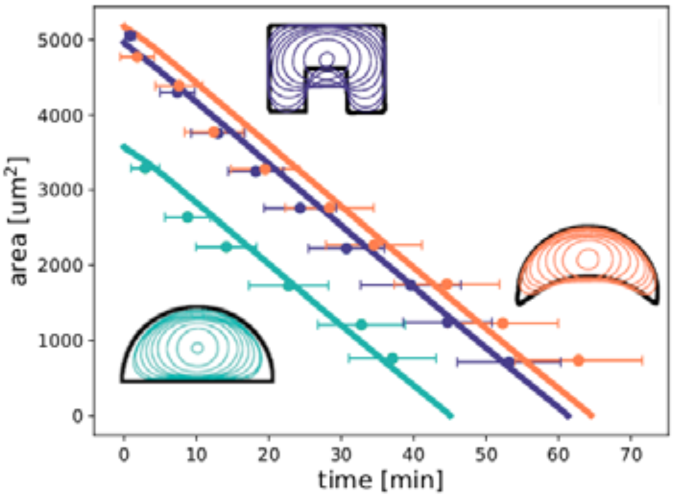

Figure 1: In-silico simulated decrease of the area over time for three differently shaped wounds: *square inset* (blue line), *half circle* (green line) and *half moon* (orange line). The horizontal bars coincides with the error bars of the experimental data extracted from [2] for each geometry. The image shows also the overlay of outlines at different time points for each of the three wound shapes.

A preliminary assessment of a new surgical procedure for the treatment of primary bladder neck obstruction through a numerical biomechanical model

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Keywords: urethral sphincter; computational biomechanics; bladder neck obstruction.

A new surgical procedure for the treatment of primary bladder neck obstruction with maintenance of anterograde ejaculation is investigated using a computational biomechanical modeling approach [1]. In place of monolateral or bilateral bladder neck incision, associated with a loss of ejaculation rate of up to 30%, the new surgical procedure consists of laser drilling the bladder neck with a number of holes and without muscle fiber disruption. The effect of this novel procedure has been studied numerically, with a simplified two-dimensional numerical model of the internal urethral sphincter, varying the position and the number of holes in the fibrotic region of the urethral tissue. The numerical model takes into account the nonlinear behavior with large deformations of the soft biological tissues, using a 5-parameters Mooney-Rivlin's material, as suggested in [2]. The material coefficients have been found by fitting an exponential law, using the set of parameters defined in [3]. Results show an improvement of the urethral sphincter opening by increasing the number of holes, ranging from about 6% to 16% of recovery. Moreover, a non-aligned position of holes positively influences the opening recovery. The concentrations of maximum principal strain and stress have been registered in the proximity of the interface between the physiologic and diseased sphincter, and in those regions where the radial thickness is significantly thinner.

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Isogeometric analysis: advances and applications with a special focus on dynamic problems

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Keywords: Isogeometric Analysis, Structural Dynamics, Transient Problems.

Isogeometric Analysis (IGA) is a successful simulation framework originally proposed by T.J.R. Hughes et al., in 2005, with the aim of bridging Computational Mechanics and Computer Aided Design. In addition to this, thanks to the high-regularity properties of its basis functions, IGA has shown a better accuracy per degree-of-freedom and an enhanced robustness with respect to standard finite elements in many applications - ranging from solids and structures to fluids, as well as to different kinds of coupled problems - opening also the door for the approximation in primal form of higher-order partial differential equations. In particular, the above-mentioned higher-regularity properties of IGA make it particularly attractive for the efficient and accurate simulation of structural dynamics and transient problems.

In this lecture, after a concise introduction on the basic concepts of isogeometric analysis and its potential advantages, some IGA recent advances in the context of structural dynamics and transient problems will be presented, along with an overview of interesting applications from different fields of Engineering.

An improved isogeometric collocation method for the explicit dynamics of geometrically exact beams

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Keywords: Isogeoemtric Collocation, Explicit dynamics, Mass lumping.

In 2010 the isogeometric collocation (IGA-C) method was proposed with the aim of keeping the computational attributes of isogeometric analysis (IGA) [1], such as high-order accuracy, robustness, geometric capabilities and, at the same time, circumventing the issues related to numerical quadrature in Galerkin IGA. Moreover, since IGA-C requires only one evaluation point per degree of freedom, regardless of the approximation degree, it results very attractive for applications where efficiency is the main goal, such as explicit dynamics [2, 3]. Beams and beam systems capable of undergoing finite motions and rotations are nowadays fundamental to model complex structures in different fields, from biomedical devices to crash dynamics. In 2019, Marino et al. [4] extended the IGA-C method to the explicit dynamics of three-dimensional beams undergoing finite motions. The formulation was based on a natural combination of the SO(3) finite rotations representation with an explicit, geometrically consistent time integrator. The focus was placed on extending the integration scheme, originally proposed in [5] for rigid body dynamics, to the geometrically exact beam case. However, that formulation was not “fully explicit” in the sense that matrix inversion was still needed. Namely, a consistent mass matrix was used within an explicit time integration scheme.

With the present contribution we aim at improving the existing formulation providing a fully explicit algorithm such that to preserve high-order accuracy in space and achieve much higher efficiency. For this purpose, the translational and rotational equations of motion are firstly decoupled, then, the mass lumping procedure proposed in [2, 3] is extended to the beam problem considering also the rotational inertia. To ensure the convergence of the algorithm, a mass scaling is performed. We also propose a possible way to enforce the Neumann boundary conditions, which are not easy to treat in dynamic formulations where the primal unknowns are the translational and rotational accelerations.

The present method is implemented using the framework introduced in [4] and verified through several benchmark tests. The results of a preliminary case study are shown in Figure 1. It is a cantilever beam with length 1 m and square cross-section with side 0.01 m, loaded with an impulsive transversal tip force F_3 with two different magnitudes (10 N and 100 N). For each of them, a comparison between the proposed lumping procedure (blue and red dashed lines in Figure 1) and the consistent mass matrix formulation (black lines in Figure 1) from [4] is provided. It can be noticed, a very good agreement between the two formulations, also when very large oscillations occur.

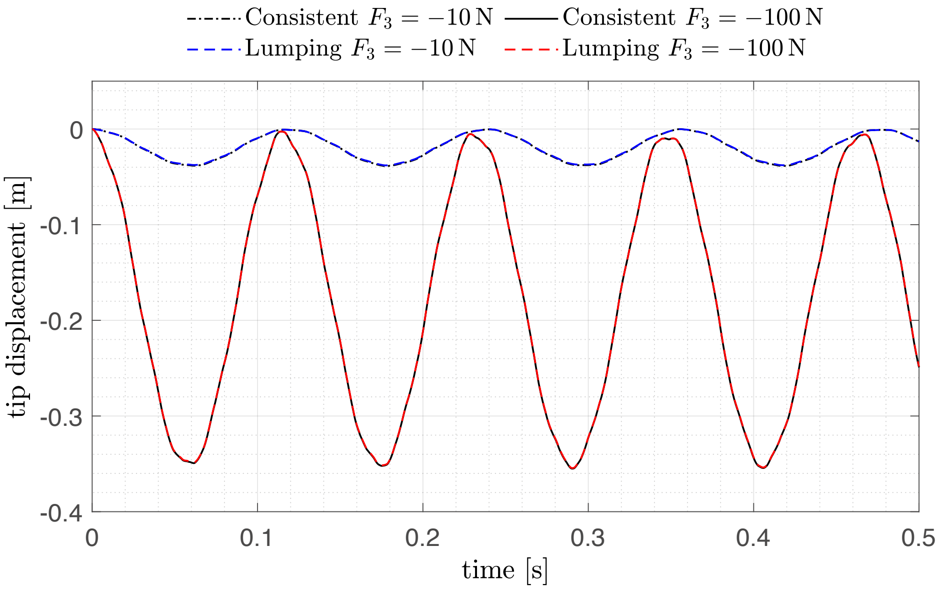

Figure 1: Cantilever beam under tip load: comparison between consistent and lumped mass matrix formulations.

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An event-driven approach for the nonlinear time-history analysis of multi-block masonry structures under seismic excitation

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Keywords: Masonry, Dynamic analysis, Rocking, Impact model, Multi-block arch.

A common approach for the seismic safety assessment of masonry arches resorts to an equivalent static analysis based on the classical Heyman assumptions [1]. Accordingly, a safe estimate of the arch vulnerability under a time-varying ground motion excitation is obtained as the minimum peak ground acceleration transforming the arch into a mechanism.

The dynamic analysis of masonry arches subjected to ground acceleration was initiated by Housner's seminal work on the rocking motion of a single rigid block [2]. Therein, the equation of motion prevailing at regular instants was derived, and the kinetic energy loss at impacts was computed assuming that concentrated impulse forces are transmitted through the pivotal points of the block. By generalizing that contribution, a first dynamic analysis of a masonry arch was carried out by Oppenheim [3], under the assumption of the arch moving along the four-hinge mechanism determined through an equivalent static analysis. In particular, direct overturning failure of the resulting single-degree-of-freedom system was investigated for an idealized ground motion pulse.

In [4], De Lorenzis and coauthors extended Oppenheim's approach for addressing the rocking motion of masonry arches. The Housner impact model was adapted to an arch behaving as a four-hinge mechanism by the assumptions that the hinges after the impact are mirrored from those before the impact and that the impulse forces at the hinge sections before the impact are located on the opposite side of the hinges across the arch thickness. As a result, it was shown that, depending on the ground impulse shape, an arch might survive the first half cycle of motion but overturn, after an impact, during the second half cycle.

A possible shortcoming of that approach, inherent to the simplification of a four-hinge mechanism, is that the thrust line may exit the thickness of the arch during the regular instants of motion [4]. The dynamic analysis of a masonry arch regarded as a system of rigid blocks has been thus undertaken in [5], assuming that hinges may open and close, and hence impact may occur, at any joint between the blocks.

In a recent contribution [6], the extension of the Housner impact model from the original case of a single rigid block to the more complicated case of a masonry arch behaving as a single-degree-of-freedom system has been re-considered. By introducing the novel concept of impulse line at impact as the analogous of the thrust line at regular instants of motion, the intuitive result that impulse forces need to be transmitted through the hinges opening after the impact has been proven. Furthermore, the minimization of kinetic energy loss at impact has been shown as the condition governing the hinge locations after the impact and the static admissibility of the resultant impulse forces.

An event-driven computational approach is here proposed for the nonlinear time-history analysis of multi-block masonry structures subjected to ground motion excitation. It is based on a novel variational formulation, which describes both the regular motion and impacts and amounts to the solution of straightforward quadratic-programming problems [7]. Numerical results are presented and compared to competing computational strategies available in the literature (e.g., see [8, 9]).

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A detailed study of high-order phase-field modeling for brittle fracture

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Keywords: Phase-Field, Brittle Fracture, Isogemetric Analysis, Higher-order models.

The evolution of brittle fracture in a material can be conveniently investigated by means of the phase-field technique introducing a smooth crack density functional $\Gamma_{d,n}$, where d represent the phase field variable and *n* the derivative order of the variable *d*.
Following Borden et al. [1] and Goswami et al. [2], two distinct types of functional are considered:

- Second-order model:

$$\Gamma_{d,2} = \frac{G_c}{2l_0}(d^2 + l_0^2|\nabla d|^2), \tag{1}$$

- Fourth-order model:

$$\Gamma_{d,4} = \frac{G_c}{2l_0}(d^2 + \frac{l_0^2}{2}|\nabla d|^2 + \frac{l_0^4}{16}(\Delta d)^2). \tag{2}$$

Although both formulations underlie the same physics, the fourth-order approach involves the bi-Laplacian of the phase field (see eq.2), posing difficulties in the approximation of the Galerkin form. Indeed, the discretization in primal form requires continuously differentiable basis functions: a condition we fulfill via Isogeometric Analysis (IgA). In this work, we propose a comparison of second-and fourth-order models through an accuracy analysis [1] using the toughness as a metric for the relative error. We perform several tests increasing progressively the complexity of the crack patterns.

Based on our results, the fourth-order approach provides higher rates of convergence and a greater accuracy (see fig.1). Moreover, we observe that fourth- and second-order models exhibit a comparable accuracy when the former method employs a mesh-size approximately two times larger than the second one, entailing a substantial reduction of the computational effort. To compute the effective toughness in the error assessment, we measure the length of the crack by means of an image-based algorithm. Our skeletonization technique automatically works for complex patterns

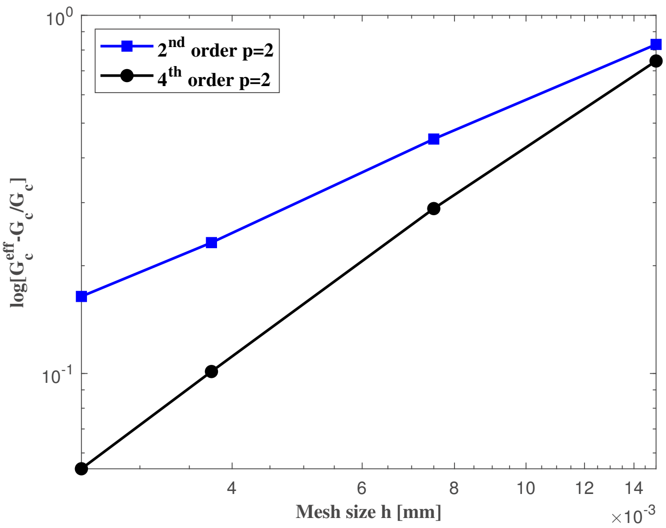

Figure 1: Example of accuracy trend in the Double Cantilever Beam [1] test.

such as curved and branched fractures. Finally, we introduce an alternative method to the initial strain-history field [3] to model a preexisting crack. The higher accuracy of the proposed method is verified simulating the center-crack plate test [4] and comparing the solution against the analytical peak reaction. In all numerical results, irreversibility is handled via the PSOR scheme [5], that is suitable to investigate both phase-field formulations since it can be used in combination with higher continuity IgA discretization.

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Integrating Neural Networks into the Parallel Rheological Framework for Improved Constitutive Modeling of Elastomers

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Keywords: Machine learning, Neural Networks, Constitutive modeling, Viscoelasticity, Finite deformations

The parallel rheological framework (PRF) is a computational framework based on the superposition of finite-strain viscoelastoplastic networks, widely used in Finite Element software and constitutive models [1]. The combination of inelastic elements in series or in parallel with elastic springs allows to simulate the complex rheological behavior of elastomers undergoing large deformations by incorporating effects such as creep and relaxation. The theoretical derivation of the PRF is based on the multiplicative decomposition of the deformation gradient into elastic and inelastic (viscous) components and by an additional constitutive assumption on the inelastic stress. Several literature models (e.g., Reese & Govindjee [2], Bergström & Boyce [3], Kumar & Lopez-Pamies [4] Yoshida & Sugiyama [5] to cite but a few) can be incorporated into this framework and distinguished only by the form of the viscosity function. This generalized framework allowed a comparison of the predicting and extrapolation capabilities of the models to fit the behavior of filled rubber, including some relevant nonlinear effects such as Payne's effect [6]. We noted that phenomenological viscosity functions are not able to exploit the potential of the experimental data in describing the behavior of the materials. Following the growing interest in using neural networks for constitutive modeling [7] [8] [9] [10], we used a neural network to exclusively describe the viscosity function, thus remaining within the PRF. We believe that this approach can reduce the data hunger of machine-learning models but take full advantage of the available data by reducing the presence of bias due to interpolating functions elaborated by experts.

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Nonperiodic masonry pattern generation and numerical analysis of cultural heritage structures

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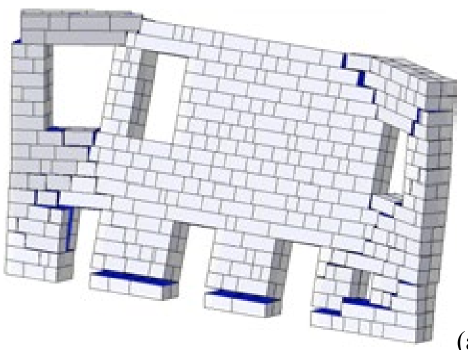
Keywords: Masonry mechanics, Nonperiodic texture, Multi-leaf masonry, Historical structures.

Block-based models represent an appealing solution for the numerical analysis of cultural heritage structures, given their high accuracy in representing masonry mechanics. Indeed, such models can account for the actual masonry pattern, and their computational efficiency has lately increased significantly. Nonetheless, historic masonries typically show complex nonperiodic multi-leaf patterns [1], and the implementation of block-by-block full-scale models is generally time-consuming or even unlikely, given the insufficiency of relevant data.

In this contribution, an algorithm for the nonperiodic masonry pattern generation of historical structures is developed through 3D solid blocks. Particularly, the 3D volume of the structure and a representative pattern of a small portion of a wall, both conveniently defined in terms of voxels, are considered as inputs. Then, the algorithm automatically generates the 3D block arrangement of the full-scale structure through a pseudo-statistical representation [2].

A meaningful cultural heritage structure benchmark, i.e. the Alcaçova wall of the Guimarães castle in Portugal [3], is used to test the efficacy of the generation algorithm. Thereby, several multi-leaf masonry patterns are generated and their structural response is compared by means of numerical analysis (Figure 1), employing the block-based model developed in [4], based on damaging blocks and cohesive-frictional zero-thickness contact interfaces.

Finally, the influence of through-thickness blocks and intralayer mechanical properties on the overall structural response is shown and discussed.


(a)

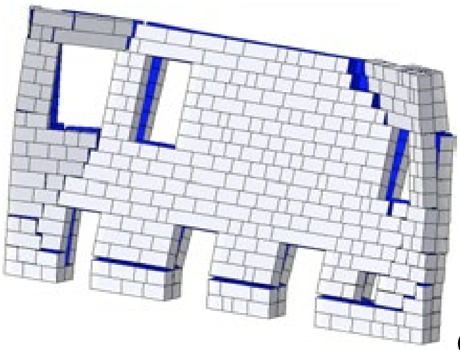

(b)

Figure 1: Crack patterns of the out-of-plane loaded benchmark (a) with and (b) without through-thickness blocks.

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A sustainable Portland pozzolana cement with recycled volcanic ash

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Keywords: Volcanic ash, pozzolanic reactivity, blended cement.

The paper summarises some of the experimental results concerning the production of a new pozzolanic cement containing recycled pyroclastic waste produced during the eruptions of the Etna volcano.

Volcanic ash (VA) is used as a pozzolanic component in the manufacture of a type IV mixed cement, according to the classification of EN 197-1. The experimental results of the tests carried out for the physical, mechanical and chemical characterisation of the new mixed cement show that although the volcanic material does not intrinsically meet the requirements dictated by the standards that are usually used to assess pozzolanic properties, such as ASTM C618 and the Italian Royal Decree n. 2230/1939 [1, 2, 3, 4], VA can be effectively used in the production of commercial pozzolanic cements as a partial, and even total replacement for the usual natural quarried pozzolans. In fact, following a performance approach, all regulatory requirements for the production of a pozzolanic cement are met, according to EN 196.

A Portland Cement (PC) type IV/A P 42.5 R SR produced by Buzzi Unicem, containing 72% of clinker, 3% of gypsum and 25% of natural pozzolan originating from the isle of Kimolos (Greece), was considered as reference mix. Six blended cement mixes were studied, varying in the reference mix the replacement percentage (10%, 25%, 35%, 50%, 75%, 100%) of the natural pozzolan with volcanic ash.

Among many others, the most significant findings are here introduced.

Following EN 196-5, the pozzolanicity is assessed by comparing the concentration of calcium ion, expressed as Calcium Oxide [CaO] present in the aqueous solution in contact with the hydrated cement, after a fixed period of time, with the quantity of calcium ion capable of saturating a solution of the same alkalinity, as a function of the concentration of the hydroxyl ion concentration ($[OH]^-$).

Figure 1 shows that all the mixes at 15 days of curing satisfy the reactivity test, lying the representative point below the saturation curve.

The cement paste strength remains almost constant and comparable to the one of the reference mix, whatever the replacement percentage, at different curing ages, from 2 to 90 days, as shown in figure 2. Differences from the reference mixture are of the order of the variance of the results.

The results of this work, beyond their scientific value, are giving impetus to the introduction of new regulatory provisions that will enable the launch of a production chain in the local area aimed at recycling the waste eruptive material that is collected during the cleaning of public and private spaces after the frequent Strombolian eruptions of Etna.

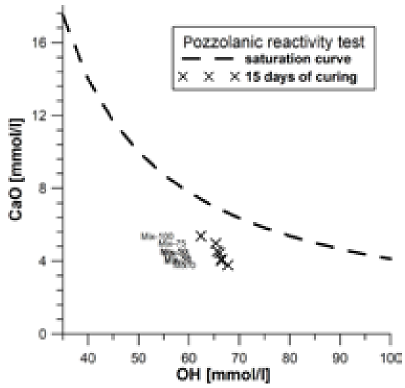

Figure 1: Comparison of reactivity test data of the mixes at 15 days of curing with the saturation curve

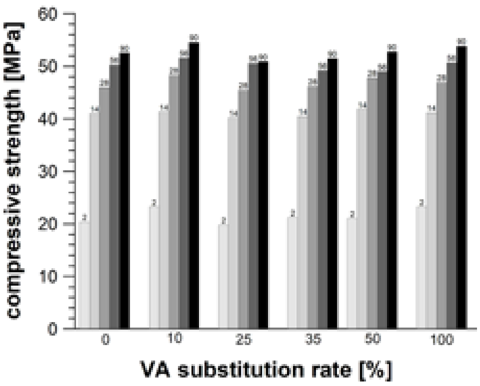

Figure 2: Average compressive strength varying the replacement percentage of pozzolana with VA at different age of curing

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Mechanical behaviour and strain localization in lattice material evaluated by means of discrete homogenization

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Keywords: Discrete homogenization, Fibre network, Anisotropic material

Fibre lattice materials are becoming widespread in engineering applications, thanks to their versatility and their efficient mechanical and physical properties. In addition to conventional fibre materials, widely used in aero-spatial technology and in civil engineering, innovative materials have been introduced by the new manufacturing technologies like additive printing. The effective behaviour of the fibre network arises from the complex local physical mechanisms that occur at the scale of the fibre arrangement.

In this context, some mechanical models have been developed. The models takes into account the micro-structure by means of a Homogenization method of Periodic Discrete Media (HPDM) in the framework of a variational approach. The lattice has been treated like an assembly of microbeams, having both extensional and bending stiffness, with different types of connection, according to the pattern and details of the network [1,2,3]. A numerical algorithm to evaluate the mechanical response of the modeled lattice materials has been implemented.

The resulting equivalent continuum presents strong directional properties, with anisotropy ratios much larger than those that can be found in natural materials [4,5].

The directionality of the response of the equivalent continuum increases with the slenderness of the fibres, leading to peculiar behaviours, like the formation of narrow bands where the strains present very large gradient.

The results of the homogenization have been validated comparing the response of the continuum with the response of discrete models, for which each element is modelled as a slender beam, and boundary conditions are accounted for in an exact way. A particular emphasis is given to anisotropy and strain gradient features in relation with the geometry of the pattern and nature of the connections.

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A linear theory for granular materials with rotating grains

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Keywords: Granular materials, micro–mechanics, constitutive laws, finite element method.

A micro–mechanical continuum model has been presented in [1, 2] for the description of dilatant granular materials with incompressible rotating grains for which the kinetic energy, in addition to the usual translational one, consists of other two terms owing to micro–structural motions: in particular, it included the dilatations and contractions of the individual granules with respect to each other, as well as the rotational movements of each grain with respect to the others.

Here, we propose suitable constitutive functionals, linear with respect to both the volume fraction, the micro-rotation gradients, and the dissipative variables, in order to obtain a general linear viscoelastic theory useful for applications and numerical checking, which generalizes the linear theory of Goodman and Cowin [3] and has the potential for applications in the area of soil mechanics, because it seems to be appropriate to analyze the dynamics and statics of sand layers. We observe that the fluctuation of the kinetic energy associated with the dilatancy of the chunks gives rise to the generation of a tensor of inertia flux in the Cauchy stress tensor, which is not necessarily symmetric, in general. Furthermore, the presence of micro–motions allows the property of granular materials to withstand shear stresses at equilibrium due to the presence of an Ericksen–type tensor in the Cauchy stress itself.

Finally, we perform numerical simulations on a simplified model of granular flows along an inclined plane (see, also, [3, 4]). We first simulate the early stage of an elastic granular dynamics, to which we add terms taking into account viscous and rotational effects to the model equations one at a time. Thus, the numerical results obtained show that viscosity plays a non–negligible role in the granular dynamics, as well as the effects due to the rotations of the granules, at least in the first phase of the implementations.

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An affine viscoelastic fully anisotropic model for composite materials with distributed fibres

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Keywords: anisotropic composite materials, viscoelasticity, fiber reorientation.

The reorganisation of the fibre structure in reinforced materials is a relevant issue in a number of applications, both in the field of material science [1] and biomechanics [2]. In this paper, we introduce a new large strain viscoelastic fully anisotropic model for composite materials, which is able to account for a distribution of fibres and for its affine evolution with the viscous part of the deformation. Specifically, the model is based on the multiplicative decomposition of the deformation gradient and on a proper constitutive assumption on the evolution of the fibre structure with viscous deformation. In addition, a generalized structural tensor is used to account for the distribution of the fibre reinforcing structure [3]. The strain energy function is chosen as the one for a standard linear solid, which is defined as the sum of a term governing the relaxation behaviour of the material and another term associated with the long-term material response. Then, the evolution of the viscous distortion is determined in a thermodynamically consistent way by solving a flow rule-like equation that depends on five characteristic times. The paper discusses the model's ability to match experimental data on epoxy-based composites [1], demonstrating its potential for accurately predicting the behaviour of these fibre reinforced materials.

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Mechanical-electrical failure correlation in metal nanowire electrodes

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Keywords: Metal nanowire electrode, nanowire damage, network failure.

Flexible transparent electrodes based on randomly distributed metal nanowires (NWs) are appealing for optoelectronic devices, solar cells, light emitting diodes, and transparent heaters. While NW electrodes are comparable to thin films in terms of electrical conductivity and transparency, they are advantageous in terms of cost and mechanical flexibility.

Metal NW electrodes are planar ensembles of interconnected NWs that form, after welding, a network capable to withstand mechanical deformations and ensure electric current conduction. The random placement of NWs makes the overall network properties spatially not uniform [1], therefore causing mechanical stress and current density localizations that result in NW breakages (local damage) [2]. These occurrences negatively affect the macroscopic response of the network, ultimately leading to mechanical and electrical performance drop (network failure).

The aim of this contribution is to track the local damage evolution process (either mechanically or electrically induced) and assess its effect on the macroscopic performance up to network failure. To this end, we make use of a computational approach to evaluate the in-plane mechanical (effective stiffness) and electrical (effective conductivity) network properties and assess the extent of the mechanical stresses and current intensity in the NWs. A Monte Carlo approach is utilized to create two-dimensional digital samples that represent NW networks. The resulting geometries are converted into beam networks and equivalent resistor networks to analyze the mechanical and electrical network responses, respectively. Finite element simulations are ultimately performed.

Our results show that the spatial distribution of damaged elements exhibits crack-like patterns that are consistent with both experimental observation [2] and numerical simulations results [3]. Although the crack pattern depends on the physics (either mechanical or electrical) driving the damage, a fully-developed crack is always detectable at failure (Figure 1). We observe that the network fail-

(a) (b)

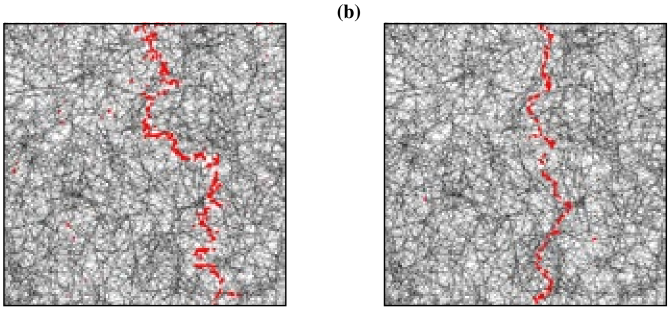

Figure 1: Distributions of damaged elements at network failure: mechanically induced (a) and electrically induced (b) failure on the same network.

ure is attained with a smaller amount of NW breakages when damaged is electrically induced. We therefore deduce that electrically induced damage is more critical to the overall network integrity compared to mechanically induced damage.

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Distal and non-symmetrical crack nucleation in reduced order peridynamic plate theory

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Keywords: crack nucleation, distal, peridynamic.

In order to characterise crack onset and propagation in thin elastic bodies that exhibit nonlocal response due to their particular micro-structure, a reduced-order formulation of peridynamic theory has been recently put forward [1]. Unlike previous models available in the literature [2], the formulation is capable of retaining information on possible cracks propagating through the thickness such as in the case of delamination failure. To achieve this result the kinematics of a thin plane element is carefully chosen to be composed of an absolutely continuous part and a zone where jumps in the displacements are allowed, i.e. the functional space in which variations in the configuration of the body are allowed is that of the functions of special bounded variation (SBV); in this way, the reduced form of the elastic bond-based peridynamic energy is explicitly retrieved and a hierarchy of terms characterising the energy stored inside the plane element is obtained.

The possibility to pass from the continuum to the discrete level is crucial in problems involving the transition from elastic to dissipative phenomena such as damage and fracture. Nevertheless, the exact equivalence between a given nonlocal model, such as the peridynamic theory, and a corresponding microstructure is usually not trivial to find. One possible interpretation, available from purely energetic arguments, can be given by means of a discrete structure [1]. Exploiting this, a straightforward interpretation is shown to be available for the various terms of the reduced energy [1]. A striking feature of the reduced energy is that, despite the small-displacement assumption, coupling between the membrane and bending terms occurs. Semi-analytical solutions for simplified settings are obtained through a minimisation procedure, and a range of nonstandard behaviours such as distal crack nucleation and curved crack paths are captured by the model. Furthermore, thanks to its nonlocal nature, fragile as well as cohesive mechanisms can be reproduced by simply calibrating the parameter defining the internal length scale - the nonlocality parameter. Finally, the convergence of the proposed reduced model to local elastic theory for vanishing internal length is determined so that a reduced-localised cohesive model for fracture is retrieved.

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Non-smooth dynamics of tapping mode AFM

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Keywords: Atomic force microscopy, tapping-mode,DMT model, pseudo-arclength continuation, bifurcations, non-smooth dynamics.

Tapping-mode is a widely used operating mode of dynamic atomic force microscopy (AFM). In this mode, the AFM oscillating cantilever tip interacts intermittently with the sample while driven close or at its resonant frequency. This approach allows routines for high-resolution imaging of a multitude of samples, e.g. DNA-protein complexes and polymers. The tip/sample interaction in tapping-mode gives rise to nonlinear dynamics. In detail, this comprises long-range nonlinear attractive forces as well as short-range repulsive forces in which the sample surface acts as a barrier defined by the elastic properties of the sample.

The AFM cantilever response can be investigated by employing the Galerkin procedure to discretize the partial differential equation governing the vibration of the cantilever into separate spatial and temporal components. Beside former and on-going intense research, only few published papers utilize a multi-degree-of-freedom (MDOF) approximation by projecting the nonlinear response onto multiple eigenfunctions of the linear system [1].

In this work the MODF dynamics of the tapping-mode is simulated using the nonlinear non-smooth Derjaguin-Müller-Toporov (DMT) model for the tip-sample interaction. The local bifurcation analysis is treated rigorously with the numerical interception of the discontinuity manifold. In addition, the validity of the smooth approximation of the discontinuous DMT model is also analysed.

Higher-order signals are capable of unraveling the characteristics of tip-sample interaction which can then potentially be exploited in simultaneous multi-parameter identifications. Furthermore, higher modes correct the prediction of nonlinear aspects such as grazing bifurcations and jumps, both being features of the rich dynamics of tapping-mode AFM [2, 3]. Evidence of different harmonic components is captured via the 2-DOF approximated analysis. Higher harmonics are being amplified to significant amplitudes by the higher eigenmodes of the cantilever. Particularly, the sixth harmonic is amplitude-magnified due to the activation of the second mode of of vibration. We remark that an augmented amplitude of the sixth harmonic is a peculiar features of AFM favoured by the microcantilever fabrication.

The multimode dynamics is found to be linked to the higher-order damping coefficients. In other words only assuming large quality-factors (i.e. low dissipation coefficients) we allow for energy transfer and higher modes of vibration to be activated as shown in Fig. 1(a). The atomic microscope also undergoes towards windows of complex motion and additional bifurcations (Fig. 1(b)).

These are considered highly dangerous conditions for tapping-mode AFM. Evaluation of this phenomenon is crucial if we consider that commercial AFM systems build their own feedback control loop on the cantilever oscillation signal locked on the primary resonant frequency.

By means of a MDOF reduced-order-model we investigated the amplitude-saturated branch in the repulsive regime as a function of the diverse dissipation mechanisms while the tip is in air or in contact with the sample. The shape and extension of the periodic solution in the repulsive region are receptive to sample properties and potentially linkable in dynamical-based identification of speci-

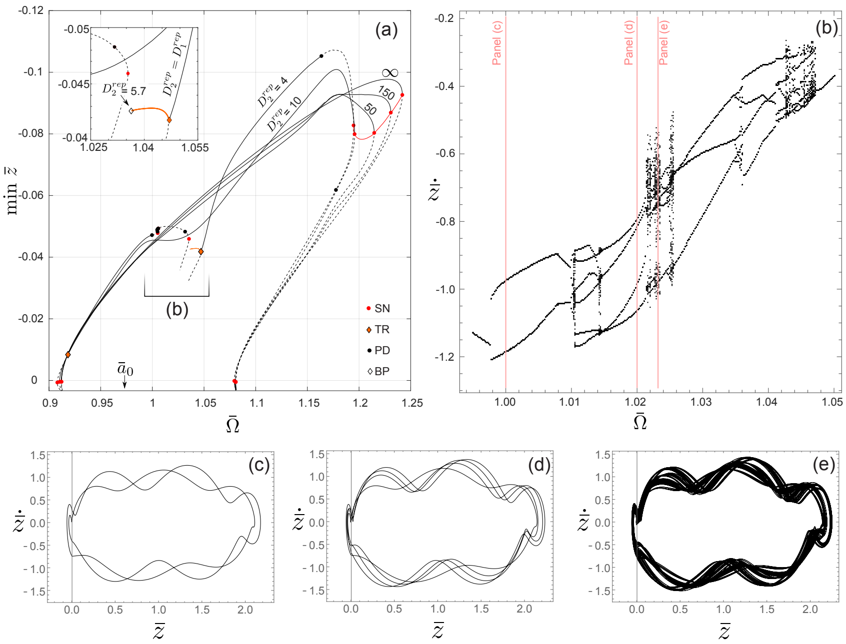

Figure 1: Dynamical response approximated with 2 modes of vibration. In panel (a) the frequency response for the amplitude-saturated response (when the cantilever overcomes the intermolecular distance $\bar{a}_0$) by varying the damping in the contact region (D_2^{rep}). The inset highlights the disappearance of the torus bifurcation (TR). Panel (b) shows the bifurcation diagram obtained via numerical integration. The span of the dimensionless excitation frequency, $0.995 \leq \bar{\Omega} \leq 1.05$, is divided in 300 steps and for each frequency we discard 600 periods and plot the last 100 dimensionless velocities of the Poincaré maps. Panel (c-e) are the phase-space portraits (tip-sample separation distance $\bar{z}$ against its velocity $\dot{\bar{z}}$) for $\bar{\Omega} = 1.00$, $\bar{\Omega} = 1.02$, $\bar{\Omega} = 1.023$, respectively.

mens in the repulsive region. By means of a multimode approximation new insights in the nonlinear dynamics have been gained. Higher modes are meaningful to unveil non-regular dynamics region that cannot be captured by a SDOF reduced-order model.

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An insight on the biaxial modelling of seismic isolators: a probabilistic assessment

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Keywords: Seismic isolators, first-excursion probability, hysteresis.

Seismic protection of structural systems by the use of isolation bearings is an effective and promising strategy that has been largely investigated in recent times. It is based on the use of devices presenting energy dissipation capacity and low horizontal stiffness.

In general, most of the commercial bearings present a complex nonlinear behavior including hysteresis phenomena and involving two horizontal components of displacements and reactions.

Within the context of the nonlinear dynamic analysis, most of the studies available in the literature, including the popular Bouc-Wen [1] and Kikuchi-Aiken [2], reproduce the bearings' response by means of two uncoupled, orthogonal springs with uniaxial response.

Although very popular in common practice, such an approximation does not take into account the dependency between the two horizontal components of the bearings' responses, thus underestimating the seismic vulnerability of the system.

For this reason, multiaxial constitutive relationships are currently investigated by the scientific community and some effective models, including the one proposed by Vaiana et al. [3] that represents the focus of this research, are available in the literature.

Such a constitutive model is the generalization of a uniaxial *Exponential Material* [4] that is ruled by 4 parameters and whose response f_t relevant to a generic displacement u_t is:

$$\mathcal{F}\left(u_t\right) = -2\beta u_t + e^{\beta u_t} - e^{-\beta u_t} + k_b u_t - s_t \frac{k_a - k_b}{\alpha}\left[e^{-\alpha\left(u_t s_t - u_j s_t + 2u_0\right) - e^{-2\alpha u_0}}\right] + \bar{f} s_t \quad (1)$$

where k_a and k_b represent the initial and asymptotic tangent stiffness, α is a transition parameter determining the amplitude of the hysteresis loop, β is a coefficient determining hardening behaviors, s_t, $\bar{f}$, and u_0 are ancillary parameters and, u_j is a history variable.

Its biaxial generalization [3] was performed by superimposing a discrete number n of horizontal springs with different orientations φ_i with $i = 1 \ldots n$ so that, fixed the horizontal components u_x and u_y of the biaxial displacement, the relevant response turns out to be:

$$\mathcal{F} = \sum_{i=1}^{n} \mathcal{F}\left(u_x \cos\varphi_i + u_y \sin\varphi_i\right)\left[\cos\varphi_i \ \sin\varphi_i\right]^T \quad (2)$$

The present research aims to investigate the influence of the bearers' biaxial behavior on their seismic vulnerability. To this end, two structural models were considered: the *coupled model* consisting in a 2DOFs oscillator modeled by the biaxial material [3] and the *uncoupled model*, where two independent uniaxial springs were used. Both models were calibrated in order to reproduce the response of a Lead-Rubber Bearer (LRB) and a High-Damping Rubber Bearer (HDRB) and were analyzed by a Monte Carlo stochastic analysis relying on simulated spectrum-compatible accelerograms [5] relevant to 4 locations with 712 and 1462 years of return periods.

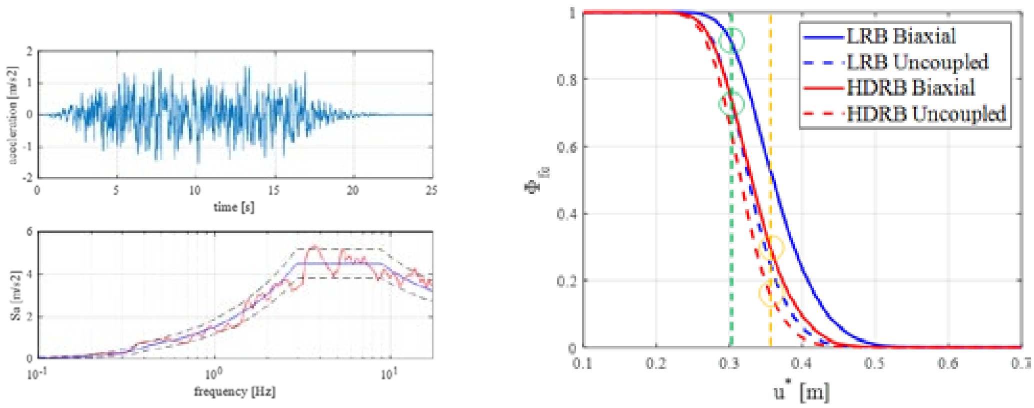

Figure 1: Realization of a spectrum-compatible accelerogram (left) and First-excursion probability comparison (right).

Figure 1 shows the comparison of first excursion probability for a significant scenario: horizontal axis reports the maximum displacement of the bearer while vertical axis reports the upcrossing probability. Moreover, solid curves are relevant to coupled oscillators while dashed graphs correspond to the uncoupled systems. As a matter of fact, first excursion probability is strongly underestimated by the uncoupled systems. This is particularly evident at the limit-state conditions, reported by the vertical dashed lined denoting the limit displacement of the bearers (the green line is relevant to the LRB, while the orange one corresponds to the HDRB).

Intersections of such thresholds with the curves represent the collapse probability of each model. As a matter of fact, uncoupled models turn out to be significantly non-conservative. Such an evidence, confirms the importance of properly account for the biaxial behavior of isolation devices for seismic analysis purposes.

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Improved pseudo-force method for time domain analysis of fractional oscillators under stochastic excitation

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Keywords: Fractional differential equation, stochastic excitation, step-by-step integration.

Fractional differential equations (FDEs) in time govern various phenomena in very different fields of science and engineering e.g., constitutive laws of materials with memory and hereditary properties, diffusion problems, control theory, etc. (see e.g., [1]).

FDEs can be solved analytically only in a few special cases. Approximate solutions are commonly obtained by applying suitable step-by-step integration schemes which require the evaluation of the fractional derivative of the relevant variables at each time step (see e.g., [2,3]). The latter involves the whole past time history due to the non-local character of fractional operators. It follows that the computational effort and the storage requirements escalate with time since an increasing number of past values of the solution needs to be considered.

Over the last decades, the analysis of fractional systems subjected to stochastic excitation has attracted increasing research interest. In spite of the large variety of analytical and numerical procedures developed to address this problem (see e.g., [4,5]), *Monte Carlo Simulation* (*MCS*) remains the most general approach to predict response statistics of non-linear systems endowed with fractional derivatives and subjected to stochastic excitation. However, the computational burden required by *MCS* becomes prohibitive due to the non-local character of the fractional operator. Thus, efficient numerical integration methods are needed to evaluate response samples.

This study presents a step-by-step procedure for the numerical integration of the FDE governing the response of single-degree-of-freedom (SDOF) systems endowed with fractional derivatives subjected to stochastic excitation. The procedure, named *improved pseudo-force method* (*IPFM*), stems from the extension of a step-by-step integration scheme proposed by the first author [6,7] for the numerical solution of classical differential equations. It has been demonstrated that this procedure is unconditionally stable [8]. The *IPFM* involves the following main steps: *i*) to use the Grünwald–Letnikov (*GL*) [1] approximation of the fractional derivative at each time step; *ii*) to treat terms depending on the unknown values of the response as *pseudo-forces*; *iii*) to handle non-linearities by performing iterations at each time step. The *IPFM* provides accurate solutions by using time steps of larger size compared to classical step-by-step integration schemes such as the *finite difference method* (*FDM*). Furthermore, to enhance the computational efficiency of the *IPFM*, the *fading memory* property of the fractional derivatives can be exploited by retaining in the *GL* approximation only a number n_T of time instants associated with the most recent time history. In the present study, the *IPFM* is applied to perform the stochastic analysis of fractional SDOF systems subjected to random excitation by *MCS*.

Numerical results concerning a linear fractional oscillator subjected to a Gaussian white noise are reported for validation purposes. The following parameters are assumed: natural circular frequency $\omega_0 = 1.0$ rad/s; fractional derivative coefficient $c_\beta = 1.0$; fractional derivative order

$\beta = 0.25$; two-sided Power Spectral Density of the white noise $S_0 = 1/2\pi$. The response obtained by applying the classical *FDM* with a time step $\Delta t = 10^{-4}$ s is assumed as reference solution. Figure 1a displays the time history of the generic sample of the displacement provided by the *IPFM* and the *FDM*. It can be seen that the *IPFM* yields a solution in excellent agreement with the reference one by using a much larger time step i.e., $\Delta t = 0.03$ s. In Fig. 1b, the time history of the variance of the displacement obtained by *MCS* ($N_s = 5000$ samples) along with the exact steady-state value (dashed line) is plotted. It can be observed that, when a time step $\Delta t = 0.03$ s is assumed, the *IPFM* provides much more accurate results than the *FDM* even when a truncation step $n_T = 500$ of the *GL* approximation is considered.

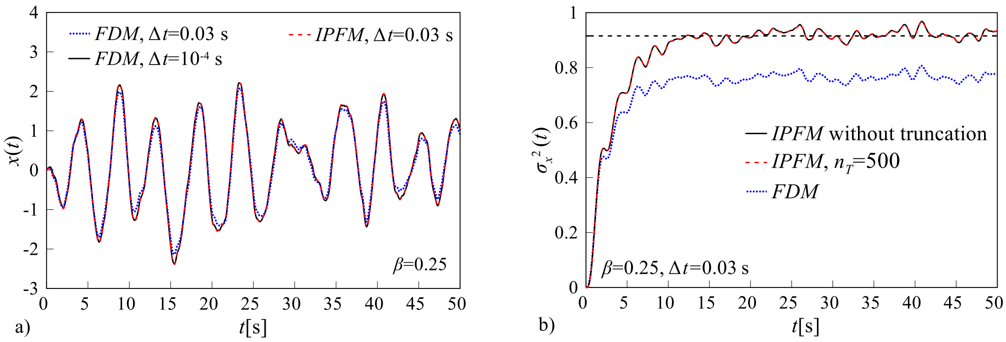

Figure 1: a) generic sample and b) variance of the displacement of the linear SDOF system under white noise excitation provided by the *FDM* and the *IPFM*.

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Dynamic identification of slender structures by means of stochastic subspace identification method.

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Keywords: stochastic subspace identification, modal identification, masonry buildings, tower bell

Since the architectural heritage is getting older, the need for structural monitoring is increasing. Structural monitoring involves the identification of the dynamic properties of the structure (frequencies, modes, damping). Vibration tests using ambient excitations are becoming more and more popular since they are reasonably inexpensive and easy to perform [1]. Several methods have been proposed, and this work investigates on the performance of the so called, stochastic subspace identification methods [2]. The main challenge in using these methods is distinguishing between true modes and artificial, mathematical, modes, that derive from noise and other imprecisions in the data treatment. Although becoming very popular, its success depends on the setting used for the implementation, and on criteria adopted for evaluating the confidence of the results [3]. The purpose of the investigation is to analyse the different parameters and criteria involved on the procedure, in order to develop a procedure for assigning confidence levels to the results obtained from the method. Some case studies will be described, related to laboratory tests, and to two slender masonry bell towers located in Eastern Sicily.

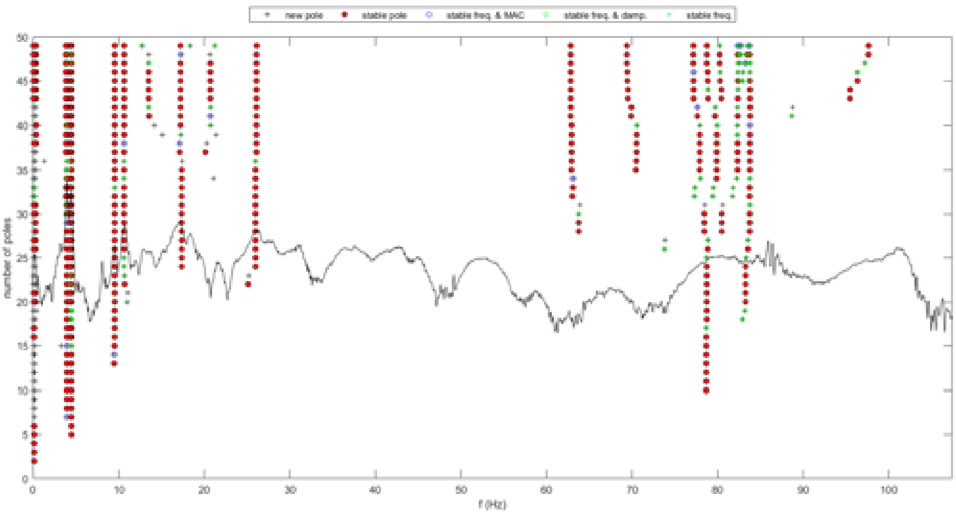

Figure 1: example of stabilization diagram.

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Energy Approach both for Fatigue Limit and Life Expectation of Rod Lift Systems

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Keywords: Sucker Rod**,** Duffing, Fatigue.

There is an obvious dichotomy of views on the role that the oil and gas industry will play in the global energy transition over the coming decades. Innovative, sustainable and disruptive artificial lift technologies are the cost-effective way seek by the energy companies to remain profitable on the market. In well with sucker rod-lift systems, see Fig.1, elastic beam vibrations induced by downhole pump operation are the main source for premature rod string failure and tubing wear also accounting for half of all well failure events, as well as, for most expensive routine well servicing cost.

This work deals with mechanical fatigue of a continuous thin elastic structure axial loaded and including axial effects (the *membrane force*) arising from sufficient deformation to cause coupling between axial and bending behaviour (the *membrane effect*). A model to enhance prediction of mechanical rod string dynamics during pumping operation has been developed and detailed in [1]. The model works on a set of forced Duffing-like differential equations with cubic non-linearity and damping, generated discretizing beam elastic behavior using vibration mode basis. Model simulation runs in the time domain [2], numerically capture relevant axial-flexural dynamic forces undergone by rod string during up and down stroke phases, as well as, rod string bending-buckling tendency and its interaction with tubing internal wall.

In the present contribution, an all-new *digital twin* model to evaluate the **fatigue endurance limit** and predict the **life expectation** of a rod-lift system in operation is proposed. New computational model combines: *specific energy* arising from the rod string dynamics during pumping operation also accounting for the material hysteresis, *Wöhler curve* of the carbon steel alloy material, and the classic fatigue endurance diagram (*Goodman diagram*). Model objectives are achieved by simulating a series of experiments under controlled conditions reflecting the nature of loading, see Fig.2 and 3.

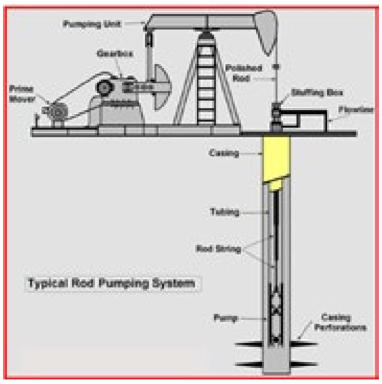

Figure 1 – The Rod Pumping System

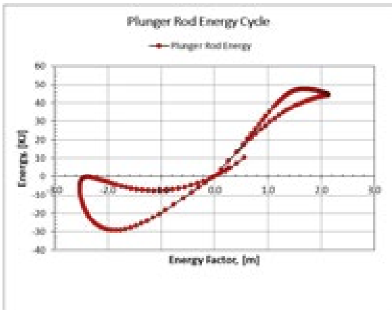

Figure 2 – Rod Energy Cycle

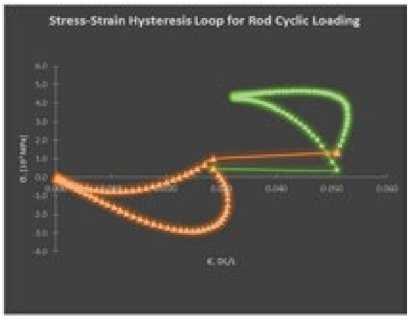

Figure 3 – Rod Stress-Strain Hysteresis Loop

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A validated biaxial test specimen design for simplifying results interpretation

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Keywords: biaxial test, cruciform specimen, shape optimization, digital image correlation.

Biaxial tensile tests are subject of growing interest in the material science community. A wider than before availability of biaxial tensile machines allows enriching the constitutive knowledge about diverse materials, from metals to polymers. Even though cruciform specimens are the most obvious choice, no universally accepted specimen shapes exist which ensure matching between common theoretical assumptions on the deformation state and the experimental conditions. The main discrepancies are represented by: the propagation of boundary conditions from the clamping to the gauge area which distort the displacement field; the practical difficulties related to the the transmission of the machine elongation towards the tested area. All considered, full field measurements via modern imaging techniques and inverse analysis often complement the mechanical tests at the expense of immediateness of results interpretation.

Figure 1: Biaxial test on cruciform specimen. The optimal shape design is validated with an in-house tensile machine. The white spots on the specimen constitute the speckle pattern used for image processing and full field measurements.

With this contribution, we propose a specimen design which guarantees a high uniformity of strain across a cruciform specimen and low discrepancy between the machine assigned macrostrain level and a large central area. This novel design is carried out via a finite element based multi-objective shape optimization procedure followed by digital image correlation validation on a range of solutions. Among different possible choices which have been demonstrated to improve the test performance as defined above, we restrict our focus on constant thickness and compact domains in order to obtain shapes that can be easily and accurately be realized in common laboratories. As a first attempt, only equibiaxial states are analyzed, but the method is robust enough to be extended to more general cases.

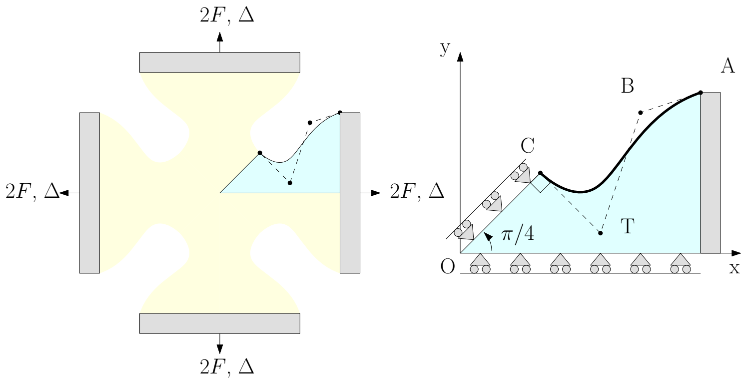

Figure 2: Cruciform specimen subjected to equibiaxial tensile test. Shape variables and reduced finite element domain thanks to symmetry in geometry and loading.

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A fluid structure interaction problem of the vibration frequencies of the eye bulb

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Keywords: ocular vibrations, fluid-structure interaction, natural frequencies.

The human eye is a pressurised organ consisting of a solid elastic shell (the corneo-scleral shell) containing a gel like substance (the vitreous humour). The intraocular pressure (IOP) is regulated by a delicate balance between fluid production by a specialised tissue named the ciliary body and resistance its drainage from the eye, into the venous system. IOP is an important clinical parameter as it is well know that high IOP values correlate with the occurrence of open angle glaucoma, a sight threatening disease and the leading cause of blindness in developed countries. IOP is routinely measured with Goldmann contact tonometers: the force required to flatten a portion of the cornea is measured and it is related to the IOP through empirical relationships. In recent years, there has been a growing interest in non-contact pressure measuring techniques and acoustic tonometry is among the most promising. The eye bulb is excited with acoustic waves and the vibration frequency of the ocular shell is measured, which allows the operator to identify natural frequencies of oscillation. The oscillation frequencies have been shown to be closely correlated to IOP, both in experimental [1,2] and numerical works [3,4]. However, a complete mechanical model that properly accounts for the interaction between the elastic corneo-scleral shell and the viscoelastic vitreous humour is still missing. We propose such a model, describing the eye wall as a spherical, prestressed elastic shell, containing a viscoelastic material. We study the eigenfrequencies of the system and the corresponding eigenfunctions, by expanding the solution in terms of vector spherical harmonics. The model allows us to single out the role of the parameters involved in the problem. IOP and Young's modulus of the shell strongly influence the vibration frequencies, whereas the vitreous rheological properties mostly influence damping.

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Active dynamics of self-contracting polymer gels subject to different chemo-mechanical environments

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Keywords: hydrogels, activity, stress-diffusion.

Biopolymer active gels are fabricated by distributing a myosin motors concentration on a network of actin filaments. The composite forms an homogeneous thin sheet of acto-myosin bonds, which is suspended in a liquid bath. This system undergoes spontaneous contraction in condition of free-swelling (i.e. without need of external stimuli)[1], or under an external dead load which is maintained, while the activity is working, when the stress-diffusion dynamics is evolving. These self-contracting materials have many potential clinical applications, ranging from artificial muscle manufacturing, wound healing speed up, to control of drug delivery in pharmaceutics.

More generally, a detailed understanding of stress-diffusion dynamics in presence of active remodeling, and under different load landscapes, is a crucial point for the coupled response of the soft material in presence of an active behaviour. We study the problem through a continuum mechanical model, based on an augmented stress-diffusion theory, which describes liquid release under bulk contraction and includes bulk sources to mimic molecular motors which cause self contraction [2]. We discuss a minimal model, let say, in terms of constitutive choices of gel elastic response and myosin motors activation, under simple assignments in terms of external applied forces and profile of bulk source, firstly to gain a deeper insight into the implications of the proposed model, and then to analyze the interplay between liquid outflow and stress-strain evolution.

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Swimming of active filaments emerging from mechanical instabilities

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Keywords: Flutter instability, Microswimmer, Biomimesis, Polyelectrolyte gels.

Many organisms propel themselves in fluid environments by beating slender, whip-like organelles known as flagella. For example, prokaryotic cells are equipped with passive flagella, whose rotational motion is imparted at the base of the filament by a complex piece of molecular machinery called *bacterial rotary motor*. Eukaryotic organisms, instead, are equipped with *active flagella*, in which the forces generated by molecular motors are distributed along the entire filament.

In the last decades, active materials have been extensively used to study and manufacture artificial flagella with applications to micro-robotics, e. g. [1]. However, these synthetic replicas were able to reproduce the periodic beating of their natural counterparts only with complicated time-varying actuation. In recent studies, dynamic instabilities have been proposed as a mean to overcome this limitation, allowing to generate a time-varying response with stationary external stimuli [2, 3].

In particular, the results in [4] show that flutter instability can be exploited to generate sustained periodic oscillations in an active polyelectrolyte (PE) gel filament subject to a uniform and constant electric field. Building upon these findings, here we show theoretically and experimentally how non-reciprocal periodic shape changes emerging from mechanical instabilities can be harnessed to achieve swimming of active gel filaments in a viscous fluid. The modelling of such active elastic filaments is based on morphoelasticity, while hydrodynamic interactions with the surrounding fluid are described by Resistive Force Theory. The linear stability analysis of the governing equations predicts the emergence of flutter and divergence instabilities when the coupling with the external stimulus is strong enough, in relation to the model parameters. Numerical simulations of the fully non-linear system confirm that instabilities corresponding to flutter lead to periodic self sustained oscillations. Interestingly, these oscillations are able to generate thrust in a viscous fluid, allowing the filament to swim. Experiments on millimetre-scale PE gel ribbons subject to uniform and constant electric field confirm the theoretical results.

This work is, to our knowledge, the first application of flutter instability in active filaments, providing a proof of concept of how complex control systems, usually necessary for swimming robots, can be embodied exploiting mechanical instabilities.

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Swimming of active filaments emerging from mechanical instabilities

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Keywords: Flutter instability, Microswimmer, Biomimesis, Polyelectrolyte gels.

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Investigating the influence of chemo-mechanical coupling in the remodelling of lipid membranes

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Keywords: Mechanobiology — Cell membrane — Lipid rafts

Membrane-mediated phenomena in living cells are essential to drive many biological mechanisms connected to cellular homeostasis and metabolism as well as to adverse processes such as phenotype mutation and infection [1]. As well known, cell membrane are highly dynamical environments showing a strong coupling between biochemical events and structural re-organization, which takes place by means of conformational changes, characterized by lipid order transitions occurring at lower scales, and associated micro-mechanical interplay of lipids with transmembrane proteins and molecular diffusion [2,3, 4]. In this framework, modelling the dynamic clustering of ordered lipids on cell membrane –denoted as lipid rafts and rich in active protein and receptors– implies a full multiphysics coupling between the kinetics of phase changes and the mechanical work performed by activating transmembrane proteins on surrounding lipids, this one being in turn mediated by the effective membrane elasticity [5]. This result in a complex interspecific dynamics in which membrane stresses and chemical potentials do compete by determining different morphological arrangements, alteration in diffusive walkways and coalescence phenomena, with a consequent influence on signalling potential and intra-cellular processes. Through in silico simulations, our purpose is to investigate this process in depth to have a quantitative predicting model for characterizing the space-time changes of rafts domains within the cell membrane to effectively observe the co-localization and synergy between the activation of membrane proteins and rafts formation. This could contribute to the attempts of testing/designing new or existing drugs by selectively controlling the mechanical properties and selectivity of the membrane to external agents, so orienting intracellular functions.

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Graded damage VS phase-field for modeling quasi-brittle fracture

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Keywords: Regularization, Damage, Gradient.

Predictive computations of failure mechanisms and ultimate load-carrying capacity of structures are among the most burdensome exercises in civil and mechanical engineering. This is a direct consequence of the intrinsic non-smooth character of damage and fracture phenomena, which render the tasks of modeling and simulation of crack initiation and growth in solid materials extremely demanding. A typical example is the analysis of concrete fracture but the same considerations apply e.g. to delamination or ductile fracture.

In recent years the family of regularized formulations known as *phase-field models* have become increasingly popular as valuable tools for simulating fracture starting from the strain localization stage, see e.g. [1] and references therein. Such models are motivated by the Ambrosio-Tortorelli (AT) approximation of the Mumford-Shah functional that has been adapted to transform the Griffith-type description of fracture into a smooth, though not convex, problem in which the global minimizer of an energy with competing volume and surface shares is sought for.

Basically, there are two reasons for the exceptional success of the AT regularization for the image segmentation problem. First is the fact that one ends up with linear (and convex) subproblems when using alternate minimization, the physical [0,1] bounds for the edge variable being satisfied *per se*. The second one is the celebrated $\Gamma-$convergence argument, for which a mathematical proof exists even for the discretized problem. However, in boundary value problems for regularized brittle fracture the above properties are quickly lost e.g. using the usual elastic energy split that prevents compressive cracking.

In this communication we work out a comparison between the classical AT phase-field models for brittle fracture and the regularized damage formulation contributed in [2]. This model is called *graded damage* to remind that we do not only penalize the gradient of damage as in phase-field, but rather we control the magnitude of it by prescribing a suitable bounding function. As a result, we obtain a generalized standard model with convex constraints in which damage is characterized as an explicit function of distance within interphases that separate the fully damaged regions of a solid body from the sound material. Finite element problems are dealt with using a staggered Newton-type solver for both models and representative numerical simulations are presented that show some distinctive features of the two approaches.

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A simple method to compute a closed-form spectral decomposition of a symmetric second order tensor

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Keywords: Computational Plasticity, Finite Deformations, Isotropy, Finite Element Method.

The spectral decomposition of a symmetric, second order tensor is widely adopted in many fields of Computational Mechanics. As an example, in elasto-plasticity under large strain and rotations, given the Cauchy deformation tensor, it is a fundamental step to compute the logarithmic strain tensor [1][2]. More in general, the spectral decomposition is a necessary step to compute the polar decomposition of the displacement gradient [1][2]. Recently, this approach has been also adopted in small-strain isotropic plasticity to reconstruct the stress tensor as a function of its eigenvalues, allowing the formulation of predictor-corrector return algorithms in the invariants space. These algorithms not only reduce the number of unknowns at the constitutive level, but also allow the correct handling of stress states in which the plastic normals are undefined [2][3][4], thus ensuring a better convergence with respect to the standard approach. While the eigenvalues of a symmetric, second order tensor can be simply computed as a function of the tensor invariants [5], the computation of its eigenbasis (i.e., of the dyadic product of each principal direction by itself) can be more difficult, especially when two or more eigenvalues are coincident (see, for example, [1][2]).

Moreover, when a Newton-Rhapson algorithm is adopted to solve nonlinear problems in computational mechanics, also the derivatives of the eigenbasis with respect to the tensor itself are required to assemble the tangent matrix. The computation of these derivatives is in general even more complicated, especially in the case of repeated eigenvalues [1].

A new, simple and comprehensive method is presented and discussed, which can be adopted to compute in closed form the eigenbasis of a second-order tensor, as well as their derivatives with respect to the tensor itself, allowing a simpler implementation of spectral decomposition of a tensor in Computational Mechanics applications.

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Form Finding of Membrane Shells with Isogeometric Analysis

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Keywords: Form finding, Isogeometric Analysis, Membrane shells.

A shell surface resists applied loads by an internal stress distribution equivalent to three distinct internal actions, i.e. membrane (in-plane), out-of-plane shear and bending-twisting stress resultants. Due to exiguous bending and torsional stiffness, the shell structural behaviour is deemed to be optimal if it experiences purely membrane stresses. Membrane shells constitute inherently an attractive architectural solution for large lightweight structures of refined aesthetic elegance since they allow for wide interiors to be enclosed unobstructedly with minimal usage of material in the absence of bending and/or twisting moments. However, randomly curved shell forms are not free from moment actions. The design procedure aimed at determining the shell form possessing such moment-free property is called *form finding*. Form-finding problems are nonlinear by nature, involving a number of interrelated unknowns. With predefined external loads, most of existing algorithms assign membrane stresses as an input, then solve for the shell form. Besides concealing the violation of trivial boundary conditions [1], the arbitrary prescription of working stresses is often limiting, especially when the resulting configuration is not satisfactory and revising the input is not intuitive [2]. At present, only few authors ([3],[4]) have computed stresses in form finding, albeit strictly fulfilling boundary conditions and ensuring working tensions of desired sign. The present work presents a novel two-step numerical form-finding procedure to determine the elevation of a shell having a prescribed covered area. First, membrane stresses are computed via a nonlinear optimization routine aimed at minimizing a specific objective function besides usual constraints. Then, the shell form is obtained by discretizing the weak form of the problem based on Isogeometric Analysis (IgA). According to Pucher [5], the complete equilibrium of an infinitesimal shell element reads:

$$\Phi_{,yy} f_{,xx} - 2\Phi_{,xy} f_{,xy} + \Phi_{,xx} f_{,yy} = q_x f_{,x} + \int q_x \, dx \, f_{,xx} + q_y f_{,y} + \int q_y \, dy \, f_{,yy} - q_z \qquad (1)$$

Here, $\mathbf{q} = (q_x, q_y, q_z)$ is the force per unit projected area, Φ the Airy potential and f the shell mid-surface. Projected membrane stress components at a point (x, y) are obtained via second derivatives of Φ. Supplemented with boundary conditions, Eq.(1) is the strong form of the problem. Let $\mathcal{F} = \{f(x, y) | f(x, y) = \bar{f}(x, y) \ \forall (x, y) \in \Gamma_c\}$ be the functional space where to look for the shell form satisfying Dirichlet conditions on the constrained boundary Γ_c, and $\mathcal{G} = \{g(x, y) | g(x, y) = 0 \ \forall (x, y) \in \Gamma_c\}$ be the set of arbitrary variations vanishing on Γ_c. Then, the equivalent weak form is obtained by algebraic manipulation of Eq. (1):

$$\int_\Omega \nabla^2 \Phi (\nabla f \cdot \nabla g) - [(\nabla f)^T \nabla (\nabla \Phi)] \cdot \nabla g - (\mathbf{h} \circ \nabla f) \cdot \nabla g \, d\Omega = \int_\Omega q_z g \, d\Omega \qquad (2)$$

Within the IgA framework, the shell domain Ω is discretized into N^e portions of B-Spline patches, i.e. elements, delimited by pairs of knot spans in the two parametric directions ξ and η. In each element, the relevant fields and their gradients are approximated as a linear combination of control point values and corresponding B-Spline local basis functions or their derivatives. Applying the mentioned scheme, the integral equation of the weak form can be formulated as:

$$\sum_{e=1}^{N^e}\left[\int_{\Omega^e}(\mathbf{L}^e\cdot\mathbf{\Phi}^e)(\mathbf{B}^{eT}\mathbf{B}^e)-\mathbf{B}^{eT}(\mathbf{C}^e\zeta^e)\mathbf{B}^e-\mathbf{B}^{eT}(\mathbf{h}\circ\mathbf{B}^e)\,d\Omega^e\right]\mathbf{Z}^e\cdot\mathbf{W}^e=\sum_{e=1}^{N^e}\left[\int_{\Omega^e}q_z\mathbf{S}^e\,d\Omega^e\right]\cdot\mathbf{W}^e$$

Assemblage over elements yields the following system of linear algebraic equations:

$$\mathbf{KZ}=\mathbf{F}+\mathbf{q} \tag{3}$$

being $\mathbf{K}$ the shell pseudo-stiffness matrix, $\mathbf{Z}$ the vector of shell control point heights, $\mathbf{F}$ and $\mathbf{q}$ the vectors of shell control point forces originated from constraint reactions and external load, in turn. Prior to solving Eq.(3) for the unknown shell form, the control point values of the Airy potential, on which $\mathbf{K}$ depends, have to be computed. This is done by solving a nonlinear optimization problem aimed at minimizing the forces transmitted to the shell supports against a user-defined limit value, while imposing null stresses on the free edges and allowing the user to choose whether the shell operates in a membrane state of pure traction or compression. Figure (1) illustrates the equilibrium shape of a shell in traction, constrained on three edges and subject to a uniform vertical load.

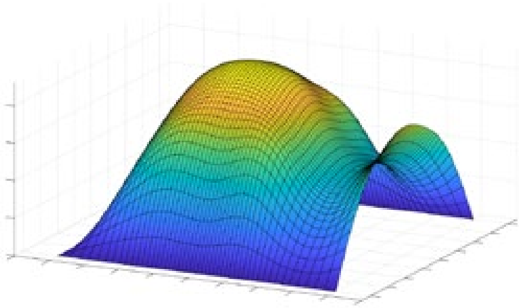

Figure 1: Isometric view of form-found shell supported at three edges

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Material point method and isogeometric analysis

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Keywords: Material Point Method, Isogeometric Analysis, Spline, Patch-wise integration.

The Material Point Method (MPM) combines a usually fixed background Eulerian grid with a collection of Lagrangian particles, referred to as material points, which are free to move over of the background grid in a non-conforming manner. The material point method (MPM) [1, 2] is a particle-based numerical technique that originates from the particle in-cell method [3]. Continuum bodies are discretized by the material points that also carry history-dependent variables such as stresses and plastic strains. The background mesh is used to solve the governing partial differential equations expressed in a weak form, and the material points serve as integration points for the weak form under consideration. MPM has been successfully applied to a collection of challenging problems involving large deformations and extreme material distortion, where conventional Lagrangian mesh-based techniques fail due to mesh entanglement and the need for frequent mesh updating or re-meshing. While linear elements, in principle, give a convergent discretization, the so-called cell-crossing instability is often observed in the MPM simulations using such elements. This instability is attributed to a discontinuity in the strain or strain rate, and the corresponding stress measure, occurring as the Lagrangian particles cross from one background element to its neighbor. More generally, this discontinuity is a direct consequence of using background FE discretizations that are C^0-continuous for the kinematic variables, which leads to strain measures that are discontinuous across element boundaries. It has been shown that cell-crossing instability may significantly affect the quality of the solution and even lead to lack of spatial convergence. Especially in problems involving large deformations and brittle damage, cell-crossing instability often leads to premature material failure and results in non-physical solutions. The use of B-Spline-based background discretizations showed the elimination of the cell-crossing instability and improved accuracy and convergence of conventional MPM.

However, even if the MPM is an increasingly popular method for tackling solid mechanics problems involving large deformations there are issues associated with applying boundary conditions in the method and, to date, no general approach for imposing both Neumann and Dirichlet boundary conditions.

The present work has three aims. The first aim is to definitively show that smooth background discretizations are key to a successful instantiation of the MPM methodology. Secondly an efficient generation of the material points initial configuration is developed by considering a patch-wise integration over the isogeometric mesh representing the body to be analyzed. Also, a general approach has been developed to efficiently apply boundary conditions. In particular as the material points per each parametric direction are also integration points, Dirichlet boundary conditions can be enforced by Lagrange multipliers or, simply, by a penalty approach. Neumann boundary conditions are included by direct integration of surface tractions along the B-spline boundary. Finally, a modified algorithm for generating patch-wise integration points, aimed to locate material points also on the boundary, is proposed in order to improve the enforcing of the Dirichlet boundary conditions directly to them in the updating phase of the solution process.

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Multiscale strategy for identification of elastic and fracture properties of polymer-based nanocomposites

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Keywords: Nanomodified epoxy-resins, Multiscale procedure, Experimental tests.

The scientific and industrial communities have recently focused their interest on the design and characterization of innovative high specific stiffness materials like composites and nanocomposites. Among them, polymer-based materials nanomodified through the addition of nanoclay platelets have become increasingly popular thanks to the possibility to significantly enhance the mechanical, thermal, and barrier properties of the polymer materials through the inclusion of low concentrations of nanofillers. In this work, the elastic properties and fracture toughness of epoxy resins reinforced with nanoclays are modeled through an innovative multiscale procedure. The proposed strategy bridges the microscopic to macroscopic descriptions at three length scales and is validated through experiments. A statistical homogenization approach (SH) is exploited to determine the effective Young's modulus of the nanomodified epoxy resins with randomly distributed nanoplatelets [1, 2]. The data obtained from the SH procedure serve then as input for a classical continuum mechanics-peridynamics (CCM-PD) coupling approach which is exploited to study the fracture toughness of the nanocomposites under consideration [3, 4]. In the coupled model, two different length scales are considered, since the small-scale heterogeneity of the crack tip zone is preserved by implementing the recently proposed intermediately-homogenized peridynamic (IH-PD) model, whereas the CCM region is modeled as fully homogeneous. The capabilities of the proposed strategy are validated by exploiting the experimental data obtained performing tensile and fracture tests on specimens composed of epoxy resin reinforced by the addition of various nanofillers. Three different inorganic nanoclays are in fact considered to study the effects of different modifiers on the overall stiffness and fracture toughness of the polymer materials. A chemical characterization of the samples is also carried out through FTIR Spectroscopy and X-Ray Diffraction, and a Thermogravimetric Analysis (TGA) is performed to analyse the effect of the different nanomodifiers on the thermal degradation of the resins. The microanalyses of the samples are performed by Environmental Scanning Electron Microscopy (ESEM), and their morphologies are studied by Transmission Electron Microscopy (TEM) (see Figure 1). Comparison to experimental results confirms the capability of the proposed approach to properly model the elastic properties and fracture toughness of nanomodified epoxies.

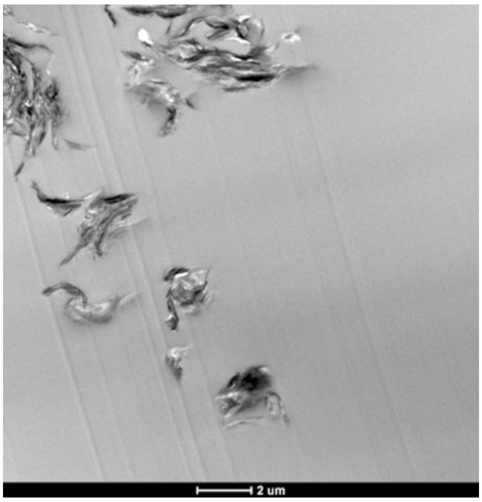

Figure 1: TEM image of an epoxy resin nanomodified through the addition of 5% wt of inorganic nanoparticles.

Acknowledgements

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Modeling of polycrystalline composites coupling virtual elements and nonlinear interface finite elements

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Keywords: Virtual Element Method, interface finite elements, polycrystalline composites.

Composite materials are nowadays largely used in many engineering fields, as they meet high requirements in terms of stiffness, strength, fracture toughness and lightness, among others. Recently, special attention has been devoted to polycrystalline composites, often obtained by interconnecting different types of crystals, also referred to as grains, with thin or thick interfaces or grain boundaries. Different macroscopic properties can be attained by varying the internal microstructure, i.e. by changing the thickness of the interfaces, the fracture properties of the interfaces and the phase density of grains [1].

In the present contribution, the response of polycrystalline composites is investigated adopting a modeling approach based on the use of the Virtual Element Method in conjunction with the Finite Element Method. The idea is to discretize each grain with a single virtual element and model the interaction behavior between grains by means of a denser mesh composed by interface finite elements with nonlinear behavior (Figure 1). In fact, it is assumed that all the nonlinear effects are concentrated at the interfaces, which are characterized by the constitutive law formulated in [2] accounting for damage, friction and unilateral contact phenomena. Hence, the advantages of the Finite Element and Virtual Element methods are exploited in a combined way, resulting in a versatile and accurate numerical approach. The reliability of the proposed modeling strategy, which avoids the usual fine finite element discretization of the polycrystals, is encouraged by data collected in [3].

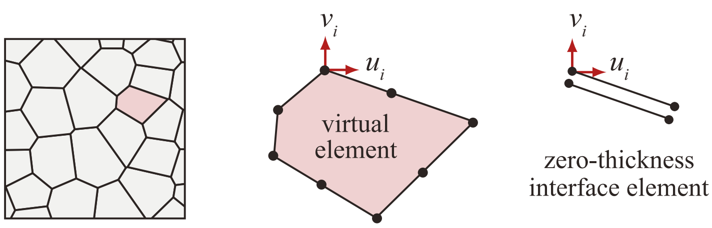
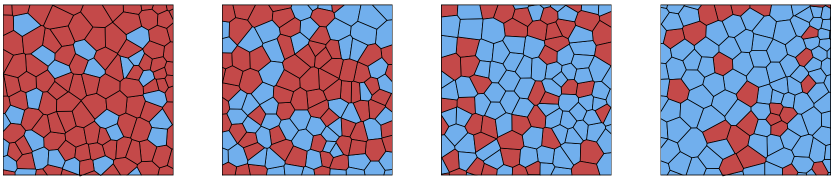


Figure 1: Modeling strategy for polycrystalline composite involving virtual elements and nonlinear interface elements.

Results of some numerical simulations are presented and discussed. Among others, the respone of Alumina/Zirconia (Al_2O_3/ZrO_2) composite is analyzed, as this is a noteworthy example of polycrystalline Ceramic Matrix Composite combining positive features of the two components, that is high hardness and low age susceptibility for the alumina, and high fracture toughness and resistance



(a) Al_2O_3 p=20% (b) Al_2O_3 p=40% (c) Al_2O_3 p=60% (d) Al_2O_3 p=80%

Figure 2: Aluminia/Zirconia specimens with different percentage p of alumina

to subcritical crack growth for the zirconia. In detail, uniaxial tensile tests are performed on the material representative volume element, whose overall size is selected on the basis of the average grain dimension and the results of literature studies concerning the homogenization of random composites [3]. Different percentages p of the alumina content (Figure 2) are considered to analyze the influence of this parameter on the response, monitored in terms of load-displacement global curves and crack propagation.

Acknowledgments

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Artificial Neural Networks for evaluation of cracks in masonry arches

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Keywords: Masonry Structures, Settlements, ANN.

Masonry structures constitute a significant proportion of the built environment worldwide. Historic architectural heritage is heavily characterized by monumental masonry structures and, in many countries, residential buildings are predominantly constructed using masonry. Preservation of historical masonry structures has spurred a growing interest in studying this construction typology and devising new computational strategies to investigate their structural behavior. A critical research area in this field concerns the investigation of damage mechanisms that occur in existing masonry structures. Although masonry buildings are highly vulnerable to the horizontal loads generated by seismic events [1], crack patterns, typically caused by differential support movements, are often observed even in non-seismic areas, and the assessment of the damage caused by foundation settling on structures has been thoroughly studied and documented in the literature.

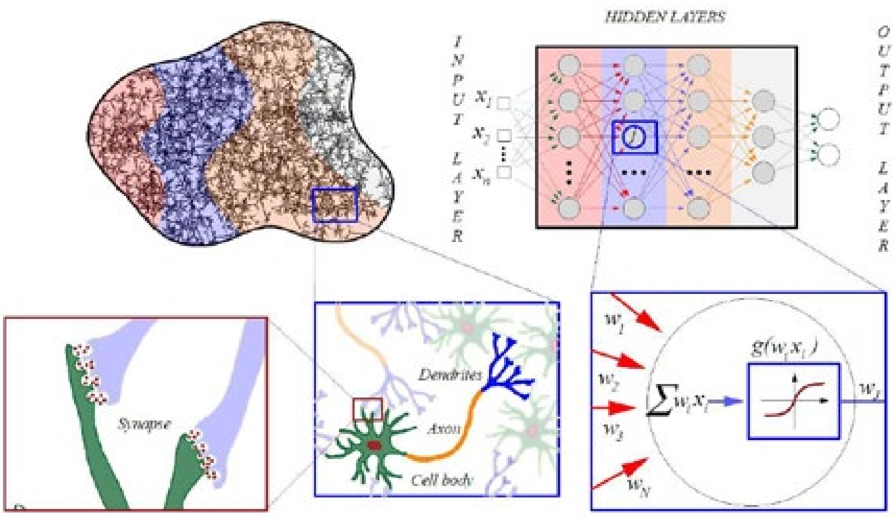

Figure 1: Natural and Artificial Neural Network Architecture.

Among the various methods for determining the causes of damage in structural mechanics, in recent years there has been a growing interest in exploring the enormous potential of Artificial Neural Networks (ANNs) and their ability to provide reliable results even for extremely complex problems. The literature on this topic is extensive and covers a wide range of fields. ANNs are computer systems inspired by the structure and function of biological neurons and consist of input nodes that receive information, output nodes that provide problem-solving responses, and hidden neurons that process input vectors and transfer them to the output vector to solve the problem. The artificial neuron, or perceptron, is the basic unit of an ANN, and it also consists of three primary components: the dendrite, axon, and cell body. In the artificial neuron, weight and bias are represented by a dendrite, denoted by w and b, respectively. The dendrite receives input signals multiplied by their corresponding weights and summed together with the bias term. The resulting value is then transmitted to the axon, an activation function that determines the output signal of the neuron. The output signal is then transmitted to other neurons or an external system (Figure 1). In this study, we proposed an ANN model using the Levenberg-Marquardt Back Propagation (LMBP) algorithm for predicting compatible settlement-induced cracks in masonry arches. We present here our preliminary results, whose quality encourages us to continue the investigation in this still unexplored world.

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Analysis of fracture propagation the Hybrid Equilibrium Element formulation

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Keywords: HEE, extrinsic interface, crack, fracture.

The present article proposes an original formulation for the analysis of propagation of a cohesive crack in elastic solids which is based on the Hybrid Equilibrium Element formulation coupled with a minimal finite element re-meshing, requiring only the rotation of the element sides, according to the orientation of maximum principal stress direction.

The hybrid equilibrium element (HEE) is an stress-based formulation developed in the variational framework of minimum complementary energy principle and it can be considered as an effective numerical tool for modelling the inter-element fracture propagation, as proposed in Ref. [5, 6] for static problems.

The inter-element cohesive behaviour is modelled by the extrinsic interface proposed in Ref. [6], which is modelled as a function of the same degrees of freedom of the HEE (generalized stress components). The interface can be assumed implicitly embedded at every element side.

In a two-dimensional problem the direction of crack is fixed normal to maximum principal stress direction and the crack is meshed as an extrinsic interface embedded at the closest element side, which is rotated around the tip in order to be geometrically co-aligned to the crack. The element side rotation is updated with the evolution of the stress field at the crack tip, as long as one point of the embedded extrinsic interface is still undamaged. The numerical problem of finding the element side orientation is strongly non-linear and the search of the crack propagation direction requires an iterative procedure. Moreover, in order to prevent erroneous crack prediction, a maximum rotation angle between two contiguous element sides along the crack path is assumed.

The HEE with the extrinsic interface embedded at the element sides is developed and implemented in an open-source finite element code, employing quadratic, cubic and quartic stress fields. Numerical simulations of some fracture propagation problems are presented.

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Validating the EUCLID Approach for Unsupervised Discovery of Hyperelastic Constitutive Laws Using Experimental Data

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Keywords: *Constitutive models; Experimental validation; Hyperelasticity; Interpretable models; Inverse problems; Sparse regression; Unsupervised learning.*

Abstract

Data-driven methods are gaining popularity in computational solid mechanics with the increasing data collection capacity of modern instruments. Recently, a new approach for automatic constitutive law discovery, called EUCLID (Efficient Unsupervised Constitutive Law Identification and Discovery) has been proposed [1]. EUCLID is capable of discovering the material model from a large library of candidates using data (applied forces and displacement fields) acquired from experimental tests. The advantages of this approach are evident when compared to classical calibration procedures (e.g., [2]), which require a significant number of tests specifically designed to induce simple stress states. In contrast, using EUCLID in combination with the digital image correlation (DIC) technique to obtain a full field displacement measurement, in principle a single test is sufficient to discover and calibrate the material model, provided that the specimen geometry is complex enough to promote a diverse multiaxial state of stress within the specimen.

Thus far, the EUCLID approach has been extensively validated with data from finite element simulations for different types of material behavior, for example hyperelasticity [1], plasticity [3] and linear viscoelasticity [4], but not with experimental data.

The aim of this work is to validate EUCLID's performance with data coming from experimental tests. To address this goal, mechanical tests on natural rubber specimens with different levels of geometrical complexity are performed (Fig. 1).

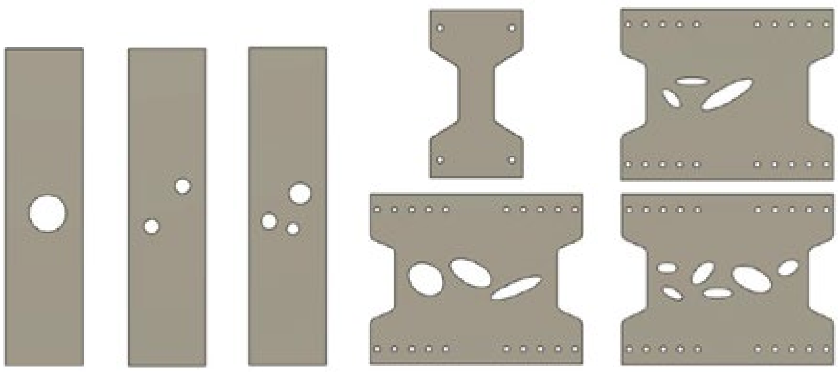

Fig. 1: Adopted rubber specimens with different levels of geometrical complexity

During the tests, a load cell measures the overall force (Fig. 2) and a DIC equipment acquires the displacement field (Fig. 3). Then, EUCLID is employed to discover the material law from a large library of hyperelastic models. Finally, the constitutive law discovered by EUCLID is validated on a set of unseen experimental data acquired through uniaxial tension and shear tests. Investigations of the influence of the specimen geometry and of the DIC noise on the EUCLID performance are carried out.

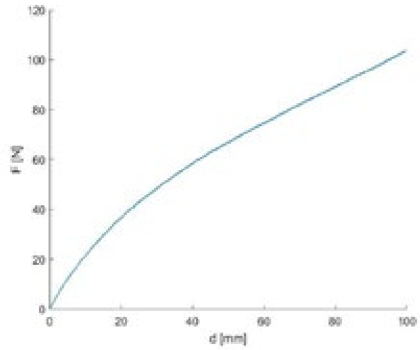

Fig. 2: Force-Displacement curve measured by the machine

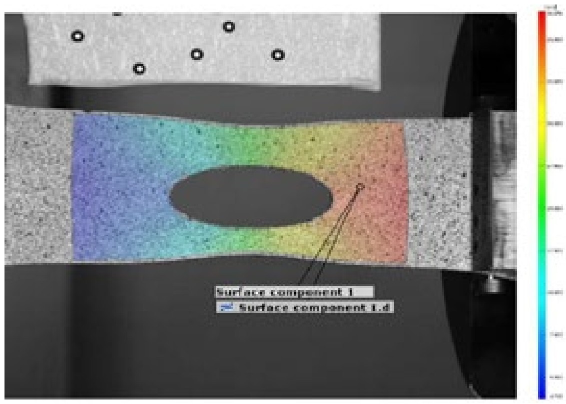

Fig. 3: Displacement field measured by the DIC equipment

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CRACK PROPAGATION PROCEDURE FOR DESIGNING HOLLOWED STRUCTURES

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Keywords: Linear Elastic Fracture Mechanics, Crack Growth, Crack Propagation, Mixed-mode, Finite Element

A novel automated and fully parametric FE procedure is proposed to compute fracture initiation and propagation in two-dimensional structures under plane stress. This methodology leverages the Hybrid Semi-Analytical Method to evaluate the mixed-mode stress intensity factors within the framework of linear elastic fracture mechanics. In particular, the Hybrid Semi-Analytical Method is based on combining the Virtual Crack Closure Technique and the generalized Clapeyron's Strain Energy Formulation, leading to a direct calculation of the stress intensity factors as a function of the nodal forces, displacements, and elements' lengths.

$$K_I = \frac{F_y^j \Delta u_y^{j-2} + F_y^{j+1} \Delta u_y^{j-1}}{2\delta \Delta u_y^{j-1} \sqrt{\Delta a_2}} \qquad K_{II} = \frac{F_x^j \Delta u_x^{j-2} + F_x^{j+1} \Delta u_x^{j-1}}{2\delta \Delta u_x^{j-1} \sqrt{\Delta a_2}} \tag{1}$$

In the proposed procedure, the fracture is assumed to start at the elastic limit of the structure, namely when the equivalent strain overcomes the yield one. The crack length increment is computed at each step, substituting the stress field at the crack tip into the von Mises yield criterion, as

$$r_p^{vM} = \frac{1}{4\pi\sigma_Y} \sqrt{\begin{array}{c} 7K_I^2 + 19K_{II}^2 + 4(K_I^2 - K_{II}^2)\cos\theta - 3(K_I^2 - 3K_{II}^2)\cos 2\theta + \\ +8K_I K_{II}(-1 + 3\cos\theta)\sin\theta \end{array}} \tag{2}$$

and the crack direction is estimated by employing the Maximum Circumferential Stress Criterion. Finally, the energy required to advance the fracture is calculated on a global-local-like approach, allowing the crack to propagate when the local strain energy at the crack tip overcomes the global one. At the end of each iteration, the geometry is modified, and an increment of the load is added to the actual one. The flow chart of the proposed procedure is shown in Figure 1.

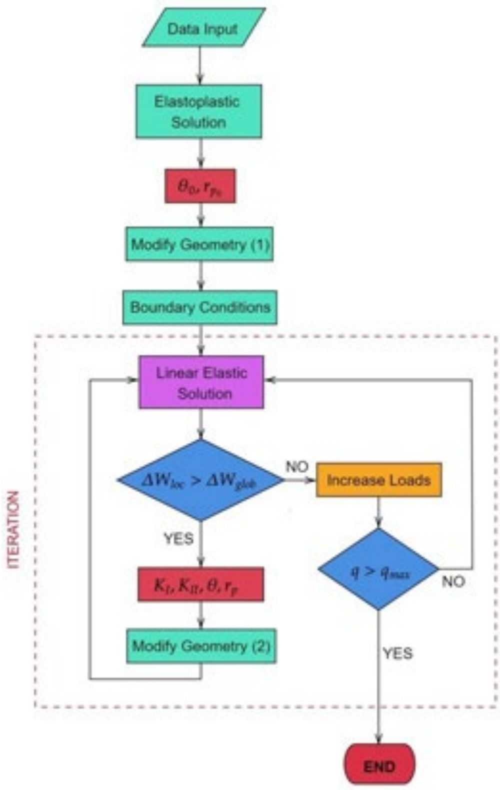

Figure 1: Flow chart of the proposed procedure.

A square hollow plate under pure tensile and shear loads, and a U-notched 4-points rectangular hollow plate (SENB specimen) are studied to demonstrate the proposed approach's effectiveness. In particular, the SENB has been analyzed by varying the holes' number, position, and notch lengths. Figure 2 shows geometry, boundary conditions, and von Mises stress for the square plate under pure tensile and shear load and the three holes U-notched rectangular plate.

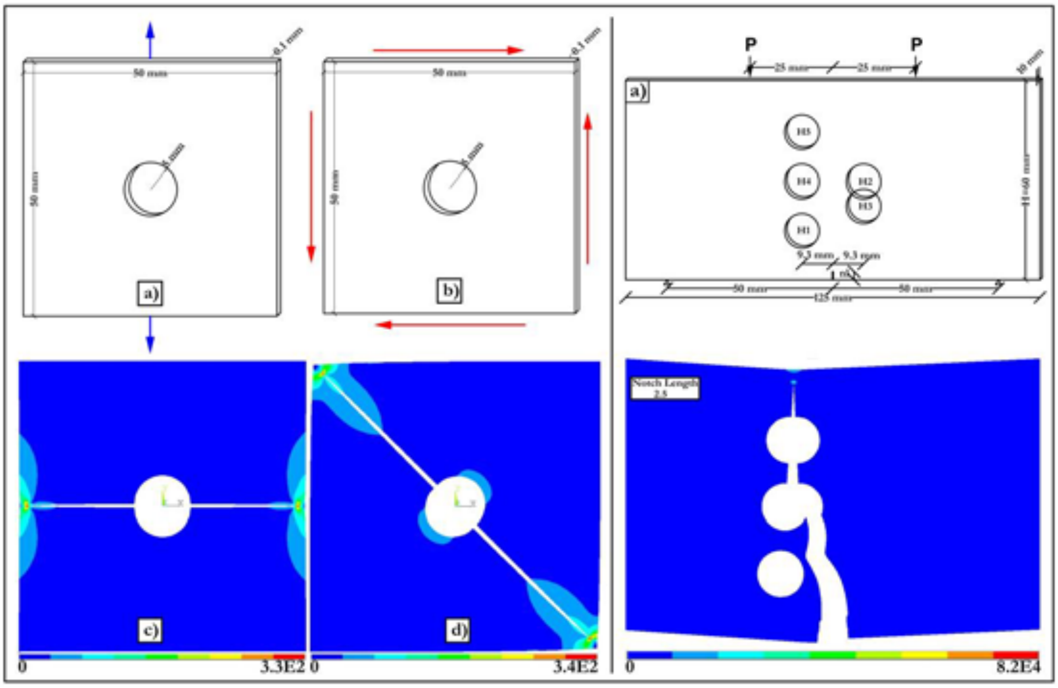

Figure 2: Square plate under pure tensile: geometry and boundary conditions (a) and von Mises stress (c), Square plate under pure shear: geometry and boundary conditions (b) and von Mises stress (d), Modified 4-points plate: geometry configurations (H1-H2, H1-H3, H1-H4, and H1-H4-H5) and boundary conditions (e), and von Mises stress in the case of three holes.

One of the main advantages of the proposed approach is that only linear elastic analyses are performed to calculate the stress intensity factors, the crack length increment, the crack direction, and the required energy to advance without refining the discretization around the crack tip or using mapped meshes, resulting in significant computational cost savings. Moreover, the strategy does not necessitate *a priori* knowledge of Young's modulus at the crack tip and embedding of the crack path nor crack increment during the crack propagation. The authors felt the proposed procedure could pave the way for designing hollowed structures and envisaging crack initiation and propagation within inhomogeneous media.

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Pre-stressed wire breakage detection using Back Propagation Neural Networks with experimental and numerical datasets

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Keywords: sound event detection, data augmentation, Finite element method

Developing an accurate and reliable real-time monitoring system for detecting prestressed wire breakage in concrete bridges is essential for ensuring the safety and longevity of our infrastructures and preventing catastrophic failures. In this context, the authors have recently proposed a novel sound event detection approach that uses Mel-frequency cepstrum coefficients (MFCCs) and back propagation neural networks (BPNN) to distinguish acoustic emission signals produced by wire breakage from those originating from environmental noise and other damage phenomena. Besides issues related to the setup and installation of the acoustic emission monitoring system and to signals processing, two are the main challenges involving numerical procedures and computational mechanics:

(1) long-term monitoring produces a large amount of data that requires accurate analysis, which can be time-consuming. Therefore, efficient and reliable data processing and analysis methods are needed to detect potential issues impairing structural safety quickly. One of the most efficient approaches to deal with this issue is utilizing machine learning (ML) and deep learning (DL)-based models. ML and DL are considered sub-fields of computer science that can build necessary algorithms based on the collected data of certain occurrences [1]. These models can be trained to identify patterns in the data, classify the data into different categories, or make predictions about future events.

(2) Developing a generalized and robust model requires a very large dataset, that is impossible to feed only with real-world data, especially for the problem at hand. Therefore, data augmentation techniques must be applied to increase the dataset size, enhancing the capability of the models and preventing over-fitting problems.

The first stage of the study consisted of: acoustic emission signals acquisition from two different bridges in Italy, their pre-processing, which includes the extraction of different representations up to obtain the MFCC (see Fig. 1), and training of different neural networks on real-world data to define a reference baseline. Then, the issue of scarcity of real-world data has been addressed by exploring two approaches to generate synthetic data: data augmentation and finite element method (FEM). In the former case, standard techniques such as mixup, time-shifting and polarity inversion were applied. In parallel, finite element models have been implemented to simulate the phenomenon of wire breakage and propagation of the elastic waves through the concrete beam taking into account the interaction between steel and concrete. As a result, synthetic datasets considering the physical behavior of pre-stressed concrete beams have been generated and used to further train the models. Two different regularizers, namely batch normalization, and dropout, were also implemented to improve the performance of BPNNs. Finally, to comprehensively evaluate the overall performance of the proposed algorithms, different measurement metrics, including precision, recall, specificity, and f1-score, were applied.

Based on the results of this study, the following conclusions can be drawn:

- FEM models and proposed augmented techniques are effective approaches for generating synthetic wire breakages and environmental noise signals. These techniques maintain the physics of the signals, ensuring that the synthetic data closely resemble the original signals. Using these techniques can lead to better classification and detection of wire cuts on the test dataset.
- the MFCCs based approach is effective in detecting and classifying AE events. This suggests that MFCC can be a valuable approach for representing the wire-cut signals and analyzing this event.
- batch-normalized BPNN performs better as it normalizes the input data for each batch before or after each hidden layer's activation function, thus helping to avoid vanishing and exploding gradient problems. This model outperforms all the others by achieving 99.30% and 99.20% for accuracy and f1-score, respectively.

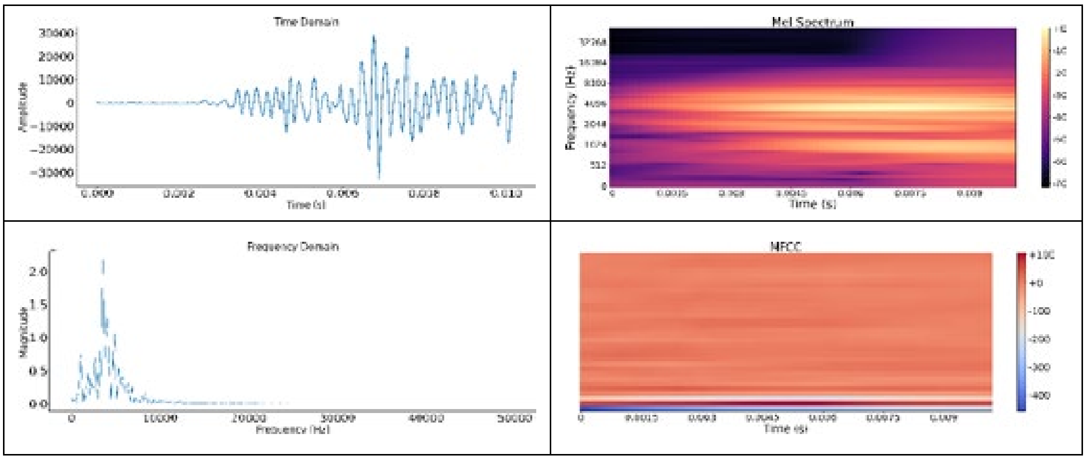

Figure 1: Wire breakage signal representations.

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Limit Analysis through Residual dislocation based Finite Elements and nonlinear compatibility domain secant aproximation with penalty factor

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Keywords: Limit Analysis, Optimization Program, Linearized Domain.

A Lower Bound limit analysis through a dislocation-based Finite Elements procedure is presented for calculating the collapse load of structures. The method allows the derivation of self-equilibrated solutions through the finite elements toward the numerization of the lower bound theorem of limit analysis in the Melàn's formulation [1-3]. To the scope, a finite element calculation of the self-equilibrated stress space is derived. This formulation is based on discrete mapping of Volterra dislocations in the structure using [4] isoparametric representation. The self-equilibrated stress state depends on the multiplicity of the equilibrium equation solutions, namely it is the null space of the balance equation [5]. Using standard finite element techniques, the linear operator $\boldsymbol{\mathcal{V}}$, that relates the self-equilibrated internal solicitation to displacement-like nodal parameters has been built through finite element discretization of displacement and strain. The derivation of the matrix $\boldsymbol{\mathcal{V}}$ has allowed to formulate the $\boldsymbol{\mathcal{V}}$FEM procedure that represents the manifold of equilibrated stress under prescribed load as the superimposition of the self-equilibrated linear variety span through $\boldsymbol{\mathcal{V}}$ and the particular equilibrated solution obtained assuming the structure made of an indefinitely elastic material. The collapse load is obtained through an optimization program [6] where the objective function is the load multiplier, and the program constraints are the structure's limit domain inequalities collocated on the element nodes. The limit domain has been linearized using the secant, say inscribed, iper-octahedron to the iper-ellipsoidal domain. Moreover, a penalty function has been introduced to consider the domain's nonlinearity. In particular, the actual stress has been penalized considering the ratio between the distance of the secant and the tangent iperplane flap to the domain along the actual stress vector direction.

A final consideration on the limit of the validity of the proposed analysis, and more in general to the applicability of limit design that does not control the ductility requirement for the method to hold, concerns the way one can estimate the dissipated energy during the process of loading since the collapse. Whether the structure ductility is limited and in any part the limit of the dissipation is reached, the structure collapses with fragile behavior for load less than the prevision of the analysis. Consequently, the limit analysis must be completed with the estimate of dissipated energy locally and globally in the structure. Some theoretical upper bound calculation for the dissipated energy is present in the literature [2]. Starting from these evaluations, it is possible to implement numerical algorithms to assess the upper bound of the actually required dissipation and compare it to the ductility performances of the structure.

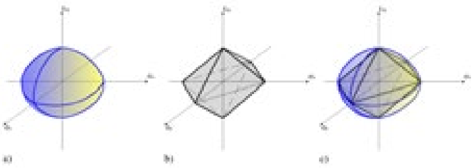

Figure 1 Non linear (a) and linear (b) domain and their superimposition (c)

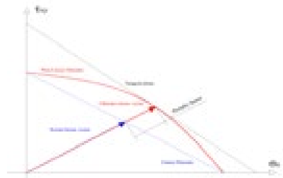

Figure 2 Penalty factor on actual stress

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