### UNIVERSITY OF PAVIA DOCTORAL THESIS

## Material behavior and manufacturing solutions for biomedical applications: from computational optimization to 3D printing

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XXX Cycle (years 2014-2017)

## **Declaration of Authorship**

I, Gianluca Alaimo, declare that this thesis titled, "Material behavior and manufacturing solutions for biomedical applications: from computational optimization to 3D printing" and the work presented in it are my own. I confirm that:

- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.

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"If in doubt, flat out"

Colin McRae

#### Abstract

This thesis investigates material behavior and advanced manufacturing solutions, with specific focuses ranging from computational optimization tools to effective component production through 3D printing technologies. The developed tools are mainly applied to biomedical field as a promising area for the use of sophisticated computational mechanics tools. In more details, the specific contributions range from the mechanical investigation of biological tissue response, in the case of a cardiovascular intervention, to the design and optimization of a medical device (Part I), including the study and the solution of rate dependent thermo-mechanical phenomena of interest in biomedical investigation (Part II). Mechanical properties of polymer-based 3D-printed components are investigated (Part III), given the new, and still not fully exploited opportunities that additive manufacturing processes may offer in terms of customization, materials and production time of dedicated patient-specific medical devices.

In particular, in Part I the impact of thoracic endovascular aortic repair (TEV - AR) on longitudinal strain and aortic tensile properties is investigated in order to better understand complications associated with TEVAR. Attention has subsequently been devoted to the problem of fatigue life in Nitinol stents. It is proposed a numerical optimization framework aiming at increasing the fatigue life reducing the maximum strut strain along the structure through a local modification of the strut profile. The adopted computational framework relies on nonlinear structural finite element analysis combined with a Multi Objective Genetic Algorithm, based on Kriging response surfaces. In particular, such an approach is used to investigate the design optimization of planar stent cell. The results of the strut profile optimization confirm the key role of a tapered strut design to enhance the stent fatigue strength, suggesting that it is possible to achieve a marked improvement of both the fatigue safety factor and the scaffolding capability simultaneously.

In Part II heat conduction in non-Fourierian conductors, as some classes of biological tissue and biomedical materials, is studied. Indeed, recent applications of physics and bio-engineering showed several unpredicted and "anomalous" effects in heat transport. An attempt to capture these effects have been reported in a paper by Cattaneo that introduced, in the well-know Fourier relation, a first order time derivative of the the heat flux and an appropriate relaxation time. We extended the Fourier conduction equation, introducing a Caputo fractional derivative with order  $\beta \in [0, 1]$ . The distribution and the temperature raising in simple rigid conductors have been also reported to investigate the influence of the derivation order in the temperature field. Then the coupled behavior of slightly deformable bodies, in which the strain is additively decomposed in an elastic contribution, and in a thermal part, is studied.

In Part III the mechanical behavior of 3D-printed FDM structural components is studied. More in detail, the influence of the extruded filament dimensions and chemical composition on mechanical behavior are investigated through experimental campaigns. We showed that FDM specimens exhibit anisotropic mechanical properties since they vary with filament extrusion direction. Accordingly, Classical Lamination Theory (CLT) and Tsai-Hill yielding criterion were found to be well capable of predicting in-plane stiffness and strength of FDM specimens. We assessed that, varying chemical composition and filament dimensions, it is possible to tune fiber properties and fiber-to-fiber bonding and, consequently, the overall mechanical properties at macro-scale, in particular the yielding strength and the strain at failure. The experimentally obtained data may be used to calibrate mechanical models to be used with computational tools as finite element analyses.

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## Introduction and outline of the Thesis

This thesis investigates both biological tissues and bio-compatible materials with the aim of contributing to the design and the manufacturing of optimized biomedical devices with particular attention to their thermo-mechanical performance. For this purpose, we conducted experimental campaigns, numerical optimizations and theoretical formulation. The proposed methodologies and the related results can be applied to other several engineering research fields. Biological tissues have been studied in terms of changes in tensile properties associated with the interaction with medical devices and in terms of non conventional heat conduction, relying on non-integer order differential operators. Biomaterials have been investigated in terms of bio-mechanical performance of Nitinol stents and in terms of polymer mechanical properties, resulting from Additive Manufacturing (AM) processes. Most of the investigations resulted in specific publications which are listed at the end of the present introduction.

**Part I** is devoted to the understating of the interaction between medical devices such as stent grafts and the vessel in which they are inserted and on mechanical performances of Nitinol stents. **Chapter 1** investigates the impact of Thoracic Endovascular Aortic Repair (TEVAR) on longitudinal strain along with aortic tensile properties in order to better understand complications associated with TEVAR. Our experimental study found that TEVAR acutely stiffened the thoracic aorta in the longitudinal direction. This resulted in a longitudinal strain mismatch between stented and non-stented segments. Uniaxial tensile testing

demonstrated that thoracic aortic tissue is more prone to rupture in the longitudinal than the circumferential direction, in particular close to the aortic arch. Such an acute strain mismatch of potentially vulnerable tissue might play a role in TEVAR-related complications, including retrograde dissection and aneurysm formation. The finding that TEVAR stiffens the aorta longitudinally may shed light on systemic complications following TEVAR, such as hypertension and cardiac remodeling. This initial study on the impact of TEVAR on longitudinal strain may serve as a base for future investigation on the interaction between aortic stent-grafts and cardiovascular biomechanics and might contribute to future stent-graft design.

**Chapter 2** deals with the problem of the redesign of self-expanding nitinol stents that, nowadays, are widely used as part of percutaneous minimally-invasive techniques aimed at treating occluded vessels. Indeed, several mechanical failures of such a class of devices have been observed; this drawback often results in a loss of scaffolding capabilities of the stent, thrombus formation, and restenosis. The majority of the mentioned out-of-service, that depend on anatomical position and the load history, occurs for cyclic loadings that induce fatigue failures.

Performing a thorough engineering analysis, we identified several relations between the stent geometry and its structural performance. Moreover, a further literature analysis showed that: i) it is possible to enhance fatigue strength acting on the stent cell design but such an improvement has its counterpart in a loss of stiffness; in other words, fatigue life and scaffolding capability of the stent are, usually, conflicting objectives ii) a tapered strut profile may enhance the stent fatigue strength, being thus an ideal starting point for the stent design optimization. Relying on the previous observations, we noted that it would have been possible to optimize stent design increasing the fatigue strength without penalizing other bio-mechanical design requirements. We then proposed a *multi-objective* optimization procedure, acting on stent cell geometry and based on the introduction of tapered strut profile. In particular, the optimization framework accounts for non-linear structural Finite Element Analisys (FEA) combined with a Multi Objective Genetic Algorithm (MOGA) based on Kriging response surfaces. Response surfaces have been used to reduce the computational effort required by the optimization procedure.

The study results confirm that the use of tapered strut profile should be a primary key factor to enhance the fatigue life of the whole stent. The selection of one design from the Pareto optimal set, that is the outcome of the multi-objective optimization, can be done selecting the trade-off point, i.e. the Pareto point that is the most appropriated with respect to the given design requirements.

As illustrative example we compared a commercial reference design with an optimized design, chosen from the obtained Pareto set, under the requirement of leaving scaffolding capability unchanged. The proposed approach suggests that the enhancement of stent fatigue life can be achieved combining tapered strut profile with an increase of the strut length and of the strut width at extremities.

Moreover, the results suggest that the width narrowing at the middle of the strut, due to the profile tapering, should be stay among 35% - 50%. Under such indications, it is possible to achieve a marked improvement of the fatigue safety factor, i.e., about 2.4 times, compared to the typical design (strut with constant section), without any loss of scaffolding capabilities. The present study underlines the value of advanced engineering tools to optimize the design of medical devices.

**Part II** is devoted to the study of heat conduction in non-Fourierian conductors as biological tissues and biomedical materials employed in medical applications. This is a key point for the assessment of suitable models able to predict thermal and thermo-mechanical response of such class of materials. The conventional theory of heat transfer is based on the classical Fourier law that involves a contemporaneous cause effect relation among the heat flux and the temperature gradient. In some recent applications of physics and bio-engineering however, experimental measures showed several unpredicted effects in heat transport. An attempt to capture these effects have been reported in a paper by Cattaneo that generalized the well-know Fourier relation with the introduction of a first order time derivative of the the heat flux and an appropriate relaxation time. In this setting the propagation of temperature waves has been related to the presence of phonon's scattering across the materials.

When the phononic propagation has a mean free path similar to the geometrical dimensions of the conductor, then a ballistic motion, related by the Cattaneo equation, may be expected. On the other hand, if the mean free path is of the order of the inter-atomic distance, a pure diffusion, ruled by Fourier equation, may be expected. The abrupt separation among the ballistic and the diffusive propagation is, however, an anomalous condition seldom encountered in applications.

Beside Cattaneo generalization of transport equation, an integral formulation has been introduced by Biot and Lord and Schulman yielding the so-called memory formalism of the heat transport equation.

Very recently the memory formalism has been specialized in a fractionalorder diffusion equation and non-local contribution of fractional order have been also introduced. Fractional-order calculus is usually referred as the generalization of the well-known ordinary differential calculus introducing real - order integrals and derivatives. It traces back to the basic definitions by Riemann as well as to successive memories of famous mathematicians as Liouville, Cauchy, Abel, Leibniz.

**Chapter 3** shows that fractional order heat transfer may be obtained introducing a self-similar, fractal type mass clustering at the micro-scale. In this setting the resulting conduction equation at the macro-scale yields a Caputo's fractional derivative with order  $\beta \in [0,1]$  of temperature gradient that generalizes the Fourier conduction equation. The order of the fractional-derivative has been related to the fractal assembly of the micro-structure. The distribution and the temperature raising in simple rigid conductors have been also reported to investigate the influence of the derivation order in the temperature field. Essentially, this is equivalent to having a distribution of masses characterized by a functionally graded hierarchy of thermal conductivities and heat capacities, scaling with a certain power law.

Results show that the solution of the fractional heat equation  $(0 < \beta < 1)$ , governed by Mittag-Leffler functions, exhibits for small times a much faster rising, and for large times, a much slower decay. Accordingly, the main property of the considered anomalous heat transfer is that the time-rate of change at which the resulting temperature field reaches a steady state, becomes higher as the discrepancy from the Fourier law increases: the thermal steadiness is consequently achieved, by anomalous conductors, employing longer times than Fourier ones. Such particular behavior represents the "long-tail memory effect", due to the power law thermal memory of such materials.

**Chapter 4** focuses on the "thermally-anomalous" coupled behavior of slightly deformable bodies, in which the strain is additively decomposed in an elastic contribution and in a thermal part. The macroscopic heat flux turns out to depend upon the time history of the corresponding temperature gradient, and this is the result of the multi-scale rheological model developed in chapter 3, thereby resembling a "long-tail" memory behavior governed by a Caputo's fractional operator. The macroscopic constitutive equation between the heat flux and the time history of the temperature gradient does involve a power law kernel, resulting in the "anomaly" mentioned above. The interplay between such thermal flux and the elastic and thermal deformabilities is investigated for a pinned-pinned truss.

While the anomalous thermal behavior in time has been extensively studied from the phenomenological and mathematical point of view, starting from the late sixties to these days, anomalous thermoelastic coupling in engineering and biomedical applications still requires thorough investigations. To this end, for the sake of illustration, a one dimensional anomalous thermoelastic truss subject to thermal loading and pinned at both ends is examined. The full analytical solution of the problem is provided obtaining the resulting displacement and temperature fields along with the internal axial force. The anomalous thermal behavior of such slightly deformable system is then investigated, thereby exploring not only the transient behavior due to its deviation from the Fourier law, but also by studying a resulting overall measure of energy rate and the interplay between the thermal flux and the elastic and the thermal deformability. Results show that the interactions, in such simply geometry, are fully coupled as the temperature and the displacement fields mutually influence one another.

The higher is the deviation from the Fourier-like behavior for the heat flux, the steeper is the resulting time-transient of each mode. The influence of the deformability on the one hand, and of the discrepancy from the Fourier behavior on the other hand, are thoroughly analyzed for the three fields mentioned above.

Measures of the overall "thermal work", and of the associate available and dissipation energy rates are evaluated, both mode-by-mode and globally, enabling the characterization of the coupled response of anomalous thermoelastic trusses. Besides determining the range of admissible discrepancies from the Fourier behavior, such quantities are shown to fully reveal the manifestation of the thermal anomaly together with the effects of the elastic and thermal deformabilities.

**Part III** deals with the manufacturing of functional components, to be employed in a very wide class of applications, with particular attention to medical ones. We focused on AM technologies, also known as 3D printing (3DP). 3DP is a disruptive technology that is changing design paradigms, distribution good chains, economical business models, paving the way to new, and even futuristic, applications. Among the many available 3D printing processes, we concentrate on direct deposition technologies, and in particular on FDM (Fused Deposition Modeling), the latter being the most widespread, flexible and economic one.

In FDM printers the material is drawn through a nozzle, where it is heated and then deposited on a building tray through a layer by layer process. In general, the nozzle can move on the horizontal plane and a platform moves down on the vertical direction after each new layer is deposited. The printing head movements, the extrusion system and all the other printing parameters are controlled by an electronic board, relying on a set of instructions known as g-code. The g-code is produced by a devoted software commonly called slicer or slicing software, that takes into account the virtual geometry, the characteristics of the printing material and the features of the specific 3D printer.

The ingredients which may boost FDM technology are the ability to process and combine large classes of materials, possibly locally changing infill patterns and density, with the final goal of producing multi-material components, eventually also characterized by spatial gradient properties. Moreover, the completely open-source nature of the FDM process, from the electronic, mechanics and software point of view, allows the user to intervene directly on the machine code controlling all the process parameters.

Besides being an open technology, FDM offers many advantages in terms of available materials, not common to other 3DP technologies. Indeed, FDM covers a wide class of thermoplastic polymers, ranging from common Acrylonitrile Butadiene Styrene (ABS) and Poly-lactic Acid (PLA) to biocompatible materials like Polycaprolactone, to high-performance materials like PEEK (Polyether ether ketone) and Ultem©, known for their recent "metal replacement" application, to high-deformable materials as TPU (Thermoplastic Polyurethane). For example,

with respect to the elastic modulus FDM materials cover about 4 orders of magnitude, from 6 MPa of TPU to 3600 MPa of PEEK.

However, FDM process is still mainly focused to non-functional components, due to the lack of knowledge on mechanical behavior, systematic design approaches and tools able to fully exploit the production methodology features for the manufacturing of parts with known and predictable characteristics.

**Chapter 5** investigates, through experimental campaigns, the influence of the mesostructure and chemical composition on structural components made of Acrylonitrile Butadiene Styrene (ABS) and obtained through FDM process.

Mesostructure is the inner geometrical structure, at a submillimeter scale, resulting from the filament deposition: it may be essentially defined through fiber thickness and width. We considered several configurations, differing in the mesostructure and in the material chemical composition. Tensile tests have been conducted varying fiber orientation with respect to the loading direction: meso-structure influence is tested on the same material, while chemical composition impact is tested using the same mesostructure. In fact, at the present day, there are no approved specific standards dedicated to the evaluation of 3D-printed objects tensile mechanical properties. Because of their pronounced anisotropy, the selection of the specimen shape is a fundamental issue.

For specimen manufacturing, first 3D models are created through a CAD software. They are then exported as STereoLithography (STL) files and subsequently loaded in the slicing software. In order to produce unidirectional specimens, gcode manipulation is mandatory, since, currently, there are no slicing programs able to directly produce them. We preliminarily used two different slicing software to produce g-codes for the single layer and for the support interface, respectively. Subsequently, we developed a custom made routine in a dedicated software environment to assembly the final g-code with the desired features.

Result confirms that FDM ABS specimens posses anisotropic mechanical properties since their response vary with filament extrusion direction. Accordingly, Classical Lamination Theory (CLT) and Tsai-Hill yielding criterion were found to be well capable of predicting in-plane stiffness and strength of FDM specimens. We assessed that, varying chemical composition and filament dimensions, it is possible to tune fiber properties and fiber-to-fiber bonding and,

consequently, the overall mechanical properties at macro-scale, in particular the yielding strength and the strain at failure.

Relying on the good consistency between experimental and estimated data, we strongly suggest the adoption of suitable standard test methods tailored on anisotropic materials in order to experimentally evaluate mechanical properties of FDM 3D-printed parts. The experimentally obtained data are useful to calibrate mechanical and yielding models to be used with numerical simulations as finite element analyses. Such computational tools would be used along with optimization techniques to design structural-optimized functional parts.

As mentioned before, this thesis presents the work done during the Ph.D. course and constitutes the compendium of the main results.

• Chapter 1 resulted in the paper:

F.J. Nauta, M. Conti, S. Marconi, A.V. Kamman, G. Alaimo, S. Morganti, A. Ferrara, J.A. van Herwaarden, F.L. Moll, F. Auricchio, S. Trimarchi. "An experimental investigation of the impact of thoracic endovascular aortic repair on longitudinal strain", *European Journal of Cardio-Thoracic Surgery*, 2016, Vol. 50, No. 15

• Chapter 2 resulted in the paper:

**G. Alaimo**, F. Auricchio, M. Conti, M. Zingales. "Multi-objective optimization of Nitinol stent design", *Medical Engineering & Physics*, 2017, Vol. 47, pp 13-24

• Chapter 3 resulted in the paper:

**G. Alaimo**, V. Piccolo, A. Chiappini, M. Ferrari, D. Zonta, L. Deseri, M. Zingales. "Fractional-Order Theory of Thermo-Elasticity I: Generalization of The Fourier Equation and Thermodynamical Consistency", *Journal of Engineering Mechanics*, 2017, in printing, DOI 10.1061/ (ASCE)EM.1943-7889.0001394

- Chapter 4 resulted in the paper:
  - V. Piccolo, **G. Alaimo**, A. Chiappini, M. Ferrari, D. Zonta, M. Zingales, L. Deseri. "Fractional-Order Theory of Thermo-Elasticity II: Quasi-Static

Behavior Of Bars", *Journal of Engineering Mechanics*, 2017, in printing, DOI 10.1061/(ASCE)EM.1943-7889.0001395

• Chapter 5 resulted in the paper:

**G. Alaimo**, S. Marconi, L. Costato, F. Auricchio. "Influence of mesostructure and chemical composition on FDM 3D-printed parts", *Composites Part B: Engineering*, 2017, Vol. 113, pp. 371–380

## Part I

# Impact of thoracic endovascular aortic repair and fatigue life in Nitinol stents

# An experimental investigation of the impact of thoracic endovascular aortic repair on longitudinal strain<sup>\*</sup>

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#### ABSTRACT

**Objectives:** To investigate the impact of thoracic endovascular aortic repair (TEVAR) on longitudinal strain and assess aortic tensile properties in order to better understand complications associated with TEVAR.

**Methods:** Twenty fresh thoracic porcine aortas were harvested and connected to a mock circulatory loop driven by a centrifugal flow pump at body temperature. Length measurements were conducted before and after TEVAR through aortic marking, high-definition imaging and custom-developed software under physiological pressure conditions (i.e. between 100 and 180 mmHg with 20 mmHg increments). Longitudinal strain was derived from length amplitude divided by the baseline length at 100 mmHg. Three groups of stent-graft oversizing were created (0-9, 10-19 and 20-29%). Finally, elastic properties of the

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aortic samples were assessed in both longitudinal and circumferential directions through uniaxial tensile testing. Longitudinal strain was compared before and after TEVAR, and stress-to-rupture was compared among specimens and locations.

**Results:** TEVAR induced a longitudinal strain decrease from 11.9 to 5.6% (P < 0.001) in the stented segments and a longitudinal strain mismatch between stented (5.6%) and non-stented segments (9.1%, P < 0.001). Stent-graft oversizing did not affect the magnitude of strain reduction (P = 0.77). Tensile testing showed that peak stress-to-rupture was lower for longitudinal (1.4 ± 0.4 MPa) than for circumferential fragments (2.3±0.4 MPa, P < 0.001). In addition, longitudinal fragments were more prone to rupture proximally than distally (P = 0.01).

**Conclusions:** This experimental study showed that TEVAR acutely stiffens the aorta in the longitudinal direction and thereby induces a strain mismatch, while tensile testing confirmed that longitudinal aortic fragments are most prone to rupture, particularly close to the arch. Such an acute strain mismatch of potentially vulnerable tissue might play a role in TEVAR-related complications, including retrograde dissection and aneurysm formation. The finding that TEVAR stiffens the aorta longitudinally may also shed light on systemic complications following TEVAR, such as hypertension and cardiac remodelling. These observations may imply the need for further improvement of stent-graft designs.

### Introduction

The use of thoracic endovascular aortic repair (TEVAR) is increasing rapidly, even in younger patients [1, 2]. However, this procedure is associated with serious complications such as retrograde dissection (with a mortality of about 40%), aneurysm formation, stentgraft induced new entry tears and rupture [3–5]. These complications might be related to different physical properties of the stentgrafts when compared with blood vessels. Current stent-grafts are several orders of magnitude stiffer than the native aorta [6, 7], most notably in the longitudinal axis. Their impact on the cardiovascular system remains unclear. Locally, segmental aortic stiffening seems to increase wall stress in segments adjacent to the

stent-graft due to a compliance mismatch [3]. This has been associated with reduced wall strength and subsequent complications [3–5]. Stent-graft oversizing reduces a ortic wall strength even further [8].

In addition to a local impact, TEVAR might affect the cardiovascular system on a systemic level. In this setting, aortic elasticity serves a critical function in damping the highly pulsatile flow coming from the left ventricle [9], known as the "Windkessel effect" [10]. Stiffening of the thoracic aorta diminishes this effect with major implications for cardiovascular disease development as it increases cardiac afterload and decreases coronary perfusion [11, 12]. It has been reported that TEVAR stiffens the aorta acutely, resulting in hypertension and cardiac remodelling in the early and late phase [2, 13]. This phenomenon may be referred to as cardiovascular remodelling and might determine long-term outcomes of TEVAR.

Aortic strain is an established measure of aortic elasticity and is traditionally reported as deformation in the circumferential direction during a cardiac cycle. This seems to diminish after abdominal endovascular repair [14]. However, aortic tissue is more prone to rupture in the longitudinal axis [15] and most intimal tears are circumferentially orientated due to the increased longitudinal stress [16].

The aim of this study was, therefore, to assess the impact of TEVAR on longitudinal strain in a controlled experimental setting, with also attention to the role of stent-graft oversizing. For this purpose, we used an ex vivo porcine aortic model connected to a mock circulatory loop driven by a centrifugal flow pump, quantifying changes of longitudinal strain for increasing pressure, before and after TEVAR. In addition, we used uniaxial tensile testing to study stress-to-rupture mechanical properties of the aortic specimens, in both circumferential and longitudinal directions, to potentially identify vulnerable aortic segments.

### Materials and methods

#### **Preparation of aortas**

Twenty fresh porcine aortas were harvested at a local slaughterhouse from young healthy Goland pigs (commercial hybrid, 10-12 months, 160-180 kg). No pigs

were sacrificed solely for this study. The thoracic aortas were transported on iced 0.9% saline solution and all experiments were conducted within 12 h from death. The aortas were procured from the origin of the left subclavian artery (LSA) to the origin of the coeliac trunk and all side branches were ligated. Subsequently, the aortas were bathed in 0.9% saline of room temperature for 15 min.

### **Experimental setup**

The prepared aortas were connected to a mock circulatory loop driven by a centrifugal flow pump (Medtronic Bioconsole BIOMEDICUS 550, Minneapolis, MN, USA), which allowed for controlled intraluminal pressurization. Water was used that was constantly heated at body temperature using a liquid heater (Nova Powerstat Protonic®, Boise, ID, USA) to preserve the biomechanical characteristics of the nitinol stents [17]. A pressure sensor (Micro Switch Pressure Sensor 40PC Series Chart, Honeywell, Freeport, IL, USA) was coupled to a 1/2-inch silicon tube just proximal to the connection with the aorta. The distal end of the aorta was connected to a 3/8-3/8-inch tube, which could move against low resistance in the longitudinal direction through a guiding half-pipe (Fig. 1). The distal 3/8-inch silicon tube was fixed at a standard appointed location to ensure similar resistance and prestretch for all aortas. A prestress of 100 mmHg was applied for all aortas prior to diameter and length measurements, which simulates mean aortic blood pressure in pigs [18].

#### Measurements of aortic dimensions and longitudinal strain

Baseline diameters and lengths were measured manually, using an electronic calliper and were repeated twice by the principal investigator and twice by a second investigator, to allow for intra and interobserver variability analysis. Medtronic Valiant stent-grafts (Medtronic Vascular, Santa Rosa, CA, USA) were used and therefore aortic diameter was based on the distance from adventitia to adventitia, as advised by the manufacturer. To capture longitudinal strain, black rubber dots with a diameter of 5 mm were sutured to the superficial adventitia along the anterior side of the aorta, starting at the origin of the LSA followed by every 5 cm distally (Levels L1 - L8, Fig. 1). Levels L1 and L8 were excluded from further


Post-TEVAR

FIGURE 1: Illustration of the mock circulatory loop connected to a porcine aorta. (A) The CFP propels the water through a soft silicon tube into the porcine aorta, with the blue arrow illustrating the direction of flow. "Fixed" marks the locations where the tube is fixed. "Pressure" shows the location of the pressure sensor. "Camera" illustrates the location of the HD-camera. The "Output Reservoir" is the water reservoir that supplies the CFP. (B) "Pre-TEVAR" shows the situation before TEVAR with the Levels L1–L8 marked accordingly. "Post-TEVAR" illustrates the situation after TEVAR with "Stent" marking the stented segments and "Total Aorta" the total aortic length. The proximal segment adjacent to the stent-graft is marked with "Prox", while "Dist" represents the distal adjacent segment. CFP: centrifugal flow pump; TEVAR: thoracic endovascular aortic repair.

analysis because they were partly covered by the tube connectors. The segment between L2 and L7 was considered the total aortic length. A high-definition webcam (Logitech HD Pro Webcam C920, Lausanne, Switzerland) was installed and fixed above the aorta and snapshots were conducted at five different pressure moments (i.e. 100, 120, 140, 160 and 180 mmHg). All measurements were conducted in threefold and means were calculated for further analysis. Snapshots were taken at a resolution of  $1920 \times 1080$  pixels. These photos were elaborated by a custom-made program developed with Matlab (The MathWorks©, Inc., Natick, MA, USA) that computed the distance between two consecutive dots through a semiautomatic procedure. The program showed the user each image of the dataset and allowed to select each dot and crop the image. The cropped area was then converted from Red–Green–Blue format to black-and-white format using a fixed threshold. A more precise detection of the centre was then performed using an automatic algorithm, which computed the centre of mass of a black region on a white background. All distances and mean values were exported into a .txt file for analysis. Longitudinal aortic strain was then calculated as

Longitudinal strain = 
$$\frac{L - L_0}{L_0}$$

where L is the final length at given pressure and  $L_0$  is the length at baseline (100 mmHg).

### **Stent-graft implantation**

The size of the stent-graft was based on the diameter at the level 10 cm distal to the LSA (Level L3, Fig. 1). To study the impact of circumferential stent-graft oversizing, the aortas were divided into three groups of 0 - 9% (n = 7), 10 - 19% (n = 7) and 20 - 29% (n = 6) of oversizing. Mean longitudinal strains per oversizing group were compared before TEVAR to ensure homogeneity between groups. Medtronic valiant stent-grafts were loaded and deployed by a custom-developed loading and deployment system, directly following the pre-TEVAR measurements. Stent-grafts were implanted with sizes 22 - 22 - 150, 24 - 24 - 150 or 26 - 26 - 150 mm, according to the appointed oversizing rates.



FIGURE 2: Specimen and results of uniaxial tensile testing. (A) Specimen location and orientation. (B) Bone-shaped specimens. (C) Bar diagrams of aortic mean peak stress-to-rupture as function of zone and orientation. (D) Top panel shows aortic specimen under stress. Bottom panel shows rupture of the specimen. Circ: circumferential aortic wall orientation; long: longitudinal aortic wall orientation.

The implanted stent-graft extended from the segments between L3 and L6 (Fig. 1). Proximal and distal landing zones were confirmed manually.

### **Tensile testing**

Uniaxial tensile testing was conducted after the experiment to study elastic properties of the porcine aortas. The specimens were preserved in a refrigerator at  $\sim 7$ °C prior to the tensile testing (time of delay1.5±0.8 days). Three zones of interest were distinguished in the excised descending thoracic aorta, i.e. proximal, central and distal (Fig. 2A). Both circumferential and longitudinal bone-shaped fragments were cut with a standardized specimen cutter. Tensile tests were performed with the MTS Insight Testing System 10 kN (MTS System Corporation, Eden Prairie, MN, USA) equipped with a 250 N load-cell, and by the ME-46 Video Extensometer (Messphysik, Fürstenfeld, Austria). Peak values of both stress and strain were computed from stress-strain curves recorded during the mechanical testing.

## Statistical analysis

Statistical analysis was performed with SPSS statistical analysis software (SPSS 22, Inc., Chicago, IL, USA). Data are shown as frequencies, percentages, mean  $\pm$  standard deviation, as appropriate. Values identified as outliers by Grubb test ( $\alpha = 0.05$ ) were excluded from the analysis. Shapiro–Wilk test was conducted to test the normality of data distribution. Statistical significance was evaluated with two-tailed paired t-tests, Pearson product-moment correlation or one-way analysis of variance. Repeatability of aortic diameter measurements was analyzed with Bland and Altman's difference against mean analysis. Statistical significance was set at the level of P < 0.05.

## Results

Pre- and post-TEVAR longitudinal strains are presented in Table 1. Time between pre-TEVAR and post-TEVAR measurements was  $0.6 \pm 0.2$  h.

## Prethoracic endovascular aortic repair longitudinal strain

The mean thoracic aortic length from the LSA to the coeliac trunk was  $325.5 \pm 29.1$  mm and the mean aortic diameter at the level of the proximal landing zone was  $20.5 \pm 0.9$  mm. More detailed aortic dimensions can be found in Supplementary Table 1. Time of delay between harvesting of the aorta and the initiation of the experiment was  $7.1 \pm 2.6$  h and the water temperature was  $37.2 \pm 0.2$  °C. Before TEVAR, we observed a significant positive linear correlation between pressure and longitudinal strain (r = 0.91, P < 0.001). Maximum strains were 11.9% in the prestented segments and 11.4% in the total aorta, observed at 180 mmHg (Fig. 3).

Aortic segment	Pressure (mmHg)	Pre-TEVAR, longitudinal strain (%)	Post-TEVAR, longitudinal strain (%)	P-value
Total aorta				
	100	$0.0 \pm 0.0$	$0.0 \pm 0.0$	-
	120	$2.0 \pm 0.9$	$1.4 \pm 0.5$	0.002
	140	$5.1 \pm 1.8$	$3.3 \pm 1.2$	< 0.001
	160	$8.5 \pm 2.3$	$5.2 \pm 1.9$	< 0.001
	180	$11.4 \pm 3.0$	$7.0 \pm 2.6$	< 0.001
Stented Segments				
	100	$0.0 \pm 0.0$	$0.0 \pm 0.0$	-
	120	$2.0 \pm 0.9$	$0.9 \pm 0.5$	< 0.001
	140	$5.3 \pm 1.7$	$2.2 \pm 1.2$	< 0.001
	160	$8.9 \pm 2.3$	$3.8 \pm 1.9$	< 0.001
	180	$11.9 \pm 3.1$	$5.6 \pm 2.7$	< 0.001
Proximal segment				
	180	$9.1 \pm 3.9$	$8.3 \pm 3.4$	0.02
Distal Segment				
	180	$11.8 \pm 3.4$	$10.2 \pm 3.6$	0.06

TABLE 1: Longitudinal strain as function of pressure per aortic segment

Continuous data are presented as the means  $\pm$  standard deviation.



FIGURE 3: Longitudinal strain as function of pressure. (A) Longitudinal strain of the stented segments as function of pressure, pre- and post-TEVAR. (B) Longitudinal strain of the total aorta as function of pressure, pre- and post-TEVAR. TEVAR: thoracic endovascular aortic repair.



FIGURE 4: Longitudinal strain per aortic segment, pre- and post-TEVAR. Mean peak longitudinal strain at 180 mmHg per aortic segment. The location of the stent-graft is marked accordingly. Dist: distal segment; Prox: proximal segment; TEVAR: thoracic endovascular aortic repair.

### Post-thoracic endovascular aortic repair longitudinal strain

After TEVAR, longitudinal strain between 100 and 180 mmHg decreased in both the stented segments (11.9 vs 5.6%, P < 0.001) and the total aorta (11.4 vs 7.0%, P < 0.001, Figs 3 and 4). Maximum longitudinal strain of the segment proximal to the stent-graft decreased after TEVAR, while this did not change in the distal segment (Fig. 4). After TEVAR, a mismatch in longitudinal strain was observed between the stented (5.6%) and non-stented adjacent (i.e. proximal plus distal) segments (9.1%, P < 0.001, Fig. 5). In addition, the positive linear correlation between longitudinal strain and pressure was reduced after TEVAR at 120 mmHg (r = 0.86, P < 0.001), and continued to be significant for all higher pressures (Fig. 3).

## Oversizing and longitudinal strain

Before TEVAR, homogeneity of longitudinal strain was confirmed between the three stent-graft oversizing groups in the total aorta (P = 0.60) and in the stented



FIGURE 5: Longitudinal strain mismatch. Post-TEVAR, a mismatch in longitudinal aortic strain is observed between the aortic segments adjacent to the stent-graft compared with the stented segments. TEVAR: thoracic endovascular aortic repair.

segments (P = 0.55). Post-TEVAR, longitudinal strain did not differ significantly between oversizing groups in both the total aorta (P = 0.77) and the stented segments (P = 0.57, Table 2).

## **Tensile testing**

Following the strain experiments, the aortas were incised along the posterior wall so that the stent-graft could be removed without damaging the aortic tissue of the anterior side. Anterior aortic specimen was then used for uniaxial tensile testing since these fragments were not interrupted by spinal side branches. Figure 2 demonstrates the results of the tensile testing. These data confirmed homogeneity of the aortic mechanical responses among all aortas, with longitudinal and circumferential peak stress-to-rupture of  $1.4 \pm 0.4$  MPa (coefficient of variation = 31.0%) and  $2.3 \pm 0.4$  MPa (coefficient of variation = 16.2%), respectively. Peak stress-to-rupture was significantly lower for the longitudinal than for the circumferential fragments in all three zones (Fig. 2C). Additionally, we found lower stress-to-rupture in proximal longitudinal fragments compared with distal longitudinal fragments (P = 0.01), while circumferential fragments showed equal

Aortic segment	Oversizing Group	Pre-TEVAR, longitudinal strain (%)	Post-TEVAR, longitudinal strain (%)	P-value
Total aorta				
	0-9%	$12.3 \pm 3.5$	$7.6 \pm 3.3$	0.002
	10-19%	$11.0 \pm 2.7$	$6.7 \pm 2.6$	0.001
	20-29%	$10.7 \pm 3.0$	$6.7 \pm 1.9$	0.001
Stented Segments				
C	0-9%	$12.8 \pm 3.5$	$6.5 \pm 3.5$	< 0.001
	10-19%	$11.9 \pm 2.6$	$5.4 \pm 2.6$	< 0.001
	20-29%	$10.9 \pm 3.2$	$4.9 \pm 1.8$	0.001

TABLE 2: Longitudinal strain per oversizing group

Continuous data are presented as the means  $\pm$  standard deviation.

stress-to-rupture in all three zones (P = 0.61).

### Intra- and interobserver variability

The intraobserver repeatability coefficient (RC) for diameter measurements of observer 1 was 2.45, and 2.01 mm for Observer 2. Differences of the measurements were smaller than the RCs and linear regression analysis was non-significant (P = 0.46 and P = 0.32, respectively), indicating good intraobserver agreement. The interobserver RC was 1.35 mm. Differences of the measurements between both observers were smaller than the RCs and linear regression analysis was non-significant (P = 0.06), indicating acceptable interobserver agreement.

## Discussion

This experimental study investigated the impact of TEVAR on longitudinal strain through an *ex vivo* porcine model and assessed stress-to-rupture with uniaxial tensile testing. The experiments were conducted in a controlled environment using fresh porcine thoracic aortas connected to a mock circulatory loop, while creating different groups of stent-graft oversizing.

We observed a significant decrease in longitudinal strain after TEVAR in the stented segments (from 11.7 to 5.6%, P < 0.001). As a result, a longitudinal strain

mismatch was observed between the stented and non-stented aortic segments. Our observed longitudinal strain before TEVAR was 11.4% between 100 and 180 mmHg. This agrees with a recent study by Krüger et al. [19] who found length changes of  $\sim 10\%$  using a similar set-up and with in vivo data of Bell et al. [20] that showed longitudinal strain ranging from 7 to 9% in the proximal aorta of the adult. However, these studies did not evaluate longitudinal strain after TEVAR. To our knowledge, the impact of TEVAR on longitudinal strain has not yet been reported.

Another main finding was that the thoracic porcine aortas were most prone to rupture in the longitudinal axis (P < 0.001), in particular in the proximal zone close to the arch (P = 0.01). This new finding may yield insight into the pathogenesis of TEVAR-related complications, such as retrograde dissection that typically occurs at the proximal end of a stent-graft.

Our observations are clinically relevant as they suggest that TEVAR causes acute segmental stiffening, which may increase wall stress in the adjacent segments [3]. Several authors proposed that such locally altered stress between the stent-graft and the aortic wall may be responsible for severe TEVAR-related complications such as retrograde dissection, stent-graft induced new entry-tear, aneurysm formation, rupture, endoleaks and stent-graft fractures and infolding [3–5, 21]. Our results showed a significant mismatch of longitudinal strain between the stented and non-stented aortic segments after TEVAR (Fig. 5). Such a mismatch may lead to the following mechanisms:

- (*i*) Repetitive pulsatile friction between the stent-graft and the aortic wall, at both the proximal and distal end, which may cause traumatic lesions to the aortic wall or the stent-graft [21].
- (*ii*) Increased wall stress along aortic segments adjacent to the stent-graft, at both the proximal and distal end, because of an increased impedance due to the stiffened stented segments [3].

Furthermore, we found that the strain mismatch between the stented and nonstented segments enlarged with rising pressure, potentially increasing the risk of aortic dissection and aneurysmal dilatation. This finding might have implications for clinical practice as it stresses the importance of strict blood pressure control in patients treated with TEVAR to minimize the strain mismatch. This supports the suggestion of others that perioperative hypertensive episodes might increase the risk of retrograde dissection after TEVAR [22], in particular in dissected aortas due to a weakened aortic wall.

During each cardiac cycle, the heart pulls the proximal aorta downwards, forcing it to stretch longitudinally [16, 20]. Stiffening of the descending thoracic aorta after TEVAR seems to limit this stretch, causing an increase in in vivo longitudinal strain in the segments proximal to the device (unpublished data). In vivo, the thoraco-abdominal aorta is proximally fixed to the heart, the supra-aortic vessels and the ligamentum arteriosum, and distally to the visceral arteries and the iliac bifurcation. Such a double-ended fixation forces the total thoraco-abdominal aorta to extend similarly before and after TEVAR. In our experimental set-up, the aortas were also double-ended fixed and prestretched; however, the distal end was allowed some freedom to be able to extend. As a result, we observed a shorter total aortic length after TEVAR when compared with before TEVAR (at 180 mmHg: 268.2 vs 280.3 mm, P < 0.001). This might explain why we did not observe an increase of longitudinal strain in the adjacent segments in this study. Further in vivo imaging studies are warranted to investigate changes in strain in segments adjacent to stent-grafts.

Uniaxial tensile testing showed that peak stress-to-rupture was lower for the longitudinal than for the circumferential fragments. These data support the study of Khanafer et al. [15]. But surprisingly, we also observed that longitudinal aortic tissue was more prone to rupture in the proximal zone than distally, while this was not the case for circumferential tissue (Fig. 2). This new finding implies that thoracic aortic tissue is more vulnerable for an acute increase of longitudinal wall stress than circumferential wall stress, in particular in proximal segments. This observation may clarify why most intimal tears are circumferentially orientated, as this is most likely the result of longitudinal intima failure [15, 16], and might indicate vulnerability of the proximal descending aorta.

Stent-graft oversizing did not determine the magnitude of longitudinal strain reduction, in our set-up. Nevertheless, we did observe a trend of increased longitudinal stiffening and severe oversizing (Table 2). Such aortic stiffening after severe oversizing might support the observation of Sincos et al. [8] who showed that device oversizing increased the risk of rupture. However, further studies are warranted to investigate the association between oversizing, longitudinal stiffening and rupture.

Stent-graft induced aortic stiffening as demonstrated by our experiments, is likely to have negative systemic effects since aortic stiffness is an established predictor of cardiovascular mortality [9, 11]. Acute aortic stiffening is also associated with important histological vascular wall changes, such as increased collagen-toelastin ratio, with elevated risk of cardiovascular disease [3, 10]. Therefore, stent-graft induced stiffening may actually be considered as extremely accelerated ageing of the cardiovascular system, leading to acute aortic stiffening and increased cardiac afterload. These findings suggest that current stiff stent-grafts might be more harmful on the long-term than currently realized. In particular extensive stent-graft coverage might, hypothetically, have a profound impact. It may therefore be advisable to minimize the length of stent-graft coverage, if possible, to decrease adverse cardiovascular effects. However, this remains to be elucidated.

To improve long-term outcomes of aortic disease, we suggest that future studies should focus on the pathophysiology of TEVAR associated complications as well as on development of more elastic stent-grafts. Large in vivo studies using dynamic imaging, such as electrocardiogram-gated computed tomography or magnetic resonance imaging, are required to clarify the association between TEVAR and cardiovascular remodelling. However, such in vivo imaging studies on the highly pulsatile thoracic aorta are associated with out-of-plane motions and cardiac/respiratory artefacts [20, 23]. Therefore, we aimed to first assess the impact of TEVAR on longitudinal strain in a controlled experimental set-up, avoiding artefacts and allowing for aortic tissue marking to overcome out-ofplane motions.

It is reasonable to assume that more elastic stent-grafts might reduce aortic stiffening, adverse cardiovascular remodelling and strain mismatches, with potential favorable long-term outcomes. Currently, stent-grafts with longitudinal connection bars are designed to be stiff in the longitudinal axis to offer better fixation through the spring-back effect. However, it is exactly this springback force that might induce bird-beaking and the formation of intimal tears [4, 5]. Longitudinally, more elastic stent-graft designs with less spring-back force, dedicated to aortic dissection, should be considered. A first modification of the Medtronic stent-grafts was the elimination of the longitudinal connecting bar from the earlier design (Medtronic Talent), which was thought to be responsible for longitudinal stiffness and the spring-back effect. However, on the basis of this study, further longitudinal elasticity might be advised for future stent-graft designs to better fit the compliant aorta, with the aim of improving clinical outcomes in patients managed with TEVAR.

### **Study limitations**

We acknowledge that the use of porcine aortas is an important limitation of this study. Nonetheless, porcine aortas are regularly used in cardiovascular research [19, 24], since their mechanical properties are comparable with those of young humans, and because they are much more widely available than human cadaveric samples. But, a porcine aorta is certainly more elastic than a diseased, often atherosclerotic, adult human aorta. However, we were not able to find data on longitudinal strain in diseased, degenerative, calcified human aortas. Moreover, we have so far not found a reproducible technique to modify the mechanical properties of aortic specimens that addresses the in vivo elastic modulus of aged diseased human aortas properly. Therefore, care should be taken when translating our results to the clinical practice. Further research focused on in vivo imaging studies of diseased adult aortas is necessary to make the step from the laboratory to clinic. Second, we used a non-pulsatile mock circulatory system, which allowed for a highly controllable experimental setting for our study purpose. However, we acknowledge that with this non-pulsatile set-up, we neglected inertial effects of pulse waves, which might have led to underestimation of in vivo strain. Nevertheless, experimental non-pulsatile mock circulatory models have widely shown to provide a valid strategy for the initial investigation of novel concepts regarding aortic elasticity [25]. Moreover, our observed strain rates were comparable with pulsatile ex vivo experimental data and in vivo patient data [19, 20].

Another drawback in this experimental study was the use of non - thrombotic blood analogue. Circulating a thrombotic agent, however, rapidly leads to clotting since there are no epithelial cells to inhibit this. Therefore, just like other ex vivo haemodynamic studies [19, 24], we used water, which sufficed for our main goal; imposing a stable intraluminal pressure. In addition, nonthrombotic fluid does not have relevant influence on the highspeed condition of the aorta [26].

It must also be noted that our findings only apply for Medtronic Valiant stentgrafts, which have interrupted stents. Other stentgraft designs, such as those with continuous stents, might show different rates of longitudinal strain. However, this was out of scope for this study, which primarily focused on a first quantification of the impact of TEVAR on longitudinal strain. Lastly, our data on longitudinal strain in the segments adjacent to the stent-graft may not totally represent the in vivo condition. After all, the in vivo aortas are fixed by multiple elastic side branches, which most likely have a different impact on the adjacent segments than the fixations in our ex vivo set-up. Future in vivo studies are therefore warranted to further elucidate dynamic changes of the total thoracic aorta following TEVAR.

## Conclusion

Our experimental study found that TEVAR acutely stiffened the thoracic aorta in the longitudinal direction. This resulted in a longitudinal strain mismatch between stented and non-stented segments. Uniaxial tensile testing demonstrated that thoracic aortic tissue is more prone to rupture in the longitudinal than the circumferential direction, in particular close to the arch. Such an acute strain mismatch of potentially vulnerable tissue might play a role in TEVAR-related complications, including retrograde dissection and aneurysm formation. The finding that TEVAR stiffens the aorta longitudinally may shed light on systemic complications following TEVAR, such as hypertension and cardiac remodelling. This initial study on the impact of TEVAR on longitudinal strain may serve as a base for future investigation on the interaction between aortic stent-grafts and cardiovascular biomechanics and might contribute to future stent-graft design.

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# Multi-objective optimization of Nitinol stent design\*

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#### ABSTRACT

**Objectives:** Nitinol stents continuously experience loadings due to pulsatile pressure, thus a given stent design should possess an adequate fatigue strength and, at the same time, it should guarantee a sufficient vessel scaffolding. The present study proposes an optimization framework aiming at increasing the fatigue life reducing the maximum strut strain along the structure through a local modification of the strut profile.

**Methods:** The adopted computational framework relies on nonlinear structural finite element analysis combined with a Multi Objective Genetic Algorithm, based on Kriging response surfaces. In particular, such an approach is used to investigate the design optimization of planar stent cell, introducing the concept of the tapered strut.

**Results:** The results of the strut profile optimization confirm the key role of a tapered strut design to enhance the stent fatigue strength, suggesting that it is

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possible to achieve a marked improvement of both the fatigue safety factor and the scaffolding capability simultaneously. The present study underlines the value of advanced engineering tools to optimize the design of medical devices.

**Conclusions:** The study results confirm that the use of tapered strut profile should be a primary key factor to reduce and uniform the strain field along the strut and thus to enhance the fatigue life of the whole stent. The obtained Pareto set allows the designer for the selection of optimized solution, according to the specific design requirements. As illustrative example we compared a commercial reference design with the optimized counterpart: increasing the strut length and the strut width at the strut extremities, it is possible to achieve a marked improvement of the fatigue safety factor, i.e., about 2.4 times, compared to the typical design (strut with constant section), without any loss of scaffolding capabilities.

## Introduction

Nowadays, self-expanding nitinol stents are widely used as part of percutaneous minimally-invasive techniques aimed at treating occluded vessels. Unfortunately, several mechanical failures of such a class of devices have been observed [1]; this drawback often results in loss of scaffolding capabilities of the stent, thrombus formation, and restenosis [2, 3]. In particular, partial or total stent fractures have been found in aortic [4], renal [5], and pulmonary [6] implants, as well as in lower limb arteries, i.e., superficial femoral artery (SFA) and popliteal artery [7–10]. Therefore, the long-term structural integrity of a given stent model should be one of the principal design parameter to be taken into account.

Given such considerations, it is necessary to optimize stent design performing a thorough engineering analysis, able to assess the relation between the stent geometry and its structural performance. Such an optimization should increase the fatigue strength without penalizing other biomechanical design requirements, such as the vessel scaffolding.

Despite several studies already addressed the analysis of Nitinol stents [11–13] and the literature provides some example of stent design optimization analysis [14–19], to the best of our knowledge, only two studies deal with fatigue strength enhancement of Nitinol stents [20, 21]. In [20] a planar lattice for the realization of a stent with smooth cell shapes is proposed in order to reduce peaks of strain induced by abrupt changes in the stent geometry. The study proposes a single-objective optimization process to minimize the curvature of the elementary unit defining the stent design, i.e., stent cell. In [21] a single-objective optimization approach, based on Kriging response surfaces, is presented; such an approach has been used to improve the fatigue strength of the stent by minimizing the strut volume without decreasing the stiffness of the stent. The algorithm considers the strut geometry (width, length, and thickness) as the design variables to be optimized. Both studies combine *single-objective* optimization methods with structural Finite Element Analysis (FEA).

Moreover, a further literature analysis suggests that: i) it is possible to enhance fatigue strength acting on the stent cell design but such an improvement has its counterpart in a loss of stiffness [22, 23]; ii) a tapered strut profile enhances the stent fatigue strength, being thus an ideal starting point for the stent design optimization [24, 25].

Relying on the previous observations, in the present study we propose a *multi-objective* optimization procedure acting on both stent cell geometry and strut shape to enhance the fatigue strength of a Nitinol stent and its scaffolding capabilities. In particular, the optimization framework accounts for non-linear structural FEA combined with a Multi Objective Genetic Algorithm (MOGA) [26] based on Kriging response surfaces.

## Materials and methods

## Fatigue strength analysis

For the purposes of our study we adopt a strain-based approach, which is the most suitable method to deal with fatigue of Nitinol stent, as suggested by Pelton and Robertson [27]. In particular, in case of time-varying cyclic loads, it is possible to define the mean and the alternating value of the first principal strain, respectively



FIGURE 6: Constant fatigue life diagram [23, 28]: shaded area represents specimens conditions that survived  $10^7$  cycles while the dashed line represents the value of  $\varepsilon_a$ , i.e., 0.4%, that we adopt in the present paper as conservative threshold.

 $\varepsilon_m$  and  $\varepsilon_a$ , as:

$$\varepsilon_m = \frac{\varepsilon_{max} + \varepsilon_{min}}{2} \tag{1a}$$

$$\varepsilon_a = \frac{|\varepsilon_{max} - \varepsilon_{min}|}{2} \tag{1b}$$

where  $\varepsilon_{max}$  and  $\varepsilon_{min}$  are respectively the maximum and the minimum principal strain values in a loading cycle.

As demonstrated by Pelton et al. [23, 28], who tested to failure planar diamondshape specimens under various combinations of  $\varepsilon_m$  and  $\varepsilon_a$ , the fatigue strength mainly depends on the alternating value of the first principal strain  $\varepsilon_a$ . As shown by the diagram depicted in fig. 6, it is possible to define a conservative threshold of 0.4% for the alternating value of the first principal strain  $\varepsilon_a$  for any value of mean strain  $\varepsilon_m$ . It is worth noting that the Damage Tolerance Analysis (DTA) is the alternative method commonly used for the study of fatigue. Such an approach essentially relies on fracture mechanics and Paris-Erdogan law [29]. As concerns Nitinol stents, very few studies have been conducted in order to evaluate the fracture strength and other parameters typical of DTA. One reason is that it holds for values of the flaw size larger than a threshold value below which there



FIGURE 7: Planar projection of a typical "v-shaped" stent obtained by a virtual unrolling of the grid: the x axis represents the axial direction, the y axis represents the circumferential direction while the z axis, orthogonal to the xy plane, is the radial direction. Global dimensions of a the stent and the elements of the cell are shown.

is no propagation of the fracture: as reported in [30] this critical flaw size is about  $15-50 \,\mu m$ . Medical devices such as stents have geometric dimensions that are comparable with this threshold value, making DTA useless: it is therefore more useful to focus on prevention rather than on control of the growth of flaws.

For these reasons it can be assumed that the DTA is more appropriate when the typical dimensions of the device are large enough to support the flaw growth or when, for example, the production-process is not sufficiently established to ensure the absence of flaws of critical dimensions [27].

### Stent geometry

In order to define the link between the overall size of a typical "v-shaped" stent and the size of the single cell, it is appropriate to refer to the planar projection of the stent obtained from a virtual unrolling, as illustrated in fig. 7. In this way, the whole stent design can be thought as a repetition of N cells along the circumference (y axis) and M cells in the axial direction (x axis). For the optimization procedure, we adopt such a simplified planar model. Accordingly, it is possible

$$l_c = \frac{\pi D}{N} \tag{2}$$

where D is the outer diameter of the stent and  $l_c$  is the length of the unrolled cell in the circumferential direction. Similarly, we have:

$$l_z = \frac{L}{M} \tag{3}$$

where L and  $l_z$  are the lengths of the whole stent and of the cell in the axial direction, respectively.

A change,  $\Delta D$ , of the stent diameter *D* leads to a variation of the cell height,  $\Delta l_c$ , (see figs. 7 and 8) that, according to eq. (2), reads:

$$\Delta l_c = \frac{\pi \Delta D}{N} = 2\delta \tag{4}$$

being  $\delta$  the displacement, along y-direction, experienced by the single strut and due to a given variation of the stent diameter  $\Delta D$ . Each cell is made up of three basic elements: strut, link, and crown. Two struts and the crown that connects them constitute the v-shape portion of the planar stent cell [31] as shown in fig. 7. Fatigue strength and scaffolding do not depend only on the cell geometry but also on strut dimensions (width w, length l, and thickness t) and on its shape (constant cross-sectional profile versus variable one). Thus, we restrict our attention in relating fatigue strength and scaffolding capabilities to such geometrical quantities: lower will be the alternating value of the first principal strain, higher would be the fatigue strength, while higher will be in-plane cell stiffness (ratio  $F/\delta$  as shown in fig. 8), higher would be stent scaffolding capability.

To this aim, let us consider a v-shape portion of the planar stent cell as shown in fig. 8, subjected to a total displacement  $\delta_{tot} = 2\delta$  in y-direction resulting from the application of a load F. We consider the strut as a cantilever beam having rectangular cross-section: from simple beam mechanics, under the assumptions of small strain approximation and linear elastic constitutive behavior [22, 23], the maximum elongation in the strut is experienced at the outer curvature. The



FIGURE 8: Stent cell "v-shape" portion with dimensions and applied loads. Axes in x and y directions are parallel to those of fig. 7.

corresponding first principal strain is:

$$\varepsilon = Z \frac{w \,\delta_{tot}}{l^2} \tag{5}$$

having the value of Z = 3/2 for rectangular cross-section. Eq. (5) shows that the principal strain  $\varepsilon$  is proportional to the strut width *w* and inversely proportional to the strut length *l*.

We also consider the opening radial force that a Nitinol stent applies to the vessel wall after the deployment, namely the Chronic Outward Force (COF) which, in case of "v-shaped" stents, can be evaluated considering the geometry and the mechanics of the single "v-shape" portion [22, 23]. Stent and vessel interact with radial forces, acting along the *z*-axis in fig 7, through the external surface of the stent and the internal wall of the vessel. However, forces applied on the vessel wall by a Nitinol stent originates from its circumferential stiffness [22, 23] and, in the same way, vessel recoil is contrasted by stent internal circumferential forces (*y*-axis in fig 7). By analogy, pressure acting on a pipe tend to



FIGURE 9: Force - diameter curve for Nitinol stent design R. The force is referred to the single cell. Dashed line: loading path A-B, continuous line: unloading path B-A, dotted line: reloading path C-D

change its diameter: such changes are opposed by the circumferential stiffness of the pipe. According to such considerations, in the present work, we evaluated COF as the force (*F* in fig 8), in the circumferential direction, resulting from a given "v-shape" displacement  $\delta$ .

A typical Nitinol stent force (per unit cell)-diameter curve is reported in fig. 9, illustrating the concept of biased stiffness. The stent is crimped at diameter of 3 *mm* into the delivery system following the loading curve (path A-B). After the release inside the vessel, the stent expands following the unloading path of the curve (path B-A). When the stent reaches the vessel diameter, i.e. 8.3 mm (point C), it continues to push outward against the vessel wall with the equilibrium force COF equal to 0.3N. On the other hand, vessel recoil is resisted through the force dictated by the reloading curve (path C-D) which is stiffer than the unloading path: the force generated by the stent to resist radial compression (point D) is the Radial Resistive Force (RRF). If the stent is unloaded, it returns to the unloading path, passing through the point C, but with a hysteresis cycle (not shown in figure). From the analysis of fig. 9 we can conclude that RRF increases rapidly with diameter changes, while COF is nearly constant at 0.3N in the neighborhood of

point C. Indeed, COF varies from 0.28N at a diameter of 8.7mm to 0.31N at a diameter of 7.9mm showing a variation less than  $\pm 5\%$  in this range of diameters. COF is proportional to the cell circumferential stiffness [23] as described by the following equation:

$$COF \propto \frac{tw^3}{l^3}$$
 (6)

Eq. (6) shows that COF is proportional to  $w^3$  and inversely proportional to the strut length *l*. Ideally, we would like to increase COF reducing, at the same time, the maximum principal strain: thus, the considered problem involve two objectives that should be simultaneously optimized. Accordingly, we focus our attention to the class of multi-objective optimization problem.

**Remark** The considerations reported in this section are valid only for qualitatively showing the influence of the considered geometrical quantities (t, w, l) on fatigue strength and stiffness of the cell. Indeed, eqs. (5) and (6) are valid only under the assumption of linear elastic mechanical behavior and small strains approximation. Otherwise, the quantity Z in eq. (5) becomes a function of material and geometry non-linearities. Similar considerations are valid for eq. (6).

## **Multi-objective Optimization**

In classical optimization problems only one objective function is considered. However, real problems often involve several objectives that should be simultaneously optimized. We consider, without loss of generality, a multi-objective minimization problem whose formulation is:

$$\begin{cases} \min\{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_k(\mathbf{x})\} \\ s.t. \quad \mathbf{x} \in \Sigma \end{cases}$$
(7)

where components  $f_i: \Sigma \longrightarrow \mathbb{R}$ , i = 1, 2, ..., k are the objective functions and  $\Sigma \subset \mathbb{R}^n$  is the feasible design domain. Furthermore, we define the objective space  $\Omega \subset \mathbb{R}^k$  as the image of  $\Sigma$ , under the mapping function  $\mathbf{f} = [f_1(\mathbf{x}), f_2(\mathbf{x}), ..., f_k(\mathbf{x})];$ 

the elements  $\omega \in \Omega$  are the objective vectors. A design vector  $\hat{\mathbf{x}}$  and the corresponding solution  $\hat{\boldsymbol{\omega}} = \mathbf{f}(\hat{\mathbf{x}})$  of problem (7) are defined trivial if:

$$\boldsymbol{\hat{\omega}}_{j} = f_{j}(\mathbf{\hat{x}}) = \min_{\mathbf{x} \in \Sigma} \left\{ f_{j}(\mathbf{x}) \right\}, \quad \forall j = 1, 2, \dots, k$$
(8)

according to definition (8), the design vector  $\hat{\mathbf{x}}$  is defined trivial if it minimizes simultaneously all objective functions  $f_j$ , j = 1, 2, ..., k. Problem (7) is defined *nontrivial* if does not exist a trivial solution and, in this case, the objective functions are said to be conflicting. When problem (7) is *nontrivial*, there exists a (possibly infinite) number of optimal solutions that can be identified introducing the definition of dominance.

A design vector  $\hat{\mathbf{x}}_1$  dominates another design vector  $\hat{\mathbf{x}}_2$  if both the following conditions are true:

$$f_i(\mathbf{\hat{x}_1}) \le f_i(\mathbf{\hat{x}_2}), \quad \forall i = 1, 2, \dots, k$$

$$(9a)$$

$$\exists j \quad \text{such that} \quad f_j(\mathbf{\hat{x}}_1) < f_j(\mathbf{\hat{x}}_2) \tag{9b}$$

eq. (9a) states that the design vector  $\hat{\mathbf{x}}_1$  is no worse than  $\hat{\mathbf{x}}_2$  for all objectives and eq. (9b) states that design vector  $\hat{\mathbf{x}}_1$  is strictly better than  $\hat{\mathbf{x}}_2$  in at least one objective.

Relying on the concept of dominance, the Pareto set is defined as the set of non-dominated solutions of problem (7). From a mathematical point of view, every design in the Pareto set is an equally optimal solution of the multi-objective optimization problem. We conclude noting that we would like to increase COF reducing, at the same time, the maximum principal strain, but the analysis of eq. (5) and eq. (6) reveals that such objectives are conflicting. Accordingly, we search for optimal solutions within the Pareto set. The selection of one design from the Pareto optimal set can be done selecting the trade-off point, i.e. the Pareto optimal point that is the most appropriated to the design context [32].

### Alternative design

In this section we introduce an alternative design, characterized by the use of a tapered strut, in order to reduce the maximum value of the first principal strain



FIGURE 10: Cantilever beam with symmetric parabolic profile.

and preserving COF, at the same time. Although it has been observed that the use of tapered profile strut may improve fatigue strength of Nitinol stent [25] and such an idea is even covered by patent copyright [24], we note that in literature, to the best of our knowledge, there are not i) any specific information about the optimal geometry with respect to the fatigue strength and COF and ii) available experimental data concerning this type of design.

As an illustrative example we consider the cantilever parabolic-profile, as shown in fig. (10), whose width w(x) is function of the abscissa *x*, as described by the following relation:

$$w(x) = w_1 \left[ \sqrt{1 - \frac{x}{l}} H\left(\frac{l}{2} - x\right) + \sqrt{\frac{x}{l}} H\left(x - \frac{l}{2}\right) \right]$$
(10)

where  $w_1$  is the height of the tips, *l* the beam length and H(x) is the Heaviside unit step function defined as:

$$H(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \le 0 \end{cases}$$
(11)

The selected parabolic-profile has been chosen to obtain a constant value of the first principal strain (and stress) along the first half of the beam, i.e. for 0 < x < l/2. Relation (10) shows that  $w_1/w_2 = \sqrt{2}$ , where  $w_2 = w(l/2)$  is the width at the center of the beam.

In order to capture the impact of the design on the strut principal strain, we compare its maximum value for the tapered and for the uniform profiles. The comparison is provided assuming the same length l and stiffness  $k = F/\delta$  for

both solutions, namely  $k_c$  for uniform profile and  $k_p$  for the tapered one, being F and  $\delta$  the force and the displacement at the free end, respectively.

The analysis is performed relying on the methodology proposed in [33]. Most recent works [34, 35] highlight that such an approach must be carefully considered because tapered beams could show a very different mechanical behavior with respect to prismatic ones. However, given the qualitative nature of the present example and considering that we are examining beam exhibiting slow cross-section variations ( $\left|\frac{dw}{dx}\right| < 0.1 \quad \forall x \in [0, l]$ ), the adopted approach may be considered sufficiently accurate. Summing up, for the constant-section beam of width *w*, the stiffness is:

$$k_c = \frac{tEw^3}{4l^3} \tag{12}$$

while, for the parabolic profile, the beam stiffness is:

$$k_p = \frac{tEw_1^3}{8l^3}$$
(13)

where *t* and *E* are the thickness and the Young modulus of the beam, respectively. The same stiffness for both designs can be obtained imposing the equality of eq. (13) and eq. (12), yielding  $w_1 = \sqrt[3]{2} w \simeq 1.26 w$ .

The expression of the principal strain  $\varepsilon_c(x)$  for the uniform profile reads:

$$\varepsilon_c(x) = \frac{3w\delta}{2l^3}(l-x) \tag{14}$$

while, for the parabolic one, we obtain the following relation:

$$\varepsilon_p(x) = \begin{cases} \frac{3w\delta}{2l^2} \frac{1}{\sqrt[3]{4}} & \text{if } 0 \le x \le \frac{l}{2} \\ \frac{3w\delta}{2l^2} \frac{1}{\sqrt[3]{4}} \left(\frac{l}{x} - 1\right) & \text{if } \frac{l}{2} < x \le l \end{cases}$$
(15)

The expressions of the normalized principal strain along the non-dimensional coordinate x/l are shown in fig. 11. Both solutions have their maximum for x = 0 and their ratio is:

$$\frac{\varepsilon_p(0)}{\varepsilon_c(0)} = \frac{1}{\sqrt[3]{4}} \simeq 0.63 \tag{16}$$



FIGURE 11: Graph of the deformation along the x axis normalized with respect to the maximum that occurs in the constant-section beam  $\varepsilon_c(0)$ .

Eq. (16) shows that, keeping the same stiffness, length l, and thickness t, the considered parabolic-profile beam (10) has a maximum value of strain which is substantially lower than the one experienced by the constant-section beam. Additionally, fig. 11 shows that, in case of constant section, the principal strain  $\varepsilon_c$  varies linearly along the beam axis while the parabolic profile (10) exhibits a constant distribution of the first principal strain along the first half of the beam and then ramps down to zero with a hyperbolic law. Clearly, when considering profiles different to (10), strain distribution along the beam x-axis will be different but, from a qualitative point of view, well-designed tapered profiles contribute to uniform strain field and exhibit lower values of the maximum first principal strain, compared to prismatic ones. Consequently, we conclude that acting on geometrical quantities such as l,  $w_1$ ,  $w_2$ , it is possible to define enhanced geometries that may provide long-term fatigue strength when considered in a structural optimization context.

**Remark** Parabolic profile (10) only depends on two independent parameters: we choose the width w and the length l of the beam. Accordingly, the corresponding beam stiffness (13) does not depend on  $w_2$ . The ratio  $w_1/w_2$  can be varied only changing the functional relationship (10).

### **Finite element model**

The considerations reported in previous sections are used to generate a virtual model of the stent-cell to be used in the structural FEA. Numerical simulations are performed using the commercial software Ansys. The optimization of the stent cell is obtained in terms of control variables corresponding to the geometrical features of the tapered profile, collected in the vector  $\mathbf{x}$  defined as (see fig. 12):

$$\mathbf{x} = [w_1, l, a, b, c]^T \tag{17}$$

where l is the length of the strut,  $w_1$  the width at the ends of the strut, and a, b and c dimensionless variables defined as:

$$a = \frac{w_2}{w_1} \tag{18a}$$

$$b = \frac{r}{w_1} \tag{18b}$$

$$c = \frac{w_k}{w_1} \tag{18c}$$

being  $w_2$  the width at the midpoint of the strut, r the crown outer radius and  $w_k$  the width of the link. Nitinol stents are usually laser-cut from a standard tube using a crimped design and then expanded and heat-treated to reach the final diameter. In crimped design, the thickness of the strut is usually constant for the convenience of the laser-cutting process and the saving of expensive materials. If the thickness is changed, the diameter of the compact design has to be also changed, thus the original tube will not be compatible. For the mentioned reason, during the optimization process, the thickness t is kept fixed, i.e.  $t = 200 \,\mu m$ .

The overall cell dimensions  $l_c$  and  $l_z$  are assumed constant during the optimization procedure because they depend on the number of cells in the circumferential and the longitudinal directions, namely N and M, as defined by eqs. (2) and



FIGURE 12: Parametric model of the stent-cell.

(3) respectively. Indeed, variations of these dimensions may result in an excessive variation of the cell surface that is an important feature for the stent performance.

Cell geometry is also defined by the angle  $\phi$  and the length of the link  $l_k$  (see fig. 12) that are related to the chosen values of  $l_c$  and  $l_z$  and to the input variables (eq. (17)) as:

$$l_c = 2l\cos\phi + 2(2b-1)w_1\sin\phi \tag{19a}$$

$$l_z = 2l_k + 2l\sin\phi + 4\left[bw_1 - w_1\left(b - \frac{1}{2}\right)\cos\phi\right]$$
(19b)

that resolved with respect to  $\phi$  and  $l_k$  yield:

$$\phi = \arctan\left[\frac{l\left(l_c w_1\left(2b-1\right)+A\right)}{l^2 l_c + (1-2b) w_1 A}\right]$$
(20a)

$$l_{k} = \frac{l_{z}}{2} - l\sin\phi - 2\left[bw_{1} - w_{1}\left(b - \frac{1}{2}\right)\cos\phi\right]$$
(20b)

where  $A = l \left(4l^2 - l_c^2 + 4 (1 - 2b)^2 w_1^2\right)^{1/2}$ . From eqs. (20a) and (20b), it can be observed that the parameters *a* and *c* do not affect the overall geometry of the cell, but they only have a local effect, in particular on widths  $w_2$  and  $w_k$ , respectively. The strut profile is represented by a spline curve.



FIGURE 13: Curve  $\sigma - \varepsilon$  for an ideal super-elastic material.

Nitinol super-elastic behavior is simulated by the Shape Memory Alloy (SMA) model available in Ansys [36]; the SMA characteristics have been assumed coincident with those reported in [37] and shown in fig. 13. More in detail,  $\sigma_s^{AS}$  and  $\sigma_f^{AS}$  are the values of stress at the start and at the end of the Austenite-Martensite (AM) transformation,  $\sigma_s^{SA}$  and  $\sigma_f^{SA}$  are the initial and final stress in the Martensite-Austenite (MA) transformation,  $E_a$  and  $E_m$  are the moduli of elasticity of austenite and martensite, v is the Poisson's ratio and  $\varepsilon_L$  is the maximum equivalent strain at the end of the AM transformation. The parameter  $\alpha$  takes into account the different behavior in tension and compression and it is defined by the following equation:

$$\alpha = \frac{\left(\sigma_s^{AS}\right)_c - \left(\sigma_s^{AS}\right)_t}{\left(\sigma_s^{AS}\right)_c + \left(\sigma_s^{AS}\right)_t}$$
(21)

where  $(\sigma_s^{AS})_c$  and  $(\sigma_s^{AS})_t$  are respectively the compressive and tensile stress at the start of the AM transformation.

The cell model is discretized with the 8-node brick element Solid185 available in Ansys element library, with full integration. A convergence analysis was performed to ensure a suitable mesh refinement. The quantity selected during the convergence analysis was the maximum value of the first principal strain on the whole strut, after the crimping inside the delivery system (end of step 1.).



FIGURE 14: Finite element model. a) Planes of symmetry  $\alpha$ ,  $\beta$  and  $\gamma$  for the unit cell. b) FE-model with boundary conditions and some detail of the mesh.

The analysis was performed decreasing the average element size in step of  $1 \mu m$  in the range  $20 \mu m - 10 \mu m$  and using several geometries of the strut. The best trade-off between solution accuracy and efficiency was obtained using an element size of  $12 \mu m$ . The adopted mesh involves a number of elements which varies, approximately, between 30000 and 40000 according to the considered design.

In fig. 14a are shown the whole cell and its geometrical planes of symmetry  $\alpha$ ,  $\beta$  and  $\gamma$ . We simulated only the strut imposing symmetry boundary conditions on the surfaces resulting from the intersection of the cell with such planes. In particular (see fig. 14b), on the surface *F* parallel to the *xy* plane, displacements  $\delta$  along *z*, due to the changes in diameter *D*, are imposed. On the surface  $A \subset \beta$  parallel to the *xy* plane, displacements in the *z* direction are prevented, on the surface  $B \subset \gamma$  parallel to the *xz* plane, displacements in the *y* direction are prevented, while on the surface  $C \subset \alpha$  parallel to the *yz* plane, displacements in the *x* direction are prevented.

The stent under investigation is characterized by a diameter D = 10.5 mmand a length L = 42 mm; then, considering a number of cells equal to N = 14 and M = 7 in the circumferential and axial directions respectively, by the relations (2) and (3) we obtain the circumferential length  $l_c$  and the axial length  $l_z$  of the cell as  $l_c = 2.4 mm$  and  $l_z = 7 mm$ . The considered loading history (fig. 15) involves four distinct steps:



FIGURE 15: Displacement history imposed on strut free end. Step 1: stent crimping, step 2: stent deployment, step 3 and step 4: stent contraction and expansion, respectively, due to blood pressure variation.

- Step 1. Stent crimping: the stent diameter goes from diameter  $D_0 = 10.5 mm$  to diameter  $D_1 = 3 mm$ . It follows (eq. (4)) that the displacement in the z direction of the surface F (fig. 14b) reads  $\delta_1 = 841 \mu m$ .
- Step 2. Stent deployment into the vessel (femoral artery): the stent diameter goes from diameter  $D_1 = 3 mm$  to diameter  $D_2 = D_s = 9.6 mm$  which coincides with the diameter of the stent at the end of the systolic phase [23]. The resulting displacement, in agreement with the eq. (4), is equal to  $\delta_2 =$  $101 \mu m$ .
- Step 3. Contraction of the stent due to the diastolic blood pressure: the stent diameter goes from  $D_2 = 9.6 mm$  to diameter  $D_3 = D_d = 9.3 mm$  coincident with the diameter at the end of the diastolic phase; the displacement at the end of this step is equal to  $\delta_3 = 135 \,\mu m$ .
- Step 4. Expansion of the stent: return to systolic diameter  $D_4 = D_s = 9.6 mm$ , corresponding to the cycle end.

In order to evaluate the change in diameter  $\Delta D = D_s - D_d$  in step 3 and 4, resulting from a pressure variation  $\Delta p$ , we set the arterial compliance as [38]:

$$C = 100 \frac{D_s - D_d}{D_d} = 3.26\%$$
(22)
corresponding to a variation in the blood pressure  $\Delta p = 100 \, mmHg$ ; similar compliance values are obtained in [39]. According to [38], the corresponding cross sectional arterial stiffness  $K_A$ , i.e. the inverse of the compliance per unit of length of the vessel is:

$$K_A = \frac{dp}{dA} = \left(\frac{1}{l}\frac{dV}{dp}\right)^{-1} = 12.1\frac{mmHg}{mm^2}$$
(23)

where A, l and V are the cross sectional area, the length and the volume of the vessel, respectively.

The quantities of interest are the alternating maximum value of the first principal strain  $\varepsilon_a$  and the chronic outward force COF. In order to evaluate them, we coded an Ansys Parametric Design Language (APDL) script. More in detail, at the end of step 3 and 4 for each element of the model the values of the first principal strain are evaluated, and then the mean values  $\varepsilon_m$  and the alternating value  $\varepsilon_a$  are calculated: the maximum value of  $\varepsilon_a$  is stored for each design point **x**. Similarly, a quantity proportional to COF, represented by the force acting on the surface *F* (indicated in fig. 14b) at the end of step 2 and necessary to keep the displacement  $\delta_2$ , is computed and stored.

**Remark** As observed in section I, COF is the opening force that the Nitinol stent applies to the vessel wall after the deployment. It can be indifferently evaluated at the end of step 2 or step 4, but not at the end of step 3, because of the biased stiffness of Nitinol stents.

### Kriging response surfaces

For completeness, a brief description of Kriging Surfaces (KS) [40–42] is given. KS predict the response  $z(\mathbf{x})$  of a function  $f(\mathbf{x})$  at unobserved design points  $\mathbf{x} \in \Sigma \subset \mathbb{R}^n$  relying on the known values  $f(\tilde{\mathbf{x}}^i)$  at all the sampled points  $\tilde{\mathbf{x}}^i$ , i = 1, 2, ..., M.

We define  $\tilde{\mathbf{f}}$  as the vector of dimension M, that contains the values of the function  $f(\mathbf{x})$  at each sampled point, namely  $\tilde{\mathbf{f}} = [f(\tilde{\mathbf{x}}^1), f(\tilde{\mathbf{x}}^2), \dots, f(\tilde{\mathbf{x}}^M)]^T$ . The general expression of KS is:

$$z(\mathbf{x}) = d(\mathbf{x}) + r(\mathbf{x}) \tag{24}$$

where  $d(\mathbf{x})$  is a polynomial function of  $\mathbf{x}$ , and  $r(\mathbf{x})$  is the realization of a normally distributed Gaussian random process with zero mean, variance  $\sigma_r^2$  and non-zero covariance. The term  $d(\mathbf{x})$  in eq. (24) is usually termed as "trend" as it globally approximates the unknown function  $z(\mathbf{x})$  over the feasible design space  $\Sigma$ , while the term  $r(\mathbf{x})$  allows for local deviations, enabling KS to interpolate the *M* sampled points. The term  $d(\mathbf{x})$  is defined as:

$$d(\mathbf{x}) = \mathbf{q}^T(\mathbf{x})\mathbf{v} \tag{25}$$

where  $\mathbf{q}(\mathbf{x}) = [q_1(\mathbf{x}), q_2(\mathbf{x}), \dots, q_m(\mathbf{x})]^T$  is the polynomial basis vector, which dimension *m* depends on the degree of  $d(\mathbf{x})$  -2 in the present work- and on the dimension *n* of the design space  $\Sigma$ ;  $\mathbf{v} = [v_1, v_2, \dots, v_m]^T$  is a vector of unknown coefficients. The covariance matrix  $\mathbf{C}$  of  $r(\mathbf{x})$  is a *M* x *M* matrix, whose elements are given by:

$$C_{ij} = \sigma_r^2 R_{ij} \tag{26}$$

where  $R_{ij}$  are the elements of **R** representing the spatial correlation functions between each pair  $(\tilde{\mathbf{x}}^i, \tilde{\mathbf{x}}^j)$  of the sampled points. The spatial correlation function used in the present work is a Gaussian correlation function defined as:

$$R_{ij} = R(\tilde{\mathbf{x}}^i, \tilde{\mathbf{x}}^j) = \exp\left(-\sum_{k=1}^n \lambda_k \left|\tilde{x}_k^i - \tilde{x}_k^j\right|^2\right)$$
(27)

where  $\lambda_k$ , k = 1, 2, ..., n, are unknown correlation parameters and the quantities  $\tilde{x}_k^i$  and  $\tilde{x}_k^j$  are the  $k^{th}$  components of the sampled points  $\tilde{\mathbf{x}}^i$  and  $\tilde{\mathbf{x}}^j$ , respectively. Given such assumptions, the vector of unknown coefficients  $\mathbf{v}$  in eq. (25) is obtained by least square regression, obtaining:

$$\tilde{\mathbf{v}} = \left(\mathbf{Q}^T \, \mathbf{R}^{-1} \, \mathbf{Q}\right)^{-1} \mathbf{Q}^T \, \mathbf{R}^{-1} \, \tilde{\mathbf{f}}$$
(28)

where  $\mathbf{Q}$  is the *M* x *m* matrix defined as:

$$\mathbf{Q} = \begin{bmatrix} \mathbf{q}^{T}(\tilde{\mathbf{x}}^{1}) \\ \mathbf{q}^{T}(\tilde{\mathbf{x}}^{2}) \\ \vdots \\ \mathbf{q}^{T}(\tilde{\mathbf{x}}^{M}) \end{bmatrix}$$
(29)

KS in eq. (24) is thus obtained as:

$$z(\mathbf{x}) = \mathbf{q}^{T}(\mathbf{x})\,\tilde{\mathbf{v}} + \mathbf{g}^{T}(\mathbf{x})\,\mathbf{R}^{-1}\left(\tilde{\mathbf{f}} - \mathbf{Q}\,\tilde{\mathbf{v}}\right)$$
(30)

where  $\mathbf{g}(\mathbf{x})$  is the correlation vector between the point  $\mathbf{x}$  and the sampled data points, namely:

$$\mathbf{g}(\mathbf{x}) = [R(\mathbf{x}, \tilde{\mathbf{x}}^1), R(\mathbf{x}, \tilde{\mathbf{x}}^2), \dots, R(\mathbf{x}, \tilde{\mathbf{x}}^M)]^T$$
(31)

Correlation parameters  $\lambda_k$  in eq. (27) are to be determined before the KS can be computed. They are evaluated maximizing, over  $\lambda_k$ , k = 1, 2, ..., n, the following functional  $\Phi$ :

$$\Phi(\lambda_1, \lambda_2, \dots, \lambda_n) = M \ln(\sigma^2) + \ln(\det \mathbf{R})$$
(32)

where  $\sigma^2$  is the estimate of variance  $\sigma_r^2$  in eq. (26), that is given by:

$$\sigma^{2} = \frac{\left(\tilde{\mathbf{f}} - \mathbf{Q}\,\tilde{\mathbf{v}}\right)\mathbf{R}^{-1}\left(\tilde{\mathbf{f}} - \mathbf{Q}\,\tilde{\mathbf{v}}\right)}{M} \tag{33}$$

The predicted deviation of the KS from the actual response, for each point  $\mathbf{x} \in \Sigma$ , is statistically represented by the root mean squared error  $E(\mathbf{x})$ , that is defined as:

$$E(\mathbf{x}) = \sqrt{\sigma^2 \left[ 1 - \begin{bmatrix} \mathbf{q}^T(\mathbf{x}) & \mathbf{g}^T(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{Q}^T \\ \mathbf{Q} & \mathbf{R} \end{bmatrix} \begin{bmatrix} \mathbf{q}(\mathbf{x}) \\ \mathbf{g}(\mathbf{x}) \end{bmatrix} \right]}$$
(34)

Typical steps in defining KS are: the evaluation of correlation parameters  $\lambda_k$  by maximizing non-linear functional (32), determination of the correlation matrix **R** by (27), evaluation of KS (30) through (28) and (31), error estimation (34).

## Optimization

We assume that the domain  $\Sigma \subset \mathbb{R}^5$  of the multi-objective optimization is bounded within the following intervals:

$$w_1 \in [80, 200]$$
 (35a)

$$l \in [1500, 2500]$$
 (35b)

$$a \in [0.35, 1] \tag{35c}$$

$$b \in [1.2, 1.5]$$
 (35d)

 $c \in [0.5, 1.5]$  (35e)

where  $w_1$  and l are expressed in  $\mu m$  and a, b and c are dimensionless. The range of variation of the input variables, has been chosen considering the typical dimensions of the strut composing commercial Nitinol stents. In particular, we chose as reference design  $\mathbf{x}_R$  the Smart stent by Cordis [43], analyzed in [23, 37], having a constant cross section strut (a = 1) with length l, height  $w_1$  and thickness t equal to  $2000 \,\mu m$ ,  $120 \,\mu m$  and  $200 \,\mu m$ , respectively; other parameters b and c are equal to 1.25 and 1 respectively. Accordingly, the reference design  $\mathbf{x}_R$  is obtained with our parametric model, employing the following design variables:

$$\mathbf{x}_{R} = [w_{1}, l, a, b, c]^{T} = [120, 2000, 1, 1.25, 1]^{T}$$
(36)

The array of the objective functions is defined as:

$$\mathbf{f}(\mathbf{x}) = \left[\boldsymbol{\varepsilon}_{a}(\mathbf{x}), COF(\mathbf{x})\right]^{T}$$
(37)

We preliminarily run a FEA to simulate the reference design  $\mathbf{x}_R$ , obtaining an alternating strain  $\varepsilon_a$  equal to 0.19% with COF = 0.24N (point *R* in fig. 18). Assuming a fatigue limit of  $\varepsilon_L = 0.4\%$  as discussed in previous sections, for the reference design the safety factor yields:

$$S_R = \frac{\varepsilon_L}{\varepsilon_a} = \frac{0.4}{0.19} = 2.1 \tag{38}$$

The multi-objective optimization aims at minimizing  $\varepsilon_a(\mathbf{x})$  and, at the same



number of refinement points

FIGURE 16: Graph of the maximum expected relative error E% vs number of refinement points relative to the Kriging surfaces. It is shown that 45 additional refinement points were needed to reach the selected value of 3% for the maximum predicted relative error. Red dashed line represents the convergence value.

time, maximizing  $COF(\mathbf{x})$ , with  $\mathbf{x} \in \Sigma$ . Furthermore, the additional constraint  $\varepsilon_a \leq 0.2\%$  is imposed to admit only  $\mathbf{x}$  (i.e. designs) corresponding to a value of the fatigue safety factor  $S \geq 2$ : in this way we consider only solutions having safety factor comparable with or higher than the reference design  $\mathbf{x}_R$ . The mathematical formulation of the considered optimization problem reads:

$$Objectives: \begin{cases} \min \{\varepsilon_{a}(\mathbf{x})\} \\ \max \{COF(\mathbf{x})\} \end{cases}$$
(39)  
$$Constraints: \begin{cases} \varepsilon_{a}(\mathbf{x}) \leq 0.2 \\ \mathbf{x} \in \Sigma \end{cases}$$
(40)

The goal of the multi-objective optimization is to evaluate the Pareto set: to



FIGURE 17: Flow chart of the optimization process. A single cycle is described by the following steps: generation of the geometry (CAD) obtained by design variable ( $\mathbf{x}$ ), finite elements analysis (FEA), assessment of the objectives  $\mathbf{f}(\mathbf{x})$ . Both Design of Experiment and Kriging surfaces refinement steps generate design points  $\mathbf{x}$  and evaluate the corresponding values of the objective function  $\mathbf{f}(\mathbf{x})$  by FEA, while the optimization process, performed by MOGA, is based on Kriging surfaces.

obtain it we use a MOGA [26, 44] based on KS. In the present work we use KS for each component of the objective vector  $\mathbf{f}(\mathbf{x})$ . KS are preliminarily built during the domain mapping phase (see fig. 17), which is essentially the selection of a set of points  $\mathbf{x}$  in which  $\mathbf{f}(\mathbf{x})$  is evaluated by FEA. Such initial set is obtained with the Central Composite Design (CCD) method [44]. According to this approach, the objective vector  $\mathbf{f}(\mathbf{x})$  is evaluated for *H* design points, with  $H = 2^m + 2m + n_c = 54$  where *m* is the number of input variables (m = 5), and  $n_c = 12$  is the number of auxiliary points that allow for estimation of second-order effects.

Once the initial mapping of  $\mathbf{f}(\mathbf{x})$  is completed (Design of experiment step in fig. 17), a first KS interpolation of the sampled points is performed, for each objective function. The greater is the number of points used to construct the surface, the lower will be its deviation from the exact value. An error estimator of KS is obtained introducing the maximum predicted relative error  $E_i$ %, defined

as:

$$E_i \% = \frac{100}{f_i^{max} - f_i^{min}} \max_{\mathbf{x} \in \Sigma} [E_i(\mathbf{x})] = \frac{100}{f_i^{max} - f_i^{min}} E_i(\mathbf{\tilde{x}}_i), \quad i = \varepsilon_a, COF \quad (41)$$

where  $f_i^{max}$  and  $f_i^{min}$  are the maximum and the minimum known values (on design points **x**) of the objective  $f_i$  under study, respectively,  $E_i(\mathbf{x})$  is the root mean square error defined in eq. (34) and  $\mathbf{x}_i$  is the design point for which the error  $E_i(\mathbf{x})$  is maximum. Clearly, the error  $E_i\%$  is not the same for both the objective functions: we define the error  $E\% = \max_i [E_i\%]$  and  $\mathbf{x}$  the point in which E% occurs. We opt for a value of the maximum predicted relative error of 3% as best trade-off between computational time needed for solving KS and accuracy. In order to obtain the requested value of E%, for each response surface refinement step, we generate the additional refinement points  $\mathbf{x}$ , and we use the corresponding  $\mathbf{f}(\mathbf{x})$ , calculated by FEA, to update KS.

This iterative process is concluded when the convergence is reached, as shown in fig. 16. As depicted in fig. 17, once the refinement of KS is obtained, i.e., the response surface phase is completed, the optimization step can be performed.

# Results

The obtained Pareto front, reported in fig. 18, shows two branches, namely *A* and *C*, characterized by different trends of input variables; in particular, the part *A* is generated by the set of arrays  $\mathbf{x}_A$  such that:

$$\mathbf{x}_{A} = [w_{1}, l, a, b, c]^{T} = [w_{1}, 2500, 0.5 - 0.6, 1.5, 1.5]^{T}$$
(42)

with  $w_1$  varying from  $80 \mu m$  to  $200 \mu m$  for increasing values of *COF*. Relation (42) states that branch A is only function of the width of the strut  $w_1$ , that may be increased when more scaffolding capabilities are requested. As concerns the length of the strut *l*, the crown radius *b* (eq. (18b)) and the width of the link *c* (eq. (18c)), their optimal values are obtained increasing them as much as possible, i.e. choosing their maximum allowed in the considered range (see eqs. (35)).



FIGURE 18: Set of Pareto optimal-points: two main different zone are present: branch A and branch C. Point R represents the constant-section strut design, point B represents the optimized tapered strut and point I represents the same geometry of the design R but with tapered profile.

Moreover, we observe that the optimal value of the input parameter a, that represents the ratio between the width at the center and at the end of the strut (see eq. (18a)), varies among 0.5 - 0.6; consequently, the optimal solutions are obtained when the strut profile is not constant.

The branch *C* is generated by the the set of arrays  $\mathbf{x}_C$  such that:

$$\mathbf{x}_{C} = [w_{1}, l, a, b, c]^{T} = [200, l, 0.6 - 0.64, 1.5, 1.5]^{T}$$
(43)

with the length *l* decreasing from  $2500 \,\mu m$  to about  $1700 \,\mu m$  for increasing values of *COF*. Relation (43) states that branch C is only function of the length of the strut *l*, that may be decreased when higher scaffolding is required. Similarly to the case of branch *A*, optimal design in branch *C* are obtained by increasing the width of the strut  $w_1$ , the crown radius *b* and the width of the link *c* up to their maximum value. The optimal value of the parameter *a* varies in the range 0.6 - 0.64.

Better results should be obtained allowing the optimization for higher value of the input variables l,  $w_1$ , b and c in the design space  $\Sigma$ . However, such extension will involve the change of the length and of the height of the unit cell, that are fundamental parameters in stent design. The parameter a for the Pareto set shows small oscillations in the reported ranges for branches A and C, without a well-defined trend. Accordingly, we considered a nearly constant. It is also important to note that the Pareto optimal set is always represented by tapered strut profiles with a ratio between the width at the center and at the end of the strut ranging in the interval 0.5-0.65.

# Discussion

In order to highlight the improvements in stent fatigue strength achieved by the proposed optimization analysis, we compare the performance of our resulting stent design with the reference design  $\mathbf{x}_R$ .

We note that all the points falling within the area  $BRR_c$ , depicted in fig. 18, are represented by design parameters that improve, compared to the reference design, the fatigue strength or the scaffolding, or both simultaneously. Moreover,

all the points that are on the portion of the Pareto front delimited by points B and  $R_c$ , represent, by definition, the solutions for which it is not possible to further improve the fatigue strength without decreasing scaffolding capabilities and vice-versa. Accordingly, such solutions are equivalent and all of them are optimal designs (in Pareto sense) in the domain  $\Sigma$ : the best design trade-off can be selected by restricting the attention to the Pareto set.

As explanatory case study, we show how we maximize fatigue strength, selecting an optimal solution from the Pareto set, under the requirement of leaving *COF* unchanged with respect to the design  $\mathbf{x}_R$ . Such optimal solution (fig. 18) is represented by the point *B* defined as:

$$\mathbf{x}_{B} = [w_{1}, l, a, b, c]^{T} = [163, 2493, 0.57, 1.49, 1.4]^{T}$$
(44)

for which we obtain an alternate strain  $\varepsilon_a = 0.079\%$  and, consequently, the fatigue safety factor yields:

$$S_B = \frac{\varepsilon_L}{\varepsilon_a} = \frac{0.4}{0.079} = 5.1$$
 (45)

Comparing eqs. (38) and (45) we observe that, with the same scaffolding capabilities, introducing the optimized tapered profile (in this case  $w_1 = 163 \,\mu m$ ,  $w_2 = 93 \,\mu m$ ,  $l = 2493 \,\mu m$ ), it is possible to increase the fatigue safety factor under pulsatile loads of approximately 2.4 times.

The effect induced by the introduction of the tapered profile only in the reference design  $\mathbf{x}_R$  is investigated considering the design resulting from the following input parameters:

$$\mathbf{x}_{I} = [w_{1}, l, a, b, c]^{T} = [120, 2000, 0.57, 1.25, 1]^{T}$$
(46)

The design  $\mathbf{x}_I$  differs from the reference design  $\mathbf{x}_R$  (eq. (36)) only for the value of the parameter a = 0.57 selected in correspondence with the absolute minimum point for the alternating strain  $\varepsilon_a$ . Therefore, the corresponding geometries are equal, except for the strut profile, which is tapered in the design  $\mathbf{x}_I$ . For such design (fig. 18) we find an alternating strain  $\varepsilon_a = 0.11\%$  and a value of the *COF* equal to = 0.19N. Assuming a fatigue limit of  $\varepsilon_L = 0.4\%$  the fatigue safety factor

Design	<b>w</b> <sub>1</sub>	1	а	b	с	$\epsilon_a$	COF
	$[\mu m]$	$[\mu m]$				[%]	[N]
X <sub>R</sub>	120	2000	1	1.25	1	0.19	0.24
<b>X</b> <sub>B</sub>	163	2493	0.57	1.49	1.4	0.079	0.24
XI	120	2000	0.57	1.25	1	0.11	0.19

TABLE 3: Geometrical features and value of the objectives for the typical  $(x_R)$ , optimized  $(x_B)$  and tapered  $(x_I)$  design.

reads:

$$S_I = \frac{\varepsilon_L}{\varepsilon_a} = \frac{0.4}{0.11} = 3.6\tag{47}$$

whereas the ratio between the *COF* corresponding to design points  $\mathbf{x}_I$  and  $\mathbf{x}_R$  is 0.19/0.24 = 0.79. Then, we conclude that only considering the tapered profile allows to increase significantly the fatigue strength but, at the same time, it involves a relative loss of scaffolding capabilities, approximately equal to 20%. Furthermore, as observed as regard to the design  $\mathbf{x}_R$ , the design  $\mathbf{x}_I$  does not belong to the Pareto set and then it is not a optimal solution in the domain  $\Sigma$ : indeed with the same scaffolding of  $\mathbf{x}_I$  it can be obtained a design with better fatigue strength (point  $I_E$  in fig. 18) or, with the same fatigue strength, better scaffolding capabilities may be reached (point  $I_C$  in fig. 18). The designs considered in this section are reported in table 3.

From an analysis of fig. 19 it is evident that the parts of the cell with higher risk of failure are near to the external part of the crown, as confirmed by other authors [45]. Moreover, the tapered profile allows to redistribute the strain along a wider part of the strut yielding a decrease of its maximum value as discussed in previous sections.

In fig (20) we show the resulting stent unit cell for both designs  $\mathbf{x}_{\mathbf{R}}$  and  $\mathbf{x}_{\mathbf{B}}$ . The length and the height of the unit cell are the same for both designs, while the corresponding geometries differ for the strut profile, crown radius and link width.

## Limitations

The major limitation of this study lies in the execution of numerical simulations considering the entire cell in a planar configuration. As already highlighted by



FIGURE 19: a) Contour plot of the alternating strain  $\varepsilon_a$  for different designs of the cell: design *B* represents the optimized profile, design *R* represents typical (constant section) profile while design *I* is equal to *R* except for the tapered profile. b) Details of the proposed designs. From top to bottom: design *B*, *R* and *I* 



FIGURE 20: Stent cell geometries. A) Typical design R. B) Optimized design B

other authors [19, 46, 47], it may be considered sufficiently accurate although i) the actual complete 3D model has curved shape and ii) stents interact with vessels, resulting in a mechanical response influenced by contact phenomena. Results much closer to the in vivo conditions may be obtained by optimizing complete models of stents. In this regard, experimental tests aimed at validate the proposed optimized design may be useful.

It is worth noting that, in addition to the time needed to implement the optimization process (parametric model, boundary and load conditions, post-processing of results), the considered problem requires non-trivial computation times; then, more realistic study require computational platforms such supercomputing.

# Conclusions

The present study discusses the use of multi-objective stent design optimization to enhance fatigue life of self-expanding Nitinol stent and vessel scaffolding capability. The results obtained through the proposed optimization study are related to a vessel with assigned compliance and blood pressure variation. The methodology introduced is still valid and can be applied also to different pressure cycles and anatomical positions. The study results confirm that the use of tapered strut profile should be a primary key factor to reduce and uniform the strain field along the strut and thus to enhance the fatigue life of the whole stent. The obtained Pareto set allows the designer for the selection of optimized solution, according to the specific design requirements.

As illustrative example we compared a commercial reference design with an optimized design, chosen from the obtained Pareto set, under the requirement of leaving COF unchanged. The proposed approach suggests that the enhancement of stent fatigue life can be achieved combining tapered strut profile with the following changes in the design of the cell:

- an increase of 25% of the strut length;
- an increase of 40% of the strut width at the strut extremities.

Moreover, the results suggest that the width narrowing at the middle of the strut, due to the profile tapering, should be stay among 35% - 50%.

Under such indications, it is possible to achieve a marked improvement of the fatigue safety factor, i.e., about 2.4 times, compared to the typical design (strut with constant section), without any loss of scaffolding capabilities.

The present study may be used as a starting point for further optimization analyses addressing the design of brand-new peripheral stent models. Further developments can address extension approach to a full 3D case or experimental validation of the achieved results by the performance of fatigue tests for the proposed stent strut design.

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# Part II

# Anomalous thermomechanical behavior

# Fractional-order theory of thermo elasticity I: generalization of the Fourier equation\*

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#### ABSTRACT

**Objectives:** The paper deals with the generalization of the Fourier-type relations in the context of fractional-order calculus. Fractional-order calculus has been also used in the theory of heat conduction to generalize the classical Fourier and Cattaneo transport equations. However, no physical ground in the formulation of neither anomalous heat transfer nor thermo-elasticity theory has been

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provided, leading to a non-physical representation of the thermoelastic phenomena reported in such studies. In the present work, a physical description of the fractional-order Fourier diffusion equation is proposed.

**Methods:** We obtain a fractional-order Fourier diffusion law from a multiscale rheological model. Indeed, the instantaneous temperature - flux equation of the Fourier-type diffusion is generalized introducing a self-similar, fractal type mass clustering at the micro-scale.

**Results:** The resulting conduction equation at the macro-scale yields a Caputo's fractional derivative with order  $\beta \in [0,1]$  of temperature gradient. The order of the fractional-derivative is found to be related to the fractal assembly of the micro-structure. The distribution and the temperature raising in simple rigid conductors have been also reported to investigate the influence of the derivation order on the temperature field.

**Conclusions:** The solution of the fractional heat equation  $(0 < \beta < 1)$ , governed by Mittag-Leffler functions, exhibits for small times a much faster rising, and for large times, a much slower decay, compared with the solution of classical heat equation, governed by exponential functions. Accordingly, the main property of the anomalous heat transfer is that the time-rate of change at which the resulting temperature field reaches a steady state, becomes higher as the discrepancy from the Fourier law increases: the thermal steadiness is consequently achieved, by anomalous conductors, employing longer times than Fourier ones. Such particular behavior represents the "long-tail memory effect", due to the power law thermal memory of such materials.

# Introduction

Fractional-order calculus is usually referred as the generalization of the wellknown ordinary differential calculus introducing real - order integrals and derivatives. It traces back to the basic definitions by Riemann as well as to successive memories of famous mathematicians, among the others (see e.g. [1]), while, more recently, other scientists focused on the feasibility of integral measures involved in fractional-order operators [2–4]. After definitions and feasibility of fractional-order operators, their introduction into continuum field theories has received significant interests worldwide [5–10]. Indeed the replacement of classical operators with their real-order counterparts  $\left(\frac{d}{dx} \rightarrow \frac{d^{\alpha}}{dt^{\alpha}} \operatorname{and} \frac{d}{dt} \rightarrow \frac{d^{\beta}}{dt^{\beta}}\right)$  with  $\alpha, \beta \in \Re$  has proved to be valuable in several engineering and physical contexts predicting phenomena with great accuracy [5, 11–13]. The use of fractional-order operators has been also reported in non-local continuum field theories of mechanics [14–20], non-local heat transfer [21–24] stochastic analysis [25–28], diffusive transport [1, 29–31], biophysics [32], rheology and many others.

Despite the wider and wider use of fractional-order operators an important question has not been answered:"What is the physics beyond the use of fractional-order derivatives?" The answer to this fundamental issue would be of great stimulus for worldwide researchers to re-derive the classical continuum field theories in terms of fractional-order operators.

On that subject, a strong effort has been profused during last years to provide a solid physical ground in the use of fractional-order derivative in the transport equations. Cases involving polymer viscoelasticity, anomalous fluid diffusion, as well as laminar flow across fractal sets have been recently provided [33–36].

Fractional-order calculus has been also used in the theory of thermo-elasticity to generalize the classical Fourier and Cattaneo transport equations [37–40]. However, no physical ground in the formulation of neither anomalous heat transfer nor thermo-elasticity theory has been provided, leading to a non-physical representation of the thermoelastic phenomena reported in such studies.

In the present work, the authors obtain a fractional-order Fourier diffusion law from a multi-scale rheological model. This is done by means of the introduction of an inhomogeneous conductor leading to an anomalous time evolution as  $t^{\beta}$  with  $0 \le \beta \le 1$  [41]. Such consideration is used in the paper to provide a physical exact description of the fractional-order Fourier diffusion equation that is also thermodynamically consistent. Numerical experiments have been reported to show the evolution of the temperature field in different domains with different boundary conditions. Anomalous thermo-elasticity is analyzed in Part II of this paper [42], where a measure of the signature of the anomaly based on a measure

# The thermodynamical model of power-law temperature evolution

In this section the authors show that anomalous rising of temperature in the form of power-law  $t^{\beta}$  is obtained using arguments presented extensively in [42].

It is assumed a distribution of n + 1 masses  $m_j = A_j \Delta z$  with j = 1, 2, ..., n + 1, where  $A_j$  represents the cross-sectional area of the  $j^{th}$  mass and  $\Delta z = l/(n+1)$ its length, being  $l = (n+1)\Delta z$  the overall length of the conductor as in Fig. 21 a). The masses, located at abscissas  $z_j = j\Delta z$  and separated by adiabatic walls from the external environment, are connected each other by a perfect conductor, so that thermal energy exchange may occur only along the *z* direction. The thermodynamic state variables describing the system are assumed as the macroscopic temperatures  $T_j(t)$  of the masses  $m_j$  for j = 1, 2, ..., n + 1.

The energy balance of the  $j^{th}$  mass  $m_j$  involves the rate of the internal energy  $U_j$  and the energy flux along the conductors  $m_j$ , namely,  $q_j(t)$  and  $q_{j-1}(t)$  that can be written as:

$$\frac{dU_j(t)}{dt} = m_j \frac{du_j(t)}{dt} = m_j C_j^{(V)} \frac{dT_j(t)}{dt} = A_{j-1}q_{j-1}(t) - A_j q_j(t)$$
(48)

where with  $C_j^{(V)} = \left(\frac{\partial u_j}{\partial T}\right)_{T_0}$  is denoted the specific thermal capacity at constant volume that is assumed to be uniform for the considered temperature interval;  $u_j(t)$  is the internal energy function density of the mass  $m_j$ .

Given the assumption that only diffusive phonon-phonon interaction yields thermal energy transport, the thermal energy flux  $q_j(t)$  of the mass located at abscissa  $z_j$  may be expressed as:

$$q_j(t) = -\chi_j^{(T)} \frac{T_{j+1}(t) - T_j(t)}{z_{j+1} - z_j} = -\chi_j^{(T)} \frac{T_{j+1}(t) - T_j(t)}{\Delta z}$$
(49)



FIGURE 21: Thermodynamical model of anomalous temperature rising: a) The concentrated mass system; b) Thermal energy balance of the  $j^{th}$  - mass

where with  $\chi_j^{(T)}$  the thermal conductivity of the  $j^{th}$  conductor is denoted. Substitution of (49) in (48) yields the thermal energy balance as an ordinary differential equation system in the temperatures  $T_j(t)$ .

$$\rho \Delta z C_j^{(V)} \dot{T}_j(t) = \frac{1}{\Delta z} \left[ \chi_{j+1}^{(T)} T_{j+1}(t) - \left( \chi_j^{(V)} + \chi_{j+1}^{(V)} \right) T_j(t) + \chi_{j-1}^{(T)} T_{j-1}(t) \right]$$
(50)

where it is assumed that  $A = A_j$  for j = 1, 2, ..., n + 1 and that the masses  $m_j = \rho A \Delta z$  (see fig. (21)) where  $\rho$  is the mass density. The energy balance equations reported in eq. (50) involve masses  $m_j$  with j = 2, 3, ..., n as the temperature of the  $m_{n+1}$  mass of the system has been set to the value  $T_{n+1} = 0$  without loss of generality. Energy balance of mass  $m_1$  of the thermodynamical system in fig. (21) b) involves an external thermal energy flux, denoted in the following formula as  $\bar{q}(t)$ , yielding:

$$C_1^{(V)} \Delta z \rho \dot{T}_1(t) + \chi_1^{(T)} \frac{T_2(t) - T_1(t)}{\Delta z} = \bar{q}(t)$$
(51)

The anomalous time-scaling of the temperature field is achieved assuming that the spatial distribution of the thermal conductivity  $\chi_j^{(V)}$  and the specific thermal capacity  $C_j^{(V)}$  varies along the masses  $m_j$  with the relations:

$$C_j^{(V)} = \frac{C_\alpha^{(V)}(j\Delta z)^{-\alpha}}{\Gamma(1-\alpha)}$$
(52a)

$$\chi_j^{(T)} = \frac{\chi_\alpha^{(T)}(j\Delta z)^{-\alpha} \Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma(1-\alpha)}$$
(52b)

where  $\Gamma(\bullet)$  is the Euler-Gamma function and the real exponent  $\alpha$  belongs to the interval  $-1 \leq \alpha < 1$  for diffusion-type phenomena. It must be remarked that the assumption of a power law variation of the thermal properties of the non-homogeneous rigid conductor is the fundamental hypothesis from which comes out the fractional constitutive relation between the heat flux and the temperature gradient. Indeed, for the case  $\alpha = 0$ , an homogeneous conductor and, consequently, the classical Fourier transport equation is obtained.

Coefficients  $C_{\alpha}^{(V)}$  and  $\chi_{\alpha}^{(T)}$  are the thermal capacity and the thermal conductivity, respectively, with anomalous physical dimensions in the International System of Units (SI) as:

$$\left[C_{\alpha}^{(V)}\right] = m^{2+\alpha} K^{-1} s^{-2} \quad ; \quad \left[\chi_{\alpha}^{(T)}\right] = kg m^{1+\alpha} K^{-1} s^{-3} \tag{53}$$

In order to show that the discrete mass system yields a power-law time rising of the temperature field it is supposed that, at the same time,  $n \to \infty$ ,  $\Delta z \to 0$  and  $l \to \infty$ . In this framework the functions  $T_j(t)$  and  $q_j(t)$  represents local values of the fields  $T_j(t) \to T(z_j,t)$  and  $q_j(t) \to q(z_j,t)$ .

Under these circumstances the balance equation reported in (48) becomes:

$$\rho C^{(V)}(z) \frac{\partial T(z,t)}{\partial t} = -\frac{\partial q(z,t)}{\partial z}$$
(54)

Eq. (54) describes the balance at location z between the rate of the thermal energy  $\dot{U} = \rho \frac{\partial u}{\partial t}$  and the difference of the outgoing thermal energy q(z+dz,t) and the incoming one q(z,t) in unit time. Introducing the following Fourier transport equation, obtained for  $\Delta z \rightarrow 0$ 

$$q(z,t) = -\chi^{(T)}(z)\frac{\partial T(z,t)}{\partial z}$$
(55)

in eq.(54), the heat equation is obtained as:

$$\rho C^{(V)}(z) \frac{\partial T(z,t)}{\partial t} = \frac{\partial}{\partial z} \left[ \chi^{(T)}(z) \frac{\partial T(z,t)}{\partial z} \right]$$
(56)

In eq.(56) the thermodynamical properties of the distributed mass system are described through the continuous counterparts of eqs. (52 a,b), i.e.  $C_j^{(V)} \to C^{(V)}(z_j)$  and  $\chi_j^{(T)} \to \chi^{(T)}(z_j)$  that read:

$$C^{(V)}(z) = \frac{C^{(V)}_{\alpha} z^{-\alpha}}{\Gamma(1-\alpha)} \qquad ; \qquad \chi^{(T)}(z) = \frac{\chi^{(T)}_{\alpha} z^{-\alpha} \Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma(1-\alpha)} \tag{57}$$

Accordingly, the boundary conditions associated to the heat equation (56) are obtained as the continuous conditions on the first mass  $m_1$  and the last mass  $m_{n+1}$ 

of the discrete system (see fig. 21) under consideration as:

$$\bar{q}(t) = \lim_{z \to 0} -\chi^{(T)}(z) \frac{\partial T(z,t)}{\partial z} \qquad ; \qquad \lim_{z \to \infty} T(z,t) = 0 \tag{58}$$

The temperature field T(z,t) may be obtained introducing the Laplace transform of (56), yielding to an ordinary differential equation in Laplace domain as:

$$\frac{d}{dz}\left[\chi^{(T)}(z)\frac{d\widehat{T}(z,s)}{dz}\right] = s\rho C^{(V)}(z)\widehat{T}(z,s)$$
(59)

where  $\widehat{T}(z,s)$  represents the Laplace transform of the temperature field T(z,t). Relation (59) can be cast, after some straightforward manipulation, as:

$$\frac{d^{2}\widehat{T}(s,z)}{dz^{2}} + \frac{\left[\chi^{(T)}(z)\right]'}{\chi^{(T)}(z)} \frac{d\widehat{T}(s,z)}{dz} - \frac{C^{(V)}(z)}{\chi^{(T)}(z)} s\rho\widehat{T}(s,z) = 0$$
(60)

Substituting for the thermal conductivity coefficient  $\chi^{(T)}(z)$  and the specific heat  $C^{(V)}(z)$  with the corresponding power-laws reported in eqs. (57), the differential equation ruling the temperature field becomes:

$$\frac{d^2\widehat{T}(z,s)}{dz^2} - \frac{\alpha}{z}\frac{d\widehat{T}(z,s)}{dz} - \tau s\widehat{T}(z,s) = 0$$
(61)

where

$$\tau = \rho \frac{C_{\alpha}^{(V)}}{\chi_{\alpha}^{(T)}} \frac{1}{\Gamma\left(\frac{1+\alpha}{2}\right)}$$
(62)

is constant with respect to space z and time t and its value changes with  $\alpha$  as shown in (62). However, physical dimensions of  $\tau$  are  $[\tau] = sm^{-2}$ , consequently they do not depend on the exponent  $\alpha$ . A canonical Bessel equation of second kind may be obtained from eq. (62) introducing the auxiliary function  $\overline{T}(z,s)$  by means of the mapping  $\hat{T}(z,s) = z^{\alpha}\overline{T}(z,s)$  yielding:

$$z^{2}\frac{d^{2}\overline{T}(z,s)}{dz^{2}} + \alpha z\frac{d\overline{T}(z,s)}{dz} - (z^{2}\tau s + \alpha)\overline{T}(z,s) = 0$$
(63)

Solution of eq. (63) involves modified Bessel functions denoted  $Y_{\beta}(z\sqrt{\tau s})$  and  $K_{\beta}(z\sqrt{\tau s})$ , respectively (see [41] for details), where  $\beta$  is related to the scaling exponent  $\alpha$  as:

$$\beta = \frac{1+\alpha}{2} \tag{64}$$

Boundary conditions in Laplace domain yield the integration constants, namely,  $B_1$  and  $B_2$  as:

$$B_1 = 0 \quad ; \quad B_2 = \frac{2^{\beta} \Gamma(2 - 2\beta) \sin(\pi\beta) \left(s\tau\right)^{-\frac{\beta}{2}}}{\pi \chi_{\alpha}^{(T)}} \widehat{\bar{q}}\left(s\right) \tag{65}$$

with  $[B_2] = K s m^{-\beta}$ , so that the temperature field of the distributed mass systems reads:

$$\widehat{T}(z,s) = \frac{2^{\beta} \Gamma(2-2\beta) \sin(\pi\beta) (s\tau)^{-\frac{p}{2}}}{\pi \chi_{\alpha}^{(T)}} \widehat{\bar{q}}(s) z^{\beta} K_{\beta} \left( z \sqrt{\tau s} \right)$$
(66)

Power-law time rising of the temperature field is obtained evaluating the temperature at z = 0 as:

$$\widehat{T}_{0}(s) = \lim_{z \to 0} \widehat{T}(z, s) = \frac{1}{R_{\beta}} s^{-\beta} \widehat{\bar{q}}(s)$$
(67)

where the anomalous thermal diffusivity coefficient,  $R_{\beta}$  reads:

$$R_{\beta} = \frac{2^{1-2\beta} \pi \chi_{\alpha}^{(T)} \csc(\pi\beta) \tau^{\beta}}{\Gamma(2-2\beta) \Gamma(\beta)}$$
(68)

and  $[R_{\beta}] = kg K^{-1} s^{\beta-3}$ . Special cases of eq. (68) can be obtained looking at some representative values of  $\beta$  ans  $\alpha$  as follows:

$$\lim_{\substack{\beta \to 0 \\ \alpha \to -1}} R_{\beta} = \frac{2\chi_{-1}^{(T)}}{\pi}$$
(69a)

$$\lim_{\substack{\beta \to \frac{1}{2} \\ \alpha \to 0}} R_{\beta} = \sqrt[4]{\pi} \sqrt{\rho \chi_0^{(T)} C_0^{(V)}}$$
(69b)

$$\lim_{\substack{\beta \to 1 \\ \alpha \to 1}} R_{\beta} = \rho C_1^{(V)}$$
(69c)

Under the assumption of stationary thermal energy flux  $\bar{q}(t) = \bar{q}_0 U(t)$ , the timevarying temperature function  $T_0(t)$  is obtained applying the inverse Laplace transform to eq. (67), yielding:

$$T_0(t) = \frac{\bar{q}_0}{R_\beta \Gamma(1+\beta)} t^\beta \propto t^\beta \tag{70}$$

that is the power-law temperature time scaling observed in fig. (21) for the discretized mass system considered in the analysis with  $\beta \in [0,1]$  (see e.g.[41] for details).

# The fractional-order generalization of Fourier heat transport equation

In this section the authors introduce a fractional-order generalization of the Fourier transport equation according to the physical model of the power-law described in previous section. To this aim, the basic framework of fractional-order calculus is first provided followed by the physical model used to generalize the Fourier equation and its compatibility with the second law of thermodynamics.

### Preliminary remarks on fractional-order calculus

Fractional calculus may be considered the extension of the ordinary differential calculus to non-integer powers of derivation orders (e.g. see [29, 43]). In this section the authors address some basic notions about this mathematical tool.

The Euler-Gamma function  $\Gamma(z)$  may be considered as the generalization of the factorial function because, when *z* assumes integer values, it follows that  $\Gamma(z+1) = z!$ . The Euler-Gamma is defined as the result of the integral as follows:

$$\Gamma(z) = \int_0^\infty e^{-x} x^{z-1} dx.$$
(71)

The Riemann-Liouville fractional integrals and derivatives with  $0 < \beta < 1$  of functions defined on the entire real axis have the following forms:

$$\left(\mathbf{I}_{+}^{\beta}f\right)(t) = \frac{1}{\Gamma(\beta)} \int_{-\infty}^{t} \frac{f(\tau)}{(t-\tau)^{1-\beta}} d\tau$$
(72a)

$$\left(\mathcal{D}_{+}^{\beta}f\right)(t) = \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \int_{-\infty}^{t} \frac{f(\tau)}{(t-\tau)^{\beta}} d\tau.$$
(72b)

The Riemann-Liouville fractional integrals and derivatives with  $0 < \beta < 1$  of functions defined over intervals of the real axis, namely f(t) such that  $t \in [a,b] \subset \mathbb{R}$ , have the following forms:

$$\left(\mathbf{I}_{a}^{\beta}f\right)(t) = \frac{1}{\Gamma(\beta)} \int_{a}^{t} \frac{f(\tau)}{(t-\tau)^{1-\beta}} d\tau$$
(73)

$$\left(\mathsf{D}_{a}^{\beta}f\right)(t) = \frac{f(a)}{\Gamma(1-\beta)(t-a)^{\beta}} + \frac{1}{\Gamma(1-\beta)} \int_{a}^{t} \frac{f'(\tau)}{(t-\tau)^{\beta}} d\tau$$
(74)

Beside Riemann-Liouville fractional operators defined above, another class of fractional derivative that is often used in the context of fractional calculus is represented by Caputo fractional derivatives defined as:

$$\left({}_{C}\mathsf{D}_{a^{+}}^{\beta}f\right)(t) := \mathsf{I}_{a^{+}}^{m-\beta}\left(\mathsf{D}_{a^{+}}^{m}f\right)(t) \quad m-1 < \beta < m$$

$$(75)$$

and whenever  $0 < \beta < 1$  it reads as follows:

$$\left(c\mathbf{D}_{a^{+}}^{\beta}f\right)(t) = \frac{1}{\Gamma(1-\beta)} \int_{a}^{t} \frac{f'(\tau)}{(t-\tau)^{\beta}} d\tau$$
(76)

A closer analysis of eq. (75) and eq. (76) shows that Caputo fractional derivative coincides with the integral part of the Riemann-Liouville fractional derivative in bounded domain. Moreover, the definition in eq. (75) implies that the function f(t) has to be absolutely integrable of order m (e.g. in eq. (76) the order is m = 1). Whenever f(a) = 0 Caputo and Riemann-Liouville fractional derivatives coalesce.

Similar considerations hold true also for Caputo and Riemann-Liouville fractional derivatives defined on the entire real axis. Caputo fractional derivative may be considered as the interpolation among the well-known integer-order derivatives, operating over functions  $f(\circ)$  that belong to the class of Lebesgue integrable functions  $(f(\circ) \in L^1)$ ; consequently it is very useful in the mathematical description of complex system evolution. It is worth noting that the Laplace and Fourier integral transforms are defined as follows:

$$\mathscr{L}[f(t)] = \int_0^\infty f(t) \mathrm{e}^{-st} dt \tag{77a}$$

$$\mathscr{F}[f(t)] = \int_{-\infty}^{+\infty} f(t) \mathrm{e}^{i\omega t} dt \tag{77b}$$

It is worth introducing integral transforms for fractional operators and, similarly to classical calculus, the Laplace integral transform  $\mathscr{L}(\circ)$  is defined in the following forms:

$$\mathscr{L}\left[\left(\mathbf{D}_{0}^{\beta}f\right)(t)\right] = s^{\beta}\mathscr{L}\left[f(t)\right] - \left[\left(\mathbf{D}_{0}^{\beta-1}f\right)(t)\right]_{t=0} \quad \text{if} \quad 0 < \beta \le 1$$
(78a)

$$\mathscr{L}\left[\left({}_{C}\mathsf{D}_{0}^{\beta}f\right)(t)\right] = s^{\beta}\mathscr{L}[f(t)] - s^{\beta-1}f(0) \quad \text{if} \quad 0 < \beta \le 1$$
(78b)

$$\mathscr{L}\left[\left(\mathbf{I}_{0^{+}}^{\beta}f\right)(t)\right] = s^{-\beta}\mathscr{L}[f(t)]$$
(78c)

In the same way, the Fourier integral transform  $\mathscr{F}(\circ)$  assumes the following forms:

$$\mathscr{F}\left[\left(\mathsf{D}^{\beta}_{+}f\right)(t)\right] = (-i\omega)^{\beta}\mathscr{F}[f(t)] = (-i\omega)^{\beta}\hat{f}(\omega) \tag{79a}$$

$$\mathscr{F}\left[\left(\mathbf{I}_{+}^{\beta}f\right)(t)\right] = (-i\omega)^{-\beta}\mathscr{F}[f(t)] = (-i\omega)^{-\beta}\hat{f}(\omega)$$
(79b)

### The fractional-order generalization of the Fourier equation

Power-law rising of temperature field described in previous sections corresponds, in the context of a linear-order heat transport to a fractional-order relation among thermal flux and temperature. Indeed, assuming that the thermal energy flux across the x = 0 cross-section is a time-dependent function, inverse Laplace transform of (67) yields:

$$T_0(t) = \frac{1}{R_{\beta}} \frac{1}{\Gamma(\beta)} \int_0^t (t-\tau)^{\beta-1} \bar{q}(\tau) d\tau = \frac{1}{R_{\beta}} \left( I_{0^+}^{\beta} \bar{q} \right)(t)$$
(80)

that is a Riemann-Liouville fractional-order integral of order  $\beta \in [0, 1]$  as in (73).

The inverse relation of eq.(80) could be obtained introducing the  $\beta$ -order fractional derivative of both sides of (80) yielding:

$$\bar{q}(t) = R_{\beta} \left( \mathbf{D}_{0^{+}}^{\beta} T_{0} \right)(t)$$
(81)

that is a fractional-order description of the temperature-flux in terms of Caputos' fractional-order derivatives analogous to fractional-order generalization of the Darcy equation ([35]).

A close observation of eq. (81) reveals that it does not correspond to the fractional-order generalization of the Fourier heat transport equation in terms of fractional derivatives, because no spatial gradient of the temperature field is involved, in spite of what occurs in Fourier equation rewritten with fractional calculus formalism, as:

$$\bar{q}(t) = -K_0 \left[ \left( \mathbf{D}_{0^+}^0 \frac{\partial T}{\partial x} \right)(t) \right]$$
(82)

where  $(D_{0^+}^0 f(t))(t) = \frac{d^0 f(t)}{dt^0} = f(t)$  is the 0<sup>th</sup>-order derivative of the function f(t) with respect to t. Fractional-order generalization of the Fourier equation will involve the presence of the real-order derivative  $D^0 \longrightarrow D^\beta$  with  $0 \le \beta < 1$  that is not present in eq. (81).

In order to provide a generalization of eq. (81) in terms of fractional-order derivative of order  $\beta$ , the authors introduce a self-similar conductor micro-structure (see, for example, [44]). In this framework, an 1D conductor with macroscopic thermal conductivity  $\chi_T$ , mass density  $\rho$  and specific heat  $C^{(V)}$  is considered. The conductor is referred to an one-dimensional abscissa *x* and it occupies the interval [0, l] of the real line (see fig. (22a) for further details) where *A* is the crosssectional area of the conductor. A spatial discretization of the conductor with interval  $\Delta x = x_{j+1} - x_j$  is considered along with a spatial thermal energy flux



FIGURE 22: a) Macroscopic thermal conductor, b) Thermal energy flux

along the positive direction of the *x*-axis (Fig. (22b). For an homogeneous conductor, the thermal energy across the cross-section at abscissa  $x_j$ , namely  $q_j(t)$ , depends only on the thermal conductivity  $\chi_T$  and on the temperature gradient  $\frac{\partial T}{\partial x}$  as in classical Fourier equation:

$$q_j(t) = -\chi \lim_{\Delta x \to 0} \frac{\Delta T}{\Delta x} = -\chi \lim_{\Delta x \to 0} \frac{T_{j+1} - T_j}{\Delta x}$$
(83)

According to eq. (83), the study of thermal energy flux across the cross-section at abscissa  $x_j$  can be conducted, without any loss of generality, assuming that  $T_j(t) = -\Delta T$  and  $T_{j+1}(t) = 0$ . The latter assumption is equivalent to the choice of the zero-temperature condition, coincident with the temperature of the cross-section  $T_{j+1}(t)$  as in Fig. (22)a.

In the following the authors assume that the mass density within the element of length  $\Delta x$  is not uniformly distributed at any resolution scale. Given such assumption and introducing a scale factor z, a self-similar cluster of massdistribution is observed as in Fig. 23(b-e). The longitudinal cross-sections of the conductor along the x-axis is shown in Fig. 23(a) assuming a Sierpinski-like mass clustering with the observation scale  $z_k$  for illustrative' sake. In passing, the authors observe that the proposed self-similar micro-structure organization is very different from the fractal mass curdling. Indeed, in the considered self-similar clustering, all the masses observed at resolution scales  $z_0, z_1, \ldots, z_{k-1}$  are present examining the mass condensation at resolution  $z_k$ .

Thermal energy exchange across the mass micro-structure is assumed in the form of phononic-phononic diffusion, ruled by the Fourier relation, in a material


FIGURE 23: Scheme of the self similar mass-distribution

with uniform thermal conductivity  $\chi_0$ . Under these circumstances, masses  $m_k$  and distances  $l_k$  at resolution scale  $z_k$  read:

$$m_k = \rho A_k l_k = \rho a^k \left(\frac{b_0}{z_k}\right)^2 \Delta z_k \Delta x \tag{84}$$

where  $\Delta z_k = z_{k-1} - z_k$ ,  $b_0$  is the edge of the conductor cross-section assumed squared at resolution  $z_0 = 1$  and  $a^k$  is the number of self-similar elements at resolution  $z_k$ ; for the proposed fractal scheme a = 2. The equivalent measure condition is achieved incrementing the resolution factor of a quantity  $z_k$  and introducing an anomalous dimension-dependent density  $\rho_d$  in eq. (84) yielding:

$$\bar{m}_k = \rho_d a^k b_0^d z_k^{1-d} \Delta z_k \Delta x = \rho_d a^k b_0^d z_k^{-\alpha} \Delta z_k \Delta x$$
(85)

where  $d = \frac{\log 2}{2\log 3}$  for the considered mass assembly at the microscale and it represents the Housdorff dimension of the geometric self-similar set describing mass curdling. Thermal energy balance of mass  $\bar{m}_k$  involves a dynamic equilibrium among the rate of internal energy and the net thermal flux across the generic mass  $\bar{m}_k/a^k$  yielding:

$$\frac{\bar{m}_{k}}{a^{k}}\dot{u}_{j}^{(k)} = \rho_{d}b_{0}^{d}z_{k}^{-\alpha}\Delta z_{k}\Delta xC^{(V)}\dot{\theta}_{j}^{(k)}(t) = -q_{j}^{(k-1)}(t)A_{k-1} + q_{j}^{(k)}(t)A_{k} = 
= -\frac{\chi_{T}A_{k-1}^{(c)}}{\Delta z_{k-1}\Delta x}\left(\theta_{j}^{(k)}(t) - \theta_{j}^{(k-1)}(t)\right) + \frac{\chi_{T}A_{k}^{(c)}}{\Delta z_{k}\Delta x}\left(\theta_{j}^{(k-1)}(t) - \theta_{j}^{(k)}(t)\right)$$
(86)

where the relative temperature  $\theta_j^{(k)}(t)$  of the mass  $\bar{m}_k$  at the  $k^{th}$  resolution scale (corresponding to the volume element located at the macroscopic abscissa  $x_j$ ) is introduced; moreover,  $A_k^{(c)} = A_k/a^k$  is the cross-sectional area of the conductor at the resolution  $z_k$ . Bearing in mind that  $A_k^{(c)} = b_0^d z_k^{-\alpha}$ , eq. (86) can be rewritten as:

$$z_{k}^{-\alpha} \dot{\theta}_{j}^{(k)}(t) = \frac{\chi_{T}}{\rho_{d} C^{(V)} (\Delta x)^{2}} \times \left[ \frac{z_{k}^{-\alpha} \theta_{j}^{(k+1)}(t)}{\Delta z_{k}} - \left( \frac{z_{k}^{-\alpha}}{\Delta z_{k}} + \frac{z_{k-1}^{-\alpha}}{\Delta z_{k-1}} \right) \theta_{j}^{(k)}(t) + \frac{z_{k-1}^{-\alpha} \theta_{j}^{(k-1)}}{\Delta z_{k-1}}(t) \right]$$

$$(87)$$

With some straightforward manipulations and letting  $\Delta z_k \longrightarrow 0$ , so that a continuous resolution scale is achieved, eq. (87) becomes:

$$z_{k}^{-\alpha} \dot{\theta}_{j}^{(k)}(z,t) = \frac{1}{\tau_{d} (\Delta x)^{2}} \frac{\partial}{\partial z} \left( z^{-\alpha} \frac{\partial \theta(z,t)}{\partial z} \right)$$
(88)

Eq. (88) is formally analogous to eq. (59) for inhomogeneous conductor presented in previous section but, it is formulated for the micro-structure observed at abscissa  $x_j$ . The boundary conditions associated with the temperature equation (88) read:

$$q_j(t) = q_j(t) = \frac{1}{\Delta x} \lim_{z \to 0} \frac{\partial \theta_j(z, t)}{\partial z}$$
(89a)

$$\lim_{z \to \infty} \theta_j(z,t) = \theta_{j-1}(z,t) = 0$$
(89b)

Solution of eq. (88), accounting for boundary the conditions (89a) and (89b) can be obtained relying on similar arguments as in previous sections, yielding:

$$\widehat{\theta}_{j}(z,s) = \frac{2^{\beta} \Gamma(2-2\beta) \sin(\pi\beta) (s\tau)^{-\frac{\beta}{2}}}{\pi \chi_{T}} \widehat{q}_{j}(s) z^{\beta} K_{\beta} (z\sqrt{\tau_{d}s})$$
(90)

where  $\beta = (\alpha + 1)/2 = (2 - d)/2$ .

Letting  $z \to 0$ , the temperature  $\hat{\theta}_j(z,s)$  tends to  $\hat{\theta}_j(s) = \hat{\theta}_j(x_j,s) = -\Delta \hat{T}(x_j,s)$  yielding:

$$-\Delta \widehat{T}(x_j,s) = \lim_{z \to 0} \widehat{\theta}_j(z,s) = \frac{1}{R_\beta} s^{-\beta} \Delta x \widehat{q}_j(s)$$
(91)

where

$$R_{\beta} = \frac{2^{1-2\beta} \pi \chi_T \csc(\pi\beta) \tau_d^{\beta}}{\Gamma(2-2\beta) \Gamma(\beta)}$$
(92)

Recasting relation (91) the fractional-order generalization of the Fourier equation is obtained as:

$$q(x,t) = -\lim_{\Delta z \to 0} R_{\beta} s^{\beta} \frac{\Delta \widehat{T}}{\Delta x} = -R_{\beta} \left( D_{0^{+}}^{\beta} \frac{\partial T}{\partial x} (x,t) \right) (t)$$
(93)

that has the formal structure of eq. (82) but also involves derivative of order

 $\beta = (2-d)/2$  that depends on the fractal-like clustering of mass micro-structure. When d = 2,  $\beta = 0$  and the classical Fourier equation is obtained.

Summing up in this section the authors observe that an approach based on a self-similar clustering of micro-scale masses in a macroscopically homogeneous conductor yields, at the macro-scale, to a fractional-order generalization of the Fourier equation in terms of Caputo fractional derivatives. The order of the derivative is related to the topological features of the microscopic set of mass clustering as  $\beta = \frac{2-d}{2}$ .

The analysis has been obtained for an 1D case and it may be generalized, straightforwardly to more complete case, repeating the analysis for an isotropic conductor in a three dimensional domain V of the Euclidean space R referred to a three dimensional coordinate system  $(O, x_1, x_2, x_3)$ . In this case identical micro-structure is observed along any direction and, therefore, the fractional-order Fourier equation may be generalized in term of the spatial gradient of the temperature field, namely,  $\nabla[\bullet] = \frac{\partial}{\partial x_k} [\bullet] i_k$  ( $i_k$  the unit vector of the coordinate system) as:

$$\mathbf{q}(\mathbf{x},t) = -R_{\beta}\mathbf{I}\cdot\left(\mathbf{D}_{0^{+}}^{\beta}\nabla T\right)(\mathbf{x},t) = -\mathbf{R}_{\beta}\cdot\left(\mathbf{D}_{0^{+}}^{\beta}\nabla T\right)(\mathbf{x},t)$$
(94)

where  $\mathbf{I}R_{\beta} = \mathbf{R}_{\beta}$  is the isotropic second-order tensor of the anomalous conductivities.

# Thermodynamical consistency of the fractional-order Fourier conduction

Thermodynamical assessment of eq.(93) must be formulated in terms of the irreversible entropy production rate  $\dot{s}_u(\mathbf{x},t)$  for unit volume, must be satisfied for any thermodynamical process at the macro-scale  $T(\mathbf{x},t)$ . In this section the authors report some basic considerations that correspond to the thermodynamical consistency of the model with a bottom-up approach from the self-similar micro-scale considered. In this circumstances the Gibbs inequality yields  $\dot{s}_u(\mathbf{x},t) \ge 0$  that must be fulfilled for any  $t \ge 0$  and at any location of the conductor  $\mathbf{x}_j \in V$  and for any micro-scale location  $z_j$ . To this aim, the second principle of thermodynamics, written for the observation scale *z*, reads:

$$\boldsymbol{\rho}(z_j)\dot{\boldsymbol{s}}(z_j,t) \ge -\frac{1}{\boldsymbol{\theta}(z_j,t)}\frac{\partial q(z_j,t)}{\partial z_j}$$
(95)

where  $\dot{s}$  represents the entropy rate. Introducing the irreversible specific entropy rate  $\dot{s}_u(z_j, t)$ , relation (95) is rewritten as:

$$\boldsymbol{\rho}(z_j)\dot{\boldsymbol{s}}(z_j,t) + \frac{1}{\boldsymbol{\theta}(z_j,t)}\frac{\partial q(z_j,t)}{\partial z_j} = \boldsymbol{\rho}(z_j)\dot{\boldsymbol{s}}_u(z_j,t) \ge 0$$
(96)

The entropy rate  $\dot{s}(z_j,t)$  could be cast in terms of the balance among the incoming and outcoming entropy flux, namely  $J(z_j,t)$ , as:

$$\dot{s}(z_j,t) = -\frac{1}{\rho(z_j)} \frac{\partial J(z_j,t)}{\partial z_j} + \dot{s}_u(z_j,t)$$
(97)

Introducing eq. (97) into eq. (96), the relevant inequality among the balance of the entropy flux and the the balance of the heat flux, at location z, is obtained in the form:

$$\frac{\partial J(z_j,t)}{\partial z_j} \ge \frac{1}{\theta(z_j)} \frac{\partial q(z_j,t)}{\partial z_j}$$
(98)

In the context of classical irreversible thermodynamics it is assumed that the entropy flux is a function of a state variable  $u(z_j,t)$  that corresponds to the specific internal energy of the conductor at location z as:

$$J(z_j,t) = \varphi(u)q(z_j,t)$$
(99)

that, after substitution in eq.(98) (omitting arguments) it leads to:

$$\left[\varphi\left(u\right) - \frac{1}{\theta}\right]\frac{\partial q}{\partial z_{j}} + \frac{\partial \varphi}{\partial z_{j}}q\left(z_{j}, t\right) \ge 0$$
(100)

Since relation (100) must be fulfilled for any thermodynamic transformation, for the linear term  $\varphi(u)$  equal to  $\frac{1}{\theta}$ , it is obtained:

$$\left(\frac{\partial \varphi(u)}{\partial z_j}\right)q = \frac{1}{\theta^2}\frac{\partial \theta}{\partial z_j}q \le 0 \tag{101}$$

Introducing the Fourier relation in (101) gives:

$$\dot{s}_{u}(z_{j},t) = \frac{\chi_{T}}{\theta^{2}} \left(\frac{\partial \theta(z_{j},t)}{\partial z_{j}}\right)^{2} \ge 0$$
(102)

Relation (102) must be verified for any thermodynamical process, for any location along the conductor, at any micro-scale resolution and for any temperature field  $\theta(z_j, t)$  yielding the thermodynamical restriction on the thermal conductivity  $\chi_T \ge 0$  so that  $R_\beta \ge 0$ .

It may be shown that the fractional-order generalization of the Fourier transport equation, reported in eq. (94), involves a state function of the form:

$$\Psi(x,t) = \int_{-\infty}^{t} \int_{-\infty}^{t} K\left(t - \tau_1, t - \tau_2\right) \frac{\partial \left[\nabla T\left(\tau_1, x\right)\right]}{\partial \tau_1} \frac{\partial \left[\nabla T\left(\tau_2, x\right)\right]}{\partial \tau_2} d\tau_1 d\tau_2 \quad (103)$$

where the kernel function  $K(t - \tau_1, t - \tau_2)$  may be written in the form:

$$K(t - \tau_1, t - \tau_2) = \frac{1}{2}G(2t - \tau_1 - \tau_2) = \frac{1}{2}\frac{K_\beta}{\Gamma(\beta)}\frac{1}{(2t - \tau_1 - \tau_2)^\beta}$$
(104)

that, after a Frechèt differentiation, it takes back the fractional-order Fourier equation reported in eq.(94). It may be observed that the expression for the free energy function in eq.(103) is obtained from the evaluation of the overall dissipation rate associated to the inhomogeneous conductor in fig.(21) (see e.g. [16] and [44] for details.

### Numerical experiments

In the present section the authors report some numerical experiments regarding the temperature field of anomalous conductors in presence of different boundary and initial conditions. In particular, in the next subsection the heat conduction problem in a one-dimensional (1D) slab with imposed initial temperature field and fixed temperature at the extremities, over time, is studied. The aim of the presented analysis is to show how the solution of the fractional heat conduction equation, i.e. the diffusion-wave equation, is influenced by the introduction of the Caputo's fractional derivative in the heat flux constitutive relation by means of problems defined in simple spatial domain.

The solution of the heat equation is obtained using the method of separation of variables: an equivalent approach has already been proposed in bounded space domains by means of the finite sine transform and the Laplace transform techniques [45]. Moreover, the Green's function approach has been thoroughly studied for the Cauchy and the Signalling problem [12, 46, 47].

In case of isotropic transport of the thermal energy across the conductor, the constitutive equation reported in eq. (94) becomes:

$$\mathbf{q}(\mathbf{x},t) = R_{\beta} \mathbf{I} \cdot \left( \mathbf{D}_{0^{+}}^{\beta} \nabla T \right) (\mathbf{x},t)$$
(105)

where **I** is the identity matrix and  $R_{\beta}$  is the "fractional" thermal conductivity with dimension  $[R_{\beta}] = kgmK^{-1}s^{\beta-3}$ . Introducing relation (105) in the energy balance equation, the three-dimensional (3D) fractional heat equation is obtained as:

$$\nabla^2 T\left(\mathbf{x},t\right) = \frac{1}{\gamma_\beta} \left({}_C \mathsf{D}_0^{1-\beta} T\right)\left(\mathbf{x},t\right)$$
(106)

Coefficients  $\gamma_{\beta} = \frac{R_{\beta}}{\rho C^{(V)}}$ ,  $\rho$  and  $C^{(V)}$  are the "fractional" thermal diffusivity, the density and the specific thermal capacity respectively, with physical dimensions reported below:

$$[\gamma_{\beta}] = m^2 s^{\beta - 1}; \ [\rho] = kg m^{-3}; \ [C^{(V)}] = m K^{-1} s^{-2}$$
 (107)



FIGURE 24: Initial parabolic temperature distribution for problem (109a)

The last part of this section is devoted to the solution of heat problem in cylindrical coordinates  $\{O, r, \theta, z\}$ ; in such a case the 3D heat conduction equation (106) is rewritten as:

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \psi^2} + \frac{\partial^2 T}{\partial z^2} + \frac{1}{2} \frac{\partial^2 T}{\partial z^2} + \frac{1}{2}$$

### Transient heat 1D problem in cartesian coordinates.

A transient boundary value problem of heat conduction for a 1D slab is considered; the initial parabolic distribution of temperature T(x,0) = F(x) is shown in Fig. (24):  $T_0$  and  $T_M$  represent, the initial temperature at the ends (x = 0 and x = L) and at the center of the slab, respectively. Moreover, the faces at coordinates x = 0 and x = L are kept, over time, at temperature  $T_0$  and there is not heat flux at the boundary lateral surfaces. The problem is to find the corresponding

temperature field T(x,t): its mathematical formulation is given as:

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\gamma_{\beta}} \left( {}_{C} \mathsf{D}_0^{1-\beta} T \right)(t) \quad \text{with} \quad 0 \le x < L, \ t > 0, \ 0 \le \beta < 1$$
(109a)

$$|T|_{x=0} = T_0, \quad \forall t > 0$$
 (109b)

$$|T|_{x=L} = T_0, \quad \forall t > 0 \tag{109c}$$

$$|T|_{t=0} = F(x) = T_0 + 4(T_0 - T_M) \left[ \left(\frac{x}{L}\right)^2 - \frac{x}{L} \right], \quad 0 < x < L$$
(109d)

The problem (109a) with boundary conditions (109b) and (109c) and initial condition (109d) can be solved shifting the temperature scale, namely defining the relative temperature as below:

$$\Psi(x,t) = T(x,t) - T_0$$
(110)

Considering equation (110), the problem (49) could be reformulated as follows:

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{\gamma_\beta} \left( {}_C \mathsf{D}_0^{1-\beta} \Psi \right)(t) \quad \text{with} \quad 0 \le x < L, \ t > 0, \ 0 \le \beta < 1$$
(111a)

$$|\Psi|_{x=0} = 0, \quad \forall t > 0 \tag{111b}$$

$$|\Psi|_{x=L} = 0, \quad \forall t > 0 \tag{111c}$$

$$|\Psi|_{t=0} = F(x) - T_0 = Q(x) = 4(T_0 - T_M) \left[ \left(\frac{x}{L}\right)^2 - \frac{x}{L} \right], \quad 0 < x < L \quad (111d)$$

The solution is found using the method of separation of variables, namely separating  $\Psi(x,t)$  into space-dependent and time-dependent functions as reported below:

$$\Psi(x,t) = \phi(t)\psi(x) \tag{112}$$

substituting (112) into (111a) and introducing the separation constant  $\lambda$ , give:

$$\frac{1}{\psi}\frac{d^2\psi}{dx^2} = \frac{1}{\gamma_\beta\phi}\left({}_C \mathsf{D}_0^{1-\beta}\phi\right)(t) = -\lambda^2. \tag{113}$$

Relation (113) is equivalent to the two following differential equations:

$$\frac{d^2 \psi(x)}{dx^2} + \lambda^2 \psi(x) = 0 \tag{114a}$$

$$|\psi|_{x=0} = 0 \tag{114b}$$

$$|\psi|_{x=L} = 0 \tag{114c}$$

and

$$\left({}_{C}\mathsf{D}_{0}^{1-\beta}\phi\right)(t) + \lambda^{2}\gamma_{\beta}\phi = 0 \tag{115}$$

The general solution of eq. (114a) is

$$\psi(x) = D_1 \cos(\lambda x) + D_2 \sin(\lambda x) \tag{116}$$

where boundary condition (114b) yields  $D_1 = 0$ , while boundary condition (114c) yields

$$\sin(\lambda L) = 0 \Rightarrow \lambda_n = \frac{n\pi}{L}$$
, with  $n = 1, 2, 3, ..$  (117)

The roots  $\lambda_n$  of relation (117) are the eigenvalues of the associated Sturm-Liouville problem [48]. As a consequence, the eigenfunctions of the problem are:

$$\psi_n(x) = D_2 \sin(\lambda_n x) = D_2 \sin\left(\frac{n\pi x}{L}\right) \tag{118}$$

After solving the problem corresponding to the space dimension, the solution for the time-dimensional problem, namely the fractional differential equation (115), is requested. Taking the Laplace transform of (115), using formula (78b), gives:

$$\widehat{\phi}(s)s^{1-\beta} - \phi(0)s^{-\beta} + \lambda^2 \gamma_\beta \widehat{\phi}(s) = 0$$
(119)

and then the solution in Laplace domain is:

$$\widehat{\phi}(s) = \frac{\phi(0)s^{-\beta}}{s^{1-\beta} + \lambda^2 \gamma_{\beta}}$$
(120)

$$\phi(t) = \phi(0)E_{1-\beta,1}\left[-\lambda^2\gamma_{\beta}t^{1-\beta}\right]U(t)$$
(121)

where  $E_{\zeta,\eta}(z)$  is the Mittag Leffler function defined as [49]:

$$E_{\zeta,\eta}(z) = \sum_{n=0}^{\infty} \frac{(z)^n}{\Gamma(\zeta n + \eta)}$$
(122)

and U(t) is the Heaviside unit-step function. Relations (118) and (121) can be combined introducing the constant  $D_n = D_2\phi(0)$  yielding, considering relation (112), the general solution:

$$\Psi(x,t) = U(t) \sum_{n=1}^{\infty} D_n \sin(\lambda_n x) E_{1-\beta,1} \left[ -\lambda_n^2 \gamma_\beta t^{1-\beta} \right]$$
(123)

where the constant  $D_n$  is defined utilizing the initial condition (111d) and noting that  $E_{\zeta,1}[0] = 1$  if  $0 < \zeta < 1$ , namely:

$$\Psi(x,0) = Q(x) = \sum_{n=1}^{\infty} D_n \sin(\lambda_n x)$$
(124)

Relation (124) is the Fourier series expansion of the function Q(x) then, multiplying both sides of such relation by  $sin(\lambda_m x)$  and integrating over the interval 0 < x < L give:

$$\int_0^L Q(\xi) \sin(\lambda_m \xi) d\xi = \begin{cases} D_m \int_0^L \sin^2(\lambda_m \xi) d\xi = D_m \frac{L}{2} & \text{if } m = n\\ 0 & \text{if } m \neq n \end{cases}$$
(125)

where the property of orthogonality of the eigenfunctions  $sin(\lambda_m x)$  for arbitrary eigenvalues  $\lambda_m$  has been used. Summing up, eq. (125) gives:

$$D_n = \frac{2}{L} \int_0^L Q(\xi) \sin(\lambda_n \xi) d\xi$$
(126)

and finally, using relations (110) and (123), the temperature field is obtained as:

$$T(x,t) = T_0 + \sum_{n=1}^{\infty} D_n \sin(\lambda_n x) E_{1-\beta,1} \left[ -\lambda_n^2 \gamma_\beta t^{1-\beta} \right]$$
(127)

Relation (127) can be converted into non-dimensional form by defining the nondimensional independent variables, through the dimensional parameters of the thermal problem, as reported below:

$$\underline{x} = \frac{x}{L} \tag{128a}$$

$$\underline{t}^{1-\beta} = \frac{\gamma_{\beta} t^{1-\beta}}{L^2}$$
(128b)

$$\underline{T} = \frac{T - T_0}{T_0 - T_M} \tag{128c}$$

$$\underline{\lambda}_n = n\pi \tag{128d}$$

Some examples of the non-dimensional temperature field are shown in Fig. (25). Compared to the time-solution  $\exp\left[-\lambda_n^2\gamma t\right]$  of the Fourier heat conduction equation  $(\beta = 0)$ , the solution  $E_{1-\beta,1}\left[-\lambda_n^2\gamma_\beta t^{1-\beta}\right]$  of the fractional equation  $(0 < \beta < 1)$  exhibits for small times a much faster rising, and for large times, a much slower decay. In view of its slow decay, the fractional thermal conduction is usually referred to as a super-slow process. Accordingly, in Fig. (25) it is seen that the main feature characterizing the anomalous heat transfer is that the time-rate of change at which the resulting temperature field reaches a steady behavior gets higher as the discrepancy from the Fourier law increases. When it comes to considering how long does it take for the body to achieve thermal steadiness, the trend shown by anomalous conductors is to employ longer times than Fourier ones. Indeed, this is exactly the "long-tail memory effect", due to the power law thermal memory of such materials.

### Transient heat problem in cylindrical coordinates.

In this example a long solid cylinder of radius b, with initial temperature F(r) is considered. For t > 0, the boundary surface at r = b is insulated; in this case the



FIGURE 25: A), B) and C) Non-dimensional temperature field  $\frac{T-T_0}{T_0-T_M}$  for different value of the exponent  $\beta$ . All the surfaces have been obtained with n = 10. d) Non-dimensional temperature field at  $\underline{x} = 0.5$ 

temperature field depends only on the position along the radius r of the cylinder. The mathematical formulation of the problem is

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} = \frac{1}{\gamma_{\beta}} \left( c \mathbf{D}_0^{1-\beta} T \right) (t) \quad \text{with} \quad 0 \le r < b, \ t > 0, \ 0 \le \beta < 1$$
(129a)

$$|T|_{r=0} \text{ bounded, } \forall t > 0 \tag{129b}$$

$$\left| \left( c \mathbf{D}_0^\beta \frac{\partial T}{\partial r} \right) (t) \right|_{r=b} = 0, \quad \forall t > 0$$
(129c)

$$|T|_{t=0} = F(r), \quad 0 < r < b$$
 (129d)

The solution of the problem (129a) with boundary conditions (129b) and (129c) and initial condition (129d) may be obtained using the method of separation of variables as in the previous example, namely by assuming a separation of T(r,t) into space-dependent and time-dependent functions as

$$T(r,t) = \phi(t)\psi(r) \tag{130}$$

substituting (130) into (129a) and introducing the separation constant  $\lambda$  give:

$$\frac{1}{\psi} \left( \frac{d^2 \psi}{dr^2} + \frac{1}{r} \frac{d \psi}{dr} \right) = \frac{1}{\gamma_\beta \phi} \left( {}_C \mathsf{D}_0^{1-\beta} \phi \right)(t) = -\lambda^2$$
(131)

relation (131) is equivalent to the two following differential equations:

$$\frac{d^2\theta(r)}{dr^2} + \frac{1}{r}\frac{d\theta(r)}{dr} + \lambda^2\theta(r) = 0$$
(132a)

$$|\theta|_{r=0}$$
 bounded (132b)

$$\left|\frac{d\,\theta}{dr}\right|_{r=b} = 0\tag{132c}$$

and

$$\left({}_{C}\mathsf{D}_{0}^{1-\beta}\phi\right)(t) + \lambda^{2}\gamma_{\beta}\phi = 0 \tag{133}$$

The general solution of eq. (132a) is:

$$\Psi(r) = M_1 J_0(\lambda r) + M_2 I_0(\lambda r) \tag{134}$$

where  $J_m$  is the Bessel functions of the first kind of order *m* defined as:

$$J_m(z) = \left(\frac{z}{2}\right)^m \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{z}{2}\right)^{2n}}{n! \Gamma(m+n+1)}$$
(135)

and  $I_0$  the Bessel function of the second kind of order zero. Boundary condition (132b) yields  $M_2 = 0$ , while boundary condition (132c) produces eigenvalues from the corresponding transcendental equation:

$$-M_1 \lambda J_1(\lambda b) = 0 \Rightarrow \lambda_n \quad \text{with} \quad n = 0, 1, 2, \dots$$
 (136)

with  $\lambda_0 = 0$ . The roots  $\lambda_n$  of relation (136) are the eigenvalues of the associated Sturm-Liouville problem [48]. The eigenfunctions of the problem are, consequently:

$$\psi_n(r) = M_1 J_0(\lambda_n r). \tag{137}$$

The solution for the time-dimensional problem, namely the fractional differential equation (133), is given by relation (121). Relations (137) and (121) can be combined introducing the constant  $M_n = M_1\phi(0)$  yielding, and taking into account relation (130), this leads to:

$$T(r,t) = U(t) \sum_{n=0}^{\infty} M_n J_0(\lambda_n r) E_{1-\beta,1} \left[ -\lambda_n^2 \gamma_\beta t^{1-\beta} \right]$$
(138)

the constant  $M_n$  is defined utilizing the initial condition (129d) and noting that  $E_{\zeta,1}[0] = 1$  if  $0 < \zeta < 1$ , namely

$$T(r,0) = F(r) = \sum_{n=0}^{\infty} M_n J_0(\lambda_n r)$$
 (139)

Relation (139) is the Fourier series expansion of the function F(r) then, multiplying both sides of such relation by  $J_0(\lambda_m r)$  and integrating over the interval

0 < r < b give:

$$\int_0^b F(\xi) J_0(\lambda_m \xi) \xi d\xi = \begin{cases} M_m \int_0^b J_0^2(\lambda_m \xi) \xi d\xi & \text{if } m = n\\ 0 & \text{if } m \neq n \end{cases}$$
(140)

where the property of orthogonality of the eigenfunctions  $J_0(\lambda_m r)$  for arbitrary eigenvalues  $\lambda_m$  has been used. Summing up, eq. (140) gives:

$$M_n = \frac{\int_0^b F(\xi) J_0(\lambda_n \xi) \xi d\xi}{\int_0^b J_0^2(\lambda_n \xi) \xi d\xi}$$
(141)

and finally, inserting relation (141) in (138) the temperature field is obtained as:

$$T(r,t) = \sum_{n=0}^{\infty} M_n J_0(\lambda_n r) E_{1-\beta,1} \left[ -\lambda_n^2 \gamma_\beta t^{1-\beta} \right]$$
(142)

The non-dimensional temperature field at t = 0 is a linear distribution as:

$$\underline{F}(\underline{r}) = 20\underline{r} + 1 \tag{143}$$

As in the previous numerical example, in Fig. (26) it is shown the non-dimensional temperature field  $\frac{T(r,t)}{F(0)}$  as a function of non-dimensional time <u>t</u> (eq. (128b)) and non-dimensional radius  $\underline{r} = \frac{r}{b}$ , for different value of the exponent  $\beta$ . Like in the case of the uniaxial thermal rigid conductor of Fig. (25), the discrepancy from Fourier's law manifests itself with higher time-rates and slower time-transients.

### Conclusions

In this paper the authors showed that the analysis of the temperature field in an inhomogeneous rigid conductor with power-law grading of the thermodynamical parameters yields a power-law time rising of the temperature at the insulated boundary of the conductor. The order of the power-law is related to the grading exponent of the physical properties of the conductor and the use of Boltzmann



FIGURE 26: A), B) and C) Non-dimensional temperature field  $\frac{T(r,t)}{F(0)}$  for different value of the exponent  $\beta$ . All the surfaces have been obtained with n = 10. d) Non-dimensional temperature field at  $\underline{r} = 0.5$ 

superposition principle for generic histories of the incoming heat flux yields a temperature-flux relation involving fractional-order operators.

The main idea that a power-law rising appears as a non-homogeneous, nonstationary flux is established in the conductor has been further expanded in the paper to yield a fractional-order generalization of the Fourier transport equation. Indeed, under the assumption of a non-homogeneous, self-similar distribution of mass micro-structure in any generic volume element of the conductor, a nonstationary flux at micro-structure level is experienced. In this setting, the assumption of a fractal mass clustering at micro-structural level with an Hausdorff dimension d yields the same kind of thermal flux, at micro-structural level, as those experienced with the non-homogeneous macroscopic conductor. As a consequence, the resulting macroscopic relation provides the heat flux by means of the fractional-order, Caputo' type, derivative of spatial gradient of the temperature field with derivation order related to the fractal dimension of the self-similar assembly as  $\beta = \frac{2-d}{2}$ .

The thermodynamic assessment of the introduced fractional-order generalization of the Fourier equation has been exploited with the same micro-structure arguments and more details are reported in a forthcoming paper. The numerical examples provided show the influence of anomalous conductivity and differentiation order for temperature fields in simple 1D and 2D domains. Indeed the obtained non-dimensional temperature fields have been compared to the timesolution of the Fourier heat conduction equation ( $\beta = 0$ ).

Results show that the solution of the fractional heat equation  $(0 < \beta < 1)$ , governed by Mittag-Leffler functions, exhibits for small times a much faster rising, and for large times, a much slower decay. Accordingly, the main property of the anomalous heat transfer is that the time-rate of change at which the resulting temperature field reaches a steady state, becomes higher as the discrepancy from the Fourier law increases: the thermal steadiness is consequently achieved, by anomalous conductors, employing longer times than Fourier ones. Such particular behavior represents the "long-tail memory effect", due to the power law thermal memory of such materials.

The proposed fractional-order generalization of the Fourier heat transport equation is used in the companion paper to formulate the fractional-order linear thermoelastic problem.

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## Fractional-order theory of thermo elasticity II: quasi-static behavior of bars \*

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#### ABSTRACT

**Objectives:** This work aims to shed light to the "thermally-anomalous" coupled behavior of slightly deformable bodies, in which the strain is additively decomposed in an elastic contribution and in a thermal part. The macroscopic heat flux turns out to depend upon the time history of the corresponding temperature gradient, and this is the result of a multi-scale rheological model developed in

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Part 1 of the present study, thereby resembling a "long-tail" memory behavior governed by a Caputo's fractional operator. The macroscopic constitutive equation between the heat flux and the time history of the temperature gradient does involve a power law kernel, resulting in the "anomaly" mentioned above.

**Methods:** The interplay between the thermal flux and the elastic and thermal deformability are investigated for a pinned-pinned truss. This allows for focusing on the effects of the deviation from the Fourier's law on the thermoelastic coupling. The full analytical solution of the problem is provided obtaining the resulting displacement, temperature, and internal axial force. The anomalous thermal behavior of such slightly deformable system is then investigated, thereby exploring not only the transient behavior due to its deviation from the Fourier law, but also by studying a resulting overall measure of energy rate.

**Results:** All the resulting fields, namely the axial stress, the displacement, and the temperature are influenced by the thermal and elastic deformability of the bar. The higher is the deviation from the Fourier-like behavior, the more rapid becomes the rise in time. This is an intrinsic feature of the anomalous heat transfer, now coupled with an elastic and thermally deformable bar. Another effect of the deviation from the Fourier behavior is the tendency to reach steady values in longer times. The higher the value of the anomaly exponent  $\beta$  in [0, 1/2) the slower this becomes.

**Conclusions:** The space-time modal analysis performed on the fractionalorder system, relying on the balance of linear momentum and on the balance of energy rate, provides the explicit solutions of the problem. The time evolution of each spatial mode, for the temperature, for the displacement and for the axial force, turn out to be characterized by modulated Mittag-Leffler functions. The higher is the deviation from the Fourier-like behavior for the heat flux, the steeper is the resulting time-transient of each mode.

### Introduction

In [1] the authors raised the most natural question about the physical grounds on which the fractional-order behavior arises in various contexts (see e.g. [2, 3] etc.). In particular, it was studied the case of rigid thermal conductors characterized by

anomalous heat transfer, in which the relationship between the macroscopic heat flux and the corresponding temperature gradient inherits a power law memory in time. This has been explained in [1] through a hierarchy of Fourierian rigid heat conductors across infinite observation scales, thereby resembling a fractal material. Essentially, this is equivalent to having a distribution of masses characterized by a functionally graded hierarchy of thermal conductivities and heat capacity scaling with a certain power. The latter can be related to the porosity of hierarchical media, where the thermal transport encounters obstacles (such as voids and a rigid solid matrix) that can heavily influence the overall heat diffusion. This is consistent with the findings in [4], where anomalous time scaling of the thermal energy has been explained through a statistical approach, thereby characterizing the evolution of its non-equilibrium excess in a one dimensional conductor. There the transient behavior of the heat flux has been found to be originated by small initial excess perturbations of the thermal energy away from equilibrium, thereby leading to an anomalous diffusion scaling in time like  $t^{\beta}$ , being  $\beta$  a real number. Anomalous heat transfer is essentially an averaged, hence macroscopic, transient phenomenon affected by the scaling discussed above. Anomalous behavior has been detected in certain materials [5] although often times such materials are treated as if both their thermal conductivity and specific heat behave non-linearly with the temperature [6].

Other works have been explaining anomalous heat transfer in rigid bodies with "billiard-like" models, quantum mechanics (see e.g. [7]), etc. It is worth noting that what is found about a connection between such methods and the hier-archical structure of the media exhibiting anomalous behavior, does not bring into play the scalings of the thermal conductivities and heat capacities at the various observation scales.

The most natural generalization of the findings in [1] is to allow for a coupled linear thermo-elastic behavior of the material under external actions. This is surely an approximate way to account for the deformability of bodies whose macroscopic thermal behavior is not Fourierian. The justification for this approach resides on the modeling of what happens at each observation scale. As a first approximation, the chain of rheological systems employed in [1] can be thought to be generalized as if associated elastic stiffness present at each observation scale would generate internal forces entering the energy balance (see e.g. eqn. (3) in [1]). If, unlike the thermal conductivities and heat capacities, such stiffnesses would not change with such scales, the overall macroscopic equations would boil down to linear thermo-elasticity with thermal memory. In physical terms this may happen whenever the time scales of thermal and mechanical exchanges significantly differ at the various observation scales. In a hierarchical

porous material this can be envisioned if stress re-distributions are much slower than the effects causing the impact between thermally excited particles and generating the anomalous spread of thermal energy in the solid matrix, as found in [4]. Small deformabilities of hierarchical solids undergoing heat exchanges are then based on a multi-scale ground. This is missing in all of the known approaches present in the literature.

Nonetheless, in [8, 9] recent phenomenological fractional-order theories for three dimensional thermo-elasticity with no such multi-scale origins were formulated and applied. Although in the present treatment the authors will focus on the space-time evolution of the system by neglecting inertia, a useful and comprehensive review about propagating waves with finite speed in thermoelastic media can be found in [10]. Here, upon removing the paradox of thermal waves propagating with infinite speed in Fourier type deformable conductors, the main focus is about the dynamics of spatially anomalous thermal response of fractal materials. To the best of authors' knowledge, a multi-scale rheological explanation analog to the one given in [1] is not yet available for such a case.

While the anomalous thermal behavior in time has been extensively studied from the phenomenological and mathematical viewpoint starting from the late sixties to these days (see e.g. [11–15]), anomalous thermoelastic coupling in engineering applications still requires thorough investigations. To this end, for the sake of illustration, a one dimensional anomalous thermoelastic truss subject to thermal loading and pinned at both ends is examined in the sequel. The full analytical solution of the problem is provided obtaining the resulting displacement, temperature, and internal axial force. The anomalous thermal behavior of such slightly deformable system is then investigated, thereby exploring not only the transient behavior due to its deviation from the Fourier law, but also by studying a resulting overall measure of energy rate. The obtained quantity corresponds to the "thermal work" introduced in [12] and studied later in several papers (see e.g.[13–15]), for the first time for rigid conductors with memory. A more extensive study of a theory for trusses and beams would have to entail a Saint Venant-type of argument, analog to the one developed in [16] for small strain viscoelasticity. Future developments of the proposed approach accounting for material hierarchies within three dimensional geometries in the presence of coupled multi-physics phenomena (such as in [3, 17], and ref.s cited therein), are envisioned in a combination between the current approach and the methodologies developed in [18–20], [21, 22], [23] and [24].

### Thermoelastic trusses and anomalous behavior

Anomalous heat conduction and its impact on evolutionary thermoelastic processes arising in one dimensional deformable solids are studied in this section. Wherever it will be not needed, the dependence on x and t in all the fields involved in the treatment will be omitted.

The constitutive equations governing the problem relate to the internal axial force (*N*)-strain ( $\varepsilon$ ) response and to the heat flux (*q*) and temperature gradient (*T*<sub>,x</sub>) behavior. The former entails the usual coupling between the axial internal force *N* arising at each cross section of the solid at the current time and the elastic strain, namely

$$N = EA(\varepsilon - \alpha(T - T_0)), \qquad (144)$$

where *E* is the Young modulus of the material, *A* is the area of the cross section of the bar,  $\alpha$  is the linear thermal expansion coefficient of the solid,  $T_0$  is a reference temperature and *T* is the current value of the temperature field. The latter constitutive equation for the heat flux has been obtained in [1], i.e.:

$$q = -K_{\beta} \left( {}_{C} D_{0^+}^{\beta} \right) T_{,x}. \tag{145}$$

In eq. (2) it is involved the time-fractional Caputo's derivative of order  $\beta \in [0, 1]$  defined as:

$$\left({}_{C}D^{\beta}_{0^{+}}\right)f = \frac{1}{\Gamma(1-\beta)}\int_{0}^{t}\frac{f'(\tau)}{(t-\tau)^{\beta}}d\tau$$
(146)

where  $\Gamma(z)$  is the Euler-Gamma function that may be considered as the generalization of the factorial function because, when z assumes integer values, it yields that  $\Gamma(z+1) = z!$ .

A general framework for the definition of fractional-order integrals in Sobolev metric space has been provided in recent mathematical literature [2, 3]. The use of fractional-order calculus to handle functions defined on fractal subsets has been reported in terms of the fundamental theorem of integral calculus involving a corrective series beside values of the primitives at the borders of the integrals [4].

The fractional operator in eq. (146) is the result of the multi-scale rheological model developed in Part 1 of the present study, thereby accounting for a "long-tail" memory behavior.

In eq. (146) it is considered the definition of the Caputo's left fractional derivative (following [25]), for which the integral lower terminal 0 is kept fixed, and the upper terminal t is varied, with 0 < t. However, it is also possible to consider Caputo's right fractional derivatives with moving lower terminal t and fixed upper terminal 0.

From a physical point of view, if the function f(t) represents the present state of a time-evolving dynamical process started at the instant t = 0, then the left derivative is an operator performed on the "past" states  $f(\tau)$  of the process being  $\tau < t$ , while the right derivative relies on its "future" states  $f(\tau)$  being  $\tau > t$ . Given such considerations, causality principle is satisfied by left derivative definition.

In this section the authors are interested in analyzing the impact of the anomalous heat transfer and of the deformability in the quasi-static thermo-mechanics evolution of the system. This is characterized by the main unknown fields u and T, namely the axial displacement of cross sections of the truss and the temperature, respectively. Standard compatibility between strain and displacement reads as follows

$$\varepsilon = u_{,x},\tag{147}$$

and it will be accounted for in the sequel. In the absence of accelerations, balance of linear momentum implies:

$$N_x + \rho \, p = 0 \tag{148}$$

where  $\rho$  is the density of the material per unit length and p is the (distributed) axial external load. Balance of energy must further be imposed, namely:

$$q_{,x} = Q - (\rho c_v T_{,t} + T_0 \alpha E A \varepsilon_{,t}), \qquad (149)$$

where Q is the heat flux source term,  $c_v$  is the thermal capacity of the material at constant volume. The whole term included in the brackets on the right hand side of such equation represents a specific enthalpy per unit length of the system. Relation (149) has been obtained in the paper by [9]. In that work, the authors start from the first law of thermodynamics (eq. 2.6) and from the balance equation of entropy density (eq. 2.7) subsequently linearized (eq. 2.27). The authors combine them and, after some manipulations, they obtain eq. 2.28 that is equivalent to eq. (149).

Thermo-mechanical coupling arises only through (144), namely the constitutive equation for N, and through (145), the balance of energy rate. Indeed, the employed constitutive equation for the anomalous heat conduction (145) does not involve any contribution coming from the mechanics. Substitution of (147) into (144) and then in (148) yields

$$EA(u_{,xx} - \alpha T_{,x}) + \rho p = 0, \qquad (150)$$

while (145) into (149) delivers

$$K_{\beta}\left({}_{C}D_{0^{+}}^{\beta}\right)T_{,xx} - \rho c_{v}T_{,t} - \alpha EAT_{0}u_{,tx} + Q = 0.$$
(151)

The obtained coupled system of nonstandard linear Partial Differential Equations (PDE) will be studied in the sequel for the case in which no sources terms  $\rho p$  and Q are present.

In order to illustrate the outcomes of the anomalous thermo-elasticity, the same initial temperature profile assumed in [1] is considered, namely:

$$T(x,0) = T_0 + 4(T_0 - T_m)\frac{x}{L}\left(\frac{x}{L} - 1\right).$$
(152)

The corresponding displacement u(x, 0) is then reconstructed through the balance of linear momentum (150). Indeed, if p = 0, upon integrating (150) twice with respect to x, the initial displacement profile takes the following form:

$$u(x,0) = C_0 + C_1 x + 4\alpha \frac{T_0 - T_m}{L} \left(\frac{x^3}{3L} - \frac{x^2}{2}\right),$$
(153)

where  $C_0$  and  $C_1$  are arbitrary constants.

It is not difficult to show that one way to solve the problem is to eliminate one of the two fields, thereby obtaining a higher order on the remaining function equation. To this end, T will be eliminated and a resulting governing equation for u will be found.

On obviously integrating (150) with respect to x, the axial internal force N turns out to depend on t alone. Hence  $N = \hat{N}(t)$  takes the following expression

$$\hat{N}(t) = EA\left(u_{x}(x,t) - \alpha\left(T(x,t) - T_{0}\right)\right)$$
(154)

thereby implying that there will be cancellation on the *x*-dependence of  $u_{,x}$  and *T*. For the sake of illustration, the following boundary conditions will be assumed for the temperature:

$$T(0,t) = T(L,t) = T_0$$
(155)

which are the same as in [1], eq.s (49b,c).

Various sets of boundary conditions can be explored. Here the pinned-pinned case and the pinned-free case will be considered.

Pinned-pinned case. This case arises when both ends are fixed in time, namely when

$$u(0,t) = u(L,t) = 0.$$
 (156)

Obviously this is a (quasi) statically undetermined problem, i.e. the time evolving internal normal force is not known a-priori and it must be determined through the full solution of the governing equations. The corresponding values of the constants appearing in (153) are the following:

$$C_0 = 0$$
 and  $C_1 = \frac{2}{3} \frac{T_0 - T_m}{EA} L$  (157)

Pinned-free. In this case one end of the bar is set free. This is a (quasi) static determinate problem and, if no external force is applied, then there is no normal force arising in any of the cross sections of the bar. The evolution of the "stress-free" movements and heat flux of the system can be determined by imposing N = 0 and either of one of the two conditions (156), e.g.

$$u(0,t) = 0$$
, and  $\hat{N}(t) = 0.$  (158)

Hence, by (153) and substituting (152) into (154) and imposing (158) give:

$$C_0 = 0 \qquad C_1 = 0 \tag{159}$$

By substituting the results in the balance of energy rate (149), it is found that the following PDE must be verified:

$$K_{\beta}\frac{1}{\alpha}\left({}_{C}D^{\beta}_{0^{+}}\right)u_{,xxx}-\left(\frac{\rho c_{v}}{\alpha}+\alpha EAT_{0}\right)u_{,tx}=\rho c_{v}N_{,t}(t).$$
(160)

For the pinned-free case it is obtained that the right-hand side is zero and (160) already represents the governing field equation for the displacement. Further differentiation of the latter relationship with respect to x allows for finding the governing PDE for the displacement in general, including the case of (quasi) static undetermined bar. This is the equation that will be studied in the sequel.

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For this purpose, the auxiliary function v, defined as follows, is introduced:

$$\mathbf{v} := u_{,xx} \tag{161}$$

and hence the corresponding resulting field equation becomes:

$$\left({}_{C}D^{\beta}_{0^{+}}\right)\mathbf{v}_{,xx}-\boldsymbol{\delta}\,\mathbf{v}_{,t}=0,\tag{162}$$

after setting

$$\delta^{-1} = \frac{\gamma_{\beta}}{1 + \frac{\alpha^2 E A T_0}{\rho c_{\nu}}}.$$
(163)

where  $\gamma_{\beta} := \frac{K_{\beta}}{\rho c_{\nu}}$  has been introduced in [1] Sect.4.1.

The behavior of rigid thermal conductors can be retrieved by simultaneously letting  $\alpha$  (the linear dilation factor) and *EA* (the axial rigidity) to tend to zero and to infinity respectively, and by requiring that  $\lim_{EA \to \infty} \alpha^2 EA = 0$ .

Relation (162) is formally analogous to the governing equation of the anomalous heat conduction obtained in [1] eqn. (49a), namely

$$\left({}_{C}D^{\beta}_{0^{+}}\right)T_{,xx} - \delta T_{,t} = 0.$$
(164)

Nevertheless the solution for such PDE obtained there is not suitable for the case under investigation, as neither the boundary conditions nor the initial ones (49b,c,d) are directly applicable to the function  $v = u_{,xx}$ . Nonetheless, the technique used to solve the above mentioned problem is obviously applicable in this case. This is based on space-time eigenmodes series expansions for both *T* and *u* in the separated variables form for solving the original coupled system (150), (151), namely:

$$T(x,t) = T_0 + \sum_{m=1}^{+\infty} f_m(t)g_m(x)$$
(165)

$$u(x,t) = \sum_{m=1}^{+\infty} v_m(t) w_m(x).$$
 (166)
Henceforth, an ansatz for v in agreement with (165) and (166) is assumed as follows

$$\mathbf{v}(x,t) = \sum_{m=1}^{+\infty} v_m(t) z_m(x),$$
(167)

where  $z_m(x) := w''_m(x)$ , where " indicates double differentiation with respect to x. Substituting such expression in (162) and imposing its validity term-by-term, does lead to the following set of two ordinary differential equations:

$$\frac{1}{\delta} \frac{z_m'(x)}{z_m(x)} = \frac{\dot{v}_m(t)}{\left(cD_{0^+}^{\beta}\right)v_m(t)} = -K_m^{-2},\tag{168}$$

where  $\dot{}$  denotes differentiation with respect to time, and  $K_m^2$  is arbitrary, to be determined by solving the associated eigenvalue problem. To this end, eq. (168) leads to the following expression for  $z_m$ :

$$z_m(x) = a_m \cos(\omega_m x) + b_m \sin(\omega_m x), \qquad (169)$$

where

$$\omega_m^2 := \delta K_m^{-2} \tag{170}$$

and hence, because  $w''_m = z_m$ , the following expression for the spatial m-mode of *u* is obtained:

$$w_m(x) = c_m \cos(\omega_m x) + d_m \sin(\omega_m x) + h_m x + l_m.$$
(171)

It is worth noting that this function carries the dimension of length, hence  $v_m$  is dimensionless. The second equation in (168), namely

$$\left({}_{C}D^{\beta}_{0^{+}}\right)v_{m}(t) + K^{2}_{m}\dot{v}_{m}(t) = 0, \qquad (172)$$

represents the associated fractional-order homogeneous initial value problem for  $v_m$ . Of course  $\omega_m$  appearing in (169), (170) and (171) can be determined through the boundary conditions on the displacement and, hence,  $K_m$  will follow according to relation (169).

Although eqn. (172) is nonstandard, it can be solved as in the case of anomalous heat transfer in rigid conductors, treated in [1]. There such equation has been recast in the following form:

$$\left({}_{C}D_{0^{+}}^{1-\beta}\right)v_{m}(t) + K_{m}^{-2}v_{m}(t) = 0.$$
(173)

Its solution has been shown to be represented as follows:

$$v_m(t) = E_{1-\beta,1} \left( -K_m^{-2} t^{1-\beta} \right), \tag{174}$$

where  $E_{1-\beta,1}$  is the Mittag-Leffler function of order  $(1-\beta,1)$ . Without loss of generality the time amplitude in (174) is set equal to 1, as the coefficient modulating each mode will be computed through a Fourier expansion technique starting from the initial data (153).

A sufficient condition for (154) is that such relation is verified term-by-term, namely:

$$EA(w'_{m}(x)v_{m}(t) - \alpha g_{m}(x)f_{m}(t)) = \hat{N}_{m}(t), \qquad (175)$$

where  $\hat{N}_m(t)$  represents the contribution of the  $m^{th}$ -mode of the axial force. Upon differentiating the last relation with respect to x it is found that:

$$\ddot{w_m}(x)v_m(t) - \alpha g'_m(x)f_m(t) = 0,$$
 (176)

and hence the following two equations are obtained

$$\frac{\ddot{w_m(x)}}{\alpha g'_m(x)} = \frac{f_m(t)}{v_m(t)} = \lambda_m,$$
(177)

where  $\lambda_m$  are real constants. It is worth nothing that such relations do force the spatial modes for the strain gradient  $u_{,xx}$  and for the temperature gradient  $T_{,x}$  to be the same.

Because of (171) and (177) the spatial form of the temperature takes the form:

$$g_m(x) = \frac{1}{\alpha \lambda_m} \omega_m \left[ -c_m sin(\omega_m x) + d_m cos(\omega_m x) + \frac{h_m + p_m}{\omega_m} \right].$$
(178)

This comes from the balance of linear momentum (150), bearing in mind (166) and (171), and also the fact that

$$g'_m(x) = \frac{1}{\alpha \lambda_m} w''_m(x).$$
(179)

Integration of the last equation yields:

$$g_m(x) = \frac{1}{\alpha \lambda_m} \left( w'_m(x) + p_m \right), \qquad (180)$$

where  $p_m$  has the meaning of a constant modal elastic strain. Indeed, revisiting (175) and knowing (180) and (171) give:

$$\hat{N}_{m}(t) = EA(w'_{m}(x) - \alpha \lambda_{m} g_{m}(x)) v_{m}(t) = -EA p_{m} v_{m}(t).$$
(181)

Because of (174), at the beginning of the evolution of the system it yields that

$$\hat{N}_m(0) = -EA \, p_m,\tag{182}$$

which explains why  $p_m$  is a constant elastic modal strain. Obviously, no axial force could develop in the bar if either each  $p_m$  would be identically zero or if  $\sum_{m=0}^{\infty} p_m v_m(t) = 0.$ 

As it was previously pointed out, the path for determining the eigenvalues  $\omega_m$  is based on the boundary conditions. The system is mechanically overconstrained. The problem is then treated in a standard way, by first removing the extra constraint and by studying a pinned-free truss undergoing the same initial conditions of the original problem. Then two cases will be considered with the idea of eventually superimposing their effects.

*Case (0)* The initial distribution of temperature and its corresponding initial displacement field will be taken to act on the pinned-free bar: here it is expected the modal strains  $p_0^{(m)}$  are zero as there is no axial force.

*Case (1)* Because of the extra constraint, an unknown axial force arises within the bar: this is the only thermo-mechanical load acting in this case.

Once the separate effects of those two cases will be worked out, the requirement for which the displacement at both ends is inhibited by the original constraint will be enforced, thereby owing the value of the axial force and the complete solution of the problem. The two cases are now examined in details.

## Case zero: Pinned-free system undergoing the initial distributions of temperature and displacement

This corresponds to the boundary conditions (158). All the quantities relative to this case are re-labeled with the superscript (0). Upon applying (158) term by term to the functions  $w_m^{(0)}$  and  $g_m^{(0)}$  introduced above, the following set of equations to be satisfied is obtained:

$$w_m^{(0)}(0) = 0 \qquad w_m^{(0)'}(L) = \frac{1}{\alpha} g_m^{(0)}(L)$$

$$g_m^{(0)}(0) = 0 \qquad g_m^{(0)}(L) = 0,$$
(183)

from (158), (155), and (165) respectively. From (171) and (183) the following relations hold:

$$c_m^{(0)} = -l_m^{(0)} \qquad \qquad d_m^{(0)} + \frac{h_m^{(0)} + p_m^{(0)}}{\omega_m^{(0)}} = 0 \qquad (184)$$

and hence  $(183)_2$  and  $(183)_3$  become:

$$-c_m^{(0)} sin(\omega_m^{(0)}L) + d_m^{(0)} cos(\omega_m^{(0)}L) + \frac{h_m^{(0)} + p_m^{(0)}}{\omega_m^{(0)}} = 0$$
  
$$-c_m^{(0)} sin(\omega_m^{(0)}L) + d_m^{(0)} cos(\omega_m^{(0)}L) + \frac{h_m^{(0)}}{\omega_m^{(0)}} = 0.$$
(185)

The last two equations imply that the modal strains  $p_m^{(0)}$  must vanish, i.e.

$$p_m^{(0)} = 0, (186)$$

and, hence, (184)<sub>2</sub> yields

$$h_m^{(0)} = -\boldsymbol{\omega}_m^{(0)} d_m^{(0)}. \tag{187}$$

Back substitution of  $(184)_1$ , (186) and (187) on either of the (185) yields an homogeneous problem which is verified if either of the following three conditions hold:

$$sin(\omega_m^{(0)}L) = 0 \text{ and } cos(\omega_m^{(0)}L) = 1, \forall c_m^{(0)}, d_m^{(0)} \Longrightarrow \omega_m^{(0)}L = 2(m-1)\pi (188)$$
  

$$c_m^{(0)} = 0 \quad \text{and hence } cos(\omega_m^{(0)}L) = 1 \text{ hence } \omega_m^{(0)}L = 2(m-1)\pi (189)$$
  

$$d_m^{(0)} = 0 \quad \text{and hence } sin(\omega_m^{(0)}L) = 0 \text{ hence } \omega_m^{(0)}L = (m-1)\pi (190)$$

for all integers *m*. In order to determine which of the three possibilities itemized above occurs, one need to appeal to the initial data of the problem. Indeed, upon applying the standard Fourier procedure, and by taking into account relations (186), (187) and (184)<sub>2</sub>, together with the initial data (152) and (153) yields:

$$c_m^{(0)} = 0,$$
 (191)

while  $d_m^{(0)}$  is certainly non-zero. Henceforth, the m<sup>th</sup>-mode for the temperature takes the following form

$$g_m^{(0)}(x) = T_m^{(0)} \left( \cos(\omega_m^{(0)} x) - 1 \right), \tag{192}$$

where  $\omega_m^{(0)} = \frac{2(m-1)\pi}{L}$  and after setting

$$T_m^{(0)} = \frac{\omega_m^{(0)} d_m^{(0)}}{\alpha \,\lambda_m}.$$
(193)

Summing up the pinned-free case, the displacement and temperature fields take the following forms:

$$u^{(0)}(x,t) = \sum_{m}^{\infty} d_{m}^{(0)} \left( \sin(\omega_{m}^{(0)}x) - \omega_{m}^{(0)}x \right) E_{1-\beta,1} \left( -\frac{\omega_{m}^{(0)\,2}}{\delta} t^{1-\beta} \right)$$
(194)

$$T^{(0)}(x,t) = T_0 + \sum_m^{\infty} \lambda_m T_m^{(0)} \left( \cos(\omega_m^{(0)} x) - 1 \right) E_{1-\beta,1} \left( -\frac{\omega_m^{(0)\,2}}{\delta} t^{1-\beta} \right), \quad (195)$$

after making use of  $(177)_2$ , relating the time dependence of the m<sup>th</sup>-mode of the temperature and the one of the displacement.

The coefficients  $T_m^{(0)}$  are determined, again, by standard Fourier procedure. Upon integrating both sides of  $T^{(0)}(x,t) - T_0$  multiplied against  $cos(\omega_m^{(0)}x)$  over the length of the bar, it is found that:

$$\lambda_m T_m^{(0)} = \frac{2(T_0 - T_M)}{\pi^2 (m - 1)^2}, \quad m \ge 2.$$
(196)

As expected, the higher is the order of the spatial mode the lower is its contribution to the temperature. The amplitudes of the modal displacements are evaluated, in an analogous way, through relation (194), to get:

$$d_m^{(0)} = \frac{\alpha(T_0 - T_m)L}{(\pi(m-1))^3},$$
(197)

Again, it is obtained that the higher is the order of the spatial mode the lower is its contribution to the total displacement field.

# Case one: Pinned-free system undergoing boundary axial forces only

The pinned-free body is now analyzed as if it would be subject to the sole unknown axial forces arising at the boundary because of the extra constraint present in the original system. Each mode contributes to such a force with its component, denoted by  $X_m$ . The initial conditions for Case 1 are then the following:

$$T_m^{(1)}(x,0) = 0$$
 and  $N_m^{(1)}(x,0) = X_m$ , (198)

where the suffix (1) emphasizes the fact that Boundary conditions $(183)_1$  are replaced as follows:

$$w_m^{(1)}(0) = 0$$
 and  $w_m^{(1)'}(L) = \frac{X_m}{EA}$ , (199)

while  $(183)_2$  still remain valid as they are. It is straightforward to show that the boundary conditions, the initial conditions and the usual Fourier procedure yield the following results:

$$\omega_m^{(1)}L = \omega_m^{(0)}L = 2(m-1)\pi, \quad l_m^{(1)} = c_m^{(1)} = d_m^{(1)} = 0, \quad h_m^{(1)} = -p_m^{(1)} = \frac{X_m}{EA}.$$
(200)

#### The pinned-pinned case

Per each index *m*, the overall spatial mode is the result of the superposition of  $w_m^{(0)}(x)$  and  $w_m^{(1)}(x)$ , namely

$$w_m(x) = d_m^{(0)} \sin(\omega_m^{(0)} x) + \left(\frac{X_m}{EA} - d_m^{(0)} \,\omega_m^{(0)}\right) x.$$
(201)

By imposing the requirement due to the pinning at x = L at all times, namely  $w_m(L) = 0$ , and by recalling that  $\sin(\omega_m^{(0)}L) = 0$ , the value of the modal axial force  $X_m$  is obtained as follows:

$$X_m = EA \,\omega_m^{(0)} d_m^{(0)} = \frac{2 \,\alpha EA \,(T_0 - T_M)}{\pi^2 (m - 1)^2}, \quad m \ge 2.$$
(202)

It is worth noting that, as expected, the series of the normal force amplitudes does converge as  $\sum_{2}^{\infty} (m-1)^{-2} = \pi^2/6$  and, hence, at t = 0 it holds that

$$\hat{N}(0) = \frac{\alpha E A \left( T_0 - T_M \right)}{3}.$$
(203)

Because of the fact that time-decaying functions multiply of each term of both the temperature and of the displacement, relations (181) reads as follows:

$$\hat{N}(t) = 2 \alpha E A \left( T_0 - T_M \right) \sum_{m=2}^{\infty} \frac{1}{\pi^2 (m-1)^2} E_{1-\beta,1} \left( -\frac{4\pi^2 (m-1)^2}{\delta} t^{1-\beta} \right),$$
(204)

after making use of (202), (200) and (174). This does imply that the axial force is certainly decaying in time, thereby keeping its value always bounded and eventually fully relaxing. Relations (201) and (202) imply that the  $m^{th}$  mode for *u* is purely sinusoidal, and hence the final displacement takes the following form:

$$u(x,t) = \alpha (T_0 - T_m) L \sum_{m=2}^{\infty} \frac{1}{\pi^3 (m-1)^3} \sin\left(\frac{2(m-1)\pi x}{L}\right) \times E_{1-\beta,1} \left(-\frac{4(m-1)^2 \pi^2}{L^2 \delta} t^{1-\beta}\right).$$
(205)

For the spatial modes of T, (192) and the results above are considered to yield the following expressions for the temperature:

$$T(x,t) = T_0 + 4(T_0 - T_M) \sum_{m=2}^{\infty} \frac{1}{\pi^2 (m-1)^2} \left( \cos\left(\frac{2(m-1)\pi x}{L}\right) - 1 \right) \times E_{1-\beta,1} \left( -\frac{4(m-1)^2 \pi^2}{L^2 \delta} t^{1-\beta} \right).$$
(206)

Here, eq. (193) is used along with the fact that, actually, the  $\lambda_m$  arising in (177) do not depend on the circumstance that either of the cases 0 or 1 are examined.

It is worth noting that a non-anomalous behavior can be achieved by letting  $\beta \rightarrow 0$ . The result does not affect the spatial modes of neither the displacement nor of the temperature.

# Thermal "work" and measures of available energy rate and dissipation

The localized form of the balance of energy rate (149) can be used for further investigating the sources of dissipation and recovery of such rate. This can be done by multiplying both sides of such equation by the rate of change of temperature at which the line density  $q_{,x}$  of heat flux arises, and by integrating over time and over the length of the bar. This gives an instantaneous measure of how much thermal "work" is done on the bar thanks to heat transfer and mechanical actions. Indeed, integration by parts in space and boundary conditions yields the

following expression of the overall balance equation:

$$\int_{0}^{t} \int_{0}^{L} q T_{,tx} dx dt = -\int_{0}^{t} \int_{0}^{L} \left(\rho c_{v} + (\alpha EA)^{2} T_{0}\right) T_{,t}^{2} dx dt + -\int_{0}^{t} \int_{0}^{L} \frac{N_{,t}}{EA} T_{,t} dx dt.$$
(207)

The interpretation of such quantity is that this is a space-time global measure of the direct expenditure of the heat flux against the gradient of the temperature rate. The dimension of such a quantity is  $F L t^{-1} T$ , hence it represents a power times a temperature.

The quantity on the left-hand side generalizes an idea of [11, 26] for rigid thermal conductors, specialized by [12] in the presence of thermal memory. This also corresponds to eq.n (4.3) obtained in [14]. Nonetheless, in the present treatment the elastic deformability of the bar explicitly manifests itself in the second term on the right-hand side of (207), besides having an effect on the expressions of T and N, as it has been highlighted in the previous section.

The case under study has a very special form of memory in time, regulated by the power law  $t^{-\beta}$ . One can show that in the absence of a heat source within the bulk (so that the first term in (6.3) in [12] vanishes), the thermal "work" done by the heat flux given by (145) can be defined as follows:

$$w_T(t) := -\int_0^t \int_0^L q(T_{,x})_{,\tau} dx d\tau.$$
 (208)

By appealing to Fubini's theorem to interchange the order of integration, and substituting (145) in the expression above, after some calculations the following expression for the thermal work are obtained

$$w_T(t) = \frac{K_{\beta}}{\Gamma(1-\beta)} \int_0^L \int_0^t \int_0^{\tau} \frac{T_{,x}(x,\tau), \tau T_{,x}(x,\rho), \rho}{(\tau-\rho)^{\beta}} d\rho \, d\tau \, dx.$$
(209)

It is worth remarking that (208) is a general notion and its definition (easily generalizable to three dimensions) does not depend on the specific solution of the Initial Boundary Value Problem under consideration. Of course neither from (207) nor from this latter expression of the overall balance of energy rates clearly appears which fraction of  $w_T(t)$  gets dissipated and which one is actually at the disposal of the thermoelastic processes available for the system.

Indeed, the direct inspection of the right-hand side of (207), which only depends on the fact that it is considered a thermoelastic truss with thermal memory coming from the multi-scale procedure derived in [1], does not directly enable one to understand if part of this global energy rate gets dissipated. In order to shed light on this issue, the authors note the formal analogy of the integrand in (208) (or (209)) and with the product  $\sigma \dot{\varepsilon}$  in relation (22) of [27]. Indeed, by setting

$$G(t) := -\frac{K_{\beta}}{\Gamma(1-\beta)}t^{-\beta}, \qquad (210)$$

upon formally identifying q with  $\sigma$  and T, with  $\varepsilon$  in such a relation, it holds

$$q(T_{,x})_{,t} = \Psi_t(x,t) + \mathscr{D}(x,t), \qquad (211)$$

where

$$\Psi(x,t) = -\frac{1}{2} \int_0^t \int_0^t G(2t - \tau_1 - \tau_2) (T_{,x})_{,t}(x,\tau_1) (T_{,x})_{,t}(x,\tau_2) d\tau_1 d\tau_2.$$
(212)

After some calculations, it is possible to show that the rate of change of such  $\psi$  takes the following form:

$$\Psi_{,t}(x,t) = q \ (T_{,x})_{,t} + \frac{1}{2} \int_0^t \int_0^t \dot{G}(2t - \tau_1 - \tau_2) (T_{,x})_{,t}(x,\tau_1) (T_{,x})_{,t}(x,\tau_2) d\tau_1 d\tau_2.$$
(213)

Finally, by making use of (210), the associated specific measure of "dissipation rate" (per unit length and per unit time) turns out to read as follows

$$\mathscr{D}(x,t) = -\frac{\beta K_{\beta}}{2\Gamma(1-\beta)} \int_0^t \int_0^t (2t-\tau_1-\tau_2)^{-(\beta+1)} \times (T_{,x})_{,t}(x,\tau_1) (T_{,x})_{,t}(x,\tau_2) d\tau_1 d\tau_2.$$
(214)

It is worth nothing that  $\psi(x,t)$  is the analog of the free energy (21) in [27], which turns out to be in the form of Stavermal and Schwarzl. The rate of change of this

last quantity represents the part of the thermal work that can be at the disposal of the body, while (214) gives the measure of the rate of dissipation during the thermo-mechanical loading of the bar. This is of particular interest as its overall value  $t = t^{2}$ 

$$\mathscr{D}_T(t) := \int_0^t \int_0^L \mathscr{D}(x,\tau) \, dx \, d\tau \tag{215}$$

will tell us how much of  $w_T(t)$  gets dissipated. Indeed, upon integrating (211) on space and time the following equation arises:

$$w_T(t) = \Psi_T(t) + \mathscr{D}_T(t), \qquad (216)$$

where the overall measure of energy rate  $\psi_T$  takes the form:

$$\begin{split} \psi_{T}(t) &= \int_{0}^{L} \psi(x,t) dx = \\ &= \frac{256\pi^{2}K_{\beta} \left(T_{0} - T_{M}\right)^{2}}{L^{5} \delta^{2} \Gamma(1-\beta)} \sum_{m=2}^{\infty} (m-1)^{2} \int_{0}^{t} \int_{0}^{t} \frac{(\tau_{1}\tau_{2})^{-\beta}}{(2t-\tau_{1}-\tau_{2})^{\beta}} \times \\ &\times E_{1-\beta,1-\beta} \left( -\frac{4(m-1)^{2}\pi^{2}}{L^{2} \delta} \tau_{1}^{1-\beta} \right) \times \\ &\times E_{1-\beta,1-\beta} \left( -\frac{4(m-1)^{2}\pi^{2}}{L^{2} \delta} \tau_{2}^{1-\beta} \right) d\tau_{1} d\tau_{2}. \end{split}$$
(217)

This global measure has been evaluated in analogy with the definition (215). Interchanging the order of integration can be done thanks to Fubini's theorem, which requires enough smoothness to do so. The correspondent measure of the overall thermal work is evaluate in full analogy with  $\psi_T$ , to get

$$w_{T}(t) = \frac{512\pi^{2}K_{\beta}(T_{0} - T_{M})^{2}}{L^{5}\delta^{2}\Gamma(1 - \beta)} \sum_{m=2}^{\infty} (m - 1)^{2} \int_{0}^{t} \int_{0}^{t} \frac{(\tau_{1}\tau_{2})^{-\beta}}{(t - \tau_{2})^{\beta}} \times E_{1-\beta,1-\beta} \left( -\frac{4(m - 1)^{2}\pi^{2}}{L^{2}\delta} \tau_{1}^{1-\beta} \right) \times E_{1-\beta,1-\beta} \left( -\frac{4(m - 1)^{2}\pi^{2}}{L^{2}\delta} \tau_{2}^{1-\beta} \right) d\tau_{1}d\tau_{2}.$$
(218)

A direct inspection of the series expansion of each term of the integrand in the latter expression shows that  $w_T(t)$  has a finite value only for  $\beta < 1/2$  (this agrees

with the fact that the original range for  $\beta$  is [0, 1) and with the convergence of the resulting singular integral). The finiteness of the global thermal work limits the degree anomaly that the heat flux can exhibit. In terms of multi-scale rheological models, there is a purely mechanical analog in [27] - Sect. 4.1, although there the value 1/2 can be achieved. This result has a direct consequence on the partition of the thermal work, thereby ensuring that both  $\mathscr{D}_T(t)$  and  $\psi_T(t)$  are finite in the same range.

## Discussion

The detailed analysis performed above and the related investigation about the global measures of the thermo-mechanical work, energy and dissipation rates allow one for comparing the consequences of anomalous heat transfer in (one dimensional) deformable bodies.

All the resulting fields, namely the axial stress (204), the displacement (205), and the temperature (206) are influenced by the thermal and elastic deformability of the bar. Two effects, namely (i) the deformability and (ii) the emerging deviation for the Fourier behavior, can be analyzed separately in the sequel.

• (i) Once  $\beta = 0$  is considered, namely the latter case, and the temperature distributions (206) and (65) in [1] are compared (see Figure 27) a noticeable difference in their time behavior is reported. The non-dimensional times with respect which the fields for deformable versus rigid conductors are plotted are  $\underline{t}_d := \frac{\delta^{-1}t^{1-\beta}}{L^2}$  and  $\underline{t}_r := \frac{\gamma_\beta t^{1-\beta}}{L^2}$ , respectively. In particular, a very significant influence on the thermal and elastic deformability on the time-rise of the temperature is detected. Indeed, from (163), because of the thermal and of the mechanical deformability, it is seen that the time dependence of the temperature (206) gains a scaling factor always less than or equal than 1, thereby reducing the value of the argument of the time modulating function  $E_{1-\beta,1}\left(-\frac{4(m-1)^2\pi^2}{L^2\delta}t^{1-\beta}\right)|_{\beta=0} = \exp{-\left(\frac{4(m-1)^2\pi^2\gamma_0}{L^2(1+\alpha^2 EAT_0/\rho c_v)}\right)t}$  for each mode. These then leads to a higher magnitudes of such modulating functions relative to the case of rigid conductors. For the only sake of illustration, numerical data such as  $\rho = 7860 \frac{Kg}{m^3}$ ,  $C_V = 502 \frac{J}{Kg^{\circ}C}$ ,  $K = 30 \frac{W}{m^{\circ}C}$ ,



FIGURE 27: Non dimensional temperature fields  $\frac{T-T_0}{T_0-T_M}$  for  $\beta = 0$ . All the surfaces have been obtained with n = 20

 $\alpha = 12 \cdot 10^{-6} \frac{1}{^{\circ}C}, E = 220 GPa$ ,  $T_0 = 125 ^{\circ}C$  and  $T_M = 25 ^{\circ}C$  have been implemented to investigate the effects of the deformability.

An interpretation of this outcome can simply be related to the fact that in the current study the bar is fully thermoelastic, which implies that there is a continuous feedback between the temperature gradient and its rates and the strain rate itself. The redistribution of temperature and displacement is indeed due to the interplay between the balance of energy rate and the one of linear momentum. Within the former, (149), the heat flux (line) density has an extra forcing supply term, which is driven by the total strain rate, given by the sum of its elastic and thermal parts (e.g. (148)). This extra supply rate then triggers a faster temperature raise with respect to the case of rigid conductors, where neither the thermal nor the elastic dilatation can take place.

• (ii) The influence of the deviation from the Fourier behavior of deformable conductors is summarized by comparing Figures 28a and 28b with the outcomes of Figure 27a. While the rapid rise in time to a regime value it is still seen here, the higher is the deviation from a Fourier-like behavior, the more rapid that rise gets. This is indeed an intrinsic feature of the anomalous heat transfer, now coupled with an elastic and thermally deformable



FIGURE 28: a) and b) Non dimensional temperature fields  $\frac{T-T_0}{T_0-T_M}$  for deformable conductors with different values of  $\beta$ , equal to  $\beta = 0.2$  and  $\beta = 0.4$  respectively; all the surfaces have been obtained with n = 20 c) Time evolution of non-dimensional axial force  $\frac{\hat{N}}{\alpha E A(T_0-T_M)}$  d) Time evolution of non-dimensional temperature fields at  $\underline{x} = 0.5$ 

bar. Another effect of the deviation from the Fourier behavior is the tendency to reach steady values in longer times. The higher the value of the anomaly exponent  $\beta$  in [0, 1/2) the faster this becomes. In particular, for higher values of  $\beta$  the temperature tends to reach  $T_0$ . This effect is more visible in the time evolution of the associate axial force, namely in Figure 28c and it is a consequence of the "long-tail memory" effect, a feature of a power law behavior given by (210). Indeed, as it is well known, the constitutive relation (145) for the heat flux can be recast as

$$q(x,t) = \int_0^t G(t-\tau)(T_{,x})_{,\tau}(x,\tau)d\tau,$$
 (219)

where the "relaxation function" G is given by (210).

A comparison among the different landscapes obtained for the displacement field for the three values of  $\beta$  mentioned above suggests a similar trend in terms of its time evolution (see Fig (29)). In fact, the higher is the discrepancy against the Fourier behavior the more pronounced is the long-tail effect on settling to a stationary value, which in this case is actually zero. Spatially, the resulting odd fluctuations relative to the midpoint of the span is essentially governed by the initial condition on u, a result of the balance of linear momentum.

The most interesting features of the anomalous thermoelastic coupling for bars comes from the comparison of the global measures of the "thermal work"  $w_T$ , of the available energy rate  $\psi_T$  and the dissipation rate  $\mathcal{D}_T$ , (209), (217) and (215) respectively. Both for the rigid and for the deformable Fourier-like cases, a smooth monotonically increase of (non-dimensional) thermal work  $\underline{W}$ , defined in Figures 30 and 31a respectively, is noted. For rigid conductors there is a smoother increase with respect to deformable ones with no appreciable asymptote before  $\underline{t} \simeq 0.5$  and with the corresponding value of  $\underline{W} \simeq 2 \cdot 10^{-3}$ . On the contrary, for deformable conductors a steady value (circa 0.7) is achieved at  $\underline{t} \simeq 0.10$  (see Figure 31), where  $\underline{t} := \underline{t}_d = \frac{\delta^{-1}t^{1-\beta}}{L^2}$ . The higher values and the sharper time rise of  $\underline{W}$ , a quadratic operator involving the rate of change of temperature gradients, is primarily due to the fact that much higher rates of temperature gradient are detected in the deformable case, as Figure 27 shows. In both cases there is a perfect equi-partition of the quotas of  $\psi_T$  and  $D_T$  (which in the figures are replaced by





FIGURE 29: Displacement fields for deformable conductors with different values of  $\beta$ . All the surfaces have been obtained with n = 20



FIGURE 30: Rigid conductors: non-dimensional thermal work  $\underline{W}$ , non-dimensional energy rate  $\underline{\Psi}$  and non-dimensional dissipation rate  $\underline{D}=\underline{W}-\underline{\Psi}$  along with non-dimensional time  $\underline{t}$ , for  $\beta = 0$ 



FIGURE 31: Deformable conductors: non - dimensional thermal work  $\underline{W}$ , non - dimensional energy rate  $\underline{\Psi}$  and non - dimensional dissipation rate  $\underline{D}=\underline{W}-\underline{\Psi}$  along with non-dimensional time  $\underline{t}$ , for different values of  $\beta$ 

their corresponding non-dimensional counterparts  $\underline{\Psi}$  and  $\underline{D}$ ) in which the thermal work is decomposed.

This fits in a striking formal analogy with linear elasticity, as  $\beta = 0$  implies  $q = -K_0T_{,x}$  like  $N = EA\varepsilon$  for the latter case. In [28] it is seen as this results from a smart re-visitation of Clapeyron's theorem for three dimensional linear elasticity. This has been rendered free of the paradox that no dissipation would have occurred even if the total work is twice the value of the strain energy at the final values of the strain in an underlying loading process. A (rate-type) viscoelastic term allowed there to consider the effect of slow loading processes, thereby retrieving the asymptotic value of the overall dissipation and matching the other missing half of the work.

Signatures of the thermal anomaly are seen in the thermal work and in the available energy and dissipation rates. First of all, it is noticeable that the higher the value of  $\beta$  the more the thermal work exhibit a discrepancy with respect to the Fourierian case. Furthermore, a deviation from equipartition between  $\psi_T$  and  $\mathscr{D}_T$  is also detected, thereby indicating that this global measure of rate dissipation rises due to the deviation from the Fourier behavior. Anomaly then introduces a further source of dissipation, most likely due to the fact that the scaling of q like  $t^{-\beta}$  resembles an hierarchy of thermal properties, as explained in [1], enhancing the possibilities of dissipating energy at the various scales. A change in signature is noticeable for  $\beta = 0.2$ , for which a softening is exhibited by <u>W</u> after  $t \simeq 0.025$ , while a plateau is then reached at <u>W</u>  $\simeq 0.95$ . The rising of the thermal work in time is analog to what it has been discussed above to the temperature, essentially characterizing the response of the anomalous thermo-mechanics evolution of the system under study.

A further extreme behavior for all the quantities  $\underline{W}$ ,  $\underline{\Psi}$  and  $\underline{D}$  is recorded for  $\beta = 0.4$ . Here the time rise becomes almost immediate, as for the corresponding temperature (see Figure 28b), and the softening behavior essentially dominates their trend. The discrepancy between the global dissipation rate  $\underline{D}$  and the corresponding  $\underline{\Psi}$  becomes more pronounced, thereby confirming the trend noticed before. Henceforth, the more the heat flux deviates from the standard Fourier behavior the higher is the likelihood of having further dissipation during the thermoelastic evolution of the system.

A modal decomposition of the global measures of energy rates is reported in Figure 32. As expected, the global measures of work, energy and dissipation rates are heavily guided by the first mode, given by m = 2, which hence gives a qualitative idea about the global measures of energy rate response of the anomalous thermoelastic system. Given the importance of the conclusions drawn above, a comprehensive thermodynamic analysis should be performed to investigate how the deviation from the standard Fourier behavior influences the performances of such systems. This is the subject for further thorough investigations involving refined measures of the actual entropy rate, that should be calculated starting from the multi-scale rheological scheme introduced in [1].

## Conclusions

In the present work the "fractional thermally-anomalous" coupled behavior of slightly deformable bodies is studied. The mentioned "anomaly" originates from the relation among the macroscopic heat flux and the time history of the temperature gradient, that involves a "long-tail" memory behavior, governed by a Caputo's fractional operator. Indeed, the macroscopic constitutive equation between the heat flux and the time history of the temperature gradient does involve a power law kernel, and it is the result of a multi-scale rheological model developed in Part 1 of the present study.

For the sake of illustration, the interplay between the thermal flux and the elastic and the thermal deformability are investigated for a pinned-pinned truss. Given the simplicity of the system geometry, together with the richness of the arising axial stress, this allows for focusing on the effects of the deviation from the Fourier's law on the thermoelastic coupling. Results show that the interactions, in such simply geometry, are fully coupled as the temperature and the displacement fields mutually influence one another.

A space-time modal analysis performed on the fractional-order system, relying on the balance of linear momentum and on the balance of energy rate, provides the explicit solutions of the problem. The time evolution of each spatial mode, for the temperature, for the displacement and for the axial force, turn out



FIGURE 32: Modal decomposition of the global measures of energy rates, for different values of  $\beta$ . a),b),c) Non-dimensional thermal work, d),e),f) non-dimensional dissipation rate

to be characterized by modulated Mittag-Leffler functions. The higher is the deviation from the Fourier-like behavior for the heat flux, the steeper is the resulting time-transient of each mode. The influence of the deformability on the one hand, and of the discrepancy from the Fourier behavior on the other hand, are thoroughly analyzed for the three fields mentioned above.

Measures of the overall "thermal work", and of the associate available and dissipation energy rates are evaluated, both mode-by-mode and globally, enabling the characterization of the coupled response of anomalous thermoelastic trusses. Besides determining the range of admissible discrepancies from the Fourier behavior, such quantities are shown to fully reveal the manifestation of the thermal anomaly together with the effects of the elastic and thermal deformabilities.

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## Part III

# Design of 3D-printed structural components

## Influence of meso-structure and chemical composition on FDM 3D-printed parts \*

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#### ABSTRACT

**Objectives:** In this study we focus on mechanical properties of Fused Deposition Modeling (FDM) 3D-printed objects. We studied the influence of extruded filament dimensions and chemical composition on mechanical behavior of FDM objects made of Acrylonitrile Butadiene Styrene (ABS) polymer.

**Methods:** The influence of filament dimension and chemical composition on mechanical behavior is studied varying fiber orientation with respect to the loading direction. All aspects are investigated through experimental campaigns: meso-structure influence, i.e. fiber thickness and width is tested on the same material, while chemical composition impact is tested using the same mesostructure.

**Results:** We verified that FDM ABS specimens show anisotropic mechanical properties since they vary with filament extrusion direction. Accordingly, Classical Lamination Theory (CLT) and Tsai-Hill yielding criterion were found to be well capable of predicting in-plane stiffness and strength of FDM specimens.

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**Conclusions:** We assessed that, varying chemical composition and filament dimensions, it is possible to tune fiber properties and fiber-to-fiber bonding and, consequently, the overall mechanical properties at macro-scale, in particular the yielding strength and the strain at failure. The experimentally obtained data are useful to calibrate mechanical models to be used with computational tools as finite element analyses. Relying on the good consistency between experimental and estimated data, we strongly suggest the adoption of suitable standard test methods tailored on anisotropic materials in order to experimentally evaluate mechanical properties of FDM 3D-printed parts.

## Introduction

Additive Manufacturing (AM) processes form three-dimensional (3D) objects from virtual models, obtained from a Computer Aided Design (CAD) software, digital scanning systems or medical imaging systems, such as computer tomography or magnetic resonance imaging. In recent years, AM processes have begun to progress from rapid prototyping techniques towards rapid manufacturing methods, where the objective is now to produce finished components [1]. AM technologies are ready to be used for industrial production and, due to a growing competition between service furnishers, they are becoming economically feasible for a great number of end-user applications [2]. In the last decade the maturity of these processes was largely increased thanks to the research on materials, the development of new equipments and the better understanding of the processes [3].

From an industrial point of view, technologies capable of producing robust parts with high strength and long-term stability are the most relevant, because they allow the direct production of end-user parts. The use of AM solutions for direct production would be possible only if mechanical properties are well known and taken into account in the design stage, depending on the process parameters. However, one of the most important open issues in rapid manufacturing is the prediction of 3D-printed parts behavior under real working conditions. In this study we focus on mechanical properties of Fused Deposition Modeling (FDM <sup>®</sup>) 3D-printed objects. Such process belongs to the material extrusion subfamilies of Solid Freeform Fabrication (SFF) technologies. In FDM processes a thermoplastic filament is heated and extruded through a robotically controlled head: the material is deployed layer by layer on a printing surface in a temperature controlled environment. Each printed layer is made of filaments known as fibers (also called "beads" or "roads") deposited in a plane parallel to the printing surface. The printing head movements, the extrusion system and all the other printing parameters are controlled by an electronic board, relying on a set of instructions (G-Code) listed in a file. The G-Code is produced by a dedicated software commonly called *slicer* or *slicing software*, that takes into account the virtual geometry, the characteristics of the printing material and the specific features of the 3D-printer.

The FDM 3D-printed object is composed by two main parts, the *internal raster* (infill) and its *outer shell*, made by perimeters and solid top/bottom layers; the direction of the deposited material is known as *fiber orientation angle*. The bonding between neighboring fibers occurs by a thermally-driven diffusion process during solidification of the semi-molten extruded fiber [4, 5].

The inner structure at a sub-millimeter scale, i.e. the *meso-structure*, is determined by the filament path deposition and process parameters. Among these, the most important are: fiber thickness and width, fiber-to-fiber overlap, fiber orientation and extrusion temperature. Figure 33 shows a schematic representation of the ideal meso-structure resulting from the FDM process. Research efforts in FDM technology have been directed towards the evaluation of the mechanical properties of the resulting part as a function of process parameters. Ahn et al. [6] showed that both fiber-to-fiber overlap and fiber orientation had a significant effect on the resulting tensile strength, while compressive strength was not affected by these parameters. Sood et al. [7, 8] investigated the functional relationship between fiber dimensions, overlap and orientation and specimen strength using response surface methodology; results show that such parameters influence fiber bonding capabilities and distortion of the printed part and, consequently, the compressive strength of test samples. Moreover, Lee at al. [9, 10] studied the influence of fiber thickness, orientation and fiber-to-fiber overlap on the strength



width

thickness

FIGURE 33: Scheme of the ideal meso-structure resulting from the filament extrusion process

DETAIL A

of FDM 3D-printed Acrylonitrile Butadiene Styrene (ABS) samples; the authors determined that the compressive strength for an axial FDM specimen is greater than for a transverse one. Rodríguez et al. [11, 12] compared elastic modulus and tensile strength of FDM printed samples with the same properties of the ABS filament feedstock; the authors concluded that parts with fibers aligned with the axis of the tension force have the greatest tensile strength.Es-Said et al. [13] investigated the influence of fiber orientation and polymer molecules alignment along the extrusion direction.

Concerning the mechanical modeling of 3D-printed parts, Classical Lamination Theory (CLT) and Tsai-Hill yield criterion have already been considered in few studies. Kulkarni and Dutta [14] applied CLT to describe the elastic moduli of FDM printed laminates. Bertoldi et al. [15] and Rodríguez et al. [4] assumed orthotropic material symmetry and obtained elastic moduli and strength values for different fiber orientations. Li et al. [16] studied the fabrication process and the mechanical properties of FDM specimens, using CLT to determine the elastic constants as a function of raster angle; experimental data were in good agreement with the results of the laminate modeling.

Literature evidence proves that CLT and Tsai-Hill yielding criterion are valuable instruments to describe the mechanical properties of FDM 3D - printed components. Accordingly, in the present work, we use both instruments to investigate



FIGURE 34: Reference coordinate system  $\{O, x, y, z\}$  for the laminate and material coordinate systems  $\{O', 1, 2, 3\}$  for the laminas

how the mechanical properties of ABS 3D-printed FDM parts are influenced *i*) by the chemical composition of the filament and *ii*) by fiber cross-sectional dimensions, maintaining the thickness/width ratio constant. The influence of filament dimension and chemical composition on mechanical behavior is studied varying fiber orientation with respect to the loading direction. All aspects are investigated through experimental campaigns: meso-structure influence, i.e. fiber thickness and width is tested on the same material, while chemical composition impact is tested using the same meso-structure.

## Mechanical modeling

#### **Elastic behavior modeling**

In this study, FDM 3D-printed objects are considered as composite laminates consisting of orthotropic laminas; each lamina corresponds to a layer made of ABS parallel filaments. We consider two right-handed coordinate systems, namely  $\{O, x, y, z\}$  and  $\{O', 1, 2, 3\}$  as in fig. 34: axis 1 is aligned to the filament extrusion direction and represents the longitudinal direction of the lamina, while axis 2 is perpendicular to fiber extrusion direction and represents its transverse direction. Axes x and y represent the loading directions of the laminate. The angle  $\theta$ , formed by axis 1 with respect to axis x in a counter-clockwise rotation, is the fiber orientation angle.

For a linear elastic orthotropic material, the constitutive relations relating stresses and strains are:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \tau_{12} \\ \tau_{13} \\ \tau_{23} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & 0 & 0 & 0 \\ Q_{12} & Q_{22} & Q_{23} & 0 & 0 & 0 \\ Q_{13} & Q_{23} & Q_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_{15} & 0 \\ 0 & 0 & 0 & 0 & 0 & Q_{16} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{13} \\ \gamma_{23} \end{bmatrix}$$
(220)

As classically done for the printed fiber [12, 16], we may assume the same mechanical behavior in direction 2 and 3, obtaining an orthotropic, transversely isotropic (in plane 2-3) material; accordingly eq. (220) becomes:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \tau_{12} \\ \tau_{13} \\ \tau_{23} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{12} & 0 & 0 & 0 \\ Q_{12} & Q_{22} & Q_{23} & 0 & 0 & 0 \\ Q_{12} & Q_{23} & Q_{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{Q_{22} - Q_{23}}{2} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{13} \\ \gamma_{23} \end{bmatrix}$$
(221)

In case of plane stress state ( $\sigma_{33} = \tau_{13} = \tau_{23} = 0$ ), relation (221) may be reduced as follows:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \tau_{12} \end{bmatrix} = \begin{bmatrix} \hat{Q}_{11} & \hat{Q}_{12} & 0 \\ \hat{Q}_{12} & \hat{Q}_{22} & 0 \\ 0 & 0 & \hat{Q}_{33} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \gamma_{12} \end{bmatrix}$$
(222)

and the quantity  $\varepsilon_{33}$  can be computed from the condition  $\sigma_{33} = 0$ . Relation (222) relates in-plane stresses and strains through the matrix  $[\hat{Q}]$  that involves four independent elastic constants, namely  $\hat{Q}_{11}$ ,  $\hat{Q}_{12}$ ,  $\hat{Q}_{22}$  and  $\hat{Q}_{33}$ . Such constants may be expressed as a function of longitudinal Young's modulus  $E_1$ , transverse Young's modulus  $E_2$ , Poisson's ratio  $v_{12}$ , and shear modulus  $G_{12}$  as shown below:

$$\hat{Q}_{11} = \frac{E_1^2}{E_1 - v_{12}^2 E_2} \tag{223a}$$

$$\hat{Q}_{22} = \frac{E_1 E_2}{E_1 - v_{12}^2 E_2} \tag{223b}$$

$$\hat{Q}_{12} = \frac{\mathbf{v}_{12}E_1E_2}{E_1 - \mathbf{v}_{12}^2E_2} \tag{223c}$$

$$\hat{Q}_{33} = G_{12}$$
 (223d)

The constitutive relations (222) can be expressed in the reference coordinate system  $\{O, x, y, z\}$  as:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{bmatrix} = \begin{bmatrix} \bar{Q}_{11} & \bar{Q}_{12} & \bar{Q}_{13} \\ \bar{Q}_{12} & \bar{Q}_{22} & \bar{Q}_{23} \\ \bar{Q}_{13} & \bar{Q}_{23} & \bar{Q}_{33} \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{bmatrix}$$
(224)

where the matrix  $[\bar{Q}]$  is

$$[\bar{Q}] = [T][\hat{Q}][M]^{-1}[T]^{-1}[M]$$
(225)

In eq. (225) matrix [M] is defined as:

$$[M] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/2 \end{bmatrix}$$
(226)

and [T] is the rotation matrix:

$$[T] = \begin{bmatrix} \cos^2(\theta) & \sin^2(\theta) & -2\cos(\theta)\sin(\theta) \\ \sin^2(\theta) & \cos^2(\theta) & 2\cos(\theta)\sin(\theta) \\ \cos(\theta)\sin(\theta) & -\cos(\theta)\sin(\theta) & \cos^2(\theta) - \sin^2(\theta) \end{bmatrix}$$
(227)

Stacking *N* laminas along the *z*-axis a laminate is obtained. In this paper CLT has been used to model the mechanical behavior of thin 3D-printed structures. CLT assumes that the generic straight segment perpendicular to the mid-plane of the

laminate remains straight and perpendicular to the mid-plane after its deformation. From this hypothesis it is possible to obtain the following expressions for in-plane strains:

$$\begin{bmatrix} \boldsymbol{\varepsilon}_{xx} \\ \boldsymbol{\varepsilon}_{yy} \\ \boldsymbol{\gamma}_{xy} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\varepsilon}_{xx}^{0} \\ \boldsymbol{\varepsilon}_{yy}^{0} \\ \boldsymbol{\gamma}_{xy}^{0} \end{bmatrix} + z \begin{bmatrix} \boldsymbol{\kappa}_{x}^{0} \\ \boldsymbol{\kappa}_{y}^{0} \\ \boldsymbol{\kappa}_{xy}^{0} \end{bmatrix}$$
(228)

where z is the distance from the mid-plane in the direction perpendicular to the mid-plane itself,  $\varepsilon_{xx}^0$ ,  $\varepsilon_{yy}^0$  and  $\gamma_{xy}^0$  are the mid-plane strains and  $\kappa_x^0$ ,  $\kappa_y^0$  and  $\kappa_{xy}^0$  are the mid-plane curvatures. Laminate normal and shear forces, namely  $N_x$ ,  $N_y$  and  $N_{xy}$  respectively, are related to mid-plane strains and curvatures through the following expressions:

$$\begin{bmatrix} N_x \\ N_y \\ N_{xy} \end{bmatrix} = [F] \begin{bmatrix} \varepsilon_{xx}^0 \\ \varepsilon_{yy}^0 \\ \gamma_{xy}^0 \end{bmatrix} + [G] \begin{bmatrix} \kappa_x^0 \\ \kappa_y^0 \\ \kappa_{xy}^0 \end{bmatrix}$$
(229)

while laminate bending and twisting moments, i.e.  $M_x$ ,  $M_y$  and  $M_{xy}$  respectively, are related to strains and curvatures as shown below:

$$\begin{bmatrix} M_x \\ M_y \\ M_{xy} \end{bmatrix} = \begin{bmatrix} G \end{bmatrix} \begin{bmatrix} \boldsymbol{\varepsilon}_{xx}^0 \\ \boldsymbol{\varepsilon}_{yy}^0 \\ \boldsymbol{\gamma}_{xy}^0 \end{bmatrix} + \begin{bmatrix} H \end{bmatrix} \begin{bmatrix} \boldsymbol{\kappa}_x^0 \\ \boldsymbol{\kappa}_y^0 \\ \boldsymbol{\kappa}_{xy}^0 \end{bmatrix}$$
(230)

in eqs. (229) and (230) matrices [F], [G] and [H] are calculated as shown below:

$$F_{ij} = \sum_{k=1}^{N} \bar{Q}_{ij}^{k} (z_k - z_{k-1})$$
(231a)

$$G_{ij} = \frac{1}{2} \sum_{k=1}^{N} \bar{Q}_{ij}^{k} (z_k^2 - z_{k-1}^2)$$
(231b)

$$H_{ij} = \frac{1}{3} \sum_{k=1}^{N} \bar{Q}_{ij}^{k} (z_k^3 - z_{k-1}^3)$$
(231c)

hence they depend on each k-th lamina stiffness matrix  $[\bar{Q}^k]$  and of distances from mid-plane to the lamina.
### **Yielding modeling**

Strength of ABS specimens is modeled using Tsai-Hill failure criterion for composite materials under multiaxial loading [17]. Tsai-Hill criterion assumes that the yielding surface is quadratic with respect to the stress components expressed in the material reference system as:

$$(B+C)\sigma_{11}^{2} + (A+C)\sigma_{22}^{2} + (A+B)\sigma_{33}^{2} - 2C\sigma_{11}\sigma_{22} - 2B\sigma_{11}\sigma_{33} + -2A\sigma_{22}\sigma_{33} + 2L\tau_{23}^{2} + 2K\tau_{13}^{2} + 2N\tau_{12}^{2} = 1$$
(232)

where A, B, C, L, K, and N coefficients are Hill's strength parameters that must be intended as yielding values for ductile materials and ultimate failure values for brittle ones. For an orthotropic, transversely isotropic lamina under plane stress, the Tsai-Hill criterion is expressed as:

$$\frac{\sigma_{11}^2}{S_1^2} + \frac{\sigma_{22}^2}{S_2^2} - \frac{\sigma_{11}\sigma_{22}}{S_1^2} + \frac{\tau_{12}^2}{S_{12}^2} = 1$$
(233)

where  $S_1$  is the strength in the longitudinal direction,  $S_2$  is the strength in the transverse direction and  $S_{12}$  is the in-plane shear strength. An admissible (elastic) stress state is obtained when the l.h.s. of the equation (233) assumes a value lower than 1.

In presence of mono-axial tensile stress  $\sigma_{xx}$  ( $\sigma_{yy} = \tau_{xy} = 0$ ), the stress components in the material reference system are given in terms of the stress in the loading direction of the specimen:

$$\sigma_{11} = \sigma_{xx} \cos^2 \theta \tag{234a}$$

$$\sigma_{22} = \sigma_{xx} sin^2 \theta \tag{234b}$$

$$\tau_{12} = -\sigma_{xx} \cos\theta \sin\theta \tag{234c}$$

Parameters	Type A	Type B	Unit
Extrusion Temperature	250-260	250-260	°C
Bed Temperature	100	100	°C
Heated Chamber Temperature	70	70	°C
Maximum Flowrate	6	5	mm <sup>3</sup> /s

TABLE 4: Main printing parameters identified during preliminary assessment

Substituting the above expressions into equation (233) and resolving for  $\sigma_{xx}$  gives the following result:

$$\sigma_{xx} = S(\theta) = \left[\frac{\cos^4\theta}{S_1^2} + \frac{\sin^4\theta}{S_2^2} - \frac{\cos^2\theta\sin^2\theta}{S_1^2} + \frac{\cos^2\theta\sin^2\theta}{S_{12}^2}\right]^{-\frac{1}{2}}$$
(235)

Equation (235), along with admissible yield stresses  $S_1$ ,  $S_2$  and  $S_{12}$  can be used to calculate the yielding strength  $S(\theta)$  against fiber orientation  $\theta$ .

## Materials and methods

#### **Preliminary material analysis**

Two different types of ABS, provided by Versalis S.p.A. [18] and indicated with letters A and B, are investigated: type A is the base ABS, while type B is a chemically additivated ABS. The 3D printer used for the present study is a 3NTR A4v3 [19]. The machine is equipped with three extruders, which can be heated up to 410 °C, through a ceramic heating component; a nozzle of 0,4 mm of diameter is used. The bed temperature can reach 120 °C, while the heated chamber can reach 75 °C. Preliminary assessment results relative to main printing parameters are shown in Table 4.

Maximum extrusion flow-rate mainly depends on nozzle diameter and on the viscosity of the filament [20] and it is about 6 and 5 mm<sup>3</sup>/s, respectively. Such values must be taken in to account for the choice of admissible printing speeds that can be used in relation to other printing parameters, namely fiber thickness and width. As an example, using a thickness of 0,2 mm and a width of 0,4 mm, a

velocity of 40 mm/s should be set (resulting in a flow-rate of 0,2 mm x 0,4 mm x  $40 \text{ mm/s} = 3,2 \text{ mm}^3/\text{s}$ ).

Thermal distortion and compatibility with the selected support material are tested through the printing of objects with a large base in contact with the bed. Type A shows an optimal compatibility with High Impact Polystyrene (HIPS), one of the most common polymers used to support ABS prints. The distance between the last layer of support material and the first layer of ABS (commonly defined as air gap) can be set to 0,1-0,2 mm. HIPS can be detached from the final object using a mechanical or chemical approach, the latter thanks to the use of a limonene solution.

Type A stitches well on a HIPS base during the printing and the support structure is extremely easy to remove after the final object has cooled down for some minutes. Type B shows a lower compatibility with HIPS: better results can be retrieved lowering the "air gap", but the printing of large objects remains difficult to be carried out. The support interface detachment is easily performed.

#### **Experimental setup**

We need four elastic constants to characterize an orthotropic lamina under plane stress (eqs. (223)), while three admissible stresses are necessary for Tsai-Hill yielding surface (eq. (233)). Such properties may be evaluated through tensile tests on specimens with fiber orientation of  $0^{\circ}$ ,  $90^{\circ}$  and  $45^{\circ}$ . Moreover, specimens must be unidirectional and, consequently, perimeters must be avoided because their direction would be different from the fiber orientation, for specimen with  $\theta \neq 0^{\circ}$ .

Longitudinal specimens (0°) are used to determine longitudinal modulus of elasticity  $E_1$ , Poisson's ratio  $v_{12}$  and yield strength  $S_1$ ; transverse specimens (90°) are used to determine transverse elastic modulus  $E_2$  and yield strength  $S_2$ .

Specimens with fiber orientation  $\theta = 45^{\circ}$  are tested to determine their elastic modulus  $E_x^{45}$  that is used to calculate the shear modulus  $G_{12}$ , as already done by Li et al. [16] and suggested in [21]. Indeed, in case of mono-axial stress state  $\sigma_{xx}$  ( $\sigma_{yy} = \tau_{xy} = 0$ ), from relations (223), (224) and (225), we obtain the elastic

Configuration	Туре	Thickness [mm]	Width [mm]
A1	A	0,2	0,4
A2	A	0,25	0,5
A3	A	0,3	0,6
B1	В	0,2	0,4

TABLE 5: Tested printing configurations differing in the filament cross-section and in the material composition

modulus  $E_x^{\theta}$  for an unidirectional specimen having fiber orientation  $\theta$ :

$$E_x^{\theta} = \frac{\sigma_{xx}}{\varepsilon_{xx}} = \left[\frac{\cos^4(\theta)}{E_1} + \frac{\sin^4(\theta)}{E_2} + \frac{1}{4}\left(\frac{1}{G_{12}} - \frac{2\nu_{12}}{E_1}\sin^2(2\theta)\right)\right]^{-1}$$
(236)

equation (236), particularized for  $\theta = 45^{\circ}$  and resolved with respect to  $G_{12}$ , gives:

$$G_{12} = \left[\frac{4}{E_x^{45}} - \frac{1}{E_1} - \frac{1}{E_2} + \frac{2\nu_{12}}{E_1}\right]^{-1}$$
(237)

We used equation (237) along with the others experimentally obtained elastic constants  $E_1$ ,  $E_2$  and  $v_{12}$ , to calculate the in-plane shear modulus  $G_{12}$ .

Similarly, we tested 45° samples to determine their yield strength  $S_x^{45}$  that is used to calculate in plane shear strength  $S_{12}$  [12, 22]. Indeed, particularizing eq. (235) for  $\theta = 45^\circ$  and resolving with respect to  $S_{12}$  we obtain:

$$S_{12} = \left[\frac{4}{\left(S_x^{45}\right)^2} - \frac{1}{S_2^2}\right]^{-\frac{1}{2}}$$
(238)

We used equation (238) along with the experimentally obtained transverse yield strength  $S_2$  to calculate the in-plane shear strength  $S_{12}$ . Moreover, we tested 20° and 70° specimens to assess prediction capabilities of CLT and Tsai-Hill yielding theory.

We consider several configurations, differing in the meso-structure, i.e. the filament cross-section, and in the material composition. Configurations are listed in table 5: the letter indicates the material, while the number indicates the filament dimensions. For type A we tested three configurations (i.e. A1, A2 and A3) in order to investigate how fiber cross-section influences mechanical properties; for

type B we consider the most common filament dimensions (i.e. configuration B1) to assess the influence of chemical composition alone on mechanical behavior. Fiber-to-fiber overlap is set to 10% of the fiber width.

It must be noted that, at the present day, there are no approved specific standards dedicated to the evaluation of 3D-printed objects tensile mechanical properties. Because of their pronounced anisotropy, the selection of the specimen shape is a fundamental issue.

Recommendations from CEN-ISO committee of AM materials have recently appeared suggesting the use of ISO-527 standard which involves the same sample shape (dog-bone) of ASTM D638 standard. However, previous studies (e.g. [6]) show that ASTM D638 [23] dog-bone shape gives rise to complications in tensile tests of 3D-printed FDM specimens. Such complications involve stress concentrations, which are produced by the termination of infill fibers used to approximate the large radii (see fig. 35a). The authors attempted to relieve the stress concentrations by using perimeters that follow the contour of the sample. This approach entails further problems such as areas where the extruded fibers are no longer in pure tension but subjected to bi-axial stress state.

Given these considerations, we observe that dog-bone specimens fail prematurely at the stress concentrations or at the bi-axial stress state zones, i.e. at radius level, while the rest of the sample remains intact. This is in contrast with ASTM D638 and ISO-527 standard requirements that actually enforce the failure to occur in the gage region (central part of the specimen), otherwise the test must be rejected.

To avoid such complications, we chose ASTM D3039 standard [24] as it is tailored to anisotropic materials. The specimen recommended by ASTM D3039 test method consists in a thin flat strip of material having a constant rectangular cross section as shown in fig. 35b.

Specimen dimensions vary with fiber orientation  $\theta$  according to table 6. To prevent gripping damage near the testing machine jaws area, ABS tabs are bonded to the specimen ends using a cyanoacrylate adhesive.

For specimen manufacturing, first 3D models are created for both samples and tabs, through a CAD software. They are then exported as STereoLithography (STL) files and subsequently loaded in the slicing software. In order to produce



(B)

FIGURE 35: Specimen shape. (a) Stress concentration zones for ASTM D638 dog-bone specimen, (b) dimensions of the adopted specimens for tensile tests according to Table 6

Fiber orientation	Specimen	Specimen/tabs	Specimen	Tabs	Tabs
	length $l_1$	width w	thickness t <sub>1</sub>	length <i>l</i> <sub>2</sub>	thickness t <sub>2</sub>
	(mm)	(mm)	(mm)	(mm)	(mm)
$0^{\circ}$	250	15	1,2	36	1,6
90°	175	25	2	25	1,6
45°	250	15	2,4	36	1,6
$20^{\circ}$	250	15	2,4	36	1,6
$70^{\circ}$	250	15	2,4	36	1,6

TABLE 6: Specimen dimensions used following ASTM D3039 - 00 standard geometry recommendations

unidirectional specimens, G-Code manipulation is mandatory, since, currently, there are no slicing programs able to directly produce them. We preliminarily used Slic3r [25] and KISSlicer [26] slicing software to produce G-Codes for i) the single layer and ii) for the support interface, respectively. Subsequently, we developed a custom made routine in Matlab environment [27] to assembly the final G-Code with the desired features.

ABS specimens are tested under displacement control, at room temperature, on a MTS Insight test system, with computer control and data acquisition. Strain is measured with a video extensometer (ME-46 video extensometer, with 1  $\mu m$  resolution and a camera field of view of 200 mm) at the mid-section of the specimen (gage section). Following ASTM D3039 recommendations, the displacement rate, is set to 2 mm/min, and it is selected to produce failure within 1 to 10 min.

## Results

Tensile tests on specimens at  $0^{\circ}$  are able to capture the mechanical response of a 3D-printed part that mainly depends on the mechanical behavior of the fiber i.e. on *intra-fiber* properties. Conversely, tensile tests at 90° are suitable for retrieving the mechanical characteristics of 3D-printed parts which primarily depend on the bonding process, i.e. on *inter-fibers* properties. During tensile tests we observed that specimens, especially longitudinal ones, exhibited whitening regions, i.e. regions where the material turn its color into lighter shades. Yielding and subsequently failure originated in proximity of these whitened zones, where we observed localized fiber delamination. Conversely, 90° specimens did not show considerable whitening, with failure always occurring at the interface between adjacent fibers.

Fig. 36 reports the experimentally obtained stress-strains curves for specimens with fiber orientation  $\theta$  equal to 0°, 45° and 90° respectively, for all configurations examined. Stress-strain curves clearly display that fiber orientation plays a significant role on the mechanical properties of the 3D-printed material. Indeed in fig. 36 we observe that longitudinal specimens (0°) show the more ductile behavior: a linear elastic part is followed by an elastic region in which the



FIGURE 36: Stress-strain curves for configurations A1, A2, A3 and B1

maximum stress value is reached, then the final part of the curve is characterized by a plastic deformation at constant stress. Transverse specimens (90°) show the more brittle behavior, almost without plastic deformation, while  $45^{\circ}$  specimens mechanical response lies approximately in the middle between 0° and 90° samples. For each configuration, elastic constants, yield stresses and ultimate strains are reported in table 7.

Fig. 37 reports elastic modulus against fiber orientation  $\theta$  as in eq. (236). Elastic response analysis of each configuration shows that Young's modulus at 0° is generally higher than Young's modulus at 90°. An unusual behavior is observed for configuration B1 for which 90° elastic modulus is higher than 0° one. Fig. 38 reports the yielding stress against fiber orientation  $\theta$  in case of mono-axial stress as in eq. (235). From the results reported we may conclude that strength modeling through Tsai-Hill yielding criterion is sufficiently accurate to describe specimen behavior. Fiber orientation significantly affects tensile yield strength:

	Config. A1	Config. A2	Config. A3	Config. B1
$E_1$ [MPa]	$1810\pm 63$	$2010\pm153$	$1953\pm83$	$1606 \pm 152$
$E_2$ [MPa]	$1695 \pm 112$	$1671\pm57$	$1752\pm 63$	$1842\pm154$
<i>v</i> <sub>12</sub>	$0,32\pm0,1$	$0,32 \pm 0,1$	$0,\!35\pm0,\!05$	$0,3\pm0,2$
$G_{12}$ [MPa]	$617 \pm 43$	$641 \pm 47$	$772 \pm 47$	$643 \pm 109$
$S_1$ [MPa]	$25,5 \pm 0,2$	$26{,}3\pm0{,}2$	$23,7\pm0,7$	$28,\!6\pm0,\!6$
$S_2$ [MPa]	$16 \pm 1$	$14,6\pm0,4$	$17 \pm 0,4$	$22,3\pm0,7$
$S_{12}$ [MPa]	$13,7 \pm 0,6$	$12\pm0,7$	$13,2 \pm 0,3$	$13,4 \pm 0,3$
$\varepsilon_1^u$ [mm/mm]	$0,\!04\pm0,\!02$	$0,021 \pm 0,007$	$0{,}016\pm0{,}002$	$0,\!31\pm0,\!07$
$\varepsilon_2^u$ [mm/mm]	$0,012 \pm 0,002$	$0{,}014\pm0{,}002$	$0{,}017\pm0{,}002$	$0{,}028\pm0{,}004$

TABLE 7: Elastic constants, yield strengths and failure strains for the different configurations tested



FIGURE 37: Elastic moduli E against fiber orientation  $\theta$ 



FIGURE 38: Ultimate yield stresses against fiber orientation  $\theta$  in case of mono-axial stress state. The area under the curve represents resistance domain accordingly to Tsai-Hill criterion

longitudinal specimens have a much higher yield strength than transverse specimens (from 25% to 45% higher). Higher data scatter can be observed in 45° and 90° specimens, while it is significantly lower for 0° specimens. This can be attributed to a transition in the failure mode from 0° samples ductile fracture to 90° samples brittle fracture, led by fiber-to-fiber bonding strength. Such transition is suggested to happen even after a slight change in the fiber angle from 0° [12].

# Discussion

Elastic modulus validation data  $(20^{\circ} \text{ and } 70^{\circ} \text{ specimen})$  show a good consistency with theoretical estimation for configuration A1 and B1, while for configurations A2 and A3 some overestimation of CLT with respect to experimental data has been observed (see fig. 37).

Validation data for Tsai-Hill criterion are also well consistent with theoretical estimation, with some slight underestimation for  $70^{\circ}$  specimens of configurations A1 and B1 (see fig. 38): the reason probably lies in the air gap parameter. For configuration A1 and B1, indeed,  $70^{\circ}$  samples could not be printed with the same air gap of the experimental data samples (namely 0,2 mm air gap), because the printing always failed. Lowering the air gap to 0,15 mm allowed the samples to be printed. The reduction of air gap increases the fiber-to-fiber adhesion in the first 1-2 layers, strengthening the whole specimen.

Comparisons between configurations have been carried out as follows: we first compared three different filament cross-sections, printed with the same material (configurations A1, A2 and A3) and then two different materials, with the same cross section (configurations A1 and B1).

Manufacturing and testing conditions were kept identical in all configuration, with the only exception of air gap parameter. Configurations A1, A2 and B1 samples have been printed with an air gap of 0,2 mm, while configuration A3, for printability reasons, has been printed with 0,1 mm air gap.



FIGURE 39: Elastic moduli for configurations A1, A2 and A3



FIGURE 40: Uniaxial tensile strength for configurations A1, A2 and A3

### Fiber cross-section comparison

The comparison between the various filament cross sections has given the following results:

- <u>elastic modulus</u> raises while increasing filament section, both at 0° and 90° (see fig. 39). This means that stiffness tends to be higher with bigger filaments, thus with a lower number of filaments in the layer (given a fixed geometry).
- Uniaxial tensile strength at 0° decreases raising filament cross-section, meaning that a higher number of smaller filaments in the layer exhibits a higher strength. Conversely, uniaxial tensile strength at 90° raises increasing filament cross-section (see fig. 40).
- <u>Ultimate strain</u> at  $0^{\circ}$  decreases increasing filament cross-section, conversely strain at failure at  $90^{\circ}$  increases with filament cross-section (see fig. 41).



FIGURE 41: Strain at failure for configurations A1, A2 and A3



FIGURE 42: Shear modulus and shear strength for configurations A1, A2 and A3

• <u>Shear modulus</u> raises increasing cross-section, while shear strength shows a trend similar to 0° uni-axial tensile strength (see fig. 42).

Tensile and shear strength values obtained for configuration A2 seem to be anomalous. Tests for such a configuration have been repeated to assess the anomalous results, previously checking G-code instructions, modality of specimen measurement and tensile test conditions. New results, not reported here, are perfectly according to the previous one, presented in study. A possible explanation for the anomalous results comes from the resolution of the motor stepper unit of the z axis (0,015 mm), responsible for the bed movement and thus for the layer height. The resolution may not allow a precise movement on the z axis of 0,254 mm, that is the nominal value so far approximated at 0,25 mm. Since the error is systematic, the resulting height of each layer may significantly vary from its nominal value. The error cannot be estimated from specimen thickness measurement, because all the specimens present a significant deviation from the nominal value, independently from filament section (0,2 x 0,4 mm: 16%, 0,25 x 0,5 mm: 13%)



FIGURE 43: Elastic modulus at  $0^\circ$  and  $90^\circ$  for configurations A1 and B1



FIGURE 44: Uniaxial tensile strength at  $0^{\circ}$  and  $90^{\circ}$  for configurations A1 and B1

and 0,3 x 0,6 mm: 18%). Thus, the anomalous values regarding configuration A2 may come from a different bonding between subsequent layers due to an incorrect layer height.

### **Material comparison**

From the comparison between materials, maintaining the same filament cross - section, we can make the following considerations:

- type B shows, compared to type A, higher elastic modulus (fig.43) at 90°, higher tensile strength (fig.44) and strain at failure (fig. 45) for both 0° and 90° orientations. Only the elastic modulus at 0° is higher for type A.
- Type B elastic modulus at 90° is higher than the elastic modulus at 0°. This behavior may depend on the optimal bonding properties of type B.
- The ultimate strain at 0° for type B is ten times higher than the corresponding type A failure strain.



FIGURE 45: Strain at failure at  $0^{\circ}$  and  $90^{\circ}$  for configurations A1 and B1



FIGURE 46: Shear modulus and shear strength for configurations A1 and B1

• Shear modulus and strength (fig. 46) do not show significant differences between type A and type B.

Type B shows a more ductile failure mode compared to type A, with much higher delamination. A brittle failure mode is found on  $90^{\circ}$  specimens, both for type A and type B.

## Conclusions

In this paper we investigated how fiber orientation, filament dimensions and chemical composition affect the mechanical properties of ABS 3D-printed components. In particular, we tested and compared i) three different meso-structures on the same material and ii) two different types of ABS using the same meso-structure.

As already highlighted by previous works, we verified how a 3D-printed material shows anisotropic mechanical properties. Accordingly, CLT and Tsai-Hill yielding theory were found to be well capable of predicting in-plane stiffness and strength at the macro-scale. Moreover, we experimentally investigated how meso-structure impact on macro-scale mechanical properties.

We assessed that, acting on chemical composition, it is possible to tune i) fiber properties and ii) fiber-to-fiber bonding and, consequently, the overall mechanical properties at macro-scale, in particular the yielding strength and the strain at failure.

Relying on the good consistency between experimental and estimated data, we strongly suggest the adoption of suitable standard test methods tailored on anisotropic materials in order to experimentally evaluate mechanical properties of FDM 3D-printed parts.

The experimentally obtained data are useful to calibrate mechanical and yielding models to be used with numerical simulations as finite element analyses. Such computational tools would be used along with optimization techniques to design structural-optimized functional parts.

# Supplementary material

In this section both the optical microscope images of the cross sections of the specimens (figure 47) and the images of the samples subjected to tensile tests (figures 48, 49, 50 and 51) for all configurations are shown. In figure 47 it is possible to observe the meso-structure, i.e. the geometry, at the sub-millimetric scale, resulting from the filament deposition process. Note the similarity between the real geometry and the idealized geometry as shown in figure 33.



(A) configuration A2, view of the cross-sectional area of longitudinal specimens, magnification 75  $\rm X$ 



(B) configuration A3, view of the cross-sectional area of longitudinal specimens, magnification 300  $\rm X$ 



(C) configuration A1, detail of the cross-sectional area of longitudinal specimens, illustrating the bonding between fibers, magnification 1000 X

FIGURE 47: Optical microscope images of the specimens



(A) configuration A1,  $\theta = 0^{\circ}$ 



(B) configuration A1,  $\theta = 45^{\circ}$ 



(C) configuration A1,  $\theta = 90^{\circ}$ 

FIGURE 48: Tensile specimens for configuration A1



(A) configuration A2,  $\theta = 0^{\circ}$ 



(B) configuration A2,  $\theta = 45^{\circ}$ 



<sup>(</sup>C) configuration A2,  $\theta = 90^{\circ}$ 

FIGURE 49: Tensile specimens for configuration A2



(A) configuration A3,  $\theta = 0^{\circ}$ 



(B) configuration A3,  $\theta = 45^{\circ}$ 



(C) configuration A3,  $\theta = 90^{\circ}$ 

FIGURE 50: Tensile specimens for configuration A3



(A) configuration B1,  $\theta = 0^{\circ}$ 



(B) configuration B1,  $\theta = 45^{\circ}$ 



(C) configuration B1,  $\theta = 90^{\circ}$ 

FIGURE 51: Tensile specimens for configuration B1

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# Conclusions

In **chapter 1** we found that TEVAR induced a longitudinal strain decrease in the stented segments and a longitudinal strain mismatch between stented and nonstented segments. Stent-graft oversizing did not affect the magnitude of strain reduction. Tensile testing showed that peak stress-to-rupture was lower for longitudinal than for circumferential fragments. In addition, longitudinal fragments were more prone to rupture proximally than distally.

This experimental study showed that TEVAR acutely stiffens the aorta in the longitudinal direction and thereby induces a strain mismatch, while tensile testing confirmed that longitudinal aortic fragments are most prone to rupture, particularly close to the arch. Such an acute strain mismatch of potentially vulnerable tissue might play a role in TEVAR-related complications, including retrograde dissection and aneurysm formation. The finding that TEVAR stiffens the aorta longitudinally may also shed light on systemic complications following TEVAR, such as hypertension and cardiac remodelling. These observations may imply the need for further improvement of stent-graft designs.

In **chapter 2** we presented an optimization framework aiming at increasing the fatigue life of Nitinol stents. The adopted computational framework relied on nonlinear structural finite element analysis combined with a Multi Objective Genetic Algorithm, based on Kriging response surfaces. In particular, such an approach has been used to investigate the design optimization of planar stent cell, introducing the concept of the tapered strut.

The results of the optimization procedure confirmed the key role of a tapered strut design to enhance the stent fatigue strength, suggesting that it is possible to achieve a marked improvement of both the fatigue safety factor and the scaffolding capability simultaneously.

The study outcomes confirmed that the use of tapered strut profile should be a primary key factor to reduce and uniform the strain field along the strut and thus to enhance the fatigue life of the whole stent. The obtained Pareto set allows the designer for the selection of optimized solution, according to the specific design requirements. As illustrative example we compared a commercial reference design with the optimized counterpart: increasing the strut length and the strut width at the strut extremities, we shown that it is possible to achieve a marked improvement of the fatigue safety factor, compared to the typical design (strut with constant section), without any loss of scaffolding capabilities.

In **chapter 3** we obtained a fractional-order Fourier diffusion law from a multi-scale rheological model. Indeed, the instantaneous temperature - flux equation of the Fourier-type diffusion is generalized introducing a self-similar, fractal type mass clustering at the micro-scale. In this setting the resulting conduction equation at the macro-scale yielded a Caputo's fractional derivative with order  $\beta \in [0, 1]$  of temperature gradient. The order of the fractional-derivative has been found to be related to the fractal assembly of the micro-structure.

The distribution and the temperature raising in simple rigid conductors have also been reported to investigate the influence of the derivation order on the temperature field. The solution of the fractional heat equation ( $0 < \beta < 1$ ), governed by Mittag-Leffler functions, exhibits for small times a much faster rising, and for large times, a much slower decay, compared with the solution of classical heat equation, governed by exponential functions. Accordingly, it was found that the main property of the anomalous heat transfer is that the time-rate of change at which the resulting temperature field reaches a steady state, becomes higher as the discrepancy from the Fourier law increases: the thermal steadiness is consequently achieved, by rigid anomalous conductors, employing longer times than Fourier ones. Such particular behavior represents the "long-tail memory effect", due to the power law thermal memory of such materials.

In **chapter 4** the "thermally-anomalous" heat conduction has been extended at slightly deformable bodies; the interplay between the thermal flux and the elastic and thermal deformability has been investigated for a pinned-pinned truss. Such simple example allowed for focusing on the effects of the deviation from the Fourier's law on the thermoelastic coupling. The full analytical solution of the problem has been provided obtaining the resulting displacement, temperature, and internal axial force. Afterward, the anomalous thermal behavior of such slightly deformable system has been investigated, thereby exploring not only the transient behavior due to its deviation from the Fourier law, but also by studying a resulting overall measure of energy rate.

All the resulting fields, namely the axial stress, the displacement, and the temperature have been found to be influenced by the thermal and elastic deformability of the bar. The higher is the deviation from the Fourier-like behavior, the more rapid becomes the rise in time. This is an intrinsic feature of the anomalous heat transfer, now coupled with an elastic and thermally deformable bar. Another effect of the deviation from the Fourier behavior is the tendency to reach steady values in longer times. The higher the value of the anomaly exponent  $\beta$  in [0, 1/2) the slower this becomes.

The space-time modal analysis performed on the fractional-order system, relying on the balance of linear momentum and on the balance of energy rate, provided the explicit solutions of the problem. The time evolution of each spatial mode, for the temperature, for the displacement and for the axial force, turned out to be characterized by modulated Mittag-Leffler functions. The higher is the deviation from the Fourier-like behavior for the heat flux, the steeper is the resulting time-transient of each mode.

In **chapter 5** we focused on mechanical properties of Fused Deposition Modeling (FDM) 3D-printed objects. We studied the influence of extruded filament dimensions and chemical composition on mechanical behavior of FDM objects made of Acrylonitrile Butadiene Styrene (ABS) polymer varying fiber orientation with respect to the loading direction. All aspects have been investigated through experimental campaigns: meso-structure influence, i.e. fiber thickness and width has been tested on the same material, while chemical composition impact has been tested using the same meso-structure.

We verified that FDM ABS specimens show anisotropic mechanical properties since they vary with filament extrusion direction. Accordingly, Classical Lamination Theory (CLT) and Tsai-Hill yielding criterion were found to be well capable of predicting in-plane stiffness and strength of FDM specimens.

We assessed that, varying chemical composition and filament dimensions, it is possible to tune fiber properties and fiber-to-fiber bonding and, consequently, the overall mechanical properties at macro-scale, in particular the yielding strength and the strain at failure. The experimentally obtained data may be useful to calibrate mechanical models to be used with computational tools as finite element analyses. Relying on the good consistency between experimental and estimated data, we strongly suggested the adoption of suitable standard test methods tailored on anisotropic materials in order to experimentally evaluate mechanical properties of FDM 3D-printed parts.

# **List of Publications**

### Other published or accepted manuscripts.

- F. Auricchio, A. Greco, G. Alaimo, V. Giacometti, S. Marconi, V. Mauri. "3D printing technology for buildings' accessibility: the tactile map for MTE Museum in Pavia", *Journal of Civil Engineering and Architecture*, accepted
- E. Massoni, L. Silvestri, G. Alaimo, S. Marconi, M. Bozzi, L. Perregrini, F. Auricchio. "3DPrinted Substrate Integrated Slab Waveguide for Single-Mode Bandwidth Enhancement", *IEEE Microwave and Wireless Components Letters*, 2017, Vol. 27, No. 6
- 3. **G. Alaimo**, M. Zingales. "Laminar flow through fractal porous materials: the fractional-order transport equation", *Communications in Nonlinear Science and Numerical Simulation*, 2015, Vol. 22, No. 1
- T. Ingrassia, G. Alaimo, F. Cappello, A. Mancuso, V. Nigrelli. "A new design approach to the use of composite materials for heavy transport vehicles", *International Journal of Vehicle Design*, 2007, Vol. 44, No.3/4 pp. 311-325

## Submitted manuscripts

• G. Alaimo, F. Auricchio, I. Bianchini, E. Lanzarone. "Applying Functional Principal Components to Structural Topology Optimization", 2017, *International Journal for Numerical Methods in Engineering*, under review

## **Conference Proceedings**

- 1. G. Alaimo, F. Auricchio, H. Giberti, S. Marconi, S. Morganti. "Additive Manufacturing for a low-cost biaxial testing machine", *Proceedings of the XXIII Conference of the Italian Association of Theoretical and Applied Mechanics, Salerno, 4-7 September 2017*
- E. Massoni, L. Silvestri, M. Bozzi, L. Perregrini, G. Alaimo, S. Marconi, F. Auricchio. "Characterization of 3D-Printed Dielectric Substrates with Different Infill for Microwave Applications", *IEEE Microwave and wireless components letters*, Vol. 27, No. 6, June 2017
- F.J. Nauta, M. Conti, S. Marconi, A.V. Kamman, G. Alaimo, S. Morganti, A. Ferrara, J.A. van Herwaarden, F.L. Moll, F. Auricchio, S. Trimarchi. "TCT-781 Thoracic Endovascular Repair Decreases Longitudinal Aortic Distensibility: Experimental Study in an Ex-Vivo Porcine Model", *Journal* of the American College of Cardiology, 66(15):B317, October 2015
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## **Book Chapter**

1. F. Auricchio, S. Marconi, G. Alaimo. "Materiali per la stampa 3D: possibilità attuali e prospettive future", in *Stampa 3D*, 2015, Filodiritto editore

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