STAMS 2022 Colloquium

SECOND COLLOQUIUM OF THE SPANISH THEORETICAL AND APPLIED MECHANICS SOCIETY

PROGRAMME

March 28 - 29, 2022

Seville, Spain

Preface

The colloquium aims to bring together leading researchers in the areas of solid and fluid mechanics to engage in in-depth and far-ranging scientific discussion of topics of current and future interest for the Theoretical and Applied Mechanics (T&AM) community in Spain. It also aims to foster and cement connectivity and networking between the Spanish and the international T&AM communities. This edition of the colloquium will cover a broad range of emerging topics including data science, artificial intelligence, medical engineering, energy, space structures and advanced materials, from mathematical and physical foundations to application. The colloquium will culminate in a discussion forum open to the free exchange of ideas and outlooks from all those in attendance. Seville is a charming venue steeped in unique history, culture and gastronomy which is sure to delight attendees, set an enchanting backdrop for the symposium and stimulate extemporaneous interactions.

Supporting Organizations

Sociedad Española de Mecánica Teórica y Aplicada (SEMTA)

Universidad de Sevilla

VI PLAN PROPIO DE INVESTIGACIÓN Y TRANSFERENCIA DE LA UNIVERSIDAD DE SEVILLA

Escuela Técnica Superior de INGENIERÍA DE SEVILLA

Colloquium Organization

Chair

Pilar Ariza Moreno
University of Sevilla

Scientific Committee

Pilar Ariza Moreno
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Michael Ortiz

Local Organizing Committee

Pilar Ariza
Héctor Cifuentes
Antonio Martínez de la Concha
Javier Ramos
José David Ríos
Guillermo Hidalgo

Colloquium Information

Conference Venue

The Second Colloquium of the Spanish Theoretical and Applied Mechanics Society is held at the Escuela Técnica Superior de Ingeniería de Sevilla, Camino de los Descubrimientos, s/n. 41092 Sevilla (Spain).

All plenary talks are held in the **Salón de Grados** on the second floor, while lunches, coffee breaks and poster sessions take place on the ground floor, as indicated in the sitemaps (see next pages), next to Elevator 2.

Registration

On Monday, from 11:00 AM to 12:00 AM. you may find the registration/information desk in the hall of **Sala Larrañeta** on the second floor. Upon your registration, you will receive an identification badge. Please wear your identification badge visible throughout the colloquium since it serves as admission ticket for events of the colloquium.

Poster Sessions

Poster Sessions are held Monday and Tuesday. Each author is responsible for mounting his/her material prior to the opening of the poster session on Monday and for removing it after lunch on Tuesday.

Authors are required to display their poster on their assigned board. Please see the number that has been assigned to each one of the **poster abstracts** in this book.

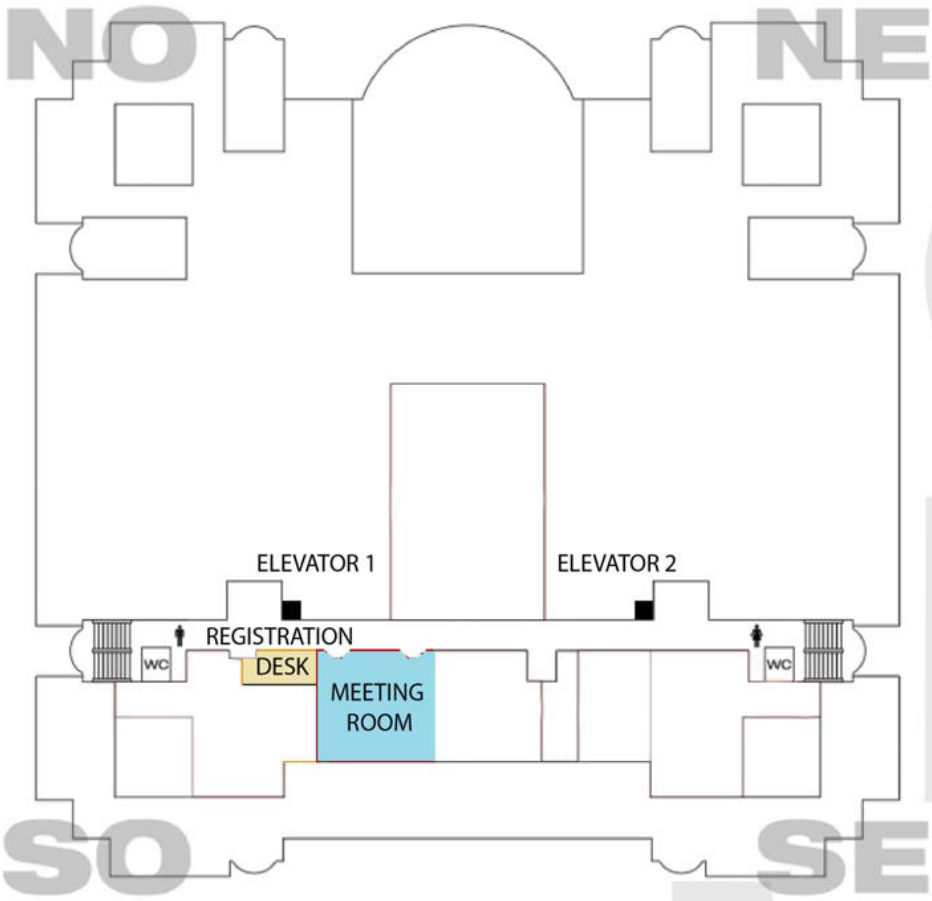
Presenting authors are asked to stand by their posters during the Poster Session time period, during which the viewers can discuss their work with them on an individual or small-group basis.

Internet Access

The University of Seville is part of the international Eduroam (educational roaming) initiative. This scheme provides and facilitates inter-institutional roaming wireless network access when one is away at another institution that also uses Eduroam.

Sitemap _ Engineering School

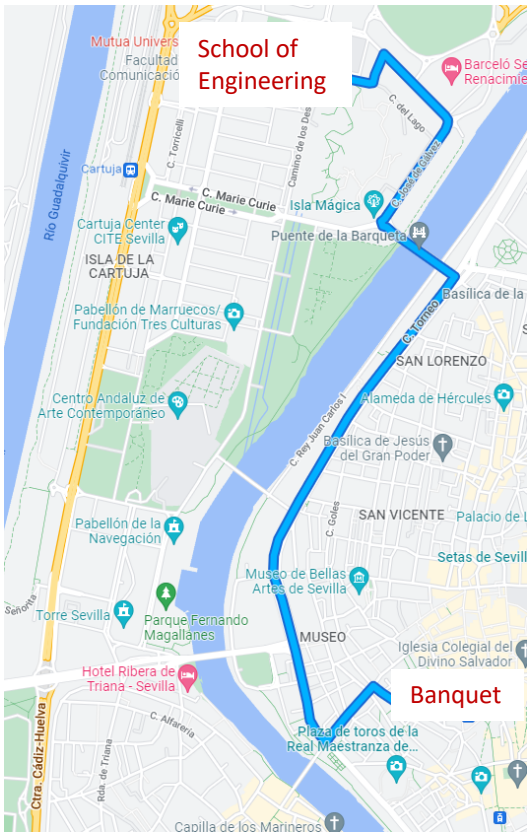
SECOND FLOOR

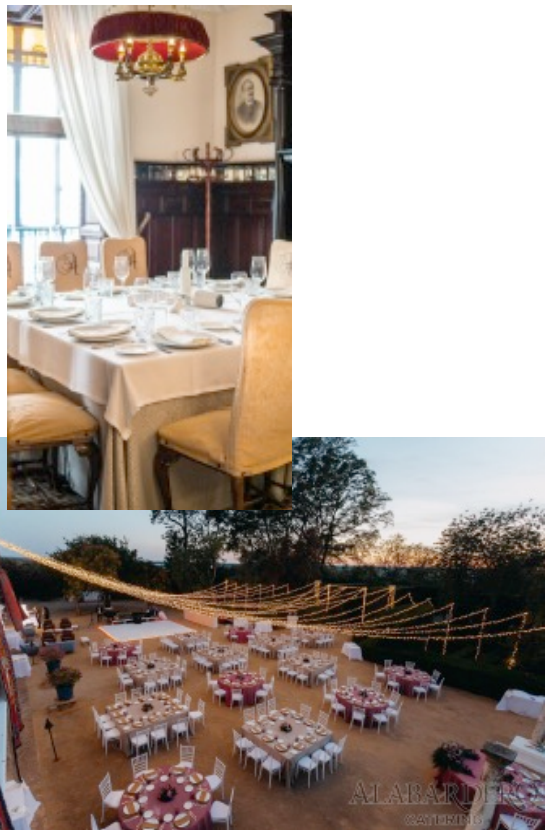


escuela técnica superior de
INGENIERÍA

Social Program

The Colloquium Banquet will take place on Monday March 28, 20:30, in the restaurant Taberna del Alabardero, a beautiful 19th century Palace House, located in Calle Zaragoza, 20, 41001-Sevilla.





Colloquium Programme

Monday, March 28

11:00	Registration
12:00	Welcome session
12:15	***A reflection on the evolution of the interaction between Mechanics and Life Sciences*** , **Manuel Doblaré**, University of Zaragoza
13:00	Lunch
14:30	**Posters session**
15:45	***Aggregation-Diffusion and Kinetic PDEs for collective behavior: applications in the sciences*** , **Jose Antonio Carrillo**, University of Oxford
16:30	Coffee
17:00	***Architected Materials: Modeling, design and performance*** , **Dennis Kochmann**, ETH Zurich

18:00	General Assembly SEMTA

20:30	**Banquet STAMS2022**

Tuesday, March 29

9:30	***Energy: Lessons learnt?*** , **Norberto Fueyo,** University of Zaragoza
10:15	***New sources of energy for a better world*** , **Jose Dominguez,** University of Sevilla
11:00	Coffee & **Posters session**
12:15	***Coilable Shell Structures*** , **Sergio Pellegrino**, California Institute of Technology (Caltech)
13:00	Lunch
15:00	***Informed and augmented learning for empowering the engineering of critical urban systems*** , **Francisco Chinesta**, ENSAM ParisTech
15:45	**Emerging Trends in Mechanics** Round table conducted by *Ignacio Romero*
16:45	Coffee

Monday, March 28, 12:15

A REFLECTION ON THE EVOLUTION OF THE INTERACTION BETWEEN MECHANICS AND LIFE SCIENCES

MANUEL DOBLARÉ
Escuela de Ingeniería y Arquitectura, University of Zaragoza

Mechanics, as the science of movement, has been applied to the study of the movement of living beings since the appearance of reasoning in humankind. Soon, early "scientists" analysed the movement of animals during hunting or flying and discovered the need of stabilizing bone fractures for proper healing. The relation between Biomedicine and Mechanics was improved along centuries, exploring the movement of internal organs like the heart and muscles, blood circulation, the hearing mechanism, and many other mechanical phenomena of importance for a healthy life. They were, however, the last decades of the XXth century when the combination of new technologies like in vivo imaging, computational approaches or new microscopic techniques gave rise to a sudden increase of our knowledge on the structural behaviour of living tissues and organs, both in healthy and in pathological conditions. A paramount new discovery, phenomenologically guessed at the end of XIXth century, has been the role of mechanical strains on cell behaviour. This discovery opened a new field of study, known today as Mechanobiology, whose objective is not only to understand the effect of mechanical deformation onto keeping the equilibrium of cells and living tissues (homeostasis), but also in provoking or preventing diseases, opening the door to new treatments and a better understanding of organ development during the foetal stage. This knowledge has also permitted to better control the development of artificial tissued composed of biological units (tissue engineering) and is also helping to better understanding the interaction between cells and their microenvironment, for example, during tumour growth and progression. From all above, it is not strange that Mechanics has been incorporated to the core of essential disciplines not only in Biomedicine, as has always been, but also in modern Biology. Long traditional biomechanical engineers are now complemented by biological engineers, with a strong knowledge of Physics (e.g., Mechanics) and Biology, who are becoming an unavoidable member of any R&D group in the Medicine of the future.

Monday, March 28, 15:45

AGGREGATION-DIFFUSION AND KINETIC PDES FOR COLLECTIVE BEHAVIOR: APPLICATIONS IN THE SCIENCES

JOSE A. CARRILLO
Mathematical Institute, University of Oxford

I will present a survey of micro, meso and macroscopic models where repulsion and attraction effects are included through pairwise potentials. I will discuss their interesting mathematical features and applications in mathematical biology and engineering. Qualitative properties of local minimizers of the interaction energies are crucial in order to understand these complex behaviors. I will showcase the breadth of possible applications with three different phenomena in applications: segregation, phase transitions and consensus.

Monday, March 28, 17:00

ARCHITECTED MATERIALS: MODELING, DESIGN AND PERFORMANCE

DENNIS KOCHMANN
Institute for Mechanical Systems, ETH Zurich

Architected materials (often referred to as mechanical metamaterials) have gained tremendous attention over the past decade. Across engineering disciplines, the modeling, design, fabrication, and characterization of such cellular solids, which derive their properties from small-scale structural architecture, has resulted in a myriad of materials systems with as-designed, optimized mechanical properties – from high stiffness- and strength-to-weight ratios to energy absorption and wave guidance all the way to active and smart reconfigurability. The dream has been to revolutionize our approach to selecting materials for engineering applications: away from property look-up tables for available materials, towards the on-demand creation of novel architected materials with controllable or extreme properties and functionality. Focusing on mechanical properties, we will discuss to what extent this has been achieved and what challenges exist. We will highlight recent examples of modeling and reverse-engineering architected materials with tunable mechanical properties, and we present experimental examples of their realization.

Tuesday, March 29, 9:30

ENERGY: LESSONS LEARNT?

NORBERTO FUEYO, ANTONIO GÓMEZ
Escuela de Ingeniería y Arquitectura, University of Zaragoza

The energy sector is Spain is often the subject of news items, and not often for a good reason. Following privatization in the mid 90's, the sector has undergone a rapid transformation that has, however, been riddled with episodes that are the telltale sign of lack of quantitative planning and sound policymaking.

The nuclear 'moratorium' of the mid 80's, the so-called 'tariff deficit' snowballing from the mid 90's, or the ill-conceived rush towards sustainability in the late 2000's have all had substantial financial impacts in families, companies and country.

As a Society, we often focus our debate in the "cost of doing": the cost of physical infrastructure, or of a policy. In this presentation we take a quantitative look at the recent past of the energy sector in Spain to assess the "cost of **not** doing" energy planning. We conclude that, while quantified energy planning is not only hard to do but also imperfect in its forecasts, it is an essential component of the policymaking toolkit.

We finally briefly reflect on the role that all the actors (politicians, media, Non-Governmental Organisations and citizens) play in this state of affairs.

Tuesday, March 29, 10:15

NEW SOURCES OF ENERGY FOR A BETTER WORLD

JOSÉ DOMÍNGUEZ
Escuela Técnica Superior de Ingeniería, University of Sevilla

During the last three decades the world has become aware of climate change and its consequences. There is a scientific consensus on the fact that greenhouse gases (GHG) produced by human activity are concentrating in the atmosphere and changing the climate with increasingly catastrophic consequences. Because of that, the United Nations Organization established the IPCC group in 1988 and the Climate Conferences of the Parties in 1995. The last one (COP26) was hold in Glasgow (Scotland) a few months ago.

Almost three quarters of the world GHG emissions come from fossil fuel energies. To change that, renewable sources of energy like wind and solar PV, have been developed to an industrial level and today their use is growing very rapidly. Wind and sun are now sources of the cheapest electricity in many parts of the world. Electric vehicles set new records of sales and performance every year. All these facts make us think that the transition to new energy sources in the world is not only essential but possible.

Nevertheless, the clean energy transition still has a long way to go and there are bad news regarding GHG emissions reduction every year. On one hand, powerful countries and companies try to control the pace of transition, the way it occurs and to maintain the status quo as much as possible. On the other hand, rapidly increasing investment and new technical developments on clean hydrogen, batteries, and transport, allow us to think we are in the good way.

The EU has set a Net Zero Emissions goal by 2050 in accordance with the International Energy Agency recommendations. Other countries have similar goals.

Looking to the problem from a completely different point of view, the recent Ukraine war has contributed to make the world, and in particular Europe, fully aware of the need and urgency of changing the energy sources as soon as possible.

Tuesday, March 29, 12:15

COILABLE SHELL STRUCTURES

SERGIO PELLEGRINO
Joyce and Kent Kresa Professor of Aerospace and Civil Engineering
Jet Propulsion Laboratory Senior Research Scientist
Co-Director, Space-Based Solar Power Project
California Institute of Technology

A wide range of behaviors of thin shells has been harnessed in new ultralight structural architectures that can be tightly packaged and are able to elastically self-deploy. Large origami-inspired polygonal structures formed from concentrically arranged, singly-curved shells are flattened and tightly coiled in a nested arrangement on a central mechanism. Their stiffness in the deployed configuration results from the transverse curvature of the shells and hence the depth of the cross-section is chosen to meet specific loading conditions. Targeting novel large solar arrays and space solar power satellites, modular structures based on this approach are built from composite laminates of extreme thinness. Areal densities comparable to thin membrane structures can be achieved, but with the advantages of modular construction, predictable deployment and a deterministic load path. The practical realization of these novel structures has presented new challenges arising from the localized buckling and stable post-buckling of thin, open-section cylindrical shells, as well as the formation of localized buckles during coiling of shells with non-uniform thickness. Understanding and correctly modeling these instabilities is key to the robust design of these novel structures.

Tuesday, March 29, 15:00

INFORMED AND AUGMENTED LEARNING FOR EMPOWERING THE ENGINEERING OF CRITICAL URBAN SYSTEMS

FRANCISCO CHINESTA
ENSAM ParisTech

Urban systems are too large, complex and uncertain to be approached by using physics-based models. At the same time fully data-driven models encounter several limitations, because of the need of large amount of data, the difficulty of explaining decisions and the unfeasibility of accessing to critical events, ... A hybrid approach combining knowledge and data, conciliates accuracy and rapidity in the diagnosis, prognosis and decision making, within a human-centric framework. Such hybrid approach can consist of informing and/or augmenting the learning. After introducing the hybrid paradigm, it will be applied in two applicative domains: drone trajectory planning and remote sensing of industrial and civil infrastructures.

POSTER 1

NON-STANDARD CONTINUALIZATION OF A TIMOSHENKO BEAM LATTICE. IMPROVED PREDICTION OF ITS DYNAMIC BEHAVIOUR THROUGH LOW-ORDER CONTINUUM MODELS

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In this work, a Timoshenko beam lattice is proposed. This system consists of a chain formed by equispaced particles with mass **m,** and straight segments of length ***d***, which is considered as the characteristic length [1]. This lattice accounts for both bending and shear deformation by means of linear rotational and transverse springs, with stiffness ***C*** and ***S***, respectively (Figure 1). Different standard and non-standard continualization techniques have been applied to the lattice system, with the aim of obtaining non-classical continuous models capable of capturing, with a lower computational cost, the size effects present in the wave dispersive behaviour of the discrete system. Continuum models with low-order governing equation are pursued, since they do not need extra boundary conditions, whose physical meaning is unclear, to be solved when finite (bounded) solids are treated. In addition, the suitability of taking the coupled discrete governing equations as a starting point for deriving new continuum models has been highlighted for the first time. The accuracy of the non-classical continuum models obtained in capturing the dynamic behaviour of the discrete one (taken as a reference) is assessed by studying their dispersion relations and the natural frequencies of two different beam configurations, *simply-supported* and *clamped-free* beams, thus treating the three common boundary conditions in a Timoshenko beam. These boundary conditions have been implemented in the discrete model through a novel edge treatment, employed here for the first time in this kind of lattices, thus making it possible to solve the *clamped-free* edges configuration. On the other hand, an exhaustive analysis of the transition frequency that initiates the shear propagation spectrum (previously studied only for the Classic Timoshenko continuum beam model [2]) has been carried out, examining its influence on both the discrete and the new non-standard continuum models. Furthermore, the occurrence of physical inconsistencies in some continuum models is discussed. Finally, it is found that some of the new continuum models proposed show a satisfactory performance, even for short wavelength waves.

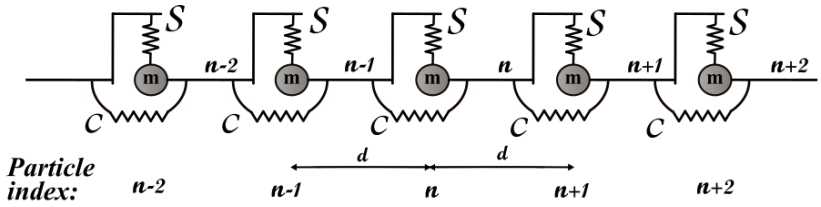

Figure 1: Timoshenko beam lattice.

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POSTER 2

DEVELOPMENT OF ENERGY HARVESTERS FOR RAILWAY BRIDGES USING ADDITIVE MANUFACTURING

J.C. CÁMARA-MOLINA [1], P. GALVÍN [1,2], E. MOLINER [3], M.D. MARTÍNEZ-RODRIGO [3] & A. ROMERO [1]

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In this work, the authors investigate the energy harvesting in railway bridges and analyse the performance under different operational conditions. The objectives of this work are within the challenge of achieving sustainable, intelligent, connected, and integrated transport. An analytical model that achieves the optimal design of a harvester for each bridge is proposed for the estimation of the energy harvested for train-induced bridge vibration. This research presents the design and development of an energy harvester device that allows to obtain electric energy from train-induced vibrations on railway bridges. This device can be used to power a monitoring system or as a sensor in railway bridges. The typology of the energy harvester studied in this work is a cantilever bimorph beam consisting of two piezoelectric patches on a substructure with a seismic mass to amplify the response. For the fabrication of the substructure, additive manufacturing is considered, and it is made by 3D printing of PLA. The design has been selected to tune the natural frequency to the fundamental mode of the bridge, finding the optimum operating point for maximum power production. The optimization problem is constrained by the integrity of the substructure, and it is solved using a genetic algorithm. Finally, the feasibility of energy harvesting is evaluated from the experimental data measured by the authors in a railway bridge from the Madrid-Sevilla High-Speed line. The results obtained allow for quantifying the energy harvested for two different train passages.

POSTER 3

QUADRATURE RULE TO VALIDATE SINGULAR INTEGRALS IN THE SOLUTION OF COMMON ENGINEERING PROBLEMS

ROCIO VELÁZQUEZ MATA
Universidad de Sevilla
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This work describes a general method to compute the boundary integral equation for common engineering problems. The proposed procedure consists of a new quadrature rule to evaluate singular and weakly-singular integrals. The methodology is based on the computation of the quadrature weights by solving an undetermined system of equations in the minimum norm sense. The Bézier–Bernstein form of a polynomial is also implemented as an approximation basis to represent both geometry and field variables. Therefore, exact boundary geometry is considered, and arbitrary high-order elements are allowed. This procedure can be used for any element node distribution and shape function. The validity of the method is demonstrated by solving a two-and-a-half-dimensional elastodynamic benchmark problem.

POSTER 4

DETERMINATION OF AORTIC DISSECTION PROPERTIES WITH COHESIVE ZONE MODELS

ITZIAR RÍOS-RUIZ [1], MIGUEL ÁNGEL MARTÍNEZ [1,2] & ESTEFANÍA PEÑA [1,2]

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Aortic dissection is a severe vascular disease with a high mortality rate [1]. Computational models can help understand the initiation and development of this pathology, mostly when supported with experimental data. A proper characterisation of the dissection properties of the vessels is required to make these models accurate and representative, but these properties are still under study. Nowadays, experimental delamination tests such as the T-peel test and the 180˚ peel test have been developed in arterial tissue in order to determine these properties [1, 2]. Only with the experimental data obtained from these tests, however, the dissection behaviour of the vessel is not fully characterised.

Therefore, we are developing computational models that reproduce both peel tests in order to determine the dissection properties of the aorta. We calibrate these models via inverse analysis with the experimental data obtained from both peeling tests performed in out laboratory.

The experimental tests were performed in porcine aortas. Enough samples were obtained from each vessel to perform a material characterisation via tension tests, as well as both delamination tests. These are performed considering the anisotropy of the vessel, i.e., the circumferential and longitudinal directions, the different interfaces that can be delaminated–the intima-media, the media-adventitia and the media within itself–and the location in the aorta, accounting for region-specific properties.

The experimental results are then reproduced computationally. Using cohesive zone modelling and a triangular traction-separation law [3], both tests are simulated following different methodologies. Models of each interface, direction and region of the aorta are developed. Force-separation curves are obtained and compared with the experimental data in terms of mean force and peak force. A proper fitting is established when the fitting error is below 10%.

Proper characterisation of biological tissue is essential in order to develop solid computational models to study the progression and possible treatments of different pathologies. With this methodology, we intend to contribute to the development of reliable numerical tools to simulate aortic dissection.

References

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POSTER 5

THERMAL AND MECHANICAL STRESSES IN SOLAR CENTRAL RECEIVERS

A. MONTOYA[1], M.R. RODRÍGUEZ-SÁNCHEZ[2], J. LÓPEZ-PUENTE[1] & D. SANTANA[2]

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Nowadays, energy production with renewable sources is fundamental. Wind and photovoltaic energy are the technologies with higher future projection due to the low cost of the energy produced. However, these technologies are intermittent and cannot be adapted to the energy demand of the society. To achieve standing alone of the renewable energy production flexible energy source is required. Then, concentrated solar power with thermal storage emerges as an important back up source of renewable energy. Within this category solar power tower, using molten salt as heat transfer fluid, is particularly relevant.

Failure in the tubes of the solar receiver is a problem that should be studied. This failure is caused by the combined action of the high temperature, stresses and corrosion. Commonly, the calculation of the stresses in the receiver tubes is carried out in the crossed sections, considering the radial and the circumferential variation of the temperature. However, the temperature gradient along the tube length has been ignored. In this study a new model for the stress calculation in the receiver tubes has been developed. This model includes the temperature gradient in circumferential, radial, and longitudinal direction, considering the movement restrictions. The results show that the mechanical boundary conditions have a large effect in the stresses of the tube, being 3 times higher than the stress when no movement restrictions have been imposed. Moreover, the stress profile is highly dependent on the temperature gradient and hence on the incident solar flux on the receiver. Homogeneous solar fluxes are then more suitable than lower levels of solar fluxes with important gradients.

This work has been performed in the framework of the projects RTI2018-096664-B-C21 and RTI2018-096664-B-C22, financed by FEDER/Ministerio de Ciencia e Innovación – Agencia Estatal de Investigación.

References

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POSTER 6

A COUPLED DIFFUSIVE-MECHANICAL MODEL FOR THE ANALYSIS OF MATERIAL DEGRADATION IN GRAPHITE-COATED ACTIVE PARTICLES OF LITHIUM ION BATTERIES

JORGE MARIN-MONTIN [1] MAURICIO ZURITA-GOTOR [1] & FRANCISCO MONTERO-CHACÓN[1]

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Current trends in portable electronic devices, electric vehicles, or renewable energy systems demand the development of lithium-ion batteries (LIBs) with improved capacity and performance. One critical component in LIBs is the negative electrode (i.e., anode), whose behavior has an important impact on the performance of the cell since it hosts the active materials in which Li intercalation (and deintercalation) takes place. One of the current strategies to prevent electrodes from the material degradation and thus enhance their electrochemical performance is the use of coatings on the active particles (APs) [1]. Coatings contribute to the stability of the electrolyte-electrode interphase and absorb the important volume changes in the active material during the battery cycling, improving the electronic conductivity through the electrode.

In this work, we present a 2D coupled diffusive-mechanical model for the analysis of coated graphite active particles. Namely, we analyze the effect of such coatings on the transport properties of LIB APs. The APs are made of graphite, a widely used electrode active material due to its low price and good cycling stability [2], while we focus on carbon-based coatings, also one of the most investigated and applied coating materials [3]. In our approach, we consider the coupled effect of Li-ion transport and mechanical stress due to volume expansions. Material damage is accounted for to foresee the conditions under which cracking occurs. Two-phase circular-shaped APs, explicitly including a thin carbon coating layer on the surface, were generated. Moreover, a single-particle model is assumed, not considering the mechanical interaction between other surrounding APs. For the numerical implementation, we adopt a lattice model approach [4]. The material is discretized as a network of nanoscopic pipe elements through which the flux of Li-ions occurs, while beam elements are considered for the mechanical problem. Material heterogeneity is included by two means: firstly, by including a randomness factor in the mesh generation, and secondly, by introducing a Weibull's distribution function on the materials properties, so as to reflect the imperfections in actual brittle material. Our model is also used to test different coating designs, including a novel Si-based nanocomposite. To analyze the interface behavior of the proposed designs, we developed a local model of the substrate-coating system.

Finally, we are able to describe the cracking evolution within APs with and without coatings. We prove that the nucleation of cracks appears at the center of the particles during lithiation, while radial outer cracks appear during delithiation. We also quantify the effect of the charging and discharging rates on the crack patterns. This information can be used to estimate the capacity fade of the electrodes due to volume changes and evaluate the suitability of the coating design.

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POSTER 7

FINITE ELEMENT SIMULATION OF CHEMO-MECHANICAL DEGRADATION OF ACTIVE PARTICLES IN DUAL GRAPHITE BATTERIES.

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The development of renewable energy (e.g., solar, wind, hydroelectric, etc.) technologies is called to play an important role in circumventing the supply dependency on fossil fuels. However, these technologies still present limitations due to their intermittent operation and dependency on external factors (e.g., sun hours, wind, water reservoirs, etc.). Developing energy storage systems is crucial for the deployment of renewable energies. In this sense, electrochemical energy storage systems may be a feasible solution for large and stationary applications. Within this group, Dual Graphite Batteries (DGB) may provide operative (economic and lifetime) and sustainability (due to a consequent reduction of metallic compounds in the electrode) advantages versus traditional Lithium-Ion batteries [1].

The working mechanism of DGB consists of the continuous insertion and extraction of anions and cations into the graphite electrodes (both positive and negative). This mass diffusion phenomenon causes the separation of graphene layers and volume changes in the material. In the case of PF_6^- intercalation, volume expansions in the range of 114% to 136% have been reported [2][3]. This cyclic massive expansion and contraction of the material may cause micro-cracks nucleation and propagation, worsening the battery performance

In our work, we propose a thermodynamically consistent model to analyze the mechanical degradation of active particles in DGB. Our model considers chemo-mechanical coupling at finite strains and characterizes the damage with a phase-field model for fracture. For the mechanical part, we consider a Saint-Venant Kirchhoff material model. We used Fick's second law to describe the mass-diffusion problem where the flux term derives from a chemical potential, which accounts for stress-diffusion coupling and limits the concentration. Additionally, the damage parameter affects the degradation of the elastic modulus and the diffusivity. Both galvanostatic and electro-chemical (Butler-Volmer) boundary conditions can be defined.

We implement the mathematical model in the open-source finite element software FEniCS. We analyze an actual 2D active particle obtained from scanning electron microscopy (SEM) images. This actual geometry is exported to GMSH and meshed. Our work reveals the influence of PF_6^- in the concentration and stress profiles and the temporal evolution of damage with the first charge/discharge cycle. Moreover, we report for the first time the effect of anion intercalation in DGB electrodes.

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POSTER 8

SEMI-ANALYTIC COMPUTATIONAL CODE FOR STRESS SINGULARITY PROBLEMS IN MULTI-MATERIAL ANISOTROPIC CORNERS

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A semi-analytic computational code in Matlab, based on the formulation presented in [1], has been developed to compute the singularity exponents and the singular stress and displacement fields in anisotropic multi-material corners under generalized plane strain. The corner is defined by the number and type of materials (isotropic, transversaly isotropic or orthotropic with any orientation), the elasticity coefficients and the polar angles of faces of each single-material wedge, and the boundary and interface conditions of the corner. The considered homogeneous boundary conditions are stress free, clamped, some restricted or allowed displacement direction, either in the face plane or in an inclined plane, and frictional sliding. The interface conditions between two consecutive materials already presented in the code are perfectly bonded, frictionless sliding and frictional sliding.

The code is successfully verified by comparing the computed results with the results obtained by applying many closed-form expressions of singularity exponents or eigenequations available in the literature for relevant special cases [2,3].

In this work we present what is behind the code, what type of problems it can solve and some of the practical cases solved with it.

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POSTER 9

A NEW DISCRETE MODEL WITH ANGLE SPRING AND ITS APPLICATION IN FRACTURE SIMULATION OF COMPOSITE MATERIALS

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In this research, we developed a new two-dimensional triangular lattice model with axial and angle springs to simulate fracture problems in unidirectional composite materials. The proposed models were based on the equivalence of strain energy between the discrete and the continuum systems. Lattice particles interact only with the nearest neighbors. Interactions were defined by axial and angle springs that depended on the stiffness matrix. Other authors [1, 2] presented discrete models for composite materials, but these models are valid to some composite materials, but not all. The proposed model in this work solves this limitation. Furthermore, the model takes into consideration the progressive damage evolution in composite materials by effectively integrating a softening constitutive law [3].

Different numerical examples are studied to show the capability of this method in modelling elastic constants, quasi-static and dynamic fracture problems in unidirectional composite materials. Results are presented in terms of elastic constants, crack pattern, and failure stress. The obtained results are compared with numerical and experimental data reported by other researchers.

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POSTER 10

DAMAGE EVOLUTION ANALYSIS IN COMPOSITE SANDWICH STRUCTURES

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In the design of structural components, the use of composite structures is now widespread due to their excellent specific properties and offering weight advantages. Specifically, in the wind energy sector, the largest parts of the wind turbine blades are usually manufactured with composite sandwich structures, which face-sheets are made of composite laminates, as they present high stiffness-to-weight ratios. As structural components, wind turbine blades are susceptible to be damaged during their service life. In this context, damage can be generated by external elements such as bird strike, debris, or hail rain. All these events can be represented as high-velocity impacts; however, these kinds of loads are not usually given by single impacts but by multiple impacts, that can be applied simultaneously or sequentially on the structure. In a multiple impact scenario, the stress waves of the different projectiles interact with each other or with adjacent damaged areas, causing the premature failure of the wind turbine blade.

It is reported that in high-velocity impacts, the impact energy of the projectile is dissipated through several energy absorption mechanisms [1], such as: elastic deformation of the laminate, frictional energy absorbed during penetration, inertia of the laminate or back-face deformation, damage generation, etc. Additionally, laminates subjected to high-velocity impact present the typical composite damage mechanisms including delamination, matrix cracking, and fibre failure [2]. In composite sandwich structures these typical failure mechanisms given for the composite face-sheets are combined with some specific failure mechanisms [3], such as the debonding between the face-sheet and core, core crushing, etc. Therefore, the objective of this work is to use a 3D finite-element model of composites sandwich structures to understand the effect of multiple impacts in composite sandwich structures. The model is implemented in Abaqus commercial code, and it is validated with results taken from the literature in terms of ballistic limit and residual velocity. Eventually, the model used to analyse the type of damage generated by high-velocity multi-impacts and to study the effect of the distance between projectiles.

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POSTER 11

ANALYSIS OF CRACK PROPAGATION IN LAYERED STRUCTURES BASED ON THIN LAYER OVER RUBBER-LIKE SUSBTRATE SYSTEMS USING A COMBINED PHASE-FIELD AND COHESIVE ZONE MODEL APPROACH OF FRACTURE

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The development of next generation high-tech products requires the optimization of structural components. One of the most exploited structural arrangements in different engineering applications such as highly stretchable electronics devices, renewable energy production systems among many others encompass layered structures and in particular thin-layer over highly deformable substrates. This study presents the analysis of the failure mechanisms that may occur in thin layer - flexible substrate systems: crack propagation through the layers, delamination at interfaces and Mixed-Mode mechanisms. The phase-field (PF) approach, formulated for hyperelastic materials, is exploited through a series of tests to prove its capabilities in assessing the mechanical performance and the crack propagation mechanism of these composite structures. While the PF approach already captures the competition between crack propagation and delamination at the interface for bilayer composites having properties mismatch, as in the case of metallic or ceramic layers on rubber-like substrates, the framework has been further enriched with a Cohesive Zone Model (CZM) approach to model imperfect interfaces. The benefit of the coupled method can be noticed especially for Mixed-Mode failure patterns, where this combination proved to be successful to capture the complexity of them.

POSTER 12

DUCTILE FRACTURE MECHANICS EXPLAINS SINGLE-ASPERITY WEAR

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Wear is a process that poses scathing environmental challenges and whose physical origins remain partially unexplained. Traditional models of wear posit [1] a linear relation between the tangential work necessary to attain relative sliding between two surfaces in contact and the volume of debris created during the process. This phenomenological law encapsulates macroscopic observations, but its validity at the microscopic level (e.g., at the level of individual asperities) remained an open question until recently. A novel numerical scheme [2], based on molecular dynamics on a basis of modified Morse potentials, enabled to simulate, for the very first time, debris formation arising from microscopic contacting asperities under shear and normal pressure. First and foremost, these simulations revealed the existence of a minimum junction size, a threshold below which plastic deformation precludes particle detachment. With this new understanding at hand, a comprehensive suite of simulations, over a range of materials and geometrical conditions, was later carried out [3]. Its outcome revealed a linear relation between tangential work and wear volume also when it comes to debris formation for isolated contacting asperities.

In this work we analyze the crack propagation process that leads ultimately to particle detachment. A new picture of the wear process emerges from this study, the relative size of the junction between asperities with respect to the characteristic length of the fracture process zone (FPZ) ahead of the crack tip being the discriminating factor among different scenarios. Our work explains the ostensible linear relation between debris volume and tangential work and generalizes it.

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POSTER 13

EFFECT OF MECHANICS IN A MECHANOBIOLOGICAL MODEL OF ATHEROSCLEROSIS

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Atherosclerosis is the process in which atheroma plaques are built up in the walls of the arteries causing narrowing, hardening of the arteries and loss of elasticity. The location of atherosclerosis is associated with flow separation and turbulence. Therefore, many studies have identified haemodynamic shear stresses as an important determinant of endothelial function and phenotype in atherosclerosis disease. Previous growth models consider the wall shear stress as the only mechanical input into convection–diffusion–reaction equations for modelling the mass balance on the artery [1]. However, the wall expansion due to blood pressure produces structural deformation of the arterial wall. As a result of the applied compression, there is a change of directional transport properties. In addition, arterial wall deformation due to growth resulting regional changes in haemodynamics at the plaque–luminal interfaces. The presented work based on the previous studies goes further and includes a fluid-structure interaction between blood flow and luminal wall and the influence of compression on the diffusion coefficient.

A mathematical model of atheroma plaque initiation and early development for coronary arteries is considered. This model uses the Navier–Stokes equations and Darcy's law for fluid dynamics, convection– diffusion–reaction equations for modelling the mass balance in the lumen and intima, and the Kedem–Katchalsky equations for the interfacial coupling at membranes, i.e. endothelium. The volume flux and the solute flux across the interface between the fluid and the porous domains are governed by a three-pore model. The main species and substances which play a role in early atherosclerosis development have been considered in the model, i.e. LDL, oxidized LDL, monocytes, macrophages, foam cells, smooth muscle cells, cytokines and collagen [1]. The material properties of the solid part were based on the experimental data [2] for the intima and media layers and the material constants were fitted by Yeoh strain energy function. The blood flow was modelled as laminar, incompressible and Newtonian. It was postulated that if the arterial wall is compressed due to vessel expansion then there must exist changes in the transport properties in radial and longitudinal directions. To consider that, the effective diffusivity coefficient D is a function of the porosity of the wall that depends of the deformation leading to an anisotropic tensor diffusion.

Our results compare atheroma plaques development for the different models analyzed, considering the porosity of the arterial wall, its tortuosity and both or none of them.

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POSTER 14

IN SILICO FORMATION OF VASCULAR NETWORKS WITHIN THE EXTRACELLULAR MATRIX

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Capillary networks perform essential functions to keep organisms alive at the cellular level. As far as their formation is concerned, a distinction can be made between vasculogenesis, primary origin of blood vessels which is produced, for example, during embryonic growth; and angiogenesis if they are created from other vessels, as during tumor growth, among others. The present study develops a discrete 3D mechanical agent-based model [1] to simulate the interactions between vascular networks and extracellular matrix (ECM). In the model, three types of cells are distinguished: Tips, located at the front, Vessels in the interior and the ECM domain, which has been modeled as a spherical distribution of points. On the other hand, the following set of forces are considered: the random force, for the heterogeneity of the medium, the chemotactic force, to calculate the gradient of the vascular endothelial growth factor, the persistent directional force, similarly to an inertial force, the angular force, to correct the instability of the proliferation and the mechanical and viscoelastic forces. These forces consider that cells are connected in the following way: network cells through a spring and network cells with matrix through a spring and a damper in parallel. The evolution of the network is analyzed in silico under different conditions of the matrix: (i) different and uniform stiffness values, (ii) different stiffness gradients and (iii) different values of viscoelasticity. In conclusion, proliferation increases as the stiffness value does. However, the opposite occurs with viscoelasticity. As the value of the viscoelastic coefficient increases, cell concentration decreases. Furthermore, when the stiffness gradient is applied, it has been observed that the network migrates towards stiffer areas, phenomenon known as durotaxis. These results are supported, qualitatively, by other experimental results found in the literature [2-4].

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POSTER 15

ASSESSMENT OF THE IMPORTANCE OF NONLINEARITY IN TRACTION FORCE MICROSCOPY

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Tractions acting on the surface of cells resulting from the mechanical interaction with their surrounding environment (ECM) pose great interest in the study of the development of certain pathologies. Traction Force Microscopy (TFM) is a hybrid experimental-computational technique that allows the computation of tractions, via tracking of the displacement of fiducial markers (in the form of fluorescent beads) distributed inside collagen hydrogels that mimic the mechanical nature of real ECMs. There are two fundamental approaches to TFM: (i) the forward method, which directly computes cell tractions from the measured displacements in the laboratory by means of the modeled hydrogel's constitutive law; (ii) the inverse method, based on a regularized minimization procedure that searches for a new displacement field close to the measured one which satisfies certain requirements. We previously developed a novel inverse method that enforces force equilibrium within the hydrogel's domain, being its performance significantly superior to that of the forward method for both linear and Neo-Hookean assumed hydrogels [1,2].

The aim of the present work is to investigate the role of nonlinear effects on traction force reconstruction, assessing the viability of employing a linear approach to TFM, due to its conceptual and computational simplicity. We performed several *in silico* simulations assuming both linear and nonlinear constitutive models and assessed traction force reconstruction accuracy of such approaches by comparing the results to previously generated ground truth reference scenarios. Simulations were performed for different cell geometries with varying degrees of cell geometrical complexity, as well as for different levels in the magnitude of the cellular pulling forces prescribed for the obtention of the ground truth solutions. The considered nonlinear hydrogel's behavior consists of a hyperelastic model that takes into account the fibrillar nature of collagen hydrogels [3]. The conclusions to be drawn from the study are the following: (i) cell traction reconstruction becomes more challenging for complex (non-spherical) cell geometries that exhibit multiple large protrusions. (ii) the inverse method significantly outperforms the forward method in every case. (iii) the selected nonlinear model shows very good performance in traction reconstruction, especially compared to that of its linear counterpart.

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POSTER 16

A MATHEMATICAL FRAMEWORK TO MODEL CELL ADAPTATION WITH INTERNAL VARIABLES

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Cells are in constant relationship with their environment. They can undergo changes in their behaviour in response to environmental changes, in processes collectively known as cell adaptation. Cell adaptation plays a crucial role in many biological processes, such as the development of cancer or the resistance to therapies [1,2], so understanding the mechanisms and quantifying the effects of these phenomena is of great importance.

In this sense, mathematical models and simulation tools can complement laboratory experiments as they allow to further understand the underlying mechanisms and interactions behind the experimental observations, and to test and propose hypotheses, saving time and resources. In the last years, different biological results have been derived from mathematical approaches, in particular in cancer progression [3]. Nevertheless, there are very few models which take into account cell adaptation to the environment in a general and flexible way.

Based on the concepts of cell state, and using internal variables to model cell stress in response to changes in the environment, we propose a new modelling framework for cell evolution. It allows to model the evolution of different cell populations, chemical species or stimuli, and internal variables using transport equations. The framework allows to incorporate cells response to changes as well as the reversibility and heritage of the stress produced. It is formulated in general and therefore allows to adapt it for a wide range of different problems. In addition, working with internal variables enables a straightforward interpretation of the model and the use of mathematical tools and techniques from other areas where working with these models is widespread.

In particular, the proposed model is able to reproduce the experimental trends in the evolution and resistance to treatment of glioblastoma, the most common and lethal brain tumour.

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POSTER 17

FRACTURE BEHAVIOR OF ULTRA-HIGH-PERFORMANCE CONCRETE REINFORCED WITH CARBON MICRO-FIBERS

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The use of concrete is increasing significantly in the field of renewable energies for the construction of the supporting towers for wind turbines, in either on-shore or off-shore wind power stations [1]. The high performance of current concretes together with the possibilities that this material offers for both precasting and in-situ production allow concrete to compete with steel reducing the economic cost and the ecological footprint of the construction of the towers [2]. These tubular structures are exposed to continuous vibrations provoked by the wind [3]. These oscillations generate compression-decompression cycles in the width of the tower section. If not correctly taken into account, periodic oscillations of a larger amplitude may produce tensile forces in the decompressed side. These loading conditions require of concrete to be as resistant as possible both to fatigue and to tensile stresses [4].

In this work, it has been analyzed the performance of the addition of different types of carbon micro-fibers in the fracture behavior and tensile strength employing an ultra-high-performance concrete matrix. Experimental tests using three types of carbon micro-fibers and different contents have been performed. All the fibers have the same diameter (7 μm) and different lengths (0.1, 3 and 6 mm). The ultimate tensile strength of carbon micro-fibers is 4200 MPa which significantly reduces the probability of failure mechanism by fiber rupture. The influence of the microstructure of the matrix on the fracture properties and tensile strength was determined using X-ray computed tomography (CT) and scanning electron microscopy (SEM) techniques. Finally, a relationship between the macroscopic and microscopic behavior as well as the influence of fibers was established. The results show the use of 3 and 6 mm fibers and a content of 6 kg/m^3 yields the highest compressive strength (18%) compared to the control concrete. However, the 6 mm fibers with 20 kg/m^3 allow the highest tensile strength and fracture energy to be achieved, with (100%) and (105%) respectively, compared to the control concrete. Longer and more fibers act as barriers to crack propagation but the distribution of fibers in the matrix is less uniform and increases the dispersion of the results.

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POSTER 18

THERMOMECHANICAL PERFORMANCE OF HEXCEM BLOCKS IN BUILDING ENVELOPES WITH ENHANCED PASSIVE INSULATION PROPERTIES

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The building sector is responsible for 40% of the primary energy requirements in the European Union and 36% of greenhouse gas (GHG) emissions in Europe [1]. For this reason, technological developments towards a nearly zero-energy approach should be embraced in both residential and non-residential buildings. In this sense, new building envelope designs are required in order to reduce the energy demand while provide thermal comfort. This can be accomplished by active/passive thermal energy management systems based on renewable sources such as solar radiation.

Phase-change materials (PCMs) present interesting thermal properties since the can absorb energy in the form of latent heat to complete a reversible solid-to-liquid phase transition, providing thermal inertia to the system. Moreover, PCMs can be embedded in cement-based materials to increase their heat capacity and improve their insulation properties in building envelopes [2].

In this work we combine the use of PCMs and additive manufacturing to design a novel cement-based block, called HEXEM (hexagonal cement), with enhanced insulation properties. Concrete elements with complex shapes are fabricated using 3D printing technology, namely, by means of tailor-made molds. This enables creating custom block geometries with optimal thermal properties (conductivity, heat capacity) and reduced weight.

The thermomechanical performance of the HEXCEM blocks is assessed following a multiscale thermomechanical procedure. In the first place, cement-based material unit cells containing PCM capsules are characterized by means of finite element simulations. The non-linear effect of the phase transition is modelled following the effective specific heat approach [3]. Different PCM volume fractions are considered, namely 0, 10 and 30%. Also, different types of PCMs can be tested by defining their enthalpy of fusion and melting point. On the other hand, the thermophysical properties evaluated with the material-level model are then upscaled into the component-level model as proposed in [4]. Thermomechanical finite element simulations of different HEXCEM designs are carried out to validate their enhanced insulation properties and predict their thermal stresses. The heat transfer simulations of the blocks are compared to experimental results, confirming the enhanced passive insulation properties.

The results obtained in this work show the feasibility of HEXCEM as an interesting alternative in building envelopes with important benefits such as improved thermal insulation, with a consequent reduction in energy consumption and GHG emissions, and reduced specific weight, and could be also used in new buildings as well as in the rehabilitation of older buildings.

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POSTER 19

FAILURE PREDICTION OF BRITTLE MATERIALS BY FINITE FRACTURE MECHANICS AND PHASE FIELD

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The development of tools for predicting the failure of brittle materials is gaining unprecedented importance as for the increasingly widespread use of brittle, high-performance materials in critical structural applications. In this sense, two approaches have aroused interest as for their capability of capturing experimentally observed phenomena: Finite Fracture Mechanics (FFM) and Phase Field (PF). The former, based on the coupling of non-local stress and energy conditions, has been proven to deliver accurate predictions for the onset of failure in a wide range of scenarios. Likewise, the latter relies on the minimization of an energy functional in which the damage is represented through a phase field, and it has been demonstrated robust for predicting failure upon complex geometries and crack patterns.

Recent advances on the aforementioned methods are herein presented, which include their extension and application to different geometries, material microstructures and loading scenarios. In particular, the size-effect on the failure of an infinite domain with a spherical void under uniaxial tensile loading is thoroughly studied by means of FFM (and other well-known models such as Cohesive Zone Model), and the resulting failure curves are proven accurate against experimental results [1]. Additionally, an extension of the FFM approach for its use under dynamic loading regimes is proposed, where FFM is modified to also consider the loading history, resulting in an extended criterion capable of replicating with great correlation the experimental results reported in the literature. Likewise, efforts are being made towards implementing the PF approach in complex scenarios, such as complex geometries or heterogeneous materials, aiming to be able to analyze complex crack propagation problems that are out-of-reach for the FFM approach.

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POSTER 20

KINETICS OF HYDROGEN DIFFUSION IN MAGNESIUM USING A DIFFUSIVE MOLECULAR DYNAMICS METHOD

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Understanding the transport of hydrogen within metallic nanomaterials is crucial for the advancement of energy storage and the mitigation of hydrogen embrittlement. Using nanosized magnesium particles as a model, recent studies have revealed several highly nonlinear phenomena that occur over long time periods. The time scale of these phenomena is beyond the capability of established atomistic models such as molecular dynamics. In this work, we present a new approach, referred to as diffusive molecular dynamics (DMD) [1,2], to the simulation of long-term diffusive mass transport at the atomic scale. The basic assumption underlying DMD is that the time scale of diffusion is much larger than that of microscopic state transitions. In terms of numerical implementation, our approach involves the numerical integration of the master equation, and the numerical solution of a highly nonlinear optimization problem at every time-step. By working with atomic fractions, the characteristic time-step size of our DMD simulations can be much larger than those based on either AMD or KMC methods. In the present work, we will focus on the characterization of thermodynamic and kinetic properties of magnesium hydride nanoparticles. Modeling phase transitions of Mg/MgH_2 systems introduce an additional difficulty due to the change of lattice structure. We also note that the scope of DMD is not limited to metal hydrides and a broad range of multi-species systems of practical interest suggest themselves as worthwhile foci for future studies.

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POSTER 21

ANALISIS OF EAM POTENTIALS FOR SIMULATION OF DIFFUSION OF HELIUM IN IRON

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Metastable Helium atoms are produced in neutron-irradiated metals as a result of (n,α) transmutation reaction from the nuclear fusion reaction of deuterium and tritium. Understanding the impact of the presence of Helium on the steel walls of the nuclear reactor is crucial for the development of fusion reactor materials. At the atomistic level, this interaction is carried out as a prelude in diffusive molecular dynamics (DMD). The Helium is trapped in small vacancy clusters, leading to the creation of helium-stabilized bubbles. In the present work, we will analyse and compare the models proposed by different authors [1-5] based on EAM and MEAM-type interatomic potentials. We have evaluated their performance under different settings, including lattice relaxations and defect formation energies.

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POSTER 22

ANALYSIS OF SELF-HEATING IN OPEN-HOLE CFRP LAMINATES UNDER TENSILE LOADING FATIGUE

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One of the most widely used composite materials in aerospace industries are Carbon Fiber Reinforced Polymer (CFRP) laminates due to their mechanical performance. Furthermore, the use of CFRP stacks with metals such as Titanium (Ti) is often found in aerospace applications. CFRP-Ti stacks and their mechanical behavior after machining are currently a subject of research [1]. On the other hand, one of the most widespread non-destructive techniques to analyze the fatigue behavior of composite materials is infrared thermography [2,3]. Different behaviors have been observed throughout the fatigue tests, depending on the type of failure that is occurring [4]. Three stages are distinguished throughout the fatigue life. A first stage in which the rupture of the matrix dominates, and rapid self-heating occurs. A second stage that represents most of the fatigue life of the component and where the temperature increases slowly. Finally, a third and final stage where a rapid self-heating occurs, accompanied by fiber breakage. In this work, the behavior of laminates belonging to CFRP/Ti stacks with different drilling orientations has been analyzed using infrared thermography. A reduction in fatigue life of more than 50% is observed between stacked drilled specimens and free drilled specimens.

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POSTER 23

DYNAMIC LOAD ALLOWANCE OF MODULAR STEEL ROADWAY BRIDGES CONSIDERING VBI

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In the present contribution, the dynamic impact (or dynamic load allowance) factor caused by moving vehicles on roadway bridges is investigated. As previous research has found, dynamic impact factor indices provided in many design codes are adequate to new-designed bridges, but they can lose accuracy when applied to existing ones, as several factors may affect the performance of the bridges in the long-term. In this sense, studies have shown that due to the road surface deterioration of existing bridges, the impact factors calculated experimentally could be higher than the values specified in many design codes [1].

In the case of modular bridges, determining the adequate impact factors is a matter of interest, as one of their main limitations is the span length between supports, which is usually limited to 60 m without operational restrictions. Recent modular bridge developments search for enlarging the available span length to 120 m and beyond, and this requires a full understanding of the dynamic effect of moving vehicles on these structures.

Thereby, the main objective of this work is to evaluate the impact factor of several steel modular bridges by means of a 3D vehicle-bridge coupled model, which is used to simulate the interaction between these two elements. The vehicle is modelled as a multi-body system and the quasistatic and dynamic excitation mechanisms generated by passage of a truck are simulated. The bridges are modelled using the finite element method. Additionally, different vehicle speeds, road/wheel irregularities and pavement imperfections and misalignments are considered. The dynamic problem is solved on the assumption that the vehicle-bridge interaction does not alter the dynamic properties of the bridges in a significant way. Therefore, modal superposition analysis can be used to reduce the computation effort. Regarding the vehicle-bridge coupled system, it is solved using a fourth order Runge-Kutta method in the time domain.

Finally, conclusions are extracted concerning the calculated impact factors for the considered steel modular bridges and those provided for the same type of structures in some of the main design codes.

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POSTER 24

PREDICTING AND UNVEILING MATERIAL RESPONSE USING PHYSICALLY-GUIDED NEURAL NETWORKS WITH INTERNAL VARIABLES

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Nonlinear material modelling using Finite Element Method presents some challenging issues. Even if many nonlinear models have been proposed for modelling elastic and inelastic solids in the last decades, model selection and parameter identification and fitting are very expensive and time-consuming processes, which rely on data obtained under very specific and controlled lab tests.

The Internet of Things has opened a new paradigm in data monitoring and acquisition, where data quantity is a frequent situation, rather than data quality and structure. With the advent of Data Sciences and in particular machine learning tools, science has progressed to extract relevant information from available unstructured data, thus allowing to make predictions with incredible accuracy [1]. In particular, in these situations with high data availability, artificial neural networks have arisen as powerful tools to deal with nonlinear problems, although they suffer from the inherent lack of explanatory capacity of "black-box" models.

Here, we exploit the recent concept of Physically-Guided Neural Networks with Internal Variables (PGNNIV) [2]. PGNNIV enable the addition of physically meaningful constraints to deep neural networks from a model-free perspective, thus resulting in fast predictions of external and especially internal variables. We use a general framework for adapting PGNNIV to continuous problems [3], to formulate infinitesimal strain solid mechanics theory, without the need of the material constitutive response prescription, which is here unveiled from the data. The presented framework leverages the use of universal equations, such as conservation laws, for obtaining interpretable values associated with some internal neurons that play the role of non-observable variable such as the stress field.

Our approach demonstrates to perform fast predictions of the mechanical system under arbitrary external stimuli, something useful when facing inverse problems and optimization, and to unveil the hidden material response, thus endowing the framework with explanatory capacity and placing it in the family of Explanatory Artificial Intelligence (XAI) [4].

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POSTER 25

A DEEP LEARNING APPROACH FOR DYNAMIC STIFFNESS OF FOUNDATIONS IN LAYERED SOILS

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The dynamic Soil Structure Interaction (SSI) effects play a major role in the design of particular structures in different engineering fields: seismic design, on-shore and off-shore wind turbines, and special energy structures. The practical computation of the impedance matrices in the frequency domain requires the use of numerical models. The Boundary Element Method (BEM) [1] is usually the best option due to its inherent properties: radiation condition and minimum mesh requirements. The main drawback of the BEM approach is its limited use to academic environments. The generalization to industrial environments requires the development of fast assessment solutions for SSI matrices, to characterize the frequency-dependent stiffness and damping matrices for each foundation mode (vertical, horizontal, rocking, torsional, and coupled terms).

In this communication it is explored the application of Deep Learning [2] to the fast computation of dynamic stiffness matrices. The analysis is limited to surface rectangular foundations. Three-dimensional homogeneous elasticity, in the frequency domain, with multilayered half space has been considered. An specific fundamental solution and traction singular functions [3] have been used to accelerate BEM results. An extensive dataset has been computed for dynamic stiffness matrices, based on Gaussian exploration of the variables, with more than 100.000 direct cases. The study has been limited to two-layer case. Deep Learning techniques have been explored to define and optimize network arquitectures, with hyperparameter tuning (optimal batch size, ReLU and modified activation functions, decaying learning rate, overfitting estimation, etc). The design and development of deep neural networks have been carried out with TensorFlow in Google Colab notebooks, based on Python and GPU processing. Error analysis in both training and testing sets have been discussed. Finally, optimal networks have been proposed, which allows the fast computation of impedance matrices with adequate accuracy (more than 95%). Such optimal networks can be stored and shared in easy way, which makes them attractive por potential applications in industry and further research studies.

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POSTER 26

MODELING OF THE BIOMECHANICAL STABILITY OF INTRAOCULAR LENSES AFTER CATARACT SURGERY

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Cataract surgery remains the most common ophthalmic procedure performed in developed countries and consists of replacing the opacified crystalline lens by an intraocular lens (IOL). In recent times, some refractive errors such as myopia, hypermyopia or astisgmatism have also been corrected during cataract surgery. This has made the surgery more complicated both due to the dificilt task of predicting the IOL power and the need to control exhaustively the IOL behavior inside the eye. The biomechanical stability of the IOL inside the capsular bag is key to avoid refractive errors that lead to a second surgery. For this reason, we developed a finite element model to predict the biomechanical stability of the IOL in the short- and long- term after surgery. The numerical model includes the implated IOL, the post-cataract capsular bag, the zonules and a portion of the ciliary body, all elements needed to simulate this phenomenon. Moreover, the connection between the anterior and posterior capsule, which occurs days after surgery, called fusion footprint, was also simulated.

A high-fidelity simulation was developed and compared sucessfully with in vitro data [1]. With the developed finite element model, different scenearios were analyzed: the size and location of the capsulorexhis, the capsular bag shrinkage and the pre-cataract geometry and the mechanical properties of the capsular bag. Moreover, three different IOL designs were evaluated: the C-loop LUCIA IOL, the double C-loop POD FT IOL, a double C-loop design and the plate AT LISA.

The results were aligned with the clinical data provided by the literature [2]. The most stiff design, AT LISA, deformed greater the capsular bag, and also presented the highest axial displacement and the lowest rotation. By contrast, the C-loop LUCIA IOL presented the lowest axial displacement and the highest rotation. The results also suggested that a larger capsulorexhis makes the post-cataract capsular bag more flexible and that the capsular bag shrinkage is key in the final configuration of the IOL inside the capsular bag.

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POSTER 27

SUBSURFACE STRESS EVOLUTION UNDER ORTHOTROPIC WEAR CONDITIONS

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Advances in computing make it possible to bring simulation closer to the reality of mechanical contact interaction. One of the most important aspects concerning contact mechanics is wear, as there are many investigations of an experimental, theoretical, computational nature, etc. In this work, simulation algorithms are developed and probed to manage three important facets. These are the orthotropic surface properties due to machining processes in most mechanical components, the tendency of stresses to be higher at the subsurface for contact problems under different friction coefficient values (i.e. low friction coefficient in metallic contact pairs or high friction coefficients in machined surfaces) and the well-known importance of wear during the life of mechanical elements. Thus, several 3D benchmark problems are solved by computing the subsurface stresses under different orthotropic contact conditions taking into account wear. The analysis of the resulting information allows us to compare the behaviors concerning subsurface stresses for different contact conditions in sliding wear and friction wear problems (i.e., gross slip and partial slip behaviors). Finally, some conclusions are presented based on the carried-out analysis.

POSTER 28

INTERFACE INCLUSION/MATRIX DAMAGE MODELLING IN LEAD-FREE PRINTABLE PIEZOCOMPOSITES

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3D printable lead-free piezocomposites offer scalable and eco-friendly solutions in many engineering applications. Typically, the composite system consists in polymeric matrices reinforced with active polycrystalline particles. The presence of interfacial inclusion/matrix damage in such composites may alter their capability to act as functional smart materials. From the mechanical point of view, an interfacial imperfection refers to displacement jump, due to, for instance, debonding or slippage. In this work, a thin interphase model to account the matrix-inclusion interfacial imperfections based on [1-3] is presented. Thus, based on a periodic unit cell, the influence of interfacial damage on the effective mechanical properties is studied.

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POSTER 29

COMPRESSIVE FATIGUE IN FIBER-REINFORCED CONCRETE: KEY ASPECTS

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Fatigue damage in concrete, especially in fiber-reinforced concrete, has its particularities in comparison with that of metallic materials. We summarize such important aspects herein based on some of our recent research works.

The experimentally measured static strength follows a Weibull distribution, thus a probabilistic fatigue model should recover such an initial distribution [1]. Factors such as the loading frequency [1,2] or the fiber content [3] play an important role in fatigue life.

There exists a significant size effect in fatigue life even though the corresponding static strength is size-independent [4]. Nevertheless, the linear relationship between the secondary strain rate per cycle and the number of cycles in the logarithmic scale, i.e., the Sparks-Menzies equation, is size-independent. In addition, it is independent of the fiber amount and is determined by the matrix alone. Such an observation offers the possibility of characterizing the fatigue properties through prematurely interrupted tests. In this way, a remarkable time and cost reduction can be achieved without the detriment of data reliability [5].

For certain compositions, maturation due to fatigue loading is observed. In other words, the residual strength is considerably improved (up to 42% observed increase) after cyclic loading. This is an interesting phenomenon that offers an alternative for the design of self-healing concrete.

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