A holistic approach to design for 4D Printing

Comlan Sossou

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Par

M. SOSSOU Germain

Une approche globale de la conception pour l'impression 4D

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Composition du Jury :

M. ANDRÉ Jean-Claude	Directeur de Recherche CNRS - Université de Lorraine	Président
M. BRISSAUD Daniel	Professeur d'université – Institut National Polytechnique de Grenoble	Rapporteur
M. BERNARD Alain	Professeur d'université – École Centrale de Nantes	Rapporteur
M. QI H. Jerry (en visioconférence)	Professeur d'université – Georgia Institute of Technology	Examinateur
M. GOMES Samuel	Professeur d'université – Université de Technologie de Belfort Montbéliard	Directeur de thèse
M. MONTAVON Ghislain	Professeur d'université – Université de Technologie de Belfort Montbéliard	Co-directeur de thèse
M. DEMOLY Frédéric	Maître de Conférences HDR – Université de Technologie de Belfort Montbéliard	Encadrant de thèse

Résumé

Titre : Une approche globale de la conception pour l'impression 4D

Mots clés : Fabrication additive ; Conception pour la fabrication additive ; matériaux intelligents ; Impression 4D ; Conception pour l'impression 4D ; Modélisation à base de voxels ; Conception avec les matériaux intelligents.

Résumé : Inventée en 1983, comme procédé de prototypage rapide, la fabrication additive (FA) est aujourd'hui considérée comme un procédé de fabrication quasiment au même titre que les procédés conventionnels. On trouve par exemple des pièces obtenues par FA dans des structures d'aéronef. Cette évolution de la FA est due principalement à la liberté de forme permise par le procédé. Le développement de diverses techniques sur le principe de fabrication couche par couche et l'amélioration en quantité et en qualité de la palette de matériaux pouvant ainsi être mis en forme, ont été les moteurs de cette évolution. De nombreuses autres techniques et matériaux de FA continuent de voir le jour. Dans le sillage de la FA (communément appelée impression 3D) a émergé un autre mode de fabrication : l'impression 4D (I4D). L'I4D consiste à explorer l'interaction matériaux intelligents (MIs) – FA. Les MIs sont des matériaux dont l'état change en fonction d'un stimulus ; c'est le cas par exemple des matériaux thermochromiques dont la couleur change en réponse à la chaleur ou des hydrogels qui peuvent se contracter en fonction du pH d'un milieu aqueux ou de la lumière. Les objets ainsi obtenus ont – en plus d'une forme initiale (3D) – la capacité de changer d'état (en fonction des stimuli auxquels sont sensibles les MIs dont ils sont faits) d'où la 4e dimension (temps). L'I4D fait – à juste titre – l'objet d'intenses recherches concernant l'aspect fabrication (exploration de nouveaux procédés et matériaux, caractérisation, etc.). Cependant très peu de travaux sont entrepris pour accompagner les concepteurs (qui, a priori, ne sont ni experts FA ni des experts de MIs) à l'utiliser dans leurs concepts. Cette nouvelle interaction procédé-matériau requiert en effet des modèles, des méthodologies et outils de conception adaptés. Cette thèse sur la conception pour l'impression 4D a pour but de combler ce vide méthodologique. Une méthodologie de conception pour la FA a été proposée. Cette méthodologie intègre les libertés (forme, matériaux, etc.) et les contraintes (support, résolution, etc.) spécifiques à la FA et permet aussi bien la conception de pièces que celle d'assemblages. En particulier, la liberté de forme a été prise en compte en permettant la génération d'une géométrie minimaliste basée sur les flux fonctionnels (matière, énergie, signal) de la pièce. Par ailleurs, les contributions de cette thèse ont porté sur la conception avec les matériaux intelligents. Parce que les MIs jouent plus un rôle fonctionnel que structurel, les préoccupations portant sur ces matériaux doivent être menées en amont du processus de conception. En outre, contrairement aux matériaux conventionnels (pour lesquels quelques valeurs de paramètres peuvent suffire comme information au concepteur), les MIs requièrent d'être décrits plus en détails (stimulus, réponse, fonctions, etc.). Pour ces raisons un système d'informations orientées conception sur les MIs a été mis au point.

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Ce système permet, entre autre, d'informer les concepteurs sur les capacités des MIs et aussi de déterminer des MIs candidats pour un concept. Le système a été matérialisé par une application web. Enfin un cadre de modélisation permettant de modéliser et de simuler rapidement un objet fait de MIs a été proposé. Ce cadre est basé sur la modélisation par voxel (pixel volumique). En plus de la simulation des MIs, le cadre théorique proposé permet également le calcul d'une distribution fonctionnelle de MIs et matériau conventionnel ; distribution qui, compte tenu d'un stimulus, permet de déformer une forme initiale vers une forme finale désirée. Un outil – construit dans l'environnement Grasshopper, un plug-in du logiciel de CAO Rhinoceros® – matérialisant ce cadre méthodologique a également été développé.

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Abstract

Title: A holistic approach to design for 4D Printing

Keywords: Additive manufacturing; Design For Additive Manufacturing (DFAM); Smart materials; 4D printing, Design for 4D Printing (DF4DP); Voxel-based modeling; Design with Smart Materials (DwSMs).

Abstract: Invented in 1983, as a rapid prototyping process, additive manufacturing (AM) is nowadays considered as a manufacturing process almost in the same way as conventional processes. For example, parts obtained by AM are found in aircraft structures. This AM evolution is mainly due to the shape complexity allowed by the process. The driving forces behind this evolution include: the development of various techniques on the layer-wise manufacturing principle and the improvement both in quantity and quality of the range of materials that can be processed. Many other AM techniques and materials continue to emerge significantly. In the wake of the AM (usually referred to as 3D printing) another mode of manufacturing did emerge: 4D printing (4DP). 4DP consists in exploring the smart materials (SM) – AM interaction. SMs are materials whose state changes according to a stimulus. This is the case, for example, with thermochromic materials whose color changes in response to heat or hydrogels which can shrink as a function of an aqueous medium's pH or of light. The objects thus obtained have – in addition to an initial form (3D) – the capacity to shift state (according to the stimuli the SMs making them are sensitive to) hence the 4th dimension (time). 4DP is – rightly – the subject of intense research concerning the manufacturing aspects (exploration of new processes and materials, characterization, etc.). However, very little work is done to support designers (who, in principle, are neither AM experts nor experts of SMs) to use it in their concepts. This new process-material interaction requires adapted models, methodologies and tools in design. This PhD on design for 4D printing aims at filling this methodological gap. A design methodology for AM (DFAM) has been proposed. This methodology integrates the freedoms (shape, materials, etc.) and the constraints (support, resolution, etc.) peculiar to the AM and allows both the design of parts and assemblies. Particularly, freedom of form has been taken into account by allowing the generation of a minimalist geometry based on the functional flows (material, energy, and signal) of the part. This methodology integrates the freedoms (shape, materials, etc.) and the constraints (support, resolution, etc.) peculiar to the AM and allows both the design of parts and assemblies. Particularly, freedom of form has been taken into account by allowing the generation of a minimalist geometry based on the functional flows (material, energy, and signal) of the part. In addition, the contributions of this PhD focused on designing with smart materials (DwSM). Because SMs play a functional rather than a structural role, concerns about these materials need to be addressed in advance of the design process (typically in conceptual design phase). In addition, unlike conventional materials (for which a few parameter values may suffice as information to the designer), SMs need to be

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described in more detail (stimulus, response, functions, etc.). For these reasons, a design-oriented database (including a design decision support) on SMs has been developed. This system makes it possible, among other things, to inform designers about the capabilities of SMs and also to determine SMs candidates for a concept. The system has been developed as a Web-service application. Finally, a modeling framework allowing quickly modeling and simulating an object made of SMs, in the early design phase, has been proposed.

This framework is based on voxel (volumetric pixel) modeling. In addition to the simulation of SMs behaviors, the proposed theoretical framework also allows the computation of a functional distribution of SMs and conventional material; distribution which, given a stimulus, makes it possible to deform an initial form towards a desired final form. A tool – based on the Grasshopper environment, a plug-in of the CAD software Rhinoceros® – materializing this methodological framework has also been developed.

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J'estime profondément que nous sommes le fruit des expériences qu'on vit et des personnes qu'on rencontre. Nombreux, sans doute, sont ceux sans qui ce travail de thèse n'aurait pu être mené tel qu'il l'a été.

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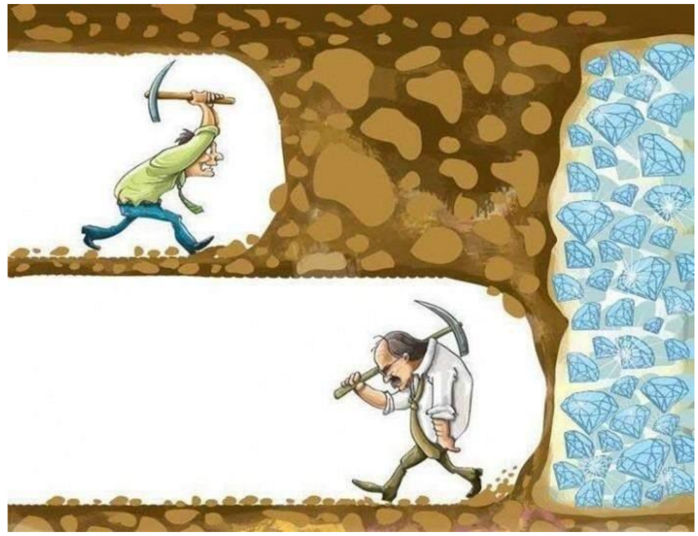
Ayez tous le sentiment d'avoir contribué d'une façon ou d'une autre à cette thèse. Alors encore une fois je vous remercie pour tout.



Ce n’est inatteignable que lorsqu’on a décidé d’abandonner. La preuve…

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4DP	4D printing
AM	Additive manufacturing
CAD	Computer Aided Design
CAE	Computer Aided Engineering
DF4DP	Design for 4D Printing
DFAM	Design for Additive Manufacturing
DLP	Direct Light Processing
DOF	Degree of freedom
DwSM	Design with Smart Materials
E	Young modulus
FDM	Fused deposition Modeling
FEM	Finite Element Method
FGM	Functionally Graded Material
G	Shear modulus
GH	Grasshopper©
PBF	Powder Bed Fusion
PRIAM	Proactive design for additive manufacturing
SCM	Shape Changing Materials
SLA	Stereolithography apparatus
SLM	Selective Laser Melting
SLS	Selective Laser Sintering
SM	Smart materials
SMA	Shape memory alloy
SME	Shape Memory Effect
SMP	Shape memory polymer

Chapter 1 Introduction

Simply speaking manufacturing is the act of turning some raw materials into useful goods. The term manufacturing is mostly applied in industrial production although it also refers to a wide range of human activities ranging from handcraft manufacturing to high tech manufacturing. It can readily be noticed how pervasive manufacturing is throughout the world and how paramount is it to mankind[1].While this thesis is not meant to be an essay on the history of manufacturing and materials, nor on their relationships with mankind, it is worth briefly looking at how things have evolved in the ways we craft stuffs from the dawn of mankind to today era. At least this would give a better appreciation of the milestone being achieved by 4D printing.

1.1 Evolution in the ways mankind crafts items

In the history of mankind, the first true manufacturing event took place about two and a half million years ago, in the Stone Age. This was when people used stones and sticks to create axes that were then used during hunting. The materials used during this period were stones and wood handles. This was the time of *Homo habilis*, and noteworthy is that the word 'habilis' is a Latin word that means toolmaker. Although there is little information about the manufacturing processes during that age, it is known that the most important manufacturing site during that age was found in Africa. In that site, stones were processed for more than a million years.

The ways we manufacture goods can roughly be classified in six main techniques which were discovered and matured in the course of mankind evolution. Making stone tools through **cutting** (2.5 million years ago) was the first milestone in the mankind ability to manufacture. It involved cutting the handles from wood and sharpening the stones. Secondly, we have been able to manufacture by **changing material properties**. The first evidence in changing material properties was observed about 120,000 years ago. In that age, people would sharpen the tip of a wooden spear and then carefully put it in fire and turn it slowly for a short time. This would ensure that the tip of the wooden spear would harden. During this period, the materials used

[1] Considering crows bending wire to catch food 1. Rutz, C., S. Sugasawa, J.E. van der Wal, B.C. Klump, and J.J. St Clair, *Tool bending in New Caledonian crows.* R Soc Open Sci, 2016. **3**(8): p. 160439. or chimpanzee crafting sticks to catch ants, the statement can actually hold for species other than humans.

were mainly wood and resins. **Joining**, which appears 72,000 years ago, is the next manufacturing technique by which people would attach arrowhead to a wooden arrow shaft using resin and other materials. Fourthly was **coating**, and this has been around for more than 30,000 years. Back then this technique was used for arts or for the purpose of documentation as it is for paints in caves. Next is **molding**: as early as 25,000 years ago figurines made through molding of clay and bone dust were crafted. Main materials which was used back then were stone, bone, wood, clay and to a lower extent metal. With **forming**, which has been used for the last 10,000 years, more and more metal parts were created.

In one way or another, all the today manufacturing processes can be traced to these primitive processes. The output of these latter was quite low and slow as they were hand operated. Mechanization was a step towards improving the efficiency and the speed of manufacturing. Egyptians seem to be among the first taking that step: thousands of years ago they created the pottery wheel and the first lathes (obviously operated by hands). However, it was only by the Industrial Revolution (in the middle of the 18th century) that manufacturing truly got mechanized. Steam power then made available by the steam engine tremendously contributed to manufacturing processes mechanization. First to be truly mechanized was the textile industry with machines such as the cotton spinning machine, the power loom (for weaving clothes and tapestry) or the cotton gin (which was used to separate cotton fibers from their seeds). The iron making industry also benefited from that mechanization. Noteworthy is the precision boring machine designed and manufactured in 1774 by Wilkinson [2]. Before then cylinder (mainly for steam engines) used to be forged with a hammer, resulting thus in a rather poor accuracy. Wilkinson's invention put on the market the technology to drill accurate cylinder. This has led to more and more built steam engines and thus more and more mechanization. In the wake of these changes, two significant iron manufacturing processes were developed: rolling (in 1783) and puddling (1784). In addition to the cylinder boring machine, other manufacturing techniques for shaping or machining metal and the like were introduced. Examples include the screw cutting lathe and the milling machine.

The Industrial Revolution had a big effect on the manufacturing industry. People stopped using their hands to manufacture goods at home and started to use machines to manufacture goods in factories. It was also during this period when steel gained worldwide use in industries. Manufacturing goods took less time as well as using fewer materials and manpower. There were major changes in the glass making, textile manufacturing, agriculture and mining among others. Through mechanization, the Industrial Revolution brought many changes and sparked inventions that laid the foundation on which modern manufacturing is based on.

Manufacturing mechanization alleviated much of the human effort required to manufacture and increased output through the introduction of machines. Nevertheless, the use of these machines did strongly rely to human intervention and monitoring (which was not really an issue back then) for every step in transforming the raw materials. That reliance of human intervention made the quality of the output inherently prone to errors. With computer power being rapidly developing as early as in the 1930s[2], another milestone for the ways we manufacture goods was on the horizon: the numerical control (NC) era or what could be called manufacturing digitization. This is when machine tools got automatized through the introduction of concepts of programmable logic. Early forms of NC involved the alteration of existing machine tools with motors that were controlled to move the machine. Typically, these were drilling machines reaching specific points whose coordinates were fed into the system with a punched tape. The first commercially available NC machine was announced in 1952 (by Arma Corporation): it was a NC lathe. With its ability to transfer design intents (such as engineering drawing or even CAD model) into machine controls and the rapidly growing computers' power, NC quickly turned into the computer numerical control and later computer aided manufacturing (CAM).

The complexity of what we are able (or what we need) to manufacture has increased, along with the repertoire of materials, in such a way that crafting goods not as a whole but as multiple parts and assembling them afterwards, became more efficient. In that regards, Henry Ford and Charles Sorensen established a major milestone in the field of manufacturing when they established the assembly line. The assembly line included people handling specific tasks. The aim of the assembly line was to ensure that cars were manufactured faster and more efficiently. Ford managed to manufacture 15 million model T cars between 1908 and 1927. This was a clear proof that the assembly line was the future of car manufacturing particularly, and manufacturing in general.

The use of robots was another major milestone in manufacturing history. The first robot to be used in manufacturing was created in the 1950s. It was used for the first time in 1961 on General Motors assembly line. Nowadays, robots are used in almost every factory. In 2008, the US Air Force developed the first all-robot squadron, a clear indication of the extent to which manufacturing has evolved throughout the history up to a point where machines are capable of operating on their own.

1.2 Imbuing static object with the capability of evolving

Most of man-made objects are thought of and designed to assume one single physical state (including generally kinematic behaviors) so as to fulfill customers' needs. They inherently static objects, and as such they are insensitive to any change occurring in their working environment. However, looking at nature one could find many living organism which are capable of state shifting (not as a result of ageing) for various reasons: adaptation and efficient use of available

[2] In 1937 a simple demonstrative binary adder built by G. Stibitz [Ritchie 3. Ritchie, D., *The Computer Pioneers: The Making of the Modern Computer*. 1986: Simon & Schuster.] proved that is was possible to apply Boolean logic to the design of computers. Two years later this proof of concept was leveraged to build the relay-based Model I Complex Calculator which was able to run computations on complex numbers.

resources (e.g. trees losing their leaves in autumn to cope with cold weather and daylight decrease), defense (as in aposematic species[3]), facilitating a new capability (for instance armadillos can curl into a ball so that they roll to move instead of walking), etc.

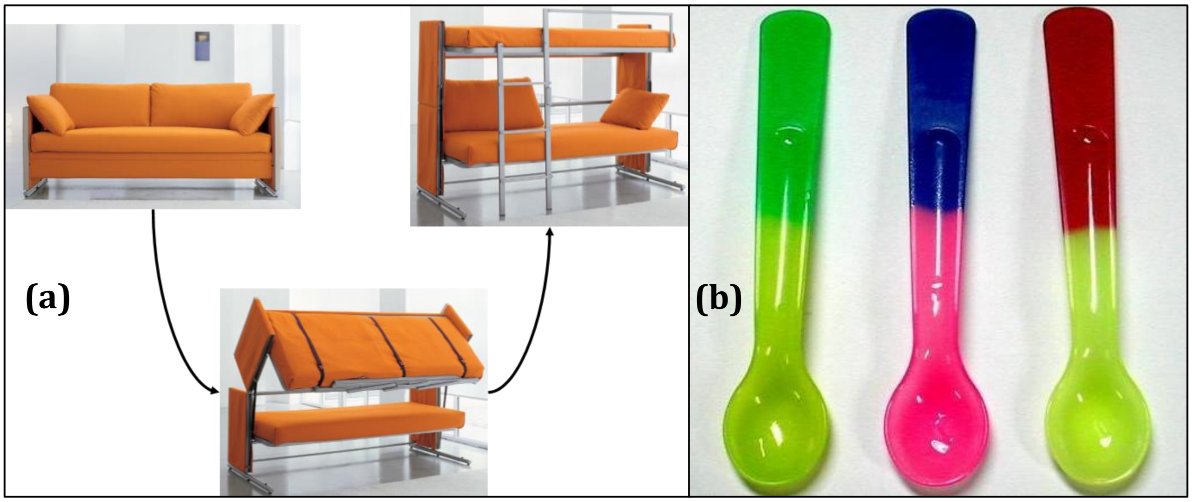


Figure 1-1: Examples of objects with the ability to change state: (a) sofa which can be turned to bunked beds - (b) temperature indicating spoon

Imbuing mane-made objects with the ability of state shifting can yield many advantages, similar to what such capability can yield in nature. In case the various states taken by the object fulfill different functionalities, this is like many objects packed in a single as in the example shown in Figure 1-1.a. Such objects also result in material and manufacturing cost saving. State changing can also mean storage space saving and portability when one of the assumed states is one with a minimum occupied state (you could think of an umbrella, a laptop, a satellite, etc.). State changing could also be a way of signaling the state of something and/or thus warning a user about a state (consider babies spoon, indicating by a color change, a food temperature as shown in Figure 1-1.b). Another advantage that can be found in such products is the ability to adapt to changing working conditions; think for instance to a pipe whose diameter could change according to the demand in water or according to drought conditions. The endeavor to instill the ability to change in objects so that they autonomously adapt to changing conditions is the driving research force in the field of the so called *smart structures* [4]. Smart structures can sense, make a decision on their own accordingly and act, abilities are likely to improve the success chances of an exploration in harsh conditions (typically in space or a celestial body).

In a nutshell, an object with the ability to change, in a controlled manner, does have many advantages. There are many ways of imbuing objects with such capabilities and the

[3] Those are species capable of changing appearance in such a way that it warns a predator.

breakthrough in manufacturing that is at the core of this thesis – namely 4D printing – is likely to be one of them.

1.3 4D printing

A new milestone is currently being achieved in manufacturing. Let's explain it.

1.3.1 3D printing or additive manufacturing

Let's put ourselves for a few moments in the place of Renault French engineer Pierre Bézier, who back in 1968 developed for Renault what could be seen as the working base of modern CAD systems: UNISURF [5]. Let's then imagine Bézier, after printing some curves on a sheet of paper, wondering: "what if, in a way similar to how I just printed these curves, I could print one of the car's parts that I just designed with UNISURF?". This, back then, futuristic vision has been turned into reality in 1983, thanks to the ingenuity of three French scientists: Alain Le Méhauté, Olivier de Witte and Jean-Claude André. Back then Le Méhauté research focus was fractals. Many of the fractals equations based on his conclusions were not backed by his fellow researchers, and the only way for him to get fully trusted was to craft his fractals. A fractal is structure whose geometrical remains invariable at various geometric scales. Examples of such structures are found in nature as shown in Figure 1-2.

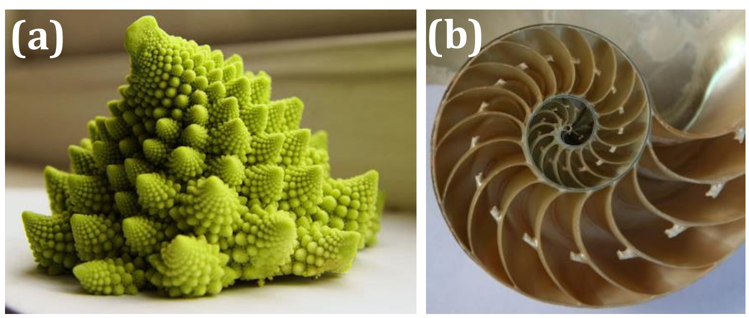


Figure 1-2 - Examples of fractals found in a nature: (a) Romanesco broccoli and (b) nautilus shell

At this moment, manufacturing such intricate structures was impossible. Le Méhauté thought the only way of getting a man-made three-dimensional fractal was by "3D printing" them. He was educated in chemistry, and particularly he knew how to turn liquid (monomer) into solid (polymer). A second spark towards 3D printing came after a discussion with his colleague de Witte who was working on lasers. They came up with the idea that by crossing lasers at a location within a resin, this latter could harden at this location. Experiments were then run to demonstrate this idea. However, these were not that conclusive, until a third spark came from Jean-Claude André: instead of curing the resin from inside (and struggling with light diffraction and deviation), why not curing it superficially, and layer-by-layer? This was the birth of 3D printing. Figure 1-3 shows on the 3D printed Le Méhauté fractal. Their invention was the first real response to the imaginary Pierre Bézier questioning.

Worth mentioning, in relating the genesis of 3D printing, is that the inventors filled a patent for their invention on the 16th of July 1984. On the other side of the Atlantic in the USA, Chuck Hull did also fill a patent three weeks later (on 8th of August) on 3D printing by the same principle of *stereolithography*. The French 3D printing patent has been abandoned few years later by Le Méhauté (and de Witte) employers, as they did not perceive the potentials of the invention, whereas the American one got maintained so far. This explains why Chuck Hull is usually credited with 3D printing's inventorship.

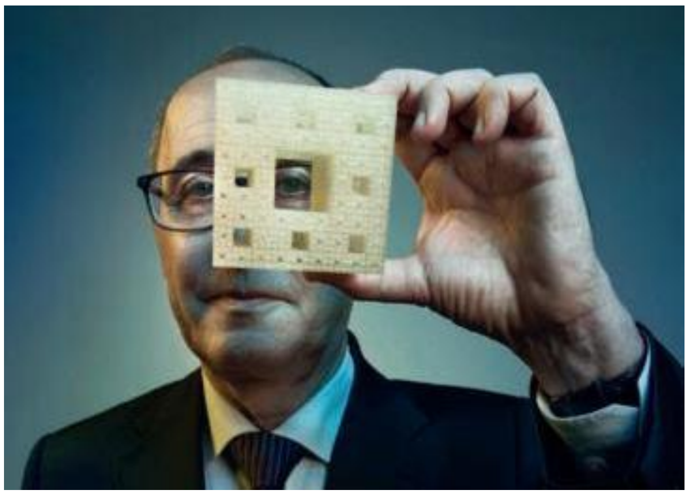


Figure 1-3 - Le Méhauté with one his 3D printed fractals

The so developed technology did not first make its way into our daily lives. It was mainly us for prototyping; and this may explain why AM is sometimes referred to as rapid prototyping. Nevertheless, the technology has matured and diversified. AM was first limited to stereolithography, but now many other AM techniques based on totally different principles have emerged. These have led to a gain in popularity of the technology both in and out of the industry in the recent years (2000s). This new way of manufacturing things is so groundbreaking that it is being taken seriously at highest level of states: USA former president Obama did acknowledge that it has "the potential to revolutionize the way we make almost everything"[4]. Firstly, used as rapid prototyping, all these AM techniques are now used to print end of use products. Indeed applications of 3D printed parts are now found in a large spectrum of industries including automotive [6], aerospace [7], electronics [8], and even health [9]. The maker movement has also largely contributed to the technology's blossoming. Indeed thanks to

[4] Extracted from President Obama February 2013 State of the Union's address

low cost machines leading hobbyist to be more and more interested in inventing and crafting at the pace allowed by 3DP. The generic process of 3D printing is presented in Figure 1-4.

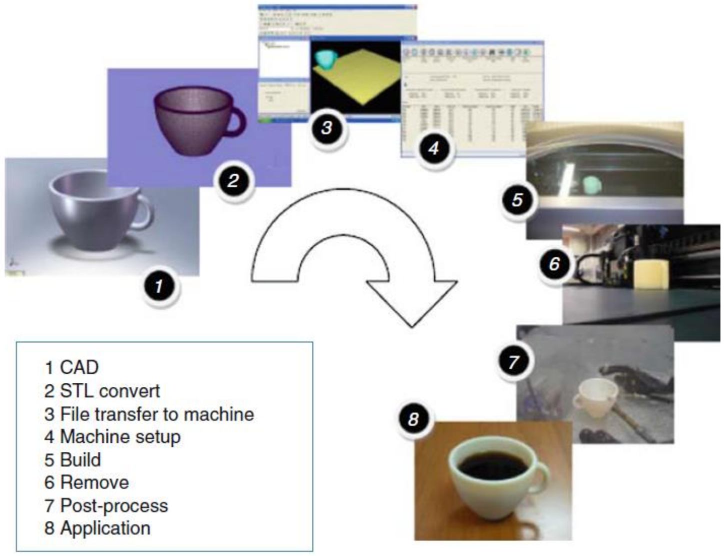


Figure 1-4 - Generic process of 3D printing (extracted from [10])

Compared to conventional manufacturing, AM techniques provide unique capabilities. Owing to the layer-by-layer building fashion of these techniques, virtually any shape can be manufactured at no significant extra cost or time. In addition to the allowed affordable geometry complexity, AM is also capable of material complexity: thanks to the emergence of multi-material 3D printers, parts with almost any material distribution can be printed. Others capabilities such as hierarchical complexity (features of any length scale – micro-, meso-, and macroscale – can be integrated into a part's geometry) and functional complexity (fully functional mechanisms – sometimes embedding electronics – can be manufactured) are also the engines of the 3D printing revolution. The material complexity allowed by AM seems to be opening a totally new dimension in the way things are thought about and manufactured.

1.3.2 Smart materials

Our customary way of conceiving materials is that they ensure what 'hold together' what is made out of them; in addition we see them as what prevent things from failure. As such our conception of materials is inherently imbued with the idea that a material is by nature static, that is, once it has been converted to an object in a desired state, it holds this state, until unpredicted conditions or aging decide otherwise. Looking at (almost) any man-made objects around us, and even many natural objects, it can wholeheartedly be asserted that this vision of material is right. Fortunately it is: what if the chair on which you are seating was changing whichever way, every hour? What if the windows of a house were able to shrink of expand randomly? What if an aircraft's fuselage were able to change shape, from cylinder to a cube, as a response to uncontrolled environmental conditions? Anyway, fortunately man-made objects are static thanks to the material they are made of.

Mother Nature, however, does not really see things this way. The necessity to adapt, to evolve, to be sustainable in order to cope with varying conditions, make that – in addition to materials that hold objects and prevent them from failure – Nature is also populated with many other materials that are sensitive and reactive to their surroundings; be them in the animal or plant kingdom. Basically, those are materials which are not static as what we are used to. Let take a look at a few of them.

An example of such material (some would say *organism*) that is sensitive and reactive to the environment and worth mentioning is the case of the chameleon's skin. As everyone would know, its color reversibly changes, almost instantly, whenever the color of the environment changes (cf. Figure 1-5.a) and depending on its mood. The change or the stimulus triggering this change of color is the environment itself: the chameleon is able to detect the color of the environment and alter its own color accordingly. The whole chameleon organism can be seen as a material that is sensitive to color changes, and reactive to these by mean of color changes. Another quite intriguing example of, say, non-static material, from mother Nature is that of plants exhibiting thigmonasty [11]. These plants move[5] themselves or their leaves, quite rapidly, when subjected to tactic stimulation. It is worth noting that the word "thigmonasty" comes from the Greek *thigganein*, meaning touch. The most famous example of such plants is the active carnivorous plant Dionaea. As shown in Figure 1-5.b, its leaves stay open until they are touched, typically by an insect which is then trapped and eaten by the plant. Here, the plant may be seen as a material in which a stimulus – touch from something in the environment – triggers a (shape) change.

[5] Such motions are referred to as *nastic* movements.

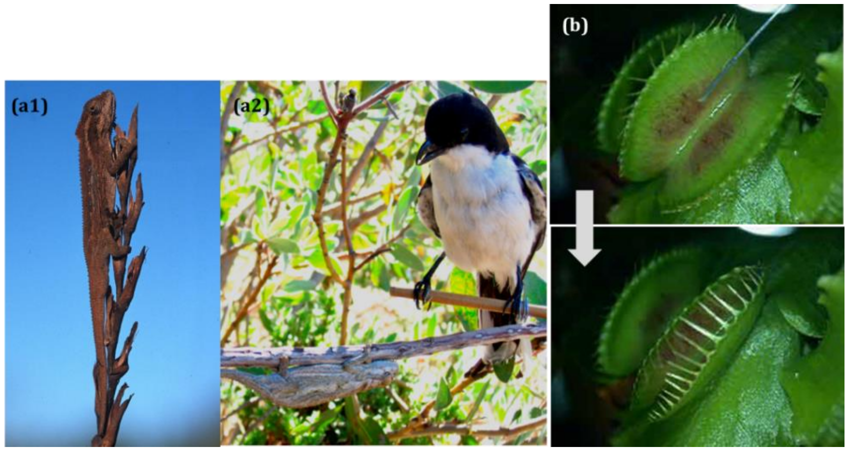


Figure 1-5 - Stimulus-responsive natural materials. (a): chameleon skin - (1) Swith's dwarf chameleon, one of the few chameleon using color-change for active camouflage; (2) A chameleon adopting a typical antipredator behavior. Adapted from [12]- (b) A Dionaea being excited by touch.

The untrained view might wonder whether such kind of materials can only be seen in animals and plants, or only in nature. Reasonably one may also question the usefulness of such behaviors. To the former questions, the answer is no. Let take a look at triboluminescent materials [13, 14]. Basically, these materials are crystals which, when subject to friction, do emit light. The first place where one may find a triboluminescent material is in a kitchen: as shown in Figure 1-6.a, sugar exhibits triboluminescence. The figure shows the light emitted by lined up sugar cubes when they are shot by a high-speed bullet. The friction caused by the bullet yields the light that can easily be seen in the dark. In the same vein, Wint-O-Green® Lifesaver, a candy popular in North America, does spark when crushed (again one's teeth); the light so emitted is so bright that it can be seen (in the dark) through the mouth. Figure 1-6.b shows image taken by a high speed camera of the candy being crushed. But obviously triboluminescence doesn't only occur in sugars or some candies. The effect can be seen in about 50% of known crystals [14] (e.g. quartz). First known use of triboluminescence by mankind dates back to the Uncompahgre Ute Indians. They crafted ceremonial rattles (cf. Figure 1-6.c) made out of buffalo skin and filled with clear quartz pebbles. When shaken at night for some rituals, the rattles produced light as a consequence of the friction of the stones impacting together and thus flashing through the translucent buffalo skin. The light emitted by triboluminescent materials is not that bright and has a wavelength between 400 and 500nm. "One of the brightest triboluminescent materials found thus far is europium dibenzoylmethide triethylammonium (EuD4TEA). This material was discovered by Hurt [15] in 1966 and is bright enough to be seen in daylight".

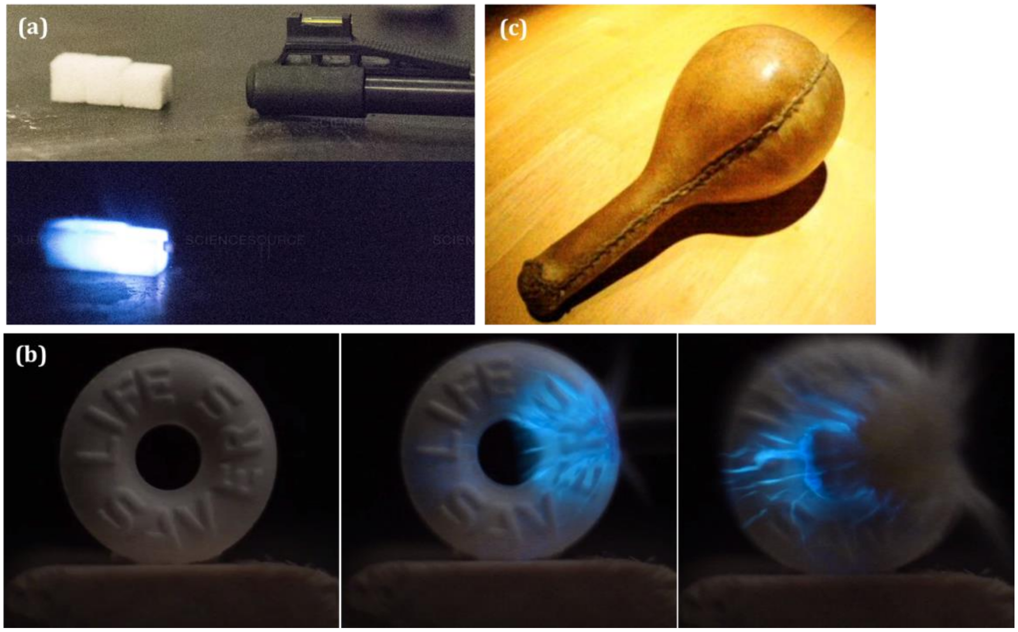


Figure 1-6 - Triboluminescence exhibited by (a) sugars and (b) LifeSaver candies [16], both being shot. (c) Uncompahgre Ute ceremonial rattle filled with quartz stones; it emits flashes of light when shaken [17].

In summary triboluminescent materials are sensitive to friction to which they respond by emitting light.

Regarding the usefulness of such behaviors, obviously they are not for fulfilling a load carrying role as it is for conventional material. Instead they fulfill functionality. Table 1-1 summarizes the discussed materials and shows what functionalities they do/can fulfill.

Table 1-1 - Example of natural stimulus responsive materials

Material	Stimulus	Response	Functionality
Chameleon's skin	Environmental color change	Color change	Camouflage Social signaling (warning, appeal, etc.) Thermoregulation
Dionaea	Touch	Shape change	Hunting
Triboluminescent materials	Friction	Light emission	1. Lighting 2. Impact detection

Materials, such as, the three aforementioned examples, are the so called *smart materials*(SM). Many definitions of SMs can be found in the literature, but a simple, and actually common one, is that they are materials which are sensitive to a stimulus and they react to it by changing their states. As shown in Figure 1-7, there are many other smart materials which differ by the stimulus they are sensitive to and how they react to it. In the engineering field, piezoelectric materials are the most popular smart materials.

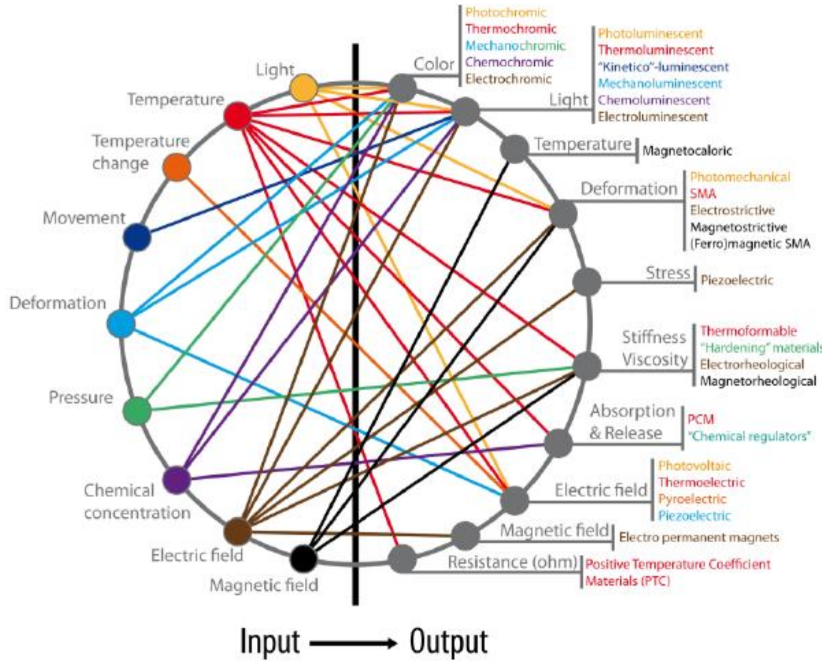


Figure 1-7- The world of smart materials as presented in [18]

It can be said that two materials age have recently occurred: the plastics age and the composite age. Somewhere in the middle of these two ages, a new era has emerged. This is the smart materials era. Whenever a breakthrough is achieved in manufacturing, materials are inherently impacted; as such breakthrough simply means new ways of processing materials. As it is shown in the next subsection, this still holds for the 3D printing revolution.

1.3.3 An introduction to 4D printing

While AM, as a new manufacturing method, is still in its infancy (despite being around since the 1980s) and, therefore, not yet fully adopted, it has yielded another disruptive technology: 4D Printing. 4D printing is the additive manufacturing of multi-material, including particularly smart materials, three dimensional objects; the 4th dimension being in reference to the ability of such objects to change their properties (shape, physical properties, etc.) and, potentially, their functionality after being printed. The temporal dimension inherent to SMs (as they are not static) adds one more dimension – time – to the three-dimensional objects. They owe such capabilities to the embedded stimuli-responsive smart materials [19]. As such, many definitions can be found in the literature:

- *4D Printing is a new process that demonstrates a radical shift in additive manufacturing. It entails multi-material prints with the capability to transform over time, or a customized material system that can change from one shape to another, directly off the print bed* [20];

- *The fourth dimension is described here as the transformation over time, emphasizing that printed structures are no longer simply static, dead objects; rather, they are programmably active and can transform independently* [20];
- *The initial configuration is created by three-dimension (3D) printing and then the programmed action of the shape memory fibers creates time dependence of the configuration – the four-dimension (4D) aspect* [21];
- *… active materials* […] *can be printed to create an active microstructure within a solid. These active materials can subsequently be activated in a controlled manner to change the shape or configuration of the solid in response to an environmental stimulus. This has been termed 4D printing, with the 4th dimension being the time-dependent shape change after the printing* [22];
- *... technology for creating dynamic devices that can change their shape and/or function on-demand and over time...* [which] *combines smart actuating and sensing materials with additive manufacturing techniques...* [23];
- *… this additional dimension only refers to the ability of a 3D printed item to switch its geometric configuration (including surface morphology) from one to another in a fully controllable manner. A particular stimulus* […] *may be applied to activate the switching process …* [24].

The ingenuity of "4D printed" objects relies on the smartly designed interactions between geometry (and more generally configuration), materials (both conventional and smart ones) and energy (either a passive one such as heat or moisture or an active one such as current). Owing to the ability of *4D printed* objects to transform (potentially in order to fulfill various functionalities); they can be seen as robotics without wires, sensors and actuators. This revolutionary technology is expected to be adopted in industries in the upcoming years. An economic report [25] predicts a commercialization of 4D printing by 2019 and a growth of 42.95% between 2019 and 2025, reaching $537.8 million.

One of the most interesting mechanical properties encountered in the smart materials realm is the shape shifting capacity as a response to a specific stimulus (heat, light, moisture, etc.). For instance, shape memory polymers (SMPs) or shape memory alloys (SMAs) can be thermo-mechanically programmed to assume a temporary shape and revert to a permanent shape once subjected to heat. This shape changing ability in SMPs is the one that has been considered the most in 4D printing studies thus far [21, 22, 26-28].

The customary way of thinking about and designing artefacts is considered as an endurantist one, that is, an artefact wholly exists at each time; thus it exhibits the same state and functionality over its lifetime. In a more and more competitive industrial global market context, driven by high profitability and new concerns such as sustainability, environment friendless, a perdurantism viewpoint of artefacts is more beneficial. Perdurantist artefacts do only exist partly at each time; they exist through their temporal parts, and as such, are able to evolve over time. 4D printing has made realistic such a philosophical vision of the world.

While understandable, the word "4D printing" as first proposed by Tibbits can be confusing. Some might see it as an evolution in printing and expect 5D printing, 6D printing, etc. to emerge. Sentences like "Unlike 3D printing, 4D printing allows the printed part to change its shape and function with time in response to change in external conditions such as temperature, light, electricity, and water" [29] may simply contribute to that vision of evolution. Furthermore, one may try to buy 4D printers. Again 4D printing is simply 3D printing (or additive manufacturing) with smart materials, among others, as "inks". There is no 4D printer, and 4D printing is not an evolution of 3D printing, instead it is an evolution in the use made of 3D printing as it is for metamaterials [30]. The expression "4D printing" is though the one being massively adopted by the scientific community, therefore instead of the explicit "smart materials based 3D printing" or "3D printing with smart materials", the term *4D printing* (4DP) will be used throughout this thesis.

1.4 General context and rationales for this PhD

Whether it is in the industry, in healthcare, or home appliance, etc. the landscape of products we are surrounded by is the outcome of many evolutions in technology, customer needs, trends, regulations. For a long period from years around the industrial revolution, companies were mainly dealing with mechanical products (assemblies of components). The main goal was to fulfill customers' needs.

Computer power rapid improvement along with its miniaturization, the Internet advent, wireless communication technologies, decreasing natural resources (such as oil and fresh water), more and more environmental concerns, materials engineering breakthrough, manufacturing methods improvements, mass production being supplanted by mass customization, an ever-increasing human's interest in space exploration have all contributed to shift the types of products produced by companies. That shift is from the basic conventional mechanical products to more autonomous and versatile objects as shown in Figure 1-8. These new types of products include mechatronic systems, connected devices, multifunctional and smart systems. In particular, over the past ten years, we have seen paradigm shifts associated with the emergence of some technologies, namely those concerned with the product-process-material interaction. These changes have occurred in products (from mechanical to intelligent products), in manufacturing processes (from conventional processes to additive manufacturing processes) and materials (from conventional materials to programmable / intelligent materials). There seems to be a common vision which aims at conceiving and realizing programmable products that are able to evolve (transformation of state, kinematics, of form, etc.) according to their environment, this in order to adapt to the need of the user during its lifecycle and consequently to postpone their obsolescence considerably.

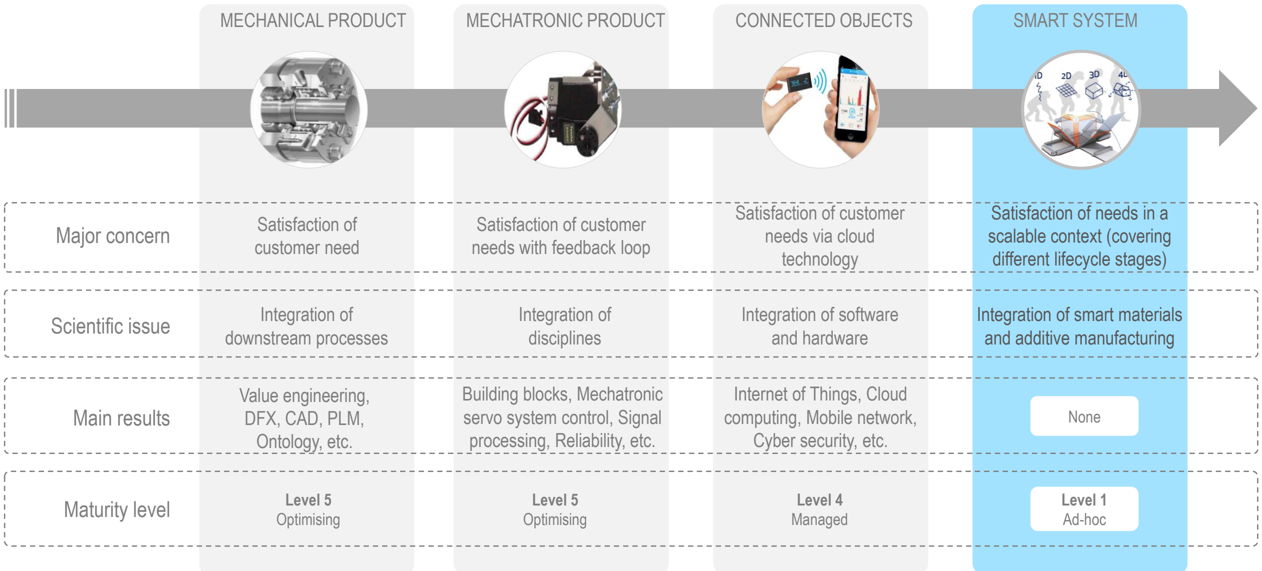


Figure 1-8 - Evolution of product kinds and related scientific challenges, results, maturity level

4DP seems to be an emerging technology in line with these evolutions. The need for adaptation in products, along with the ever rising additive manufacturing technologies' capabilities have somehow lead to explore that integration of smart materials and additive manufacturing. 4DP is a promising technology that is still at the Innovation Trigger stage in the latest Hype cycle [31] as shown in Figure 1-9. Companies cannot stay competitive and profitable without following these waves. Companies and governments seem to have already realized the potential of this technology. Many of the state-of-the-art studies are funded by the US Department of Defense. Airbus Group[6] is working with the Massachusetts Institute of Technology not to stay on the sidelines of this evolution. BMW also seems to want to contribute to the emergence of technology. Staying competitive in such a dynamic environment entails, on top of, investing in the new related technologies, rethinking the whole development cycle of products. In other words, part of efficiently embracing this new technology involves putting forth new design models, design methodologies and tools.

This PhD project is targeted on the additive manufacturing oriented design of mechanical and smart products, using smart materials. It aims at helping designers to understand this new way of thinking and to design the products to be realized via this new revolutionary manufacturing technology and which are evolving in their use's context.

[6] https://www.airbus.com/newsroom/news/en/2016/03/digital-materials.html

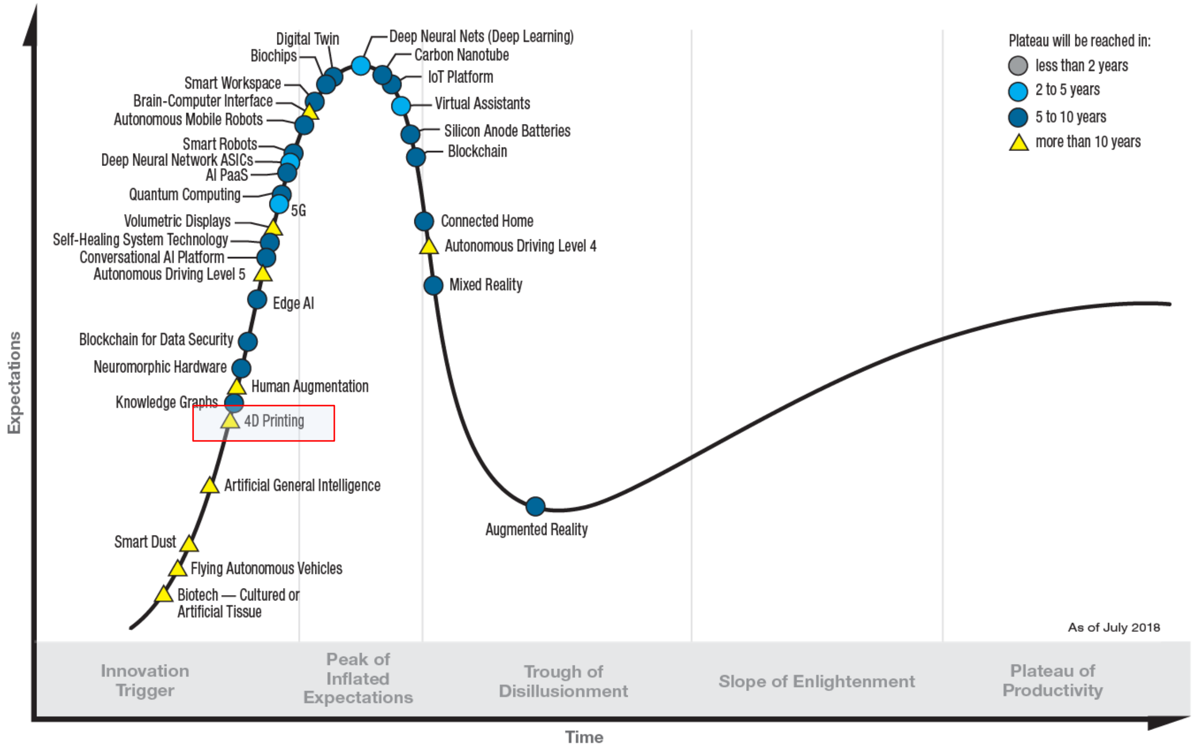


Figure 1-9 - Gartner Hype Cycle for Emerging Technologies 2018, © Gartner [31]

1.5 Motivations and objectives

Once a new technology is discovered, we are more concerned (and enthusiastic) with its physical and tangible aspects than its essence and how we can efficiently use it to improve our lives. This is quite natural, as somehow said in Alfred Nobel's saying: "One can state, without exaggeration, that the observation of and the search for similarities and differences are the basis of all human knowledge". Experimentation can also be added to these cornerstones of human knowledge. 4DP does not seem to escape this natural tendency: as the thesis literature review will point out, most of the research now undertaken on 4DP is targeted at manufacturing and materials issues; issues that are actually important to make the technology more mature and to push further our knowledge of it. It is noteworthy to highlight that to date there is not yet a single application of 4DP that is commercially available.

Before 4DP is fully industrially adopted a number of challenges will have to be overcome. These obstacles are of a tangible and immaterial nature. Tangible scientific problems include, and are not limited to:

- **Deformation and rigidity**. Most of the 4DP studies are now targeted at shape changing materials, materials which are actually soft. The more a structure is deformable (here programmatically) the less it is rigid and therefore able to carry loads. This should not really impact the emergence of 4D printing in the long run. There are indeed already 3D printing studies where fibers are used as reinforcements of the material [32, 33]. The use of metallic SMs could be envisaged: the selective laser melting (SLM) process has already been used (not for the sake of 4DP) with SMA powder [34, 35]. This approach nevertheless poses, for the moment, many problems including: (i) a small deformation (whereas SMPs allow deformations up to 400%, the SMA's deformation is around 10-15%), (ii) the shape memory effect of SMA is extremely sensitive to the composition of the material, which varies during melting.

- **Control of stimuli outside the laboratory**. The demonstrations currently done are in a controlled environment and considered as proof-of-concept. What will happen to the structure if the level of stimuli is not exactly what is expected? How to make sure that the sensory part of the structure is properly exposed to the stimulus, and not screened from it by an inert part?
- **Speed of change of state**. The changes currently observed are slow, which may not be appropriate for some applications.
- **Reversibility**. Most of the materials used today do not allow autonomous (and intelligent, that is, response to another change or withdrawal of excitation) return to the initial state. This may mean that only one autonomous reconfiguration is possible.

Scientific problems of immaterial nature are about all the thoughts or the engineering that need to occur before a 4D printed product is made real. Briefly stated, these (not independent) problems include:

- **Design**: a change in what we are able to manufacture should trigger a change in how things are designed, simply for improving the efficiency of the process leading from the idea (or the need) of a product to its final design. In the case of 4DP, manufacturers (smart material experts, AM processes experts, chemists) are mainly the ones able to design (and manufacture) 4D printed demonstrative artifacts. It can reasonably be stated that today or tomorrow design engineers - which are more likely to find innovative applications bridging the gap between laboratories and industry - are not ready to embrace this new design freedom allow by 4DP.
- **Modeling**: crucial to any design process is the capability to model the under designed item. Are current design tools able to handle the capabilities now afforded by AM (regarding, for instance, shape complexity and material complexity)? Are they able to model stimulus responsive behaviors of SMs? Because these modeling tools were not meant to suit of these new emerging technologies, it cannot be asserted that these are efficient to accompany designers into the 4DP revolution.

- **Simulation**: before a designed artifact can be manufactured and commercialized, it ought to me somehow tested; this explained why computer aided engineering (CAE) tools are so important in most design projects.

The thesis is more focused on solving the aforementioned immaterial problems; through the creation of a design environment allowing/facilitating the design of this type of products (obtained by additive manufacturing and intended to evolve). Before being able to state a problem and define more concisely the voids to be filled on this aspect, it is necessary to investigate the related themes that fall under the design for 4D printing. Given the definitions encountered in 4D printing, core topics to be investigated include:

- **Design with smart materials.** The question of (conventional) material comes classically at a time when a fairly precise knowledge of the final product exists, because the material only plays a structural role. However as explained in the introductory section on SMs, SMs do also play a functional role. This is why the question of how to design with SMs needs to be elucidated.
- **Design for additive manufacturing**. Because this manufacturing process eliminates the constraints specific to conventional processes, it is important to review the way in which one conceives, a way currently somewhat restrained and/or unjustly guided by the knowledge that a designer has of conventional processes.
- **Design for (mechanical) evolution.** Inert mechanical evolution and smart mechanical evolution (sensitive and reactive). What are the products we are talking about and what is there to facilitate the design of these products? Evolution – or change – in a product may be of a nature different from mechanical as well.

The PhD research work has been done within the ICB (in French: Laboratoire Interdisciplinaire Carnot de Bourgogne) UMR 6303 CNRS laboratory, especially in the COMM (Design, Optimization and Mechanical Modeling) department, lead by Prof. Samuel GOMES. In this departement, I was involved in the design-oriented team which focuses its efforts on product lifecycle management, knowledge-based engineering, proactive design for X, advanced computer-aided design and knowledge description and representation to name a few [36-39]. Overall the last five years, promising research initiatives have been made on the need of qualitatively describe technical objects over time to fully track their semantic paths, to capture and understanding the design evolution in the overall product development process and also to fully describe the product from an assembly process perspective. This has been a logical and natural opportunity to address 4D printing issue that gathers all these aforementioned scientific issues through additive manufacturing technologies and smart materials. Recently, this research action has been identified as a strategic ones at the ICB and CNRS levels, and falls under a cross-disciplinary theme called “Design, modeling, optimization for 3D and 4D printing” led by Dr. Frédéric DEMOLY in order to structure and bring together the multiple competencies of the people involved in COMM department.

1.6 Thesis structure

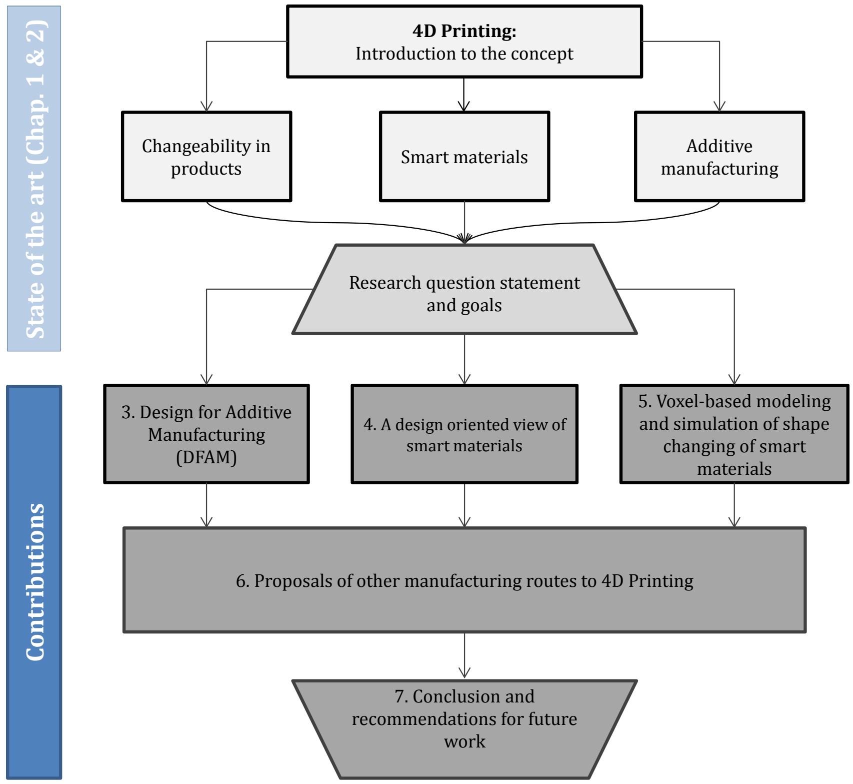


Figure 1-10 - Thesis outline

After this introducing chapter, a literature review will be conducted to gain an in depth understanding of the concept and also look at it from a design perspective. Then three main contributions will be made to fill the highlighted gaps identified in the literature review (chapter 3, 4, 5 and 6 mainly).

- Chapter 3: designing for additive manufacturing, this chapter aims at putting forth a design methodology taking into account the design freedom allowed by AM while abiding by its specific constraints.
- Chapter 4: considerations of SMs purely from a design perspective. This chapter addresses how the capabilities of SMs can be made available in such a way that they benefit designers.
- Chapter 5: simulation of smart materials behaviors on a voxel basis. The goal is to provide a modeling framework easing the simulation of SMs distribution and also for computing materials distributions.

- Chapter 6: this chapter provides alternative routes for 4D printing; a machine for easily processing SMs in resin form is presented.

Finally conclusions will then be drawn and work still needed to be done will be stressed out in the last chapter.

Chapter 2 State of the art, research question and proposal

The thesis introducing chapter has briefly introduce 4D Printing (4DP) after looking back into how the way we manufacture things has evolved, delineating 3D Printing and smart materials. This chapter goes deeper into the topic. To ease the understanding of 4DP, first background on its main physical constituents, that is, additive manufacturing (AM) and SMs, is provided. In addition to ease the understanding of 4DP, this background information is also meant to review the state of the art regarding these building blocks. The purpose of this thesis is not really about manufacturing, but rather about design methodologies. As such we found it worth explaining what undertaking research in design methodologies was about and why such research is important.

Once the background information has been established, the chapter delineates all that has been done so far regarding 4DP, not only manufacturing wise but also – if any – design methodology wise. It is worth noting that, before the Tibbits 2012 Ted talk[7] introducing the buzzword *4D printing* the interaction AM-SMs was already under investigation; as shown in Figure 2-1, there has been an acute surge in publications on the topic from 2014.

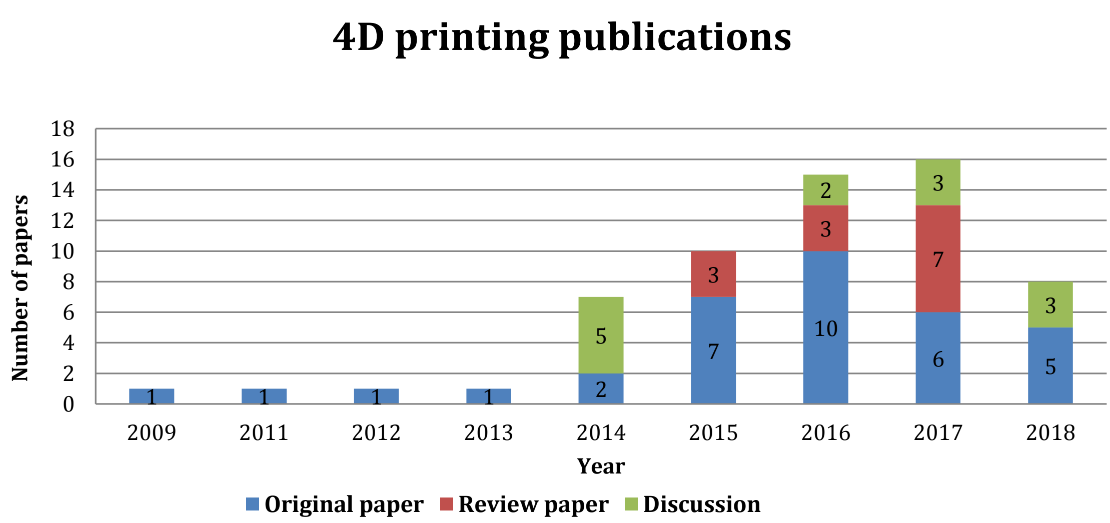


Figure 2-1 - 4D printing studies breakdown by year and type of contribution

[7] https://www.ted.com/talks/skylar_tibbits_the_emergence_of_4d_printing

Independently to what can be found in the 4DP literature, an analysis of the field from a design related point of view has been conducted. Based on the conducted analysis and on the identified gaps, the research question motivating this PhD has been clearly stated and our proposal to solve it has been outlined.

2.1 Background information

2.1.1 Additive manufacturing technologies

Table 2-1 - Additive manufacturing processes classification

Family process	Description	Typical processed materials	Typical techniques
Material extrusion	A material is semi-solid state is extruded through a nozzle/needle, and is cured.	Polymers, ceramics, metals,wood	FDM, Direct Ink Write (Robocasting)
Powder bed fusion	A thermal source selectively fuses layers of powder.	Polymers, ceramics, metals	Selective Laser Sintering (SLS), Selective Laser Melting (SLM)
Photopolymerization	Layers of photopolymers are selectively cured upon exposure to a radiation.	Photocurable polymers	Sterelithography Aparatus (SLA)
Directed energy deposition	A focused high power laser beam melts a material powder as it is being deposited.	Metals	Laser Engineered Net Shaping (LENS), Direct Metal Deposition (DMD), 3D laser cladding
Sheet lamination	Material sheets are bonded; each sheet (representing a cross section of the CAD model) is selectively cut with an energy source.	Papers, metals, polymers	Laminated Object Manufacturing (LOM), Ultrasonic Consolidation (UC)
Material jetting	Droplets of a material (or a mix of two materials) are selectively deposited in thin layers from a print head and cured either by a source of energy or by environmental conditions.	Polymers, wax	Multi-Jet Modeling (Drop-On-Demand), PolyJet
Binder jetting	A binder is selectively deposited, from a printhead, onto a powder bed, forming a section of the CAD model.	Plastics, metals, composites, ceramics, polymers	3D printing

As its name suggests, through additive manufacturing (AM) one can craft parts by adding materials – layer-by-layer – rather than removing it, as it is for some conventional (subtractive) manufacturing processes such as milling. This manufacturing method originated from stereolithography (as explained in the introducing chapter). Since then AM has evolved and many other kinds of manufacturing processes relying on the principle of bonding material layer by layer have been developed. Depending on the way these processes form matter, they can be classified in seven families [34], each including different techniques as shown in Table 2-1. Over 70 manufacturers across the world are providing AM machines with various capabilities and for various niches. The repertoire of types of materials that can be processed by AM has also expanded: almost all the materials can now be processed by AM, these include polymers, metals [40], ceramics [41], concrete (for construction) [42], foods [43], other organic materials such as wood [44], biomaterials[45], and also smart materials. As such AM technology is being considered and adopted as a key enabler for the so-called new industrial revolution. Many papers and books [10, 46, 47] do explain in great details the AM real. Nevertheless, for the sake of completeness we find if worth briefly outlining the current seven AM processes, as these will be evoked throughout the thesis.

2.1.1.1 Powder bed fusion processes

In powder bed fusion processes, a part is basically formed by turning material fed in powder form into a solid. There is one or two feedstocks at both sides of a platform. The powder is dispensed and even from either of the feedstocks onto the platform and in a thin layer (typically around 0.1mm); this powder is kept at a high temperature below the material melting point. An energy source (generally a laser) is then used to selectively melt or sinter the powder according to the part's section being manufactured. Once the section is complete, another layer of powder is dispensed onto the previous one and the process is repeated until all the part's sections are built. The energy source is high enough to melt (or to sinter) the powder and to bond layers together. Typical techniques of this process are SLM which typically processes metals powders and ceramics powders, and selective laser sintering (SLS) which is commonly used to process polymer powder such as nylon polyamide. The latter has the great advantage of being a support-free technique in that uncured powder acts as support material. This can also be the case of SLM, but owing to the high energy laser there can be high temperature gradient along the build direction between layers, leading to part's deformation. To avoid this, supports are printed (with the part material) and they are used both as heat sinks and also to support overhangs.

2.1.1.2 Photopolymerization

Behind the first 3D printing machine is the photopolymerization principle. A platform is first immersed for a small distance down into a vat of a photocurable resin. Such a resin cures once exposed to a specific light. The thin layer of resin that is on top of the platform is then selectively exposed to a light (typically an ultraviolet light) according to the part cross section, which is thus crafted. As the name suggests this process is limited to polymers, however the polymer can be reinforced by filling the resin to obtain specific properties such as hardness. Typical techniques include: stereolithography (SL) in which a laser spot is used to cure the resin; microstereolithography (μSL) which works the same way, except that it is suitable for complex shaped parts of size not bigger than a millimeter; mask projection SL (aka direct light processing or DLP), whose particularity lies in that a single layer is create at a time by projecting bitmaps on the resin, thus a faster process. Photopolymerization techniques are inherently single-material one, unless altered as in [48]. Owing to this characteristic, support structures are made out of the same material as the printed part.

2.1.1.3 Directed energy deposition [49, 50] (also known as beam deposition)

The principle governing direct energy deposition (DED) is close to welding, except that the raw material can also be provided in powder form. A material powder – typically a metal – is projected on a spot; meanwhile a laser (a plasma arc or an electron beam) is focused on that same spot. The powder is basically melted, deposited and solidified almost simultaneously. The principle is similar to the one behind extrusion based processes. The motion of the depositing head is governed by the part cross section being manufactured. While DED processes are mostly used with metal powder, they can also be used to process polymers and ceramics. Owing to the predominance of metals, these processes are sometime referred to as 'metal deposition'. This process makes it possible to print multimaterial part, even with continuously varying material properties as shown in [51, 52].

Within this family of AM techniques, there is almost no variation in the way matter is formed. Many companies have developed DED machines (embodying the same principle) and which are referred to as: Laser Engineered Net Shaping (LENS®), 3D Laser Cladding, Laser-Based Metal Deposition, Directed Light Fabrication, Laser Consolidation, etc. The differences that may be seen in them lie in laser power, laser spot diameter, type of laser, the way powder is delivered, and the motion of the nozzle (most of the system are 3-axis systems which work only of flat substrate, but there also 4- or (- axis systems which can work on any 3D substrate).

2.1.1.4 Sheet lamination processes

The principle on which is based sheet lamination is simply sheet bonding: sheets of material are bonded one on another and/or one aside another. Each stack of sheets roughly represents a cross section of the manufactured part. The way the sheets are bonded and shaped characterizes the four main techniques making up the sheet lamination process family. The 1st approach is glue bonding where the used sheets are coated on one side with an adhesive, forming a layer can be made according to two ways: *bond-then-form* (in which the sheet is cut into the object's contour by laser or knife cutting after being bonded) and *form-then-bond* (the reverse). The 2nd technique uses thermal bonding, mainly with a form-then-bond approach. In Sheet Metal Clamping, the 3rd technique, bonding is simply realized by mechanical clamping force: the sheets are cut into a desired shape allowing at least one stackable side, and are subsequently clamped (through bolt clamping for instance). Finally, sheet lamination is also realized through ultrasonic consolidation (UC), illustrated in Figure 2-2. This can be seen as a hybrid (additive and subtractive) manufacturing technique. Thin (typically 100-150µm) foils of a material (mainly metal) are laid side-by-side on previously formed matter, a rotating sonotrode then travels on them. The force applied by the sonotrode along with the friction induced by its motion at the interface allow for plastic deformation and ultimately consolidation to occur. A milling system is then used to cut the formed layer into the desired shape. The process is repeated until all the cross sections are made.

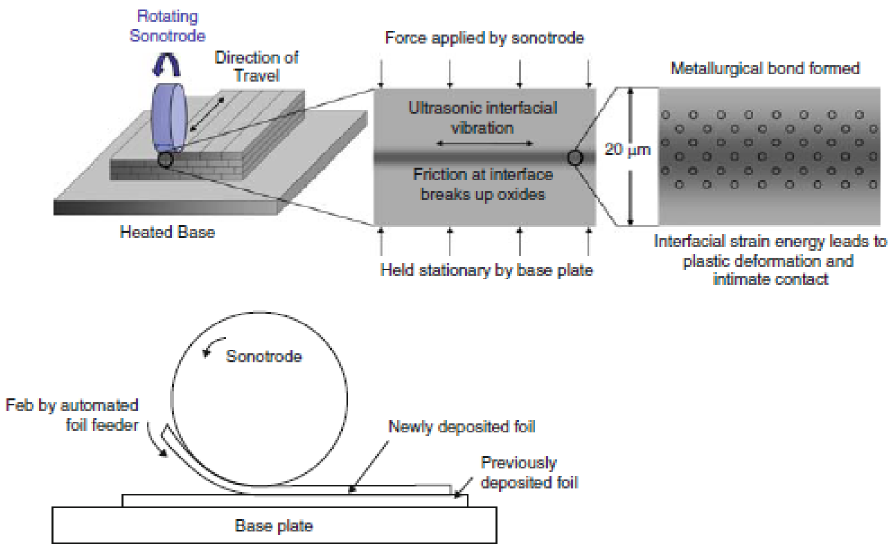


Figure 2-2 - The ultrasonic consolidation technique (extracted from [10])

Typically any material which can be made available in sheet form, with the sheet capable of being laser (or knife) cut and bonded is processable by sheet lamination; nevertheless some techniques namely those based on thermal bonding and UC are limited to metals.

2.1.1.5 Binder jetting processes

The material jetting princess could have been termed (more explicitly) as *selective powder binding* as depicted in Figure 2-3. Indeed, it works by selectively binding a material in a powder form. A layer of powder is first laid on a platform; secondly tiny drops of an adhesive are selectively deposited onto the powder according to the part's cross-section being printed. Another of layers of powder is then laid on the previous one and the process is repeated until all the cross sections are manufactured. This principle is very close to how (2D) inkjet printing works. And this explains why the only one technique within this family is the one truly named "3D printing". The parts obtained by the aforementioned process are usually post-processed to enhance material properties: for instance, thy can be infiltrated and/or fired to increase mechanical strength and density. As for 2D printing, the adhesive (the ink's counterpart) may actually be a collection or a mixture of two or three different base materials, thus the possibility of printing multimaterial parts in general, and particularly multi-color parts. The material properties of the green body depend both on the powder (which can be of polymer, metals or ceramics) and the binder.

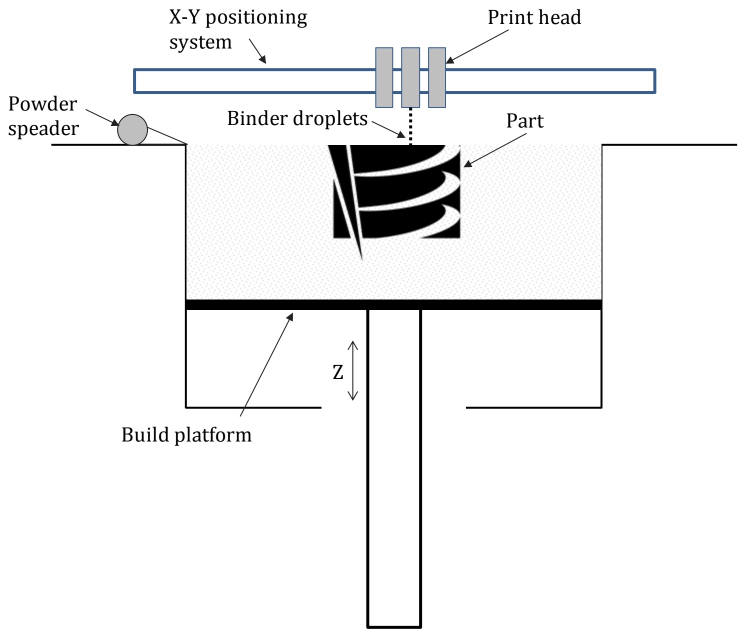


Figure 2-3 - Schematic of the binder jetting technique

2.1.1.6 *Material jetting processes*

The material jetting principle is similar to the binder jetting one, in that it works similarly to 2D printing – as a matter of fact, the classification used in the reference book [10] gathers these two principles in a single family referred to as printing processes – expect that material jetting does not use raw material in powder form and what is sprayed onto the platform is the raw material in liquid form. Basically, the principle is depositing droplets of the material from a print head onto the platform; the deposited droplets are then cured. Techniques based on this principle differ according to how the deposition is made by the print head: this could be point-wise (as in earlier forms) or line-wise. Variation among the techniques also comes from how many materials could be deposited in a single layer. While first printers (such as the ModelMaker by SolidScape) were limited to printing basic wax material that was liquefied, recent printers (such as the Connex500 of Stratasys or 3D Systems machines) can print with (photo-)polymers with different material properties (e.g. color, hardness, melting point). Finally, the way the deposited material is cured is another factor which differentiates material jetting techniques: curing can be made through solidification (as in systems where the deposited material is wax) or through photopolymerization. Worth highlighting is the PolyJet technique (the MultiJet Modeling technique is similar) embodied by many of the Stratasys printers. In this technique, droplets of a photocurable resin are first selectively deposited on a platform, and then a UV light flashes the resin which cures immediately. The process is then repeated until all the layers are printed. The droplets are deposited from a print head which extends over the whole platform length (line-wise deposition) and which can have over 1500 nozzles. The technique is shown in Figure 2-4. One of the deposited materials is used for support material that can easily be removed post-fabrication. The other base materials can be mixed into any proportion for varying material properties within the same part, the obtained materials are the so-called *Digital Materials*.

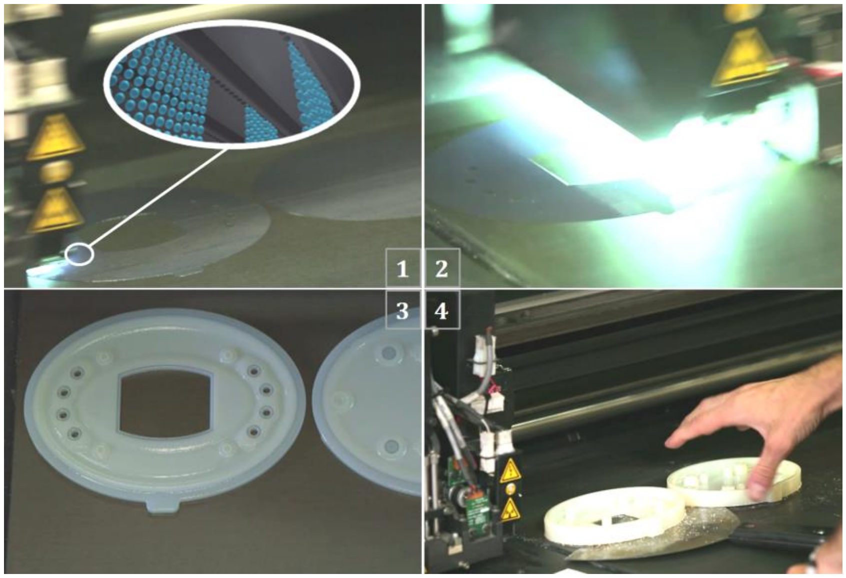


Figure 2-4 - The PolyJet technique with a Stratasys printer [53].

2.1.1.7 Extrusion-based processes

As suggested by the name, techniques within this family work by depositing a material by extruding it through a nozzle. The material (with an appropriate viscosity) is extruded while the nozzle scans a platform (which is heated or not, depending on the technique and the material) according to part cross section being printed; the so deposited cross-section is immediately cured and the process is repeated onto the previous layer until all the layers are printed. There are seven key features that distinguish AM techniques based on extrusion: loading of material, material liquefaction, the way pressure is applied to move the material through the nozzle, the deposition strategy (to print the same cross section, many different paths may be taken), the ability to generate support structures, bonding between layers. Typically materials used with extrusion based techniques are polymer and to a lower extent organic materials (such as food or living cells in solution for tissue engineering). The main technique within this family is Fused Deposition Modeling in which the raw material is fed in the form of filament which is forced through a heated nozzle so that it melts before being deposited. Materials used are mainly polymers but their properties can be expanded by filling the polymer with specific filler to enhance a property (such has electrical conductivity).

2.1.2 Smart materials

Since the discovery of piezoelectricity and the shape memory effect [54], the range of SMs properties has significantly expanded, in terms both of stimuli and responses. This section is intended to briefly review the SMs realm. Many definitions of SMs are found in the literature, however all of them are in agreement with the fact that these are materials whose properties (be them physical or chemical) are altered as a response to a specific change – a stimulus – in their environment. Behind such properties, can be seen the research endeavor to incorporate intelligence into matter so that it behaves autonomously by sensing, reacting and adapting to the environment, as does any biological system. Many matters possessing such capabilities are termed as smart materials; however for this review we provide other characteristics which define the scope of our investigation. We consider as SMs:

- Materials which sense and react to stimuli at their own, that is, which do not need another material to perform such functions. This excludes for instance dielectric elastomers[8] [55], because even though they do expand in response to a potential difference, they are formed by the combination of the dielectric material sandwiched between two electrodes.
- Materials whose response is not encountered, as a physical phenomenon in a conventional material. Thus are excluded, materials such as electrocaloric materials which – like any resistive materials exhibiting the Joule effect – show a reversible temperature change as a response to an electrical current.
- Materials whose response to a stimulus is different from the stimulus itself. Ferroelectric materials are thus excluded, as these materials which respond to an electric field by becoming permanently electrically charged.

Depending on how they respond to a stimulus, SMs fall in any of the following groups:

- **Shape changers:** these are those which respond to stimuli by strain or stress. While some of them simply exhibit change in size (e.g. hydrogel, piezoelectric material, etc.) other, such as shape memory materials, react by changing shape.
- **Optical sensors:** within this group are materials whose response is optically perceivable; this includes for instance thermochromic materials, triboluminescent materials or switchable mirrors.
- **Converters:** these materials are those whose response is typically a signal that can be used as a stimulus for another SM or to provide information about a medium's state. Examples of such materials include piezoelectric material, thermoelectric material or photovoltaic material.

[8] Nevertheless those are considered as *smart material systems*.

- **State changers:** SMs usually have a single condition; state changers are those whose conditions change in response to a stimulus. Examples of these are electro-/magneto-rheological fluids or shear thickening fluids.

Figure 2-5 shows these groups of materials along with their basic behaviors when subjected to the stimulus.

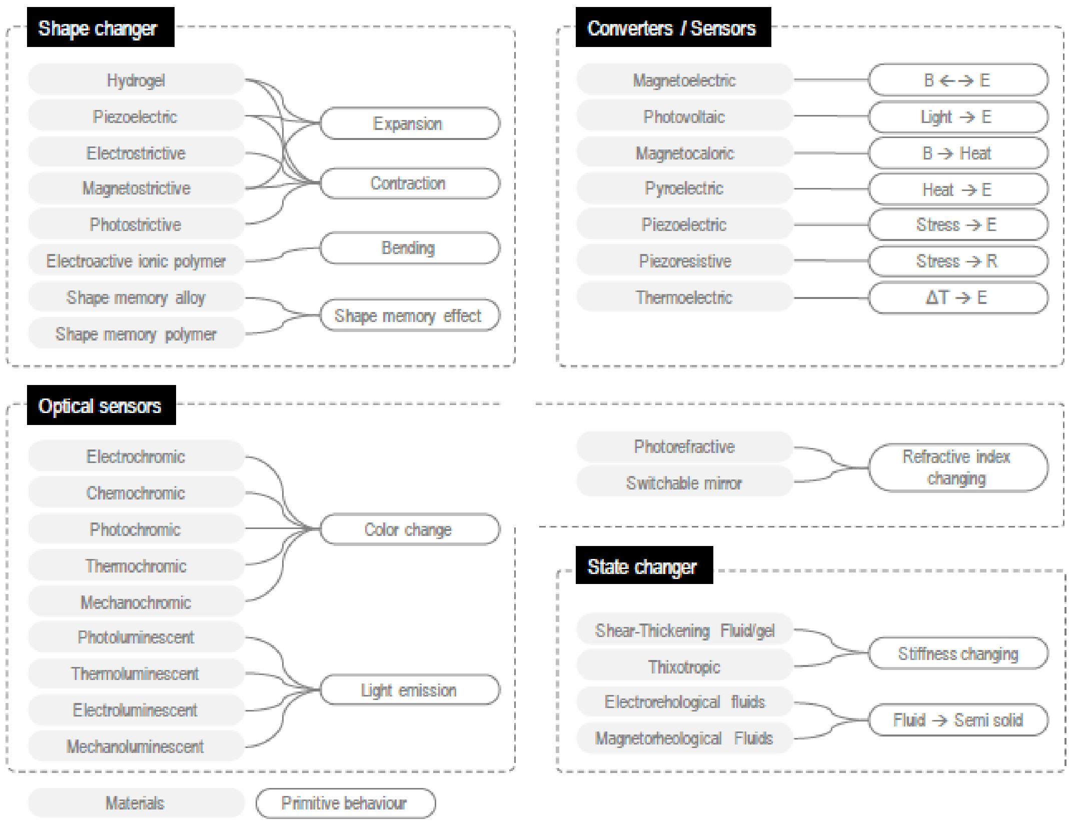


Figure 2-5 - Proposed classification of the smart materials [56]

Shape changing materials (SCM) are those which respond to a stimulus by producing a strain (or equivalently a stress), in others words their smartness lies in their ability to change size or shape as a response to a stimulus. Within this group of SMs it is worth distinguishing two subgroups: programmable SCMs and non-programmable SCMs. While in non-programmable SCMs the way the material can change shape is predefined during fabrication, in programmable SCMs the shape change pathway can be changed to yield a desired effect post-fabrication. Yet, the term *programmable* has been used with non-programmable materials. By means of a sophisticated processing/manufacturing method, Kim et al [57] were able to introduce heterogeneities in a hydrogel sheet, which exhibits complex shape change behavior (more elaborate than simple shrinking and swelling); the way the manufacturing has occurred could be referred to as the "programming" of the material. However, no matter how much complexity is involved in the shape change behavior, the pathway of shape change is definite and cannot be changed after fabrication, unlike programmable SCM. Nevertheless, these terms are here described for the sake of consistency and to avoid any confusion. They do not reflect any standardized or official terminology.

Programmable SCMs change shape according to a pathway that can be altered regardless of how they were manufactured. In other words, after manufacturing they can be trained to shift shape between almost any shapes. These materials are typically shape memory materials. They are formed into one permanent shape, and can be thermomechanically trained (or programmed) to assume one (or several) temporary shape(s) from which the permanent shape can be recovered. Two types of shape memory effect (SME) mechanism can be found: the one in SMA and the one in SMP.

In SMA, the SME is due to phase transformation between two phases referred to as austenite (stable at high temperature) and martensite (stable at lower temperature). Usually at room temperature, a SMA is totally made of martensite. It can be deformed (apparently) plastically (up to 10%) into any desired shape (the temporary shape). Once heated above a certain temperature (A_{finish}, a temperature at which the SMA is totally composed of austenite) the phase transformation triggers a total shape recovery back to its initial ("memorized") shape. This is the one-way SME (OWSME), which is not reversible: cooling the sample does not deform it back to the deformed shape again. There is nevertheless a two-way SME (TWSME) or reversible SME in which the SMA can "remember" its shapes at both high and low temperature. However TWSME is less used as it requires a more complex thermomechanical training process and the recovered strain is less than the one that can be found in OWSME, in addition the strain quickly deteriorates over the cycles.

In SMP, shape change is also the result of heat induced phases change within the material but the thermomechanical training works differently. The material must first be heated above a switching temperature T_W (which is either glass transition temperature or melting temperature) and then deformed into a desired shape. It is then cooled below T_W while the deforming strain is maintained; upon release of the deforming stress (after cooling) the sample keeps the deformed shape. It recovers the permanent ("memorized" or as manufactured) shape when heated again above T_W. The so described process is the OWSME in SMP. The TWSME is also possible in SMP [58].

The aforementioned SMEs (in SMA and SMP) are the classical dual shape memory effect in which the material changes shape between two shapes: the permanent one and a deformed one. But there can also be multi-shape memory effect (both in SMP [59] and SMA [60]). This can be achieved through more complex manufacturing and thermomechanical training steps. SMAs are essentially sensitive to heat, however there are also magnetic SMAs [61] in which the shape recovery is triggered by a magnetic field. In SMP the base stimulus is also heat, but they can also be made sensitive to light (either through light induced heating or chemical reactions and changes induced by light irradiation). Their chemical tunability and compatibility to other materials makes them capable of being sensitive to other stimuli [62].

Non-programmable SCMs are those whose shape change behaviors are predefined by the fabrication process and usually involve affine transformations (shrinking, swelling, etc.). Their extreme shapes (and thus, change pathways) are intrinsically embedded in their behavior at the time they are manufactured. They are also distinguishable from programmable SCMs in that their response is a continuous function of the stimulus: the shape change is triggered once the stimulus is sensed (regardless of its value), and as soon as this latter is turned off (or removed), they return to their initial shape. These materials include:

- Hydrogels [63]. Polymeric gel like materials which shrink isotropically in response to heat (as shown in the figure below). They are *easily* chemically tunable which has led to hydrogels responsive to light, electricity, chemical concentration (e.g. pH or glucose) and biocompatible hydrogels. They are good candidate for soft actuators [64]. The strain developed in response to heat can be up to 800%.

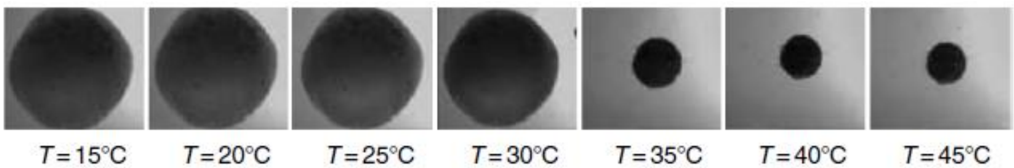


Figure 2-6 - Collapse transition of a bead of hydrogel. The diameter of the gel bead is 1.87mm before the collapse transition [65]

- Piezoelectric materials. These materials are sensitive to electricity and pressure. The *direct piezoelectric effect* found in some ceramics is when the material generates voltage when stressed. The reverse piezoelectric effect refers to the generation of a stress and equivalently a strain when the material is subjected to an electric field. Piezoelectric materials are essentially ceramics in which the generated deformation is rather small (0.1% - 0.3%) but precise. They are nevertheless (synthetized) piezoelectric polymeric materials, namely the ferroelectric polymer polyvinylidene fluoride (PVDF). These materials are used for sensors and microactuators application and more and more for energy harvesting.
- Electrostrictive materials. In a way similar to piezoelectric materials, these materials are responsive to electric field. They develop strain when subjected to an electric field but they do not have a “direct effect”, that is, pressing them does not generate a voltage. The strain developed by electrostrictive materials is rather small, common electrostrictive ceramic materials exhibit strain between 0.1 to 0.2%.
- Magnetostrictive materials. These are the magnetic counterparts of electrostrictive materials: they basically elongate in the direction of an applied magnetic field. Though they also differ from electrostrictive materials in that there is a “reverse” effect: deforming a magnetostrictive material generates a magnetic field. The effect is found in

ferromagnetic[9] materials and it does require quite strong magnetic fields for strain ranging from 0.001% to 0.1% for Terfenol-D, the predominant magnetostrictive material.

- Photostrictive materials: upon exposure to light these materials exhibit a non-thermal change in dimensions, a phenomenon referred to as photostriction. It is found in many types of materials including ferroelectrics, polar and non-polar semiconductors, and polymers. The effect is most important in polymeric photostrictive materials where the developed strain is up to 400% [66].

2.1.3 Research in design

For almost any activity carried out by humans, there is a thinking process (whatever its duration) which precedes, at least for deciding what actions will be taken and how these will be taken. This could be for finding directions, fixing a device, writing a thesis, cooking a meal, crafting a tool or an aircraft, etc. Simply speaking, design – as the activity – could be defined as that thinking process preceding the concretization or realization of a project. More specifically design is the process by which knowledge and creativity are converted into a representation of an object (be it physical or not); a representation that is detailed enough to ease its concretization. Depending on the field the definition may be furthered. In engineering, design is defined as "the process of devising a system, component or process to meet desired needs"[10]. Mechanical design is dedicated at designing components and systems of a mechanical nature using knowledge from mathematics, physics, material sciences, etc. Finally worth mentioning is that, design is a decision making process for solving problems (usually stated qualitatively) which do not have unique solution. As such the process is prone to iterations.

For a long time devising an object has been considered as an art rather than a science. But at some point, it turned into a scientific discipline. The goal of that science (usually referred to as Design Theory and Methodology (DTM) or Design science) was to somehow rationalize the activity. Such rationalization is for improving the performance of the output and for increasing the efficiency of the whole output's development phase (e.g. iteration count reduction). This has led to the development of a number of methodological approaches to the design process, namely: the axiomatic design by Suh [67], the systematic approach to engineering design by Pahl and Beitz [68] to name a few.

In mechanical design – which this thesis is mostly concerned with – one of the main reasons of design iterations, is manufacturing. Owing to the lack of information exchange between the workshop floor and design office, a solution – despite being innovating and theoretically performant – may simply be unfeasible with the current (or available) manufacturing

[9] Metal that can be permanently or temporarily magnetized or that is capable of being attracted by a magnet.

[10] Accreditation Board for Engineering and Technology (ABET)

techniques' capabilities. A situation usually referred to as the Over The Wall engineering, and which is illustrated in Figure 2-7.

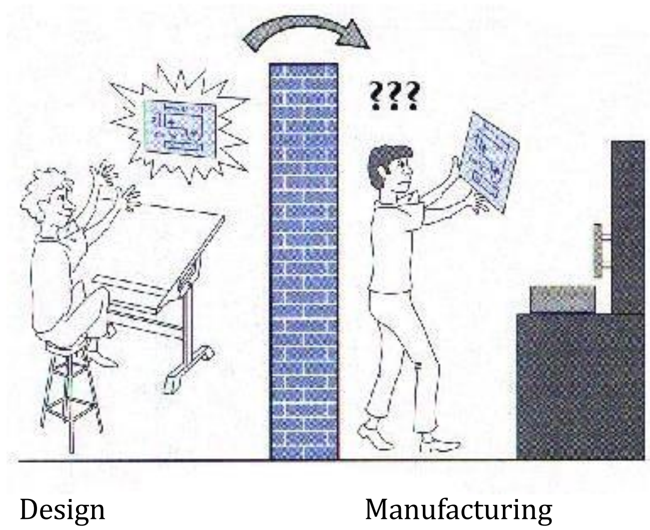


Figure 2-7 - *Over The Wall* engineering

On the other hand, a design may not be optimized up to the capabilities of the manufacturing workshop. These situations have prompted academia and industry to expanding design science by considering another approach, namely concurrent engineering [69] in which stakeholders of a product development process works concurrently rather than sequentially. It is that same vein that Design For X (DFX) [70] becomes a major research branch of DTM. The X standing for a lifecycle stage of the product (e.g. manufacturing, assembly, recycling, etc.). The goal of DFM being, basically, tailoring what is conceivable to what is manufacturable.

2.2 4D printing studies

To review how 4D printing has been investigated so far, a breakdown of the contributions has been done according to which AM processes and techniques have been used.

2.2.1 Photopolymerization-based techniques

Photopolymerization techniques basically are AM techniques through which a photopolymer (photocurable resins) is selectively cured by a light source. By nature, materials processable by these processes are polymeric; nevertheless the properties of these resins can be expanded by filling them with specific fillers [71, 72]. While the range of commercial resins for photopolymerization is expanding (in term of properties), there are currently very few commercial SMs in a form suitable for these processes. Despite this, 4DP is also being given research interest from a photopolymerization processes point of view. In most of the case – as with extrusion based techniques – works achieved in that regard consist in synthesizing a SM resin and using it with a commercial or proprietary printer.

2.2.1.1 SLA based 4D printing

In [27] shape memory thermosets were developed; influence of the chemical content on the mechanical properties was gaged. Shape recovery ratio of more than 93% and shape fixity ratio[11] higher than 98% were reported. The developed resins were used in a commercial SLA printer to print complex shape memory structures. Noteworthy in their approach is that as the whole geometry of a part is made of SMP, many different transformation pathways are therefore possible as shown in Figure 2-8. The SME was triggered with hot air flow, but also with electricity as, one of their examples was coated with a carbon nanotubes (CNT) layer acting as electrical heater. Compared to many other 4DP approaches, this study shows a 3D↔3D shape change (not limited to bending motion) which has been leveraged to many complex shape objects. However the viability to print the whole structure with the SM is questionable in terms of material use and cost efficiency. Using a commercial SMP photocurable epoxy resin on a commercial SLA machine, Lantada et al. [73] printed micro actuators. The originality of their approach lies in how heat has been provided to trigger the shape recovery. Heat was provided internally: micro channels were designed into the parts' geometries, and hot water was injected in these. Worth mentioning is that SLA proved efficient at accurately building the channels with diameter as small as 0.6mm.

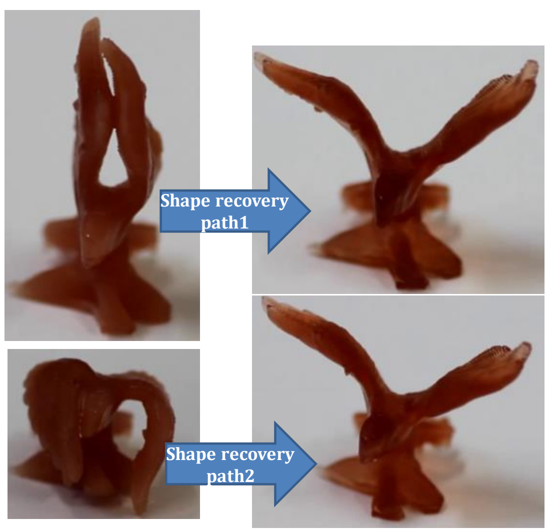


Figure 2-8 Different paths of shape memory recovery for the same SMP part (adapted from [27])

[11] Shape recovery ratio is measure (based on strain) accounting for how the recovered shape does match with the initial (not deformed) shape. Shape fixity ratio is a similar measure which quantifies how the sample keep its deformed shape once the deforming stress is removed and the temperature is decreased below Tg.

Functional performance of a SMP parts can be assessed by a number of characteristics including shape fixity and recovery properties, the thermomechanical degradation in terms of shape memory cycle life. These properties determine the suitability of a SMP for industrial applications where robustness of the shape memory performance over multiple cycles is paramount. Noticing that these properties, especially functional fatigue[12], were not investigated in SLA-based SMP, Choong et al. [74] conducted parametric experimental studies to develop an efficient SLA processable SMP resin. The SMP exhibited shape memory performance with 100% full recovery and stable shape memory properties over 14 thermomechanical cycles. The shape memory effect showed degradation by the 22th cycles which could be considered as a long lifecycle for SMP. In a similar study [75] shape memory properties (recovery rate, shape fixity and shape recovery ratios, durability) and mechanical properties (strength, toughness and glass-to-rubbery modulus) rate were investigated for a SLA printed proprietary SMP photocurable resin.

Piezoelectric materials are well known materials which have good smart properties for actuators and sensors applications. They are commercially available in limited shapes, and shaping them to a desired shape with conventional method is quite cumbersome (especially because they are brittle). With the ability to readily shape these materials in virtually any complex shape, a new route for exploring and expanding their performance can be achieved .This is what was done in [76], where the goal was to demonstrate a low-cost and accurate route for AM of piezoelectric material. They prepared a suspension with a piezoelectric powder with a suitable photocurable resin. The so prepared suspension was used on a proprietary microstereolithography (µSL) machine to print parts. Parts were finally sintered, acquiring thus a density close to those found in conventionally obtained ceramic. The piezoelectricity of the printed parts was investigated. Particularly values for the d_{33}[13] coefficient were close to those of the same ceramic conventionally formed. Nevertheless it was found that the anisotropy introduced by the layer-wise manufacturing does propagate into the piezoelectricity properties.

2.2.1.2 *Projection microstereolitography (PµSL) and direct light projection based 4D printing*

One the features that make SMP a hot research topic in 4DP is their tunability: by properly mixing some base chemical constituents one can achieve a wide range of both mechanical and shape memory properties. This is well illustrated in [48] where a family of photocurable methacrylate based polymers were printed using a proprietary PµSL printer. Mechanical properties such as failure strain were reported to be 300% higher than values found in existing printable SMP. Noteworthy in their study is that their printer allows multimaterial printing thanks to an automated material exchange system. Finite Element simulations were run and shown results in good agreement with the experiments both for single and multimaterial parts.

[12] Basically, it refers to the degradation of the SME over the cycles.

[13] The highest coefficient linking the strain and the applied electrical field.

Among the endeavors pursued by 4DP is the one to mimic nature. This was literally realized in the work by Invernizzi et al. [77]. They developed a photocurable SMP resin which has been used in a proprietary DLP machine. The particularity of their 4D printed parts is that, in addition to exhibit the heat triggered shape memory effect, the parts are also capable of self-healing: cracks in these parts self-heal upon exposure to heat, a behavior common in natural tissues.

In contrast to most of the photopolymerisation-based 4DP studies, Han et al. [78] have used as SM a heat responsive hydrogel. The developed photocurable hydrogel was processed with projection microstereolitography (PμSL). The effects of printing parameters (such as layer thickness, light intensity) and the chemical composition on the LCST[14] and swelling/shrinking ratio were evaluated. These investigations yielded insights into how to print parts embodying variable shrinking properties (which can be seen as multimaterial parts). Particularly these insights showed how to achieve sequential deformation as shown in Figure 2-9.

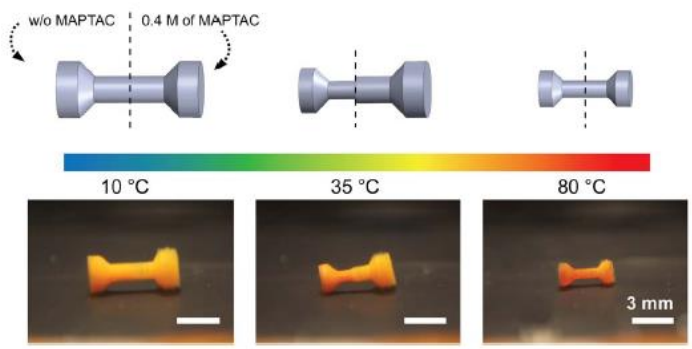


Figure 2-9 - Sequential shape changing in a multimaterial hydrogel - PμSL printed part. The two halves of the part were made with various compositions hydrogel (extracted from [78])

2.2.2 Extrusion-based processes

For now 4DP seems to be confined to research environment; it has not (yet) made its way into the maker movement. This may be related to the fact that AM machines commonly used by hobbyists mainly include fused deposition modeling (FDM) machines for which there are almost no SMs commercially available. Nevertheless, there have been a few commercial initiatives[15] and research effort aimed at filling this gap or, equivalently, at introducing 4DP into FabLabs.

[14]Lower critical solution temperature, it is the lower threshold by which such hydrogels start swelling/shrinking.

[15]In 2015, a US company working in the field of SMP turned one of its SMP resins into filament form for 3D printing, the aim was to launch a fundraising campaign to better develop this filament and market it (for domestic applications). 79. Scott, C. *New Essemplex Shape Memory 3D Printing Filament Can Be Reshaped Again and Again*. 2015 [cited 2018 30/07/2018].

2.2.2.1 FDM-based 4D printing

Most of the studies presented here, are in the form of producing proprietary SMP filament and then printing it with commercial FDM machine sometimes with some alterations to the machine. Using SMP in pellets form, Yang, et al. [80] produced their own SMP filament to be used in (commercial) FDM machine. Their study is mainly concerned with manufacturing process parameters for producing high quality (fully dense and bubbles free) SMP filaments. A commercial FDM machine was used – after some alterations – to print with the so produced filament; different printing parameters (e.g. extrusion temperature, printing speed) were evaluated in regards to the printed part quality. While this study was mainly focused on manufacturing process, a few simple functional parts were also printed to demonstrate the complex shape capability of AM harnessed to shape memory effect. Namely a gripper has been printed. In the same vein, Chen et al. [81] crafted a SMP filament that can be used in commercial 3D printers. Though, the aim of their study was to develop SMP that can exhibit a kind of multi shape memory effect. Basically, a sample of such SMP is sequentially trained at different regions under different temperature; these regions then recover their original shapes at their corresponding programming temperature. The so developed SMP filament consists in a blend of three base chemical components. A few parts were printed to demonstrate the feasibility of using the developed filament in a commercial FDM machine. Noting that most of 4DP studies using SMP are done with the PolyJet® technology and acknowledging the highly expensive initial investment required (along with other technical drawbacks compared to FDM), Ly and Kim [82] have found in FDM a more accessible alternative to SMP printing. Noteworthy in their study is that in addition to produce conventional SMP filament, they also produced a SMP/CNT composite filament. The conducted investigations were about the printed SMP recovery time *versus* the triggering temperature and the triggering voltage. This latter stimulus influence was investigated in the SMP/CNT composites: electricity was used to trigger the shape recovery as the samples act as resistor, thus generating heat by Joule effect. It was found that increasing the triggering temperature increases the recovery speed. Similar to this latter study and as a demonstration of an alternative to heat-based SMP triggering is the study led by Garces and Aryanci [83] which developed a SMP composite with graphene as filler. Using a dual extrusion FDM machine, a proprietary SMP filament (made from pellets) and a commercially available PLA-graphene conductive filament, they printed SMP composites. The matrix was made of SMP and the fibers which extend from side to side were made of the conductive PLA-graphene. Such SMP composites can therefore be activated by electricity with to Joule heating. A quite different approach was taken in [84]: SMP was used in the form of thermoplastic polyurethane pellets and was directly fed into a proprietary extrusion based 3D printer. A number of geometry parameters and manufacturing parameters were investigated to gage their influences on recovery time and recovery force.

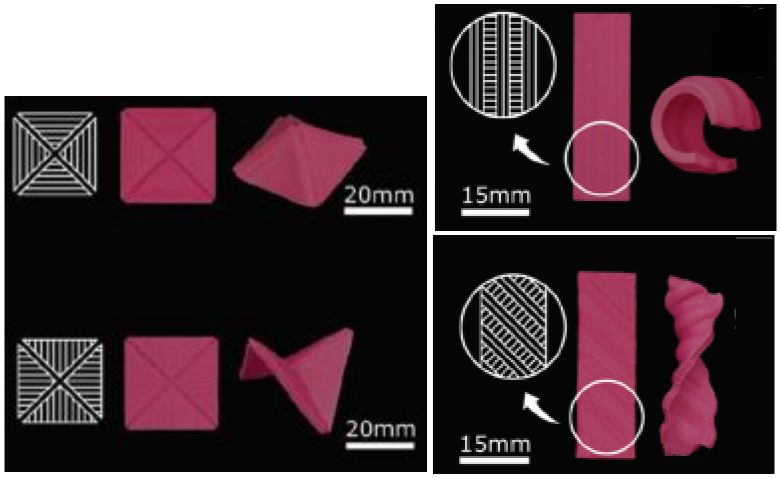


Figure 2-10 - Complex self shape-shifting with 3D printed PLA (adapted from [85])

Shape memory effect in SMP conventionally involves a thermomechanical training that occurs after the part has been manufactured. A novel route for SMP 4D printing and that is inherent to the FDM technique is what could be called *during deposition thermomechanical training* or *embedded thermomechanical training*: basically the thermomechanical training is done while the part is being printed. Printing parameters such as deposition speed, deposition temperature, deposition paths (which may differ from one layer to the next one), all contribute to induce a prestrain in the part. It is this prestrain combined with the heat provided that act as the training step. Heating the part after it has cooled down releases the prestrain leading to a deformation, thus a kind of SME. This route for FDM based 4DP has been demonstrated with polymers which are not conventionally used for SME and even which are not seen as SM, as shown with PLA [85]. In this study run with hobbyists FDM machine and off-the-shelf PLA material, layer printing orientation and layer thickness were taken as design parameters to understand self-folding and self-twisting. Based on these insights, more complex shape-shifting behaviors were designed. These include 2D (flat) surfaces to 3D complex shapes as shown in Figure 2-10. A quite stunning approach in that vein is the one demonstrated in [86], in which PLA is printed onto a sheet of paper. In addition to the above described SME effect initiated during the printing, the difference in coefficient of thermal expansion between PLA and the paper also contributes to the shape shifting behavior. Noteworthy is the fact that the so printed self-foldable composites have a reversible behavior. The (embedded thermomechanical training) route has also been used with SMP. This latter case can be seen in the study led in [87]. The printed parts are capable of 1D-to-2D (strand) bending and 2D-to-3D flat surface bending. In addition to the experimental study they derived constitutive model for the SMP and non-linear FE governing equations for the printed objects. The implementation of their FE model proved accurate at estimating the prestrain induced during the printing and at simulating the 1D-to-2D and 2D-to-3D bending. Quite a similar study from the same group is the one led by [88] in which insights gained from the FEM modeling was used to design other structures. Worth mentioning in the same vein is the work done by Bodaghi et al. [89] in which the as-printed shape is considered as a first temporary shape, which is then plastically deformed into another (second temporary) shape. The shape recovery path then exhibits two different temporary shapes, thus a triple shape memory effect as shown (with a different AM technique) in [90].

Most of current 4DP studies seem to be dedicated at considering shape changing materials, while the range of SMs is beyond these. In contrast to that main stream, Peterson et al. [91] explored the interaction of AM with a color changing SM: mechanochromic material. This material changes color once it is stressed. Depending on the stress value the color change may be reversible.

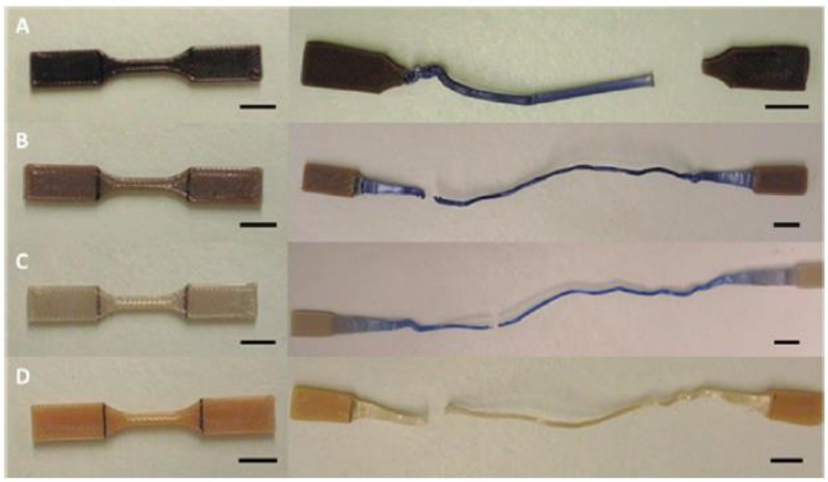


Figure 2-11 - 3D printed tensile test specimens with mechanochromic material; scale bars are of 1mm. (extracted from [91])

2.2.2.2 *Bioprinting or Liquid Deposition Modeling*[16]

Bioprinting is an extrusion-based technique which basically involves the deposition from a syringe of a material in resin form and the subsequent curing. The curing occurs right after the material has been deposited. Another family of smart materials that is of interest in the 4DP domain is hydrogels [63]. These materials work in liquid environments and owe their smartness to their ability to swell or shrink in response to environmental stimuli such as heat, change in pH or even electric field. Using a Bioplotter (an extrusion process based 3D printer that processes biomaterials) and a heat responsive hydrogel as 'ink', Bakarich et al. [23] were able to design and print a smart valve to control water flow as shown in Figure 2-12. Parts of the valve were printed in the hydrogel, and others were rigid. With water at 20°C the hydrogel parts were swollen and water could flow through the valve. Water at 60°C leads the hydrogel sections to

[16] This terminology is not an official one but was introduced by the author to avoid the medical connotation associated with biopritting.

contract and block the water, reducing the flow rate up to 99%. Reversibility was demonstrated with cooler water flowing through the valve normally and again hot water being blocked.

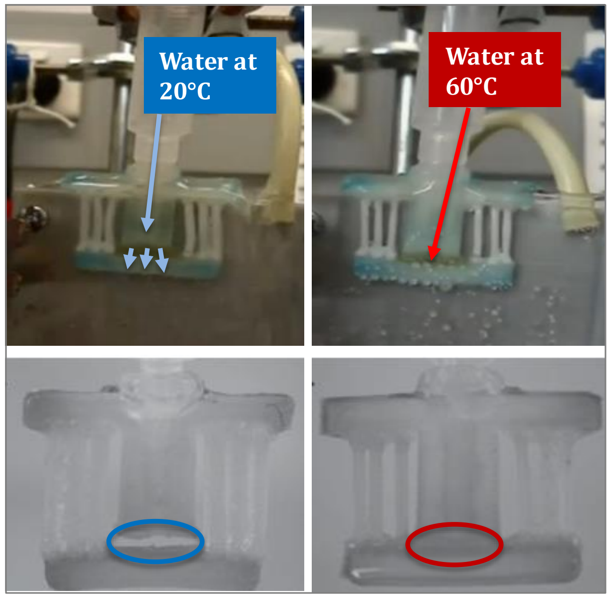


Figure 2-12 - 3D printed hydrogel smart valve (adapted from [23])

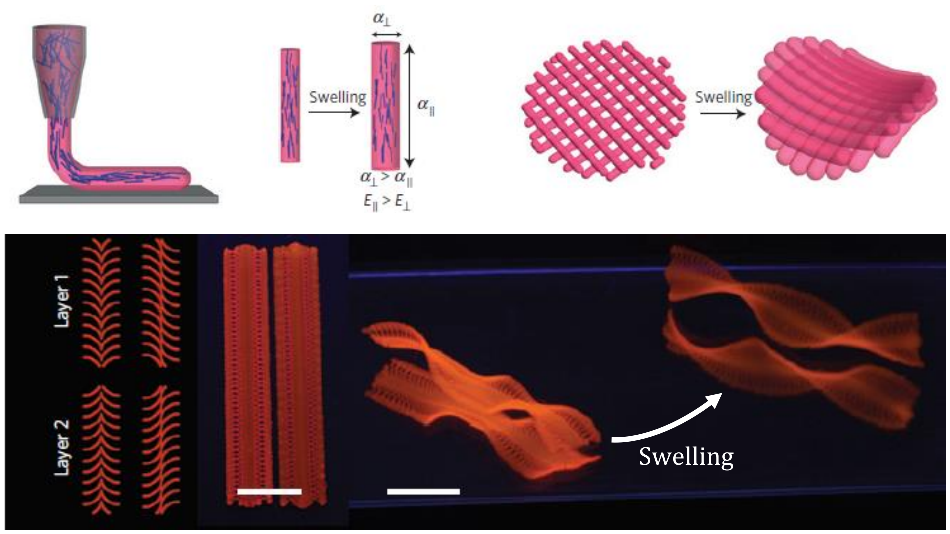


Figure 2-13 - Bioprinting with hydogel composites. [92]

Hydrogels owe their smartness to their ability to shrink or swell in response to a stimulus. This smartness can be expanded by making the swelling/shrinking behavior anisotropic. This is the route followed in [92]. Hydrogel composites were made by mixing the hydrogel with some fibers (see Figure 2-13). A proprietary LDM machine is used to deposit the so obtained composite. During the deposition, fibers are aligned in a layer along the deposition direction.

This leads to an anisotropic behavior: strain along the deposition direction is lower than strain in the transverse direction. There is therefore a difference is swelling behavior between two layers deposited (one on the other) at different direction. Bilayers encoded with anisotropic swelling can therefore be created to achieve a desired shape change upon immersion in water. They developed a predictive model capable of tackling both the forward and inverse design problem.

2.2.3 Powder bed fusion based and binder jetting based 4D printing

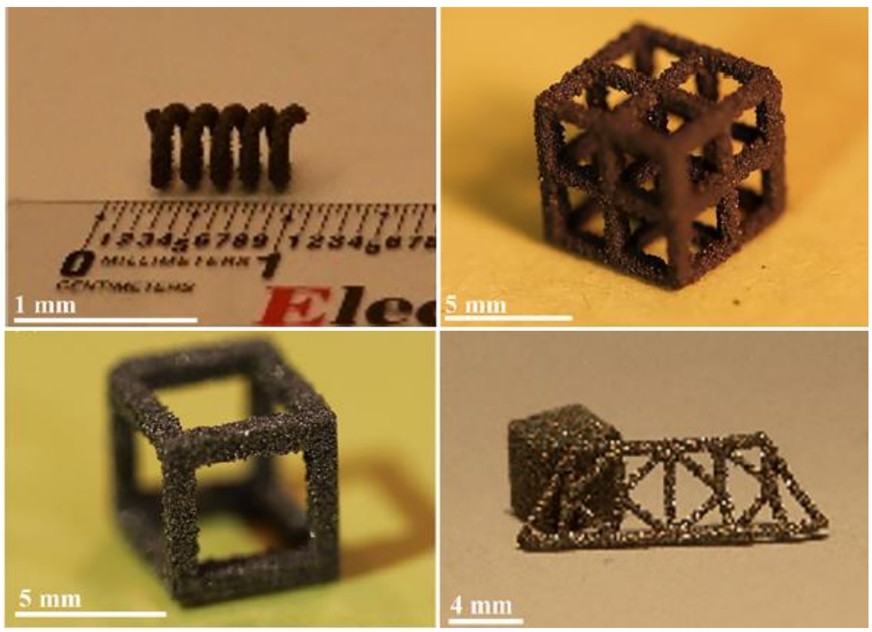


Figure 2-14 - 3D printed magnetic shape memory alloy parts (adapted from [93])

4DP has barely been scrutinized with the powder bed fusion (PBF) processes. This may be due to the limited availability of SMs in powder form and/or to the fact that the energy required to melt or to sinter the powder may affect the smart behavior of the material, as it is for SMA. One of the features of what can be called mainstream 4DP, that is polymeric 4DP, is the softness of the materials. In many applications, this may not be an issue; however when the active structures are also load carrying structures this softness can be a drawback. This issue may be solved by some PBF processes. Even though they were not meant to be a 4DP demonstration, noteworthy are the works presented in [34, 35, 94]. The SME effect was not particularly investigated (except in [94]) but the purpose of these studies was to demonstrate SMA powder processing with SLM as an easy alternative to conventional SMA processing, but also as a new venue for complex shape parts made of SMA.

Most of the studies of AM of SMA powder have used as AM technique either selective laser sintering/melting or direct energy (laser) deposition [95]. Prompted by the fact that magnetic-field-induced strains (MFIS) in magnetic SMA can be increased by porosity, and that 3D printing[17] (a binder jetting process) allow more control on this latter, Caputo et al. [93] have taken another route for metallic 4DP. In their study Ni-Mn-Ga alloy, a magnetic SMA, has been processed by binder jetting followed by curing and sintering. The so obtained parts were mechanically strong and exhibited the SME induced by magnetic field. The obtained strains were quite low (around 0.009%) but can still be useful in some applications such as microactuators. Nevertheless, it was a good demonstration of AM of magnetic SMA without a loss of the SME. Examples of the so printed parts are shown in Figure 2-14.

It is worth noting that regarding AM of metallic SMs, the term 4D printing has not been used except in [93], the other studies were mainly concerned into the processing of SMA with SLM/SLS but not into the shape-memory functionality.

2.2.4 Material jetting based 4D printing

Material jetting processes are technically dominated by the Stratasys PolyJet® technique [53]. Owing to its multi-material printing capabilities and its high resolution (in any direction), the PolyJet® technique has been quite prolific in the 4D printing demonstrations. In addition to the allowed geometry complexity, PolyJet® printers allow another degree of design freedom: the so-called *Digital Materials*. These polymer materials are generated as a specific combination of 2 or 3 base (polymer) materials, in a way similar to how data are generated with bits. A large spectrum of material properties, including those of some smart materials, can therefore be obtained, and multi-material parts can readily be printed. Particularly, PolyJet® printers can generate shape memory polymers with continuously varying glass transition temperature, even within a single part. It is this ability of the technique which has been alleviated to 4D printing.

Ge, et al. introduced *printed active composites* (PACs) [21], which are 3D printed composites with SMP fibers in an elastomeric matrix. The intelligence of these composites relies on the design of the lamina and laminate configuration, and the post-printing thermomechanical training process. They designed and printed the PACs in form of thin plate which are programmable to assume various temporary shapes including bent, coiled, and twisted strips and complex shapes of spatially varying curvature; the plate shape is recovered once the composite is heated. The design is depicted in Figure 2-15.a. They showed how PACs can be combined with conventional materials parts to design smart components capable of shape shifting. Using the PACs as hinges, in a subsequent study [22], they designed and fabricated active origamis, that is, flat sheets that can self-fold from the flat sheet configuration to a 3D structure or vice versa once triggered by heat. The printed parts include two origami airplanes, a box and a pyramid. In addition, they printed a box which after being deformed to a flat plate recovers the box configuration once heated. The PAC hinges were fabricated by creating their CAD model including the fiber and

[17] 3D printing here refers to the 3D printing technique as explained in section 2.1.1.5

matrix configuration. A theoretical model has been developed to assist in choosing design parameters (length, fiber dimensions, etc.) and the thermomechanical programming steps to achieve any desired folding angle. Another research group further investigated the thermomechanical behavior of the Polyjet printed PAC construct [96]. In the same vein, Bodaghi et al. [97] developed an unit actuator made of SMP fibers embedded in an elastomeric matrix; their proposed architecture differs from the previous PACs in that two kind of SMP fibers – particularly with different Tg and stiffnesses – are used. The architecture and the material distribution allow for a sequential shape recovery (after programming step consisting of pulling) which is made of a slight expansion followed by shrinking to the permanent shape. After experimental studies to characterize the thermomechanical behavior of the developed unit actuator and finite element method (FEM) modeling, more complex structures (both planar and tubular) made a lattice-based repetition of the unit actuators were designed and printed. In the aforementioned studies, the embedded fibers responsible of the SME were all printed at the same time of the matrix deposition. Ge, et al. [98] demonstrated another way of manufacturing the PACs; the novelty of the presented approach lies in which fibers were embedded and how were they embedded. Channels (at a given orientation) are designed into the matrix and by interrupting the printing at a specific height (and removing sacrificial material), the channels are filled with a SMP melt. After smoothing the latter surface, the printing is resumed, thus encapsulating the fibers. The thermomechanics behavior along with anisotropy of the so-printed composites were investigated.

SMPs are characterized (among others) by their glass transition temperature Tg, that is, the temperature at which the shape recovery effect occurs. A part embodying different SMPs can therefore exhibits a sequential shape shift when subjected to a temperature higher than all the Tg. This has been considered by Yu, et al [28, 99] in 4D printing. SMPs were used as active hinges to perform folding. They designed and printed parts exhibiting sequential shape recovery, using the active hinges. The parts include a helical structure, an inter-locking structure and an interlocking box. The basic idea of their approach is that by printing SMPs with carefully chosen Tg at specific locations of a part, sequential shape recovery (after deformation from the permanent as-printed shape) can be achieved. The helical parts were printed in their helical shape; they were deformed to a line shape at high temperature and cooled. Once heated they successfully revert to their original shape in a sequential manner. The shape recovery scheme was similar for the box. The ability for PolyJet® printers to generate *Digital Materials (DMs)* is at the core of the success of such smart objects. Using similar methods in a separate study [90], they printed parts exhibiting multi-shape memory effects, that is, parts taking different shape at different times.

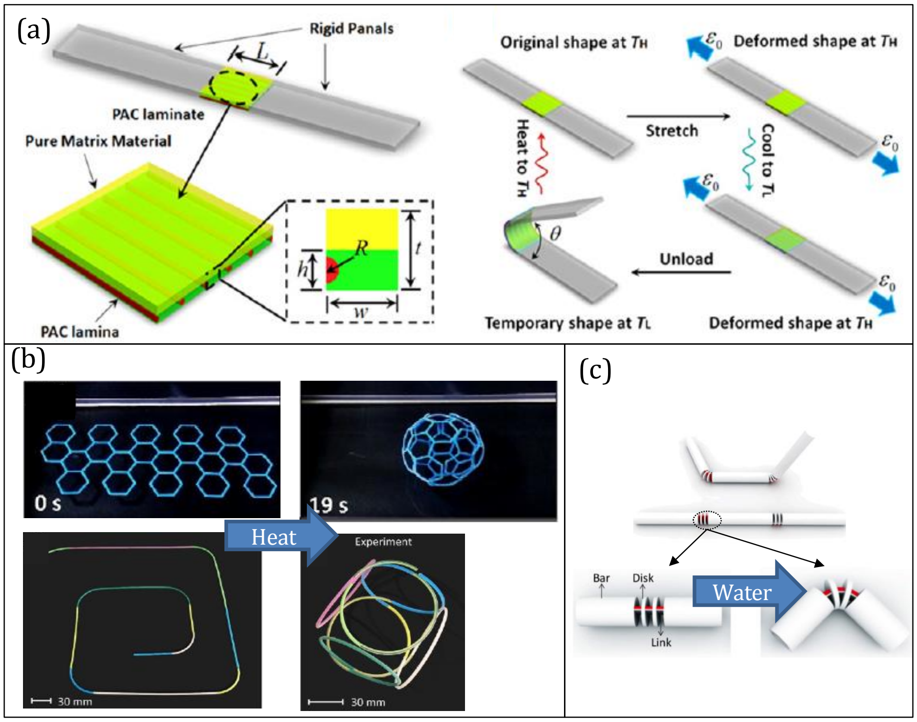


Figure 2-15 - 4D printing with PolyJet® technique. (a) SMP *printed active composite* [22] - (b) *4D rods* made of a glassy polymer printed with an elastomer [100] – (c) Folding primitive printed with a hydrophilic polymer [101]

The SMPs obtained as DMs of PolyJet® are, again, combinations of two base materials: Vero (which is a glassy polymer) and Tango+ (which is an elastomer). Taken alone, these materials do not exhibit a noticeable SME; as such they can be seen as conventional polymers. Nevertheless, in a way similar to how "SMs-free 4D printing" has been done with PLA using FDM machines [85, 86], Ding et al. [100] have also printed self-shape-changing structures using (glassy polymer) Vero® and (elastomer) Tango+®. Their design concept is a rod capable of either bending or twisting once heated. Each cross-section of the rode is made of two separate domains consisting of the glassy polymer and the elastomer. While the elastomer is being deposited and cured, a prestrain is introduced (up to 4%), but after printing, as the glassy domain is way stiffer, the rod remains straight in its plane. The shape shifting upon heating is due to two mechanisms: first the glassy section softens and the prestrain in the elastomer is released, secondly as coefficient of thermal expansion is different in two materials, heat does also introduce eigenstrain. Experimental studies along with *ad hoc* computational modeling for simulating the shape shifting behavior of the rods gave insights into how to design and print more complex shape shifting behaviors as shown in Figure 2-15.b.

One of the drawbacks of common SMPs is that the SME is a one way one: after the permanent shape recovery is triggered by the stimulus, removing this latter does not lead back to the (deformed) temporary shape; to get the temporary shape another thermomechanical training is required. This drawback has been circumvented by Mao et al. [102] in a study where SMP has been associated with hydrogel. Thanks to the multimaterial capability of a PolyJet® printer, a SMP, an elastomeric (inert) polymer and hydrogel were printed in a specific distribution within the same part, in such a way that the SME of the SMP is reversible. Basically, in their design, the swelling force of the hydrogel (due to water absorption) is used to yield the SMP deformed (temporary) shape; this is facilitated at high temperature by a decrease in the other materials' stiffnesses. As swelling and shrinking of the hydrogel are autonomous, the SME cycle can be repeated by simply by applying the right stimuli (heat and moisture).

Water (or more generally moisture) can also be used as a stimulus for smart materials, that is the case for instance for hydrophilic materials whose volume can dramatically expand (up to 200% of original volume) once immerged in water, they can recover their size once fully dried. Shape change mechanisms, including two stretching primitives and one folding primitive (shown in Figure 2-15.c), have been designed and printed by Raviv, et al[101] using a highly hydrophilic polymer. The actuation principles of these mechanisms are due either the expanding capacity of the material or both that capacity and mismatch deformation with another (inert) material. Objects designed and printed with these primitives include: a 1D part in the shape of the connected letters "MIT" self-transforming into the shape "SAL", 2D grids deforming into a sinusoidal wave, a hyperbolic surface, and a saddle like shape. All the transformations occurred as the objects were immerged in water.

2.2.5 Synthesis

4DP is currently being given tremendous research efforts. The reviewed work revealed that most of the contributions are targeted at the shape changers SMs group with a particular focus on SMP as shown in Figure 2-16. Worth mentioning is that with seven families of AM techniques and about 30 SMs (according to the classification given in [18]), there are potentially more than 207 ways of exploring 4DP. Given the reviewed work it can therefore be said that we are definitely still at the beginning of the exploration. Today's work on the topic is mainly concerned with proofs-of-concept in laboratories, so this technology can be placed at level 3 (out of 9) of the TRL (technical readiness level) scale. This level corresponds to a technology in which "analytical or experimental evidence[s] of the main functions and/or characteristics of the concept" are shown.

The current state of 4DP research does not yet show any concrete application of 4D printing. Industrial applications are only considered in a vague way (*structures involving complex deformation permutation*, *spontaneous configuration changing applications*, *self-assembling structures*, etc.). This finding cannot really be seen as research gap, but to increase the acceptability of this new technology, a reflection must be conducted to specify the industrial products that can benefit from 4D printing.

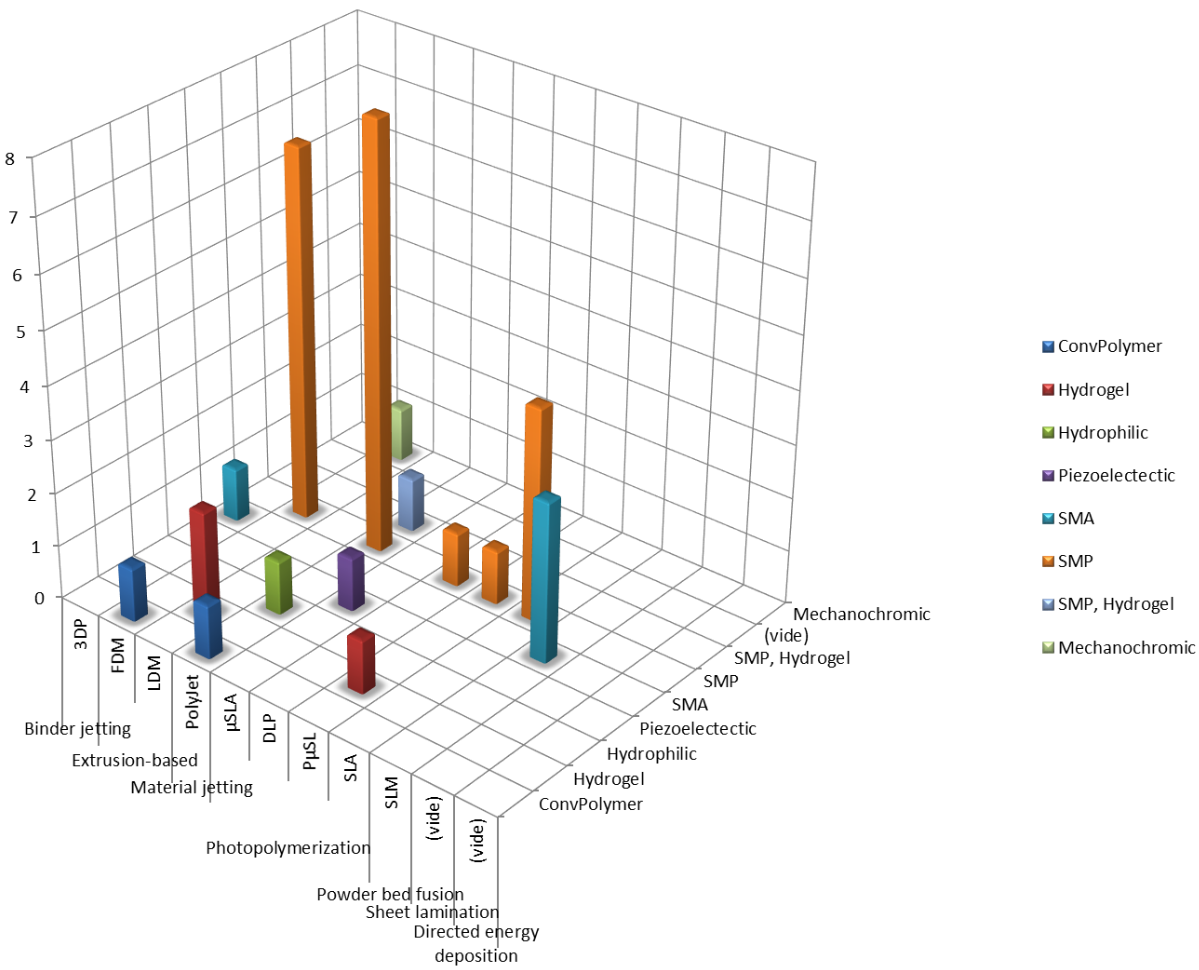


Figure 2-16 - Additive manufacturing and smart materials interaction

While it cannot be claimed that the conducted review on 4DP studies is exhaustive, it does at least provide a broad view of what is now manufacturable with the new material-manufacturing process interaction being realized by 4DP. The interaction is still in its infancy. We conducted a breakdown of the reviewed work according to what was the main concern of these works. Two main concerns can clearly be identified:

- Manufacturing: the main concerns of the presented research is about providing physical proof-of-concept for 4DP. The focuses of these studies include: chemistry, demonstration of a new way of processing a SM, material characterization.
- Manufacturing and design: in addition to physically demonstrate the concept, these studies also propose some mathematical/computational modeling supported by their experiments. The goal being to support the design of parts made of the investigated SMs and printed with the used AM technique.

As shown in Figure 2-17, 4DP is currently mainly scrutinized from a manufacturing point of view, which is needed for the technology to be established. However, scrutinizing it from a design methodology perspective is also part of the journey towards its establishment, that is, its industrial adoption. The following section is dedicated at reviewing the literature in this regard.

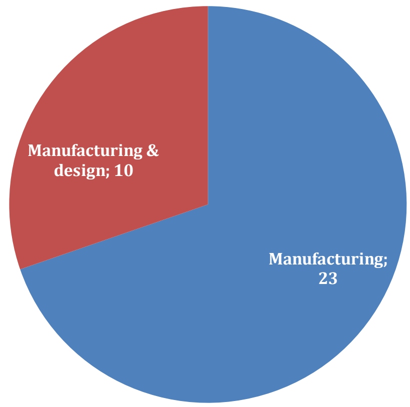


Figure 2-17 - Breakdown of the reviewed 4D printing papers according to main concerns

2.3 Design with smart materials

Conventionally, over the course of the process of designing a product, material's concerns arise at a time when a detailed geometry is already defined. Given that geometry and the loads, materials are selected to ensure the integrity of the product during its operation. SMs play a more important role because they are functional: for example, a mechanism that is conventionally made of an assembly of several parts can be realized with a single component made totally or partly of a SM. Burman, et al. [103] use the term *functional materials* instead of the usual *smart materials*. When SMs is to be considered, material concerns must be shifted earlier in the design process, particularly these should occur in the concept generation phase. To realize a mechanism, the designer can propose several concepts based on established technological solutions (hydraulic, pneumatic, electromechanical, etc.) and others based on SMs. A step of evaluation and selection of the concepts then follows. However, the value of a SMs-based concept cannot be measured without the properties, shape and dimensions of the considered material. This shows that in order to gage a SMs-concept, the designer must have a good understanding of the factors governing the smartness of the material.

Most of the research on SMs is targeted at their syntheses, their characterizations (notably the derivation of constitutive relationships), the development of SMs systems[18], and their shaping

[18] These are arrangements combining conventional and smart materials and which exhibit a smart behavior (that is, they are sensitive and reactive to a stimulus). An example is electro-active polymers.

processes. Considering the remarks made in the previous paragraph, efforts must be made to facilitate designing with SMs. Few research efforts have been made in this direction.

The most scientifically and industrially (they are easily found in the trade and are the basis of several applications) established SMs are the shape memory alloys (SMAs). In order to determine the state of the art on designing with SMs, we, therefore, elected to focus specifically on SMAs. A relatively recent review article [104] on the state of the art of SMA cited 565 references, but only five of them are cited as dealing directly or indirectly with design (from a purely engineering point of view). As a matter of fact as early as in 1997, Abrahamsson and Møster [105] explicitly considered SMAs from a strictly design perspective. Based on an international survey (16 countries) conducted in two stages, they established a set of requirements to facilitate the use of SMAs by designers. Figure 2-18 shows a table extracted from their paper and which presents these requirements. SME was neither explicitly nor implicitly mentioned in their text, which supports the choice made to generalize the conclusions resulting from their study to all the SMs. The groups that are directly relevant to design are those of the requirements on design tools and on the information about SMs. Some work has been undertaken in these regards and it can be divided into two types: selection tools and design aids (which provide technical and functional knowledge).

I – Information:	(I_1)	Extensive and reliable material property data provided by the manufacturer – especially on transformation temperatures, applicable force, hysteresis, and fatigue life.
	(I_2)	Literature offering more detailed descriptions of product development projects utilizing SMAs.
	(I_3)	Networks involving designers and metallurgists for discussions and advice.
M – Material:	(M_1)	A wide range of commonly available materials providing different ranges of transformation temperatures.
	(M_2)	More stable material properties – especially those concerning the functional behavior, such as fatigue, hysteresis, transformation, ageing and deterioration temperatures.
	(M_3)	Materials offering low hysteresis, high working temperatures and high energy efficiency.
P – Performance:	(P_1)	Better understanding of the phenomenological (macroscopic) behavior and properties – structural as well as functional.
	(P_2)	Constitutive equations describing the material behavior, such as relations between stress, strength, temperature, hysteresis, fatigue etc.
D – Design tools:	(D_1)	Design tools describing the functional behavior, such as computerized constitutive material models, product geometry models and material property databases.
	(D_2)	Design guidelines, such as guidelines regarding overheating protection, fatigue protection, control of operating temperature, joule heating and cooling.
	(D_3)	Design procedure models more properly benefiting utilization of SMAs.
O – Operation:	(O_1)	Adaptive systems measuring the changes of material properties or product behavior and adapting the operational conditions to the properties and / or behavior changed.
S – Standardization:	(S_1)	Standardized materials.
	(S_2)	Standardized methods for testing phenomenological properties.
	(S_3)	Standardized methods for joining, soldering and welding.

Figure 2-18 - Requirements to promote SMA adoption (extracted from [105])

2.3.1 Selection tools

An extension of CES software provides information about actuators, with some specific information about SMA actuators. TechOptimizer ™ provides a set of tools (to help designers generate concepts) including a library of SM effects. These effects are presented in the form of description text, figures, some important formulas, examples. The advantages and limitations of each effect are described. However, it seems that this tool is no longer marketed. On a principle similar to that of Ashby's graphs, [106] proposed a list of SMA performance indicators and selection graphs based on these indicators.

2.3.2 Design aid tools

In response to the problem of overly specialized information, a team of German researchers has developed the K&M-base$_{SMA}$[19] tool [107] (see Figure 2-19). It is a design support tool with SMAs for designers with little or no knowledge of SMAs, and it includes a knowledge base and methods on these materials. The knowledge available in the tool comes from a literature and patent analysis. The tool is supposed to help the designer throughout the entire product development process (see Figure 10.a). A graphical interface provides knowledge on:

- SMAs' effects, which are presented as basic information and described from a purely technical point of view;
- Solution principles encountered in existing products. They correspond to general possibilities on how to realize actuators, dampers, release mechanisms, etc;
- The properties of materials and detailed information are provided to allow selection and sizing of components. Application examples, links to suppliers;
- Design rules;
- Other quantitative and qualitative information such as the influence of thermal cycling on the material, test results interpretation on specific samples, manufacturing processes.

This tool does not allow interactivity, the formulas for sizing are just provided.

[19] Knowledge and Method Base for SMAs

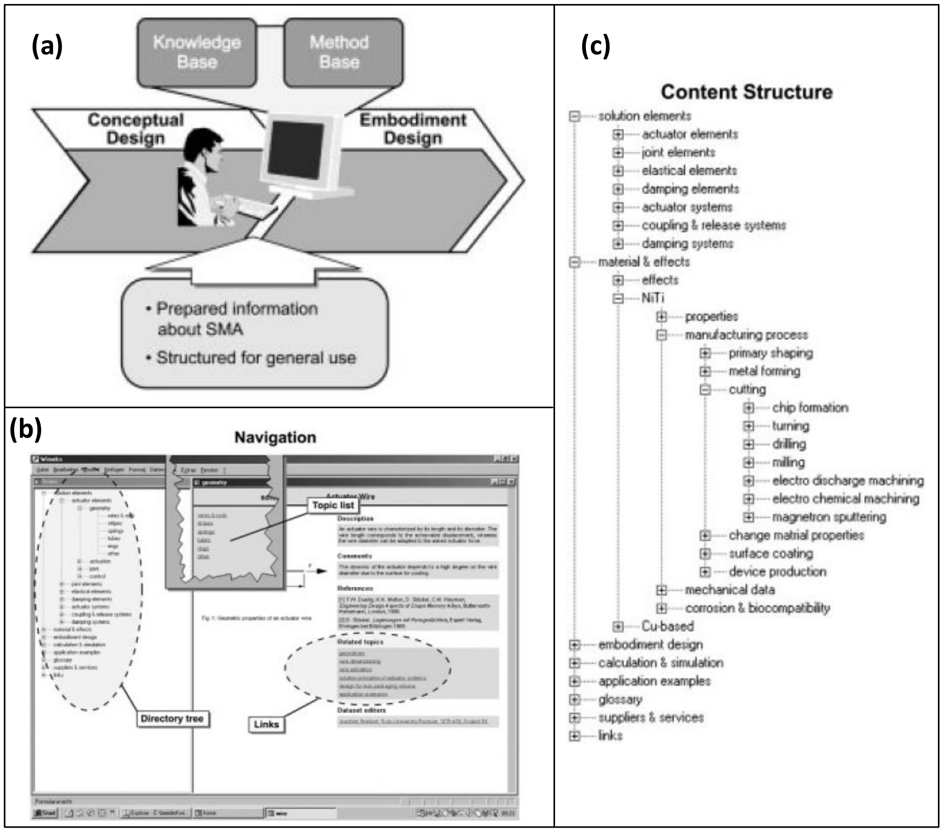


Figure 2-19 - K&M baseSMA tool - (a) design phases supported by the tool. (b-c) Information provided by the tool [107]

Park [108] has developed a database of several SMs, including SMA, piezoelectric materials (ceramics and polymers), thermoelectric materials, and electro- and magnetorheological fluids. In addition to information on the properties of materials, the base also incorporates actuators and sensors made from these materials (and commercially available), and analytical models for their dimensioning. A computer tool [109, 110] has been developed to make this database (see Figure 2-20) easily usable. The tool makes it possible to select materials, but also to size some components made of them. Particularly, it allows to know the possible performance of a type of actuator/sensor for a (geometric) configuration and excitation chosen by the user. For the designer familiar with these actuators/sensors, the tool will be very useful because it is already in detailed design where a technical solution has already been selected and where the goal is just to determine what dimensions, materials to choose, what response can be expected for a given excitation or for a desired response, what stimulus must be provided. The tool does not allow to make innovative design.

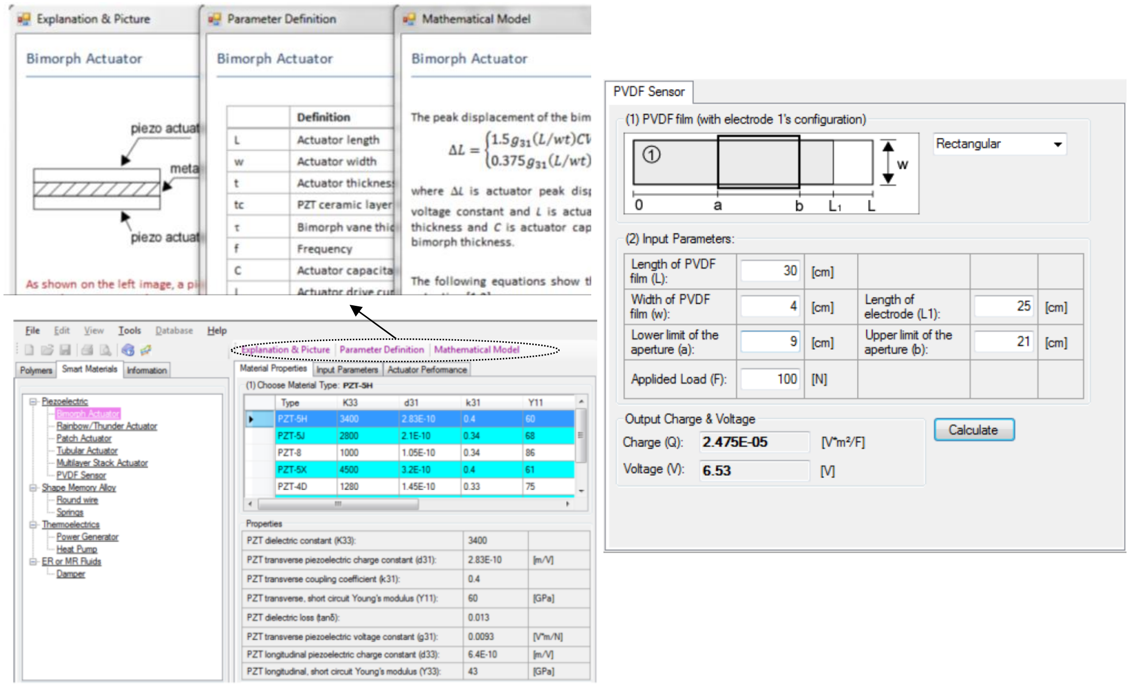


Figure 2-20 - Selection and sizing tool by Park [108]

It is important to note that the intelligence of mechanically active SMs (i.e. those with some deformation or constraint in their response) is not really useful by itself. The ingenuity of a component made of SMs comes from the way the SMs is assigned within the component and the way it (possibly) interacts with other SMs and conventional materials. Figure 4-1 (page 90) where hydrogel (whose smartness lies, inter alia, in its ability to contract in an aqueous medium under the effect of heat) interacts with an inert polymer, illustrates this vision. This view is also supported by the concept of a composite proposed by Kuksenok and Balazs [111] and for which the matrix is a heat sensitive gel and the fiber a light sensitive material. When the material of the fiber is uniformly distributed in the gel, heat and light all have the effect of uniformly contracting (no bending) the gel, but when the fibers are used and the composite is not fixed on a surface (Figure 5-2.c at page 110), it contracts like an accordion under the effect of heat and flexes when illuminated.

One can therefore think that the challenge to be taken up in designing with the SMs is the capacity to distribute them to realize a desired deformation considering their activity. In other words, we are looking for the answers to the questions: how to use the contraction of a hydrogel? The swelling of a hydrophilic polymer? The shrinking of an electrostrictive? The shape recovery of a SMA or a SMP? Etc. This does not mean that the standard knowledge base tools and data on SMs are useless, but the designers would benefit if these tools could also "educate" the material and simulate the behavior.

The ingenuity of the actuators is in the way the SMs are arranged, the attention of the designer must be focused on this fact, not so much on the intrinsic properties of the material. This fact is even more true with AM which makes it possible to deposit material "anywhere".

2.4 Design for additive manufacturing

Because AM eliminates many manufacturing constraints related to conventional (subtractive) manufacturing processes, designing objects to be manufactured by this new family of processes requires a paradigm shift. The freedoms that the AM offers can be listed as follows [10]:

1. Complexity of shape: almost any shape can be made,
2. Hierarchical complexity: a variation of the complexity at different scales (macro, meso, micro) within the same part can be realized,
3. Functional complexity: functional assemblies of parts can be manufactured,
4. Complexity of the material: the possibility of depositing material point by point or layer by layer gives a freedom on the disposition of the material and the possibility of manufacturing multi-material parts.

However, AM also has constraints, which when not considered can lead to design a part whose manufacture is of poor quality or even unfeasible. These constraints include, among others, the minimum / maximum achievable dimensions, the anisotropy, the presence of support materials (which can impact the surface quality).

Designing effectively for AM should therefore meet two types of objectives: taking into account the constraints of the process (to maximize the manufacturability of the part) and capturing the opportunities offered by the process (to maximize the performance of the part). Many studies have already been undertaken in this direction, to allow designers to follow this paradigm shift. This work can be classified into three main groups:

- Design rules specific to the various processes [112-114]. These are compilations of recommendations mainly on geometry and materials, similar to handbooks on design for manufacture and assembly.
- Top-down design approaches [115-118]. These approaches are global design methods which, based on the product specifications and the capabilities of the process under consideration, allow the geometry of the product to emerge.
- Re-design approaches [119, 120]. In this case, the goal is to redesign a product (typically made of several assembled components) by integrating the functions and merging some of the component (part consolidation)

It has already be shown that SMs play a functional role. The material considerations of these different approaches are purely structural because they are based on conventional materials.

This does not necessarily mean that they are all useless for 4D printing, but it may be necessary to extend them to account for SMs as well, especially the top-down design approaches.

In the proofs of concept provided on 4D printing, apart from the freedom that additive manufacturing offers on the positioning of materials, we see in the simplicity of the geometries that the question of additive manufacturing-oriented design is not addressed. The design of the active parts (based on SMs) could be made more optimally by taking advantage of the capabilities of the AM to, for instance maximize deformation or for a given deformation minimize the volume of material required. It is noted that the bimetal effect, to achieve bending, is used in several studies but in the configurations used there is no difference compared to the way in which the bimetal effect is conventionally achieved (combination of two homogeneous layers of different materials). The studies [121, 122] – performed in a context unrelated to 4D printing – consider the bimetal design with an approach based on topological optimization.

2.5 Research question and proposal

The literature review conducted in this chapter has revealed the multidisciplinary aspect of 4D printing. It has been explained why designing for 4D printing requires:

1. mastery of what smart materials are capable of, and especially how to arrange them for useful functionality,
2. Consideration of the advantages and constraints specific to AM processes to design optimized geometry (at the level allowed by AM).

Besides, in the reviewed literature on 4DP, none of the contributions that could be deemed as design-oriented tackles the problem from a global perspective.

The research question of this thesis can therefore be stated as:

Given a product's specifications involving the need for the structure to change state geometrically (in order to possibly change functionality) when subjected to a stimulus, how to determine a suitable geometry that is sensitive and responsive, and that takes advantage of the freedoms allowed by the AM while abiding by its constraints?

Our goal to solve this question is to create a methodological framework that allows designers to design efficiently for 4D printing. The goal is not to design automatically but to create methods, models and tools to accompany the designer so that he knows what to do, when and how. To reach this goal, this PhD project aims at:

- Putting forth a design methodology aimed at helping designers embracing the design freedom allowed by AM, and at making aware of the limitations of AM;
- Making designers aware of what SMs are truly capable of.

- Creating a design and simulation environment for actuators based on SMs. This environment, in addition to integrating data on SMs (allowing in particular the simulation of their behaviors), would integrate a method to determine a distribution of SMs whose activation would allow a desired change.

Chapter 3 Designing for additive manufacturing

3.1 Introduction

Most of the work achieved in 4DP seems to be mainly focused on the "4D" aspect, which is the change occurring post-manufacturing in the printed item. This still holds even when a methodological approach is taken to design the items: what is mainly sought is the part's changeability. However this vision of 4DP has been hindering the fact that a 4D printed item is inherently an additively manufactured one, and as such freedoms allowed by AM must be seized and constraints peculiar to it ought to be taken into account. The rather spartan shapes encountered in (most of) the printed items in the 4DP works reviewed in the literature review chapter, is a clear indication that at least the shape complexity allowed by AM was not leveraged (to improve the 4DP aspect performance for instance).

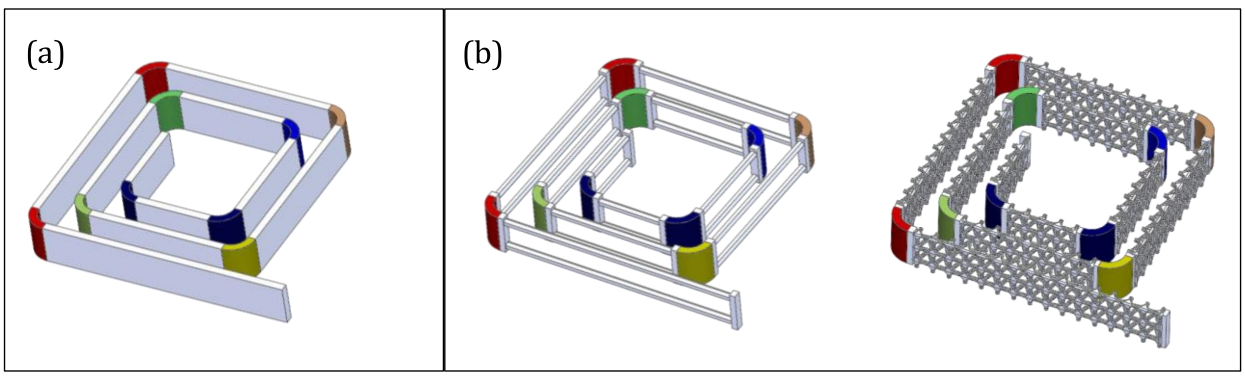


Figure 3-1 - (a) Typical 4D printing design. (b) 4D printing designs with a DFAM strategy

The separation of a 4D printed part into an active structure (made of SMs) and an inert structure exacerbates this lack of pure AM vision in the context of 4DP. This can be illustrated with the helical part presented in [28, 99]. This part is made of an inert polymer material and many other shape memory polymers (SMP) (which differ by their glass transition temperature, a specific temperature at which shape recovery is triggered). In this part, depicted in Figure 3-1.a, there are (inert) rigid sections which basically hold the whole part and (active) SMP sections responsible for the whole part shape change. The material distribution is such that the part behavior is sequential: at a temperature higher than all the Tg, the hinges' shape recoveries (from their deformed straight shapes to the permanent bent shapes) occur sequentially, ensuring thus a successful shape recovery of the whole part. As shown in Figure 3-1.b, with a better DFAM vision the inert sections could have been designed otherwise without decreasing the shape changing performance of the part, but with less material and a higher shape recovery ratio and speed.

Nevertheless, these lacks cannot truly be considered as lacks in the reported works, as the authors weren't investigating how to efficiently design their parts for them to fully benefit from AM capabilities while not violating its constraints. They were instead investigating manufacturing and/or (both smart and conventional) materials issues, which we acknowledge to be fully part of the 4DP way out to the industry.

Furthermore 4DP as is it, is focused on parts. However looking at everything around us, it can readily be realized that parts rarely work on their own, they are usually part of a whole assembly.

Based on these highlighted gaps in the knowledge regarding 4DP from a design perspective, this chapter aims at putting forth a design methodology for additive manufacturing. The contribution which has been made in the DFAM field took a global, or product/assembly, point of view and was regardless of whether the designer using it, is solving a design problem considering 4DP or not. As such the contribution may benefit purely DFAM (that is, AM with conventional materials) and Design for 4D printing (DF4DP), especially when an active and an inert structure make the whole product.

3.2 Premises

3.2.1 Additive manufacturing design related characteristics

The ultimate goal of DFAM is about harnessing the unique capabilities offered by AM to maximize products' performance while taking into account the constraints related to these processes to ensure a seamless manufacturing. This subsection is about clarifying these capabilities and constraints, and also it is aimed at providing a comparison between processes' families regarding these characteristics. In addition, this clarification is also intended to specify the levels of a product (e.g. part level) which are likely to be impacted by these characteristics. It will then provide insights into how and when to guide designers, or raise their awareness about specific aspects of AM.

3.2.1.1 Assembly related additive manufacturing characteristics

AM is usually described as having the unique capabilities of shape complexity, hierarchical complexity, material complexity, and functional complexity [10]. All these capabilities are mostly considered at part level, except for the functional complexity one which may be considered at product level. More specifically, at this level, the unique capabilities of AM can be enumerated as:

- **Multimaterial manufacturing [123, 124]:** the capability to directly manufacture multiple material component either discretely or continuously throughout a part volume (which yields a new route for functionally graded materials). Processes fully capable – that is, without any hardware alteration – of this property include DMD [52], LENS[51] for the metals, and FDM [125], 3DP, and PolyJet for the polymeric materials.
- **Kinematic joint printing [126]:** the capability to manufacture directly assemblies with moving parts. This has been referred to as non-assembly fabrication, in situ fabrication, or assembly free fabrication. The printing of historical Reuleaux kinematic models [127] is a great illustration of this AM capability. Table 3-1 shows some kinematic pairs and specific joints which have been additively manufactured. Critical to this capability to be conveniently taken into account is the clearance between the moving parts and access to these clearances for uncured or support material to be removed.
- **Around insert building [128]:** in some cases it is likely that groups of components are not (or cannot be) manufactured with AM (e.g. engines, batteries, etc.), but are required to be embedded into a part. Some AM processes have this capability to be paused, for a complete part to be laid on the part being manufactured, and to be resumed. This can be viewed as another route for multimaterial printing.
- **Electronics printing:** the capability to deposit electronics components (conductive inks, sensor, etc.). This ability is somewhat related to the machine capability. In various ways, these capabilities can ease a product architecture. It is the case for example for the Voxel 8 machine [129].

Table 3-1 - Non-assembly additively manufactured kinematic

	SLA	SLS	FDM	SLM	PolyJet
Revolute	[130-132]	[130, 131]	[133, 134]	[135-137]	[138, 139]
Prismatic	[131]	[131]			
Cylindrical				[135]	
Spherical	[130, 131]	[130, 131]			
Gear				[137]	[139]
Universal joint	[131]	[131]		[136]	[138]

3.2.1.2 Part related characteristics

There are number of characteristics which distinguish AM techniques as regards the features and the quality of the output without considering any post-processing step. These are described as follows:

- **Material type:** as shown in Table 2-1 materials processed by AM machines include plastics, metals, ceramics and composites. Whereas some techniques such as SLM or

LENS do only process metals, techniques such as PolyJet or SLA are limited to plastics. As such choosing a type of material is an implicit way of selecting an AM technique.

- **Resolution:** the features details and minimum wall thickness of a part strongly depend on the machine resolution (XY resolution and layer height or vertical resolution). Resolution varies between techniques, as shown in Figure 3-2, and for the same technique it can also be a matter of hardware.
- **Maximum size:** any AM technique is limited in buildable size by the machine embodying it, therefore so are the parts (or the number of parts) that can be manufactured at once. This limitation may lead to break down the CAD model to manufacture it in smaller chunks and then reassemble them afterwards [140]. The largest AM machines have built dimensions ranging from 90cm×60cm×30cm (Merke IV) to 40m×10m×6m (Windsor) and even to (theoretically) infinite dimensions. Knowing which machine will manufacture the part before designing it will definitely restrain the design space, and conversely with a rough idea of the overall dimensions of the part a proper machine may be selected.
- **Surface quality:** Numbers of factors do affect part's surface finish. Owing to the layer-wise manufacturing method peculiar to AM, stair step effect makes orientation and layer thickness very influential regarding surface finish. On a single part many different surface finishes may be encountered, varying by a more than 9 factor in terms roughness (Ra). Nevertheless the technique itself does also influence the surface quality. In techniques processing plastics for instance, SLA machines do provide a better surface quality than FDM ones; in metals SLM parts have better quality than those manufactured with LENS.

Figure 3-2 - Part printed with the same layer thickness using a FDM machine (left) (right) (adapted from [141])

3.2.2 Concepts underpinning the approach

3.2.2.1 Functional interfaces

A functional interface (FI) (of a product or a component) is an interface that characterizes the relationship that two spatial regions must have for a function to be fulfilled. That relationship may require an actual physical contact – subject to a certain clearance – between two components (e.g. sliding components) or it may be contact free. A FI may be a surface (either planar or three-dimensional), a point, or a line. A component's FIs are basically where its geometry "grows" from, and as such they must be carefully identified in order for the component's dimensions to be as much as possible close to the bare minimum. There are three kinds of FIs that can be distinguished:

- Contact free FI: it may fulfill functions related to aesthetics, gas or water tightness, heat dissipation (such as cooling fins), fluid deviation (such as aircraft's wings surfaces), etc.
- Handling FI: it can be for the product use (lever, button, etc.) or for the product to be assembled, transportable or maintained, and as such the physical contact is not permanent.
- Part-to-part contact relationship FI: this kind of FI may be required to perform positioning in an assembly, to provide guidance or for load transmission between parts. They can be generated using the Skeleton geometry-based Assembly Context Definition (SKL-ACD) approach [142]. Based on the kinematic pairs between parts, this approach can compute the generic surfaces on which the required FIs can be laid or the required FI itself along with geometric entities controlling its orientation and location.

3.2.2.2 Functional flows

The overall function performed by a product is associated with flows. In their lowest level of specificity these are energy, material or signal [68]. Conceptually these flows are closely associated with basic functions (e.g. transfer, channel, separate, etc.). Hirtz et al. [143] have classified the basic functions within eight groups including: branch, channel, connect, control magnitude, convert, provision, signal and support. The reader is advised to refer to [143] for a thorough list of the basic functions along with their definitions.

Components, as the physical embodiments of the functions, are ultimately "flows processors". While some functions may, explicitly, require a flow to get through a component, others may just require the flow to bypass it. For instance within the *signal* functions group – defined as "To provide information on a material, energy or signal flow as an output signal flow" – there is the basic function *detect* whose definition is: "to discover information about a flow". A component fulfilling such a function is not necessarily crossed by the flow, and as such the matter forming it, is not critical to its performance; instead it is the component's interface in contact with the flow which is critical. On the other hand, a component fulfilling the *transmit* function – defined as "To move an energy from one place to another" – is a "flow crossed" component, and as such has its matter critical to the performance. Nevertheless, it is worth mentioning that the working mechanism chosen to fulfill a function may still dictate whether the flow is to bypass or to get through the component. Given a component whose function(s) require(s) a flow to cross it, the material, its shape and its dimensions determine how well is (are) the function(s) fulfilled. Components' interfaces are the "gates" of the flows.

3.2.3 Overall Description

When considering AM at product level, the ultimate goals should be the possibility to consider part consolidation and/or to design an as*sembly-free* product (or *non-assembly* mechanisms [126, 130, 131]), that is, a product which after a few minor post-processing tasks is ready for use. Illustrations of such mechanisms include the fully assembled 3D printed *28-geared Cube* made by the *maker* Alexander Maund as shown in Figure 3-3, the historical mechanisms printed by Lipson et al. [127], or the bearings manufactured by SLM in [135]. As shown in section 3.2.1, this vision is sometimes made possible for single material mechanisms. Furthermore multi-components products have been printed by some AM machines such as the Voxel8[129] which, during the same print job, can process multiple polymers (including hard, soft and flexible) and print electronics components as well. However as the previous AM characteristics analyses have shown, none of the available AM techniques is capable of all the enumerated assembly related characteristics at the same time. Besides, some components in a product may prove more economically viable if manufactured by conventional processes or simply if outsourced. For these reasons we posit that:

- Owing to the heterogeneous nature of a product, assembly-free AM is not, generally, possible in the current state of art. The AM of a product may involve many AM processes, even in some cases other conventional manufacturing processes as well (*hybrid manufacturing* [144]), and a few assembly operations.
- The possibility to consider part consolidation cannot be made regardless of the specific characteristics of available AM techniques.

Figure 3-3 - Assemble-free *28-geared Cube* [145]

The goal that should, therefore, be sought is to find a product architecture, or an engineering bill of materials (eBOM) in case of redesign, which is minimal (while still functional) – that is, with the least separate components – and which is manufacturable with a single AM process or with the least AM processes. Besides, once the product architecture is minimized a strategy must be retained for the way the parts will be designed to take advantage of the selected AM processes' characteristics. Our strategy is that, once a part's functional interfaces (surfaces, points, etc.) are identified, these are connected both to ensure structural integrity and a proper conveyance of the flows getting through the part, abiding by any design space and manufacturing constraints. Thus, AM-ready parts' geometries can emerge.

At the core of the proposed design framework are the aforementioned premises. The framework is dedicated at helping designers mainly through embodiment and detail design stages. It aims at three main goals:

- Ensuring that the product architecture is kept to its supreme boundary by considering the available AM processes' specific part consolidation capabilities.
- Determining a manufacturing plan along with any *in situ* (during manufacturing) or subsequent assembly operations.
- Providing what could be called components' control structures – such as functional interfaces, functional flows and design spaces – (based on the architecture and the manufacturing plan) to be used for the detail design of the parts with the retained strategy so as to generate AM-ready product geometry.

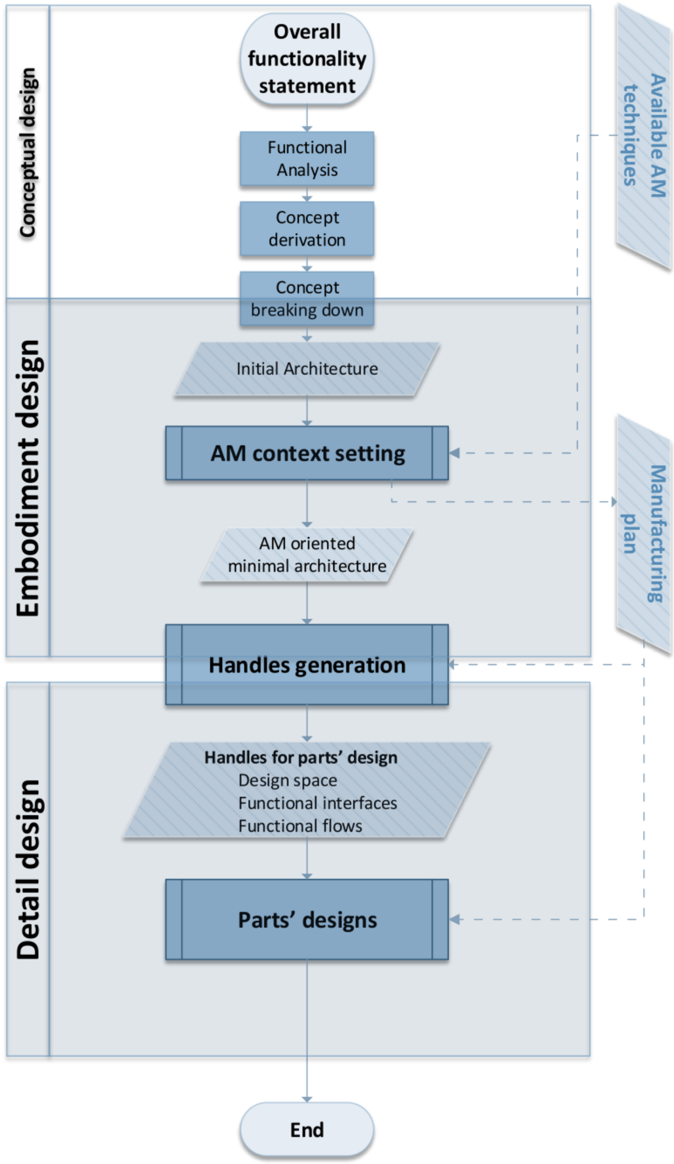
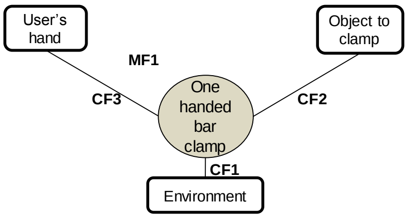


Figure 3-4 - Flowchart of the proposed framework

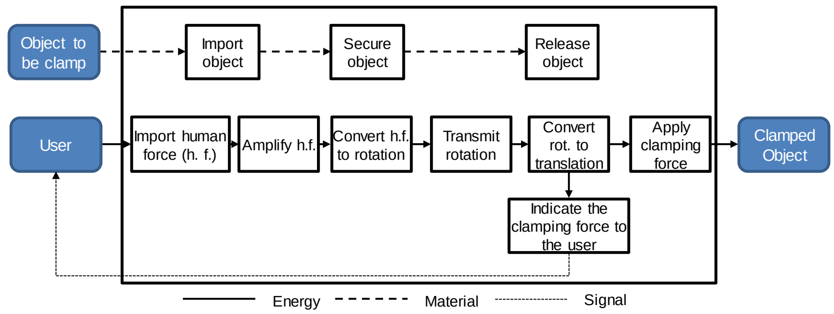
As shown in Figure 3-4, these goals are reached through 3 main steps, which are described in the following section. Since the proposed design framework is adapted for new product development, the way functional analysis is to be conducted is first described for the sake of clarity and consistency.

3.3 Assembly-oriented DFAM

3.3.1 Initial product architecture derivation



Main functions	MF1: convert human hand's force to clamp an object
Constraints functions	CF1: Protect from dust (to avoid failure) CF2 : Prevent the object from wear CF3 : Be ergonomic



(a) (b)

Figure 3-5 - Gripper's functional analysis. (a) External functional analysis – (b) Functional decomposition

The framework is dedicated to new development of products mainly manufactured and assembled with AM. As such it is intended to guide the product architect and designer from the overall functionality statement of the product to the detail design of the product. A first stage is to get an enhanced product architecture from a comprehensive functional analysis (both external and internal). This stage is structured in five steps described as follows:

- **Step 1 – External functional analysis**. The product environment – that is, everything it is to interact with in order to fulfill its functionality – is analyzed and enumerated (e.g. human, air, raw material, etc.) in terms of external elements (EEs). Such analysis can be summarized using a diagram like the one presented in Figure 3-5.a (for the gripper case study). In this case study, EEs include the user's hand, the object to clamp and the environment that the product is surrounded by.
- **Step 2 – Functional structure.** Two kinds of top level functions are then to be identified: main functions which are those whose action is related to two EEs, and constraints functions which act on a single EE (as shown in Figure 3-5.a), these do not actively participate in the overall functionality but are required for the product to be conveniently usable (e.g. maintain gas tightness, stand on a plane platform). The flows (energy, material, or signal) to be conveyed by the product are enumerated. Using standardized basic functions from the Reconciled Functional Basis [143], each top level function is decomposed to its lowest level and the basic functions derived from it are arranged in an order allowing the fulfillment of the overall function. Finally, the flows

are routed through all the standardized functions. The outcome of this step can be summarized with a block diagram (Figure 3-5.b).

- **Step 3 – Concept derivation and breaking down**. A concept is derived for the product with a close attention to the fact that each basic function is fulfilled by one or many components and that many components may fulfill a single function. The derived concept is abstracted with a product architecture which combines three views:
    - Part-to-part kinematics relationships view: all the components are enumerated and the kinematic pairs between them are specified.
    - Functional flows view: components in the part-to-part relationships graph are first clustered according to the basic functions they fulfill, and then the corresponding flows are routed from the EEs through the components. Some flows may have to be split, while others may be required to merge.
    - Spatial relationships view: using the mereotopological primitives descriptors to describe the physical connections between spatial regions (denoted x and y) such as developed in [37, 146-148] as "*x is part of y*", "*x is tangent of y*", and "*x overlaps y*".

Step 4 – Specific requirements. Specific information is added for the components. Firstly, maintenance/repair requirements and production requirements (3D printable, not to be 3D printed, or outsourced component) are specified. Then for each component candidate to AM, a number of desired characteristics are to be specified. These characteristics (or requirements) are used to generate suitable AM techniques and materials. Figure 3-6 delineates a data structure for the characteristics of a part to be additively manufactured, along with some values of the characteristics. It is worth highlighting that some of these characteristics (such as minimum wall thickness for instance) are conventionally known after a part's detailed geometry has been made, or these may be constraints set by the available AM machines. However in our proposal the designer using the approach is prompted to think about them beforehand, and to somehow commit to them. Nevertheless, not all the characteristics must be specified, one may choose to simply ignore the less crucial ones; the aim of that strategy is to get the proper AM techniques that will manufacture the parts and designing the product geometry accordingly (and avoid time consuming design iterations). This choice is consistent with the proactiveness of the proposed approach: the way(s) the product is to be additively manufactured will be known before efforts are put into its detail design, so that the designer is aware of how the designs can fully leverage the specific capabilities of the selected AM techniques while abiding by their constraints. In addition to direct detail design, these specific requirements will also be used to influence decisions made about part consolidation.

The information contained in the so derived initial product architecture is:

- For the parts themselves: indication of whether the component will be outsourced or is not to be additively manufactured (e.g. battery, engine, bearings, etc.), indication of whether the component would need to be maintained (in case of a weary component) or often moved, characteristics for AM techniques/machines selection.
- For the part-to-part relationships: kinematic relationships, spatial relationships and flows.

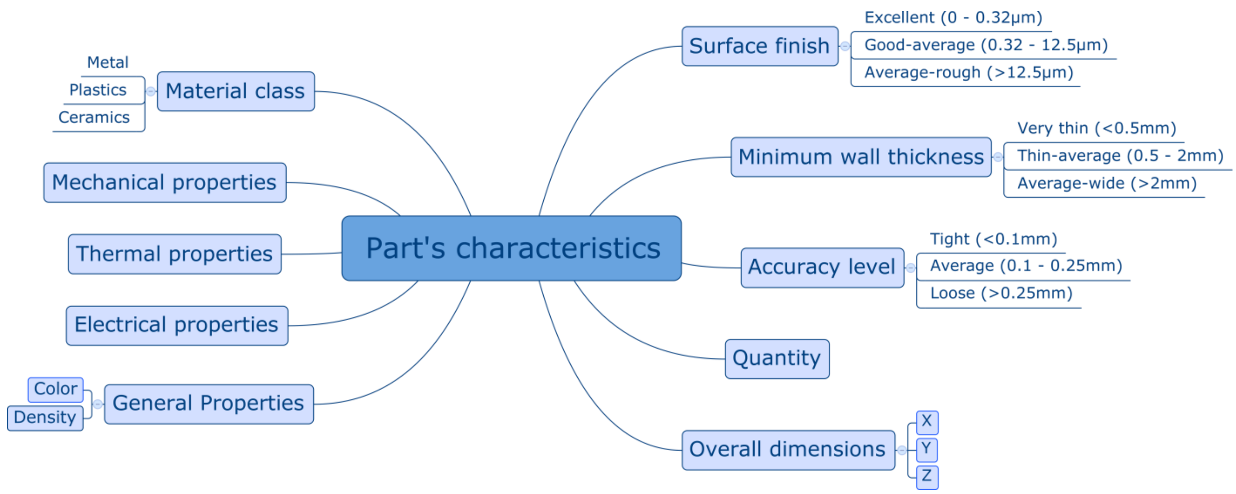


Figure 3-6 - Part's characteristics for AM techniques selection

3.3.2 Additive manufacturing context setting at product level

We define a minimal product architecture as an architecture containing the minimum necessary separate parts. This stage of the methodology is intended to make sure that AM capabilities and constraints are taken into account at product level by setting up an AM context. More specifically it aims at:

- Determining an architecture with the least components based on the available AM techniques' capabilities.
- Maintaining functionality regardless of how components have been combined.
- Determining a manufacturing plan (including assembly operations) so that the detail design stage is made accordingly, abiding by the selected processes' constraints. Another rationale underpinning this goal is that, those components that are to be manufactured together (be them moving relatively to each other or not) must be designed together (or at least with the same awareness of how manufacturing will occur), since manufacturing direction will be the same for them.

As the product concept is generated regardless of any conventional manufacturing constraint, it is likely that standalone components have to be so for various reasons (i.e. functionality, maintenance, etc.). As such a product architecture – which is derived within an AM context – may already be a minimal one, that is, without unnecessary standalone components like fasteners. However, to ensure that unnecessary standalone components are eliminated, any architecture should be checked. The proposed framework can be used for that purpose. It is notable that the method may also be used for redesign cases where the product has been originally designed to be manufactured by conventional processes.

Hence, setting an AM context is based on the initial product architecture (as described in section 3.3.1) and it requires knowledge about the specific characteristics of the available AM techniques (as described in section 3.2.1). The stage is organized in 3 steps.

3.3.2.1 *Preliminary processes selection and manufacturing plan generation*

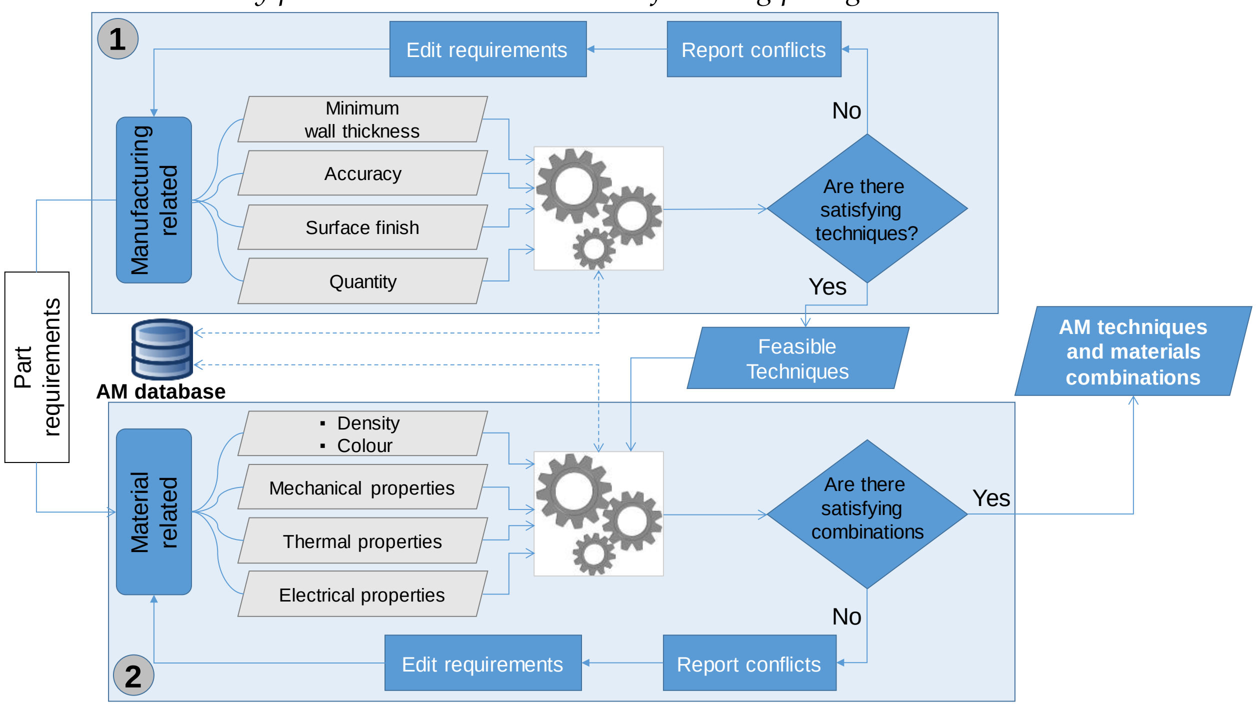


Figure 3-7 - Additive manufacturing preliminary techniques selection (at part level)

A number of studies have been carried out about AM process selection for parts [149, 150]. As this aspect is not the core of our proposal, we elected to build on previous work addressing this issue. This preliminary technique selection is achieved through two sub-steps:

1. Materials and techniques selections for each part individually based on the specific requirements stated for each of them. This is where research work from [149] on a decision support system has been harnessed to our contribution.
2. Techniques choice for the whole assembly. Each of the part to be additively manufactured is likely to be manufacturable by more than one AM material-technique

combinations. This sub-step is, basically, intended to determine the combinations that will suit most of the parts, as a way to streamline the manufacturing of the whole assembly.

The procedure for techniques and materials selection at part level is made through two main steps as depicted in Figure 3-7. Requirements on part which has an influence on the AM technique are first used to generate a set of feasible techniques (taken from the available AM techniques); these requirements are used to find techniques satisfying them individually, then the so found sets of techniques are crossed to find techniques meeting all the requirements. In case there is no available techniques meeting all the requirements, those which are conflicting are highlighted and either they are edited or the part is deemed not manufacturable by the available AM techniques. Each technique has a set of required materials that it can process. Techniques generated from the first step, along with parts' requirements related to materials are used to select techniques and materials combinations possible for the part. Similarly to the previous step, when no combination is found, either material requirements are edited or the part is deemed not additively manufacturable. For each component C_i, candidate to AM (that excludes outsourced components or those required to be manufactured by a conventional process), a set S_i of available AM techniques that can, possibly, manufacture it, is therefore generated.

As an attempt to streamline the product's manufacturing, the maximum intersection of the selected AM techniques sets (that is, the largest set where the sets S_i overlap), which is denoted $S = \bigcap S_i$ is determined. S is then ranked according to the assembly related characteristics described in section 3.2.1. The best process is then selected and designated as the *main AM technique*. The same procedure is repeated for the remaining components (those whose S_i elements are not included in S) to find a *secondary AM technique*. The process may be repeated again in case there are still parts not manufacturable by the selected secondary AM technique. In order to keep the manufacturing scheme simple, a criterion for limiting the number of repetition – that is, the number of secondary AM techniques – is decided. In case where the criterion is not met either the requirements on parts are revised, or the whole concept is deemed as not easily additively manufacturable and have to be altered.

At the end of this stage, a new view is then generated for the product architecture: a manufacturing view indicating whether a component is manufacturable by the main AM technique, manufacturable by a secondary AM technique, or not additively manufacturable.

3.3.2.2 *Architecture minimization between mating components*

Once the processes by which components are to be manufactured are determined, decisions are made both about how they can be consolidated to generate a minimal architecture and about how will the whole product be manufactured and assembled. In others words, the purpose of this step is to provide an answer to the following question: given two parts non-moving relatively to each other, how can these parts be consolidated in order to simplify the product architecture? As shown in Figure 3-8, three outcomes can result from this analysis: the parts are simply merged (*merging*), or one of the parts is laid inside the other, while this latter is being manufactured (*part embedding*), or they are regularly assembled. The process is as follows:

1. Components without relative motion are first clustered within sub-assemblies.
2. Consolidation is made by components' pairs comparisons in each sub-assembly. Four cases can then occur, as regards manufacturing and materials requirements:
    - Case 1: components are of the same material and are manufactured by the same AM process. In such case they are simply merged as a single component and their respective functional flows are combined.
    - Case 2: components are of different materials processed by the same process. In that case, they are also merged and flows are combined.
    - Case 3: components are of different materials processed by different processes. In this case, spatial relationships between the components (read from the architecture's spatial relationships view) along with the abilities of the two processes of building around insert are used to make a decision as shown in Figure 3-8. The two components are either tangent or overlapping at some region. In case they are tangent, they are simply manufactured separately and regularly assembled (requiring therefore assembly features for a rigid kinematic pair). If they are overlapping, let's denote 2 the outermost component in the regions where the parts are overlapping. If the process manufacturing 2 is capable of building around insert, then 1 and 2 are assembled in such a way that 1 is embedded in 2 while this latter is being manufactured; otherwise they must be regularly assembled, that is, manufactured separately and assembled afterwards.
    - Case 4: one of the components is outsourced or non-additively manufacturable. We assume that two adjacent outsourced components are considered as a single outsourced component, the case where both compared components are outsourced is thus excluded. In case the 2 parts are overlapping and the outermost component is the outsourced one then the parts are regularly assembled. Otherwise the outcome is the same as for case 3.

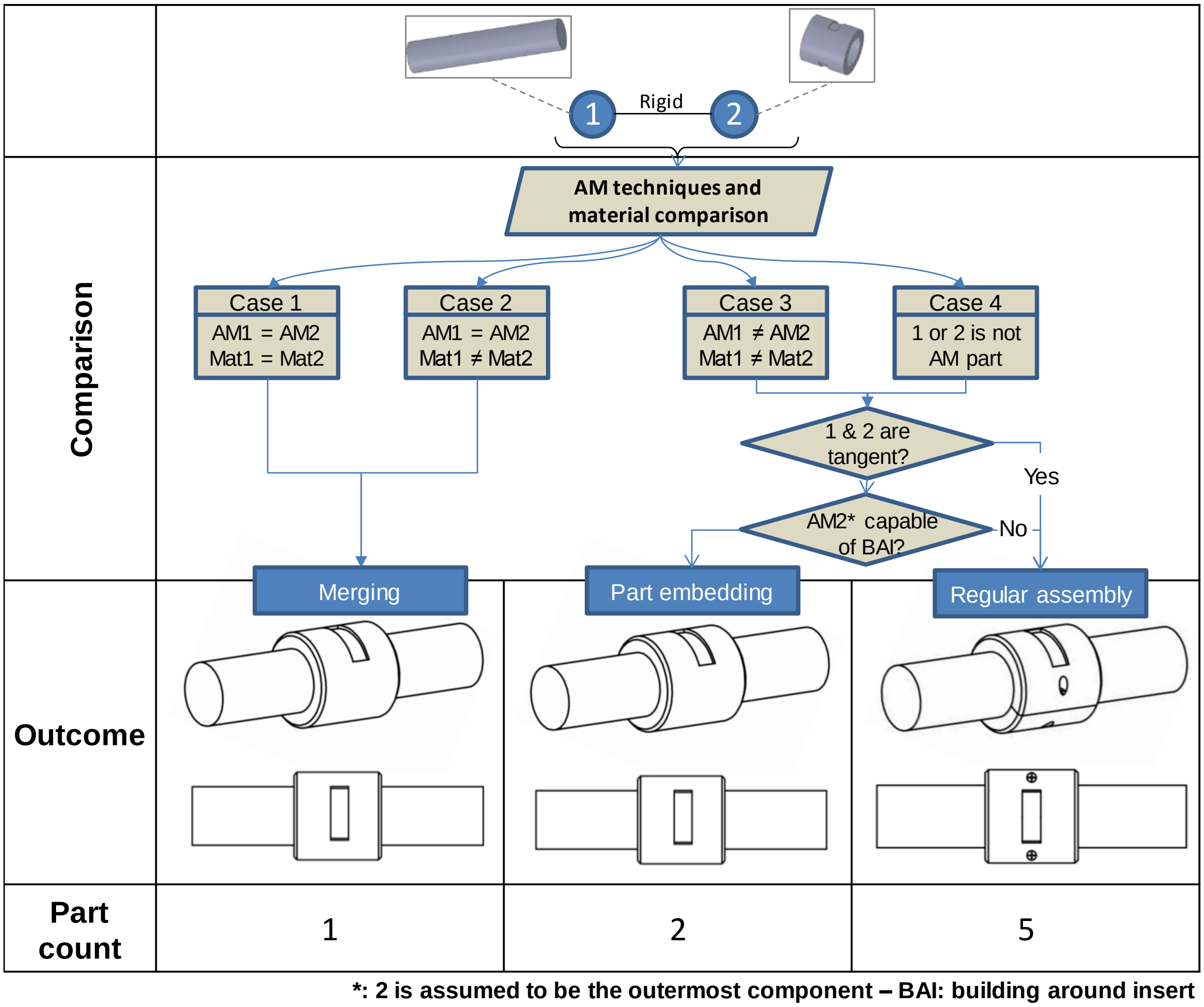


Figure 3-8 - Product architecture minimization between mating components

3.3.2.3 Architecture minimization between moving components

Components moving relatively to each other are conventionally manufactured separately and assembled afterwards, however as shown in section 3.2.1, depending on the kinematic pair linking them and the selected AM processes, the adjacent components can be manufactured together while still be able to move relatively to each other. This step is about identifying all these moving components that can be manufactured together. It will have implications on the final design, in that manufacturing a joint may requires a particular orientation and consequently alterations of a conventional joint's design [130]. The step is conducted by comparing pairs of moving components A and B, which are related by joint J: A–J– B. The possible situations are as follows:

- A and B are manufacturable by the same process. If kinematics pair J is also manufacturable by the process then the whole assembly is consolidated during manufacturing. Otherwise – that is, if the kinematics pair is not manufacturable – the components are assembled afterwards and assembly features must be integrated in their designs.
- A and B are not manufacturable by the same process. In that case they are assembled normally.

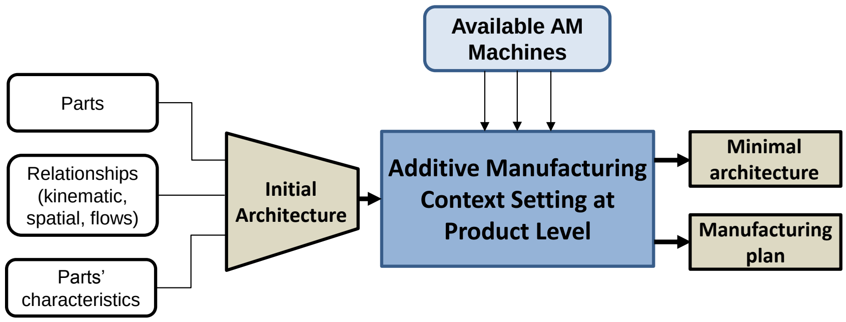


Figure 3-9 - Summary of the AM context setting at product level stage

As depicted in Figure 3-9, at the end of this stage, the enhanced product architecture derived in the previous stage (section 3.3.1) has been used to generate a minimal architecture and a manufacturing plan based on the available AM machines' capabilities. The so derived minimal architecture shows parts that have been combined, flows which have been merged. The manufacturing plan tells which part is to be manufactured by which AM machine and how are the parts to be assembled. The minimized architecture and the manufacturing plan are then the basis of the components designs stage, which is described in section 3.5.

3.4 The case of mechanisms to be manufactured by the same process, in a single print job [151]

It is likely that groups of components, be them moving relatively to each other or not, are to be additively manufactured and assembled together (it is actually one of the sought goals of our proposal) within the same AM machine. Besides, situations where the whole product can be manufactured and assembled in a single print job, may also arise. This section aims at providing a methodology to handle these cases. Within the whole proposal (as depicted in Figure 3-4), it is part of the "handle generation" step. The purpose of this step is to derive a design context in which both the product's functionality is maintained and AM constraints are proactively considered.

3.4.1 Design spaces definition

For each of the components identified in the part-to-part relationships graph a design volume is specified by the designer in the form of a rough shape (cylinder, cube, etc.). Then design spaces are positioned relatively to each other according to the derived concept. Since AM is capable of complex shapes, components without relative motion, could all be consolidated. However, some components may be subject to wear and therefore required to be usually changed, they may be required to be removable, they may be outsourced (such as standard components), or they may be required to be manufactured either in a material that is not processed by the chosen AM technique, or by a different manufacturing process. In these cases, a separate design space defined for these components is removed from their mating components' design spaces and new FIs specific to a rigid kinematic pair, are defined on the design space of the components they are attached to.

3.4.2 Emergence of functional interfaces

For each component, the relationships with its neighboring components and (possibly) with external elements are analyzed and the corresponding FIs are picked and positioned. Positioning a FI between two components affects the design space of both components. The process is repeated until all the relationships are physically instantiated by the FIs in the design spaces. At this stage, each design space (or equivalently each component to be additively manufactured) is associated with its FIs and the whole product is modeled in a layout form.

3.4.3 Additive manufacturing contextualization

The time required for post-processing an additively manufactured assembly should not outweigh the one required to manufacture (by AM or not) the assembly's components separately and to assemble them as it is conventionally done. Therefore care should be given to the process specific constraints so that the mechanism is successfully manufactured and post-processed (if needed). Once the developed concept has been abstracted in a layout form and functionality has been assured through the right FIs, AM specific constraints must then be taken into account. These constraints are considered through the steps of clearances setting, printing configuration, printing orientation choice, and accessibility to the clearances.

- **Step 1 - Clearances settings.** To ensure a successful manufacturing (and a seamless post-processing) without impeding the functionality related to the joints, care must be given to clearances within pairs of sliding FIs. The chosen clearance is related to the required joint performance, and the printing resolution. Clearance between sliding surfaces must be tight enough to ensure joint performance (avoidance of instability, vibrations, and unwanted DOFs). They must also be large enough to prevent mating surface from merging during the manufacturing. Depending on the mating surfaces geometries, clearances values differ. For flat surfaces (involved in prismatic pair mainly), reported successful values include 0.3 mm with a SLA and a SLS machines [131]. For circular surfaces, reported successful values are 0.5mm (SLA and SLS [131]) - 0.2 mm with a PolyJet machine [152] - 0.2 mm and 0.05mm (with alterations to the journal's shape of a revolute joint) with FDM [133] - 0.2 mm with SLM[136]. Because they are specific to the

AM machines (accuracy, layer thickness) and the materials used, these values cannot be considered as normative; though they can be used as a rough estimate of successful joint clearance. Besides there are some AM services providers [153] which publish for each of their processed materials, the right clearance value. All the sliding FIs are then to be spatially constrained using the required clearances. This may involve offsetting some FIs.

- **Step 2 - Printing configuration.** As components can move relatively to each other and are *in situ* assembled, they can be manufactured in different configurations. To reduce as much as possible the need of support structure (or unprocessed raw material) within the clearances and to allow as much as possible access to the clearances, components – wherever possible – should be moved in such a configuration that mating surfaces have the lowest facing area as shown in Figure 3-10. In addition when possible, the components should be moved such that clearances which are along a single direction (e.g. for the kinematic pairs prismatic, cylindrical, etc.) are mostly all aligned along one single direction. Indeed, in such configuration, selecting a printing direction to avoid support structure within the clearances requires less compromise. Nevertheless, while choosing a configuration, care must also be given to the available printing volume so that the product does not exceed it.

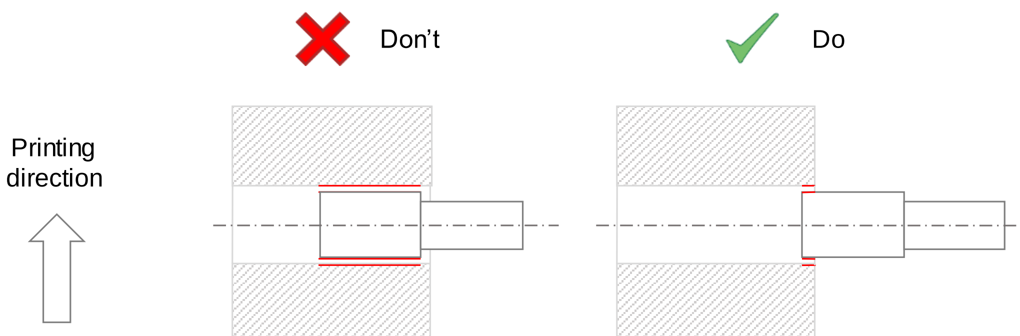


Figure 3-10 - Preferential printing configuration for a pair of components

- **Step 3 - Printing Orientation.** Printing orientation affects number of parameters of the printed item, these include dimensional accuracy, surface finish quality, strength, build time, support structure, and eventually cost. As such determining a manufacturing direction is quite a cumbersome task, which involves many competing goals: while a direction may yield the lowest build time, it may be the one leading to the poorest surface quality on a surface that is critical to the item's performance. Many studies have tackled this task for parts [154, 155] whose geometries are explicitly defined. However when considering assemblies, we posit that the main concern must be about the clearance gaps, especially about avoiding as much as possible support structure (or unprocessed raw material) within them, since they are critical to the joints' performance.

In order to choose an optimal printing orientation which minimizes post-processing effort, an indicator should be used so that different orientations can be compared quantitatively. Requirements for such metrics include:

- It must depend on all the assembly's joints.
- It must provide a measure of the trapped matter within the joints' clearances, and as such its minimal value would indicate the best orientation.
- As it is easier to remove loose (unprocessed) raw material (in the form of powder or resin) than to remove cured support structure, be it dissolvable or not, the measure must account for support structure and loose material differently. Support structure presence should then be penalized by a value higher than the one yielded by loose raw material presence.
- For a single joint, it must be able to differentiate printing orientations based on the volume of trapped material. Thus, even though there must be support (or unprocessed) material in any two orientations, there is still the possibility to know which one is likely to yield the least. See Figure 3-11, where this requirement is illustrated with a prismatic joint. Using the trapped material's volume (weighted depending on the material's state) would easily indicate that the orientation on the left (orientation 1) would require less support than the one on the right.

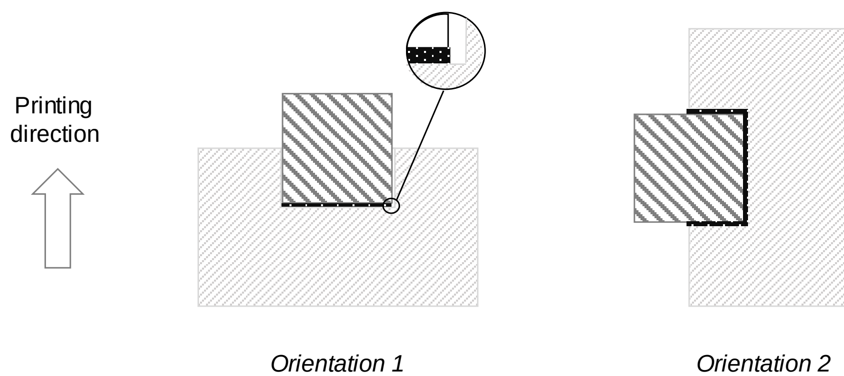


Figure 3-11 - Distinguishing two build orientations requiring support

To account for all these requirements, we propose the following metrics. For joint i, a measure of how much in between material, printing it in orientation $\vec{u}$, would require is:

$$J_i(\vec{u}) = k_{uc} v_{i,uc}(\vec{u}) + k_{ss} v_{i,ss}(\vec{u})$$

Where :

$v_{i,uc}$: volume of uncured material

$v_{i,ss}$: volume of support structures

In order to penalize support structures, k_{uc} and k_{ss} are two coefficients such that $k_{uc} \ll k_{ss}$. The measure that is then to be used for the whole assembly is an increasing function of the all the $J_i(\vec{u})$:

$$S(\vec{u}) = f(J_1, J_2, \cdots, J_n)$$

The simplest ways of constructing f being by summing or multiplying the J_i. An illustration is provided with a single revolute joint in Figure 3-12 with $k_{uc} = 1$ and $k_{ss} = 100$.

Once S is evaluated for each printing orientation in the selected configuration, the best orientation is the one yielding the lowest value of S.

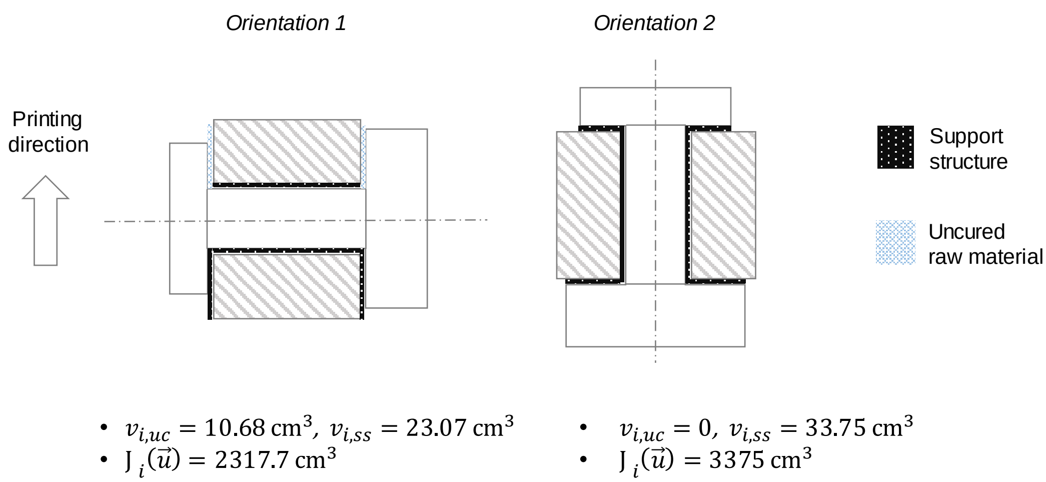


Figure 3-12 - Trapped material measure illustration

- **Step 4 - Accessibility to the clearances.** Even though a printing orientation has been selected to minimize both uncured material and support structures within the clearances, chances are that there are still clearances filled with support and/or loose materials (subsequently referred to as *in-between materials*). Care must then be given to the clearances, so that depending on what they are filled with, there is a way to clean them, especially there is an access for what is used for removal. This is the purpose of this step. Ways for clearances cleaning depend on the clearance, the kind of in-between material, and the kind of tools used for removal.

- Table 3-2outlines the possible situations. The most critical in-between material being the rigid metallic support structure which is required for powder bed fusion processes. Despite a recent report of dissolvable metallic support structure[156] for the LENS process, metallic support structures are mostly removed from parts by using pliers or chisels. Given the values of successful clearances (which are less than a millimeter), such tools may not be useful in cleaning the clearances. Alternative solutions for hard support removal may be:
  - *Micromilling*: high precision milling tools can have tips of diameter of as low as 0.1 mm and can process materials as hard as very hard steel (HRC 55) (which is quite harder than the typical porous metallic support structures). However such solution may be limited by cutter's length. Indeed, typical the cutter's lengths found in high precision milling tools are in the range of 1 mm which may not be long enough to reach the whole clearance.
  - *Laser cutting*: lasers' tips diameters can be in the range of micrometer, and their power can be adjusted so that they only destroy the support structures. There is no limitation as regards the depth the laser can attain. Such route can be beneficial in that it can also improve the surface quality of the facing surfaces. Though, issues related to thermal cutting processes may arise, especially the heat-affected zone (HAZ) issue.
  - *Water jet cutting*: high precision technologies using high pressure water such as Microwaterjet® [157] have cutting accuracy in the range of 0.01mm, can be positioned with an accuracy of ±3 μm, can provide a surface quality of N7 (Ra 1.6 μm), and can cut almost any material between rubber and steel. Such solution for support removal has the advantage of being "cold", thus avoiding issues related to thermal solution like lasers.

The identified solutions are those that allow access to tiny interstices (in contrast to conventional tools used to remove support structures under overhangs) and that are still effective at breaking away hard materials. As long as access is provided for the tool's energy (be it mechanical or thermal), any of these solutions can be used to clean the clearance from possible support structures. This is what makes the step of accessibility to the clearances, of high importance in the proposed methodology.

Table 3-2 - In between materials removal

Type of in-between matter	Techniques	Removal methods	Requirement for removal
Uncured resin	SLA	Gravity based flow, suction	Access for fluid flow from inside
Unprocessed powder	SLM, SLS, 3DP	Gravity based flow, suction	Access for the powder flow: holes in dimensions of a few times particles' size
Water soluble support structure	FDM, PolyJet,	Washing away in solution, jetted hot solution,	Access for fluid flow through the support
Rigid polymer support structures	FDM, SLA,	Breaking away with hands or tools	Access for tools
Rigid metallic support structures	SLM, LENS	Breaking away with hands or tools	Access for tools

3.5 Part-oriented DFAM

3.5.1 Foundations of our strategy for harnessing AM shape complexity to part's performance

Any system, sub assembly or component is designed to fulfill a function which represents what the device must do. The device's shape, form or architecture answers the question of how is the function fulfilled. This shows why a device's function must be fully understood before time is spent on its embodiment design. Tightly related to a device's function is the notion of flow which basically is what the device operates on for the function to be fulfilled. Systems, even those made of a single component, rarely fulfilled their function(s) in an isolated manner. In other words, they always fulfill their function by interacting with their surroundings (be it made of a user or others components) by means of one or several flows exchange. The interaction between a component and its surroundings occurs at its interfaces, which can be seen as the flows' "gates". It can be summarized that a component is fully defined firstly by its functions (which is what it does), the flows it processes for the functions to be fulfilled, its interfaces through which the flows are exchanged and its shape holding the interfaces together. This breakdown of component is depicted in Figure 3-13.

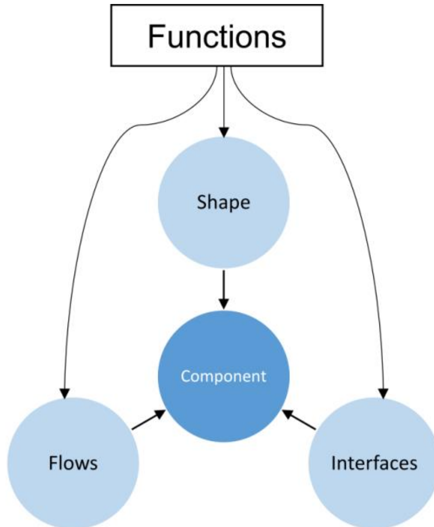


Figure 3-13 - Elements characterizing a component

Once flows getting through a component are identified, it is of interest to determine what impact (if any) they have on the shape and interfaces of the component. Again, at their lowest level of specificity, flows are either energy, material or signal [68, 143]. Functions associated with material flows are basically functions that process the materials by somehow changing its state. These are categorized by Ullman [158] in three groups: through flow functions (e.g. rotate, translate, move, lift, channel, etc.), diverge flow functions (disassemble and separate) and converge flow functions (mix and attach). A Component fulfilling such function must "clear the way" for the materials and as such its shape is not crucial for the flow conveyance. However when the processed flow is energy, say in a mechanical form (load for instance), it is obvious that shape, along with interface, play a key role.

Ullman [158] has stated that:

"It has been estimated that fewer than 20% of the dimensions on most components in a device are critical to performance. This is because most of the material in a component is there to connect the functional interfaces and therefore is not dimensionally critical. Once the functional interfaces between components have been determined, designing the body of the component is often a sophisticated connect-the-dots problem."

The premise governing the methodology proposed to leverage AM shape complexity capability to design effective components is profoundly related to that statement. The extra 80% of components' dimensions that are not critical to the performance may be due to conventional (subtractive) processes' limitations. Furthermore, to better suit our approach the statement can be extended as "... *a sophisticated connect-the dots problem* in order to assure a structural integrity and a proper conveyance of the flows related to the component's functionality". Another important statement of the Ullman book, highlighting the importance of interfaces, in agreement with the aforementioned statement and which is worth quoting reads:

"Components grow primarily from interfaces."

In a nutshell, a component is bounded by its functional interfaces (FI), these must be connected to ensure structural integrity and to ensure that flows entering or leaving interfaces are conveniently conveyed. The AM shape complexity gives way to ensure that connectedness with the bare minimum matter. This minimalist vision of part design is illustrated in Figure 3-14 for an aircraft hinge plate; a comparison is made between how this component has been designed for conventional processes and how it could have been designed for AM.

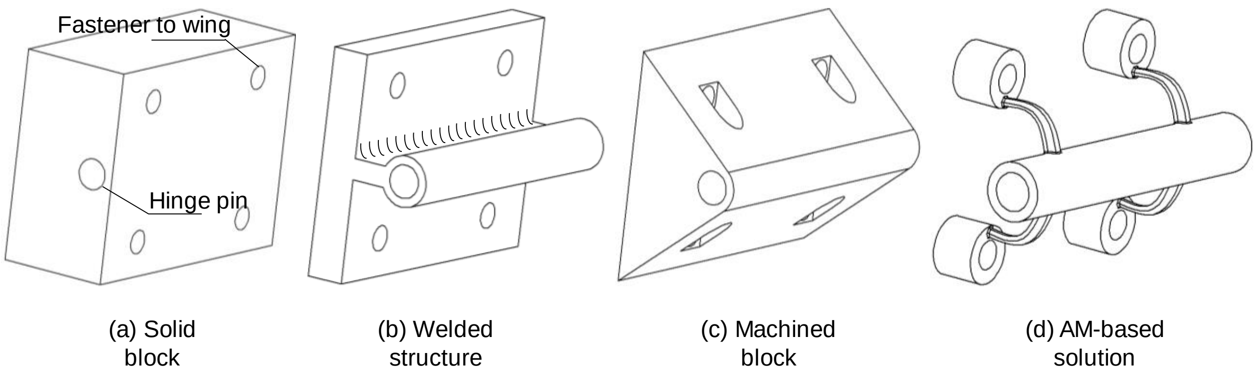


Figure 3-14 - Aircraft hinge plate designs according to various manufacturing processes including AM

3.5.2 The proposed methodology for part oriented DFAM

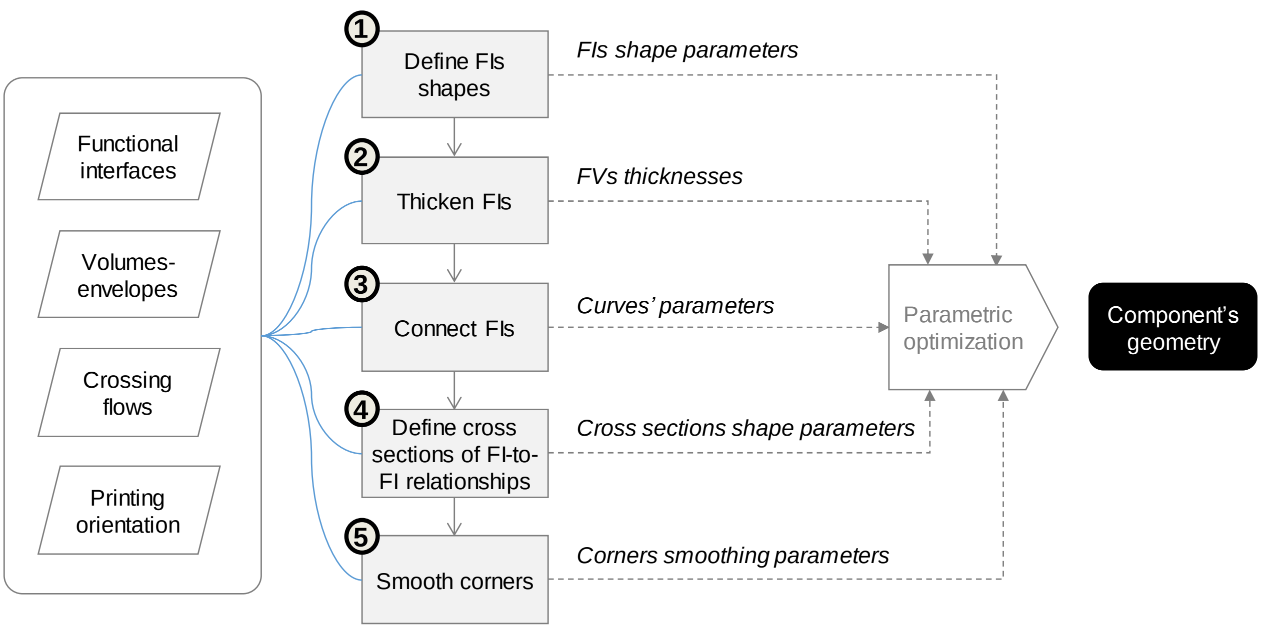


Figure 3-15 - The proposed methodology for part's design

Consistent with the aforementioned philosophy, a five-steps-strategy is proposed to design the geometry in a minimalist way, as outlined in Figure 3-15. The selected AM techniques constraints are taken into account as well. First, the component's FI shapes are drawn. Second, the FIs' shapes are thickened into functional volumes (FVs); the thicknesses can be governed both by resolution of the considered AM process and tolerances related to the considered FI. In the third step, paths joining the FVs are defined; this can be done either to ensure the component's connectedness, or to ensure a way for a specific flow (or even a combination of flows), or both. Fourthly, the connecting elements' shapes along the previously defined paths are designed. To improve the performance of the component, the section can be of different types including solid cross-section, solid cross-section with lattice structure, hollowed cross-section, hollowed cross-section with lattice structure, etc. To avoid sharp corner (and equivalently, stress concentration), corners are smoothed in the fifth step. Each of these steps leads to some geometric parameters. Those are then finally optimized to generate a component that behaves and conveys the flows appropriately. The following scheme has been retained for the parametric optimization:

- Choice of each parameter's bounds.
- Specification of any constraint on the parameters. These can be geometric constraints such as relationships between parameters, or constraints ensuring a proper behavior such as maximum stress or minimal natural frequency. The functional flows conveyed by the part on one hand, and the chosen material on the other hand can provide indication on what constraints related to an appropriate behavior must be met.
- Definition of the component's mass as an objective function. Choosing the component's mass as an objective function to minimize is consistent with the endeavor to design components with the bare minimum matter. Others objective functions which are sensitive to the chosen parameters and which are relevant to the sought performance may also be chosen.

3.6 Case study

The proposed framework has been illustrated with a one handed bar clamp, similar to the one that is discussed in chapters 7 and 9 of [158]; another illustration on the case of assembly manufactured with a single AM process at once can be found in [151]. The main steps have been shown.

3.6.1 Initial architecture derivation

After a functional analysis, as explained in section 3.3.1 and a concept generation, an architecture with 17 components have been retained. The concept's bill of material, along with the requirements for each component, can be found in Table 3-3. Figure 3-16.a shows the part-to-part kinematics relationships view combined with the functional flow view.

3.6.2 Minimized architecture and manufacturing plan

We used a scenario of an AM factory that has 6 machines based on the following techniques: FDM, SLA, PolyJet and SLS. Details of the available machines can be found in Table 3-4. All components candidate to AM were found manufacturable with the available machines. Based on the assembly related characteristics, and especially the capability to build around inserts, the Ultimaker 3 Extended (U3E) machine has been found to be the best AM machine. The combination U3E-PLA has been selected for the components: 1, 2, 4, 5, 8, 9, 12, 14 and 15 (cf. Table 3-3). For components 6 and 7 (pads), a different material – TPU 95A – has been selected; it is a semi-flexible and soft (shore A 95) material with high wear and tear resistance. These choices have led to a generated minimized architecture with 13 separate components, as shown in Figure 3-16.b. The manufacturing plan is delineated in Table 3-5.

Table 3-3 - Parts' requirements

		AM	Material class	Surface finish	Minimum wall thickness	Accuracy level	Overall dimensions	Mechanical properties	
								Yield strength (MPa)	Durometer
1	Main body	Y	Plastics	Average-rough	Thin-average	Average	100x150x30	10-20	Shore D 60-70
2	Trigger	Y	Plastics	Average-rough	Thin-average	Average	40x90x30	10-20	Shore D 60-70
3	Bar	N							
4	Tail stock	Y	Plastics	Average-rough	Thin-average	Average	50x50x30	10-20	Shore D 60-70
5	Lock	Y	Plastics	Average-rough	Thin-average	Loose			
6	Pad1	Y	Plastics	Good-average	Thin-average	Loose			Shore A 40-100
7	Pad2	Y	Plastics	Good-average	Thin-average	Loose			Shore A 40-100
8	Roll pin	Y	Plastics, metals	Average-rough		Average			
9	Knurled pin	Y	Plastics, metals	Average-rough		Average			
10	Release trigger spring1	N							
11	Release trigger spring2	N							
12	Release trigger	Y	Plastics, metals	Average-rough	Thin-average	Average		10-20	Shore D 60-70
13	Power spring	N							
14	Jam plates1	Y	Plastics, metals	Average-rough	Thin-average	Average		10-20	Shore D 60-70
15	Jam plates2	Y	Plastics, metals	Average-rough	Thin-average	Average		10-20	Shore D 60-70
16	Split pins1	N							

17	Split pins2	N							

Table 3-4 - Available AM machines

Machine name	Technique	Minimum wall thickness	Accuracy	Surface finish	Max XxYxZ (mm)	Materials types	Processed materials	Multimaterial	Capability to print electronics	Capability to build around insert	Printable kinematics pairs
Ultimaker 3 Extended	FDM	Very thin	Average	Good-average	197x215x300	Polymers	Nylon, PLA, ABS, CPE, CPE+, PVA, PC, TPU 95A, PP, Breakaway	Yes	No	Yes	Oui
Ultimaker 2+	FDM	Very thin	Average	Good-average	223x233x205	Polymers	PLA, ABS, CPE, CPE+, PC, Nylon, TPU 95A, PP	No	No	Yes	Oui
Objet30	PolyJet	Very thin	Tight	Excellent	294x192x149	Polymers; Wax	VeroWhitePlus™, VeroGray™, VeroBlue™, VeroBlack™, Durus	Yes	No	No	Oui
Form 2	SLA	Very thin	Tight	Excellent	145x145x175	Polymers	CLEAR FLGPCL03, HIGH TEMP FLHTAM01, TOUGH FLTOTL03, DURABLE FLDUCL01, FLEXIBLE FLFLGR02, DENTAL SG FLDGOR01, CASTABLE FLCABL02	No	No	No	Non
EOS P 77	SLS	Very thin	Tight	Good-average	700x380x580	Polymers	Alumide, PA 1101, PA 1102 black, PA 2200, PA 2201, PA 3200 GF, PrimeCast 101, PrimePart FR (PA 2241 FR),	No	No	No	Oui
FORMIGA P 110	SLS	Very thin	Tight	Good-average	200x250x330	Polymers	PA 2200, PA 2201, PA 3200 GF, PrimeCast 101, PA 2105	No	No	No	Oui

Table 3-5 - Manufacturing plan

Step	Parts or sub-assembly	Machine-Material	Comments
1	• 4-5-8-9 • 14-15 • 1-2-12	Ultimaker 3 Extended - PLA	*In situ* assembly for (1, 2,5) *In situ* assembly for 1-2 and 1-12
2	6, 7	Ultimaker 3 Extended - Nylon	Regular assembly after AM
3	3, 16, 17	(not AM)	Regular assembly to (4-5-8-9)
4	10, 11, 13	(not AM)	Regular assembly to (1-2-12) and 3

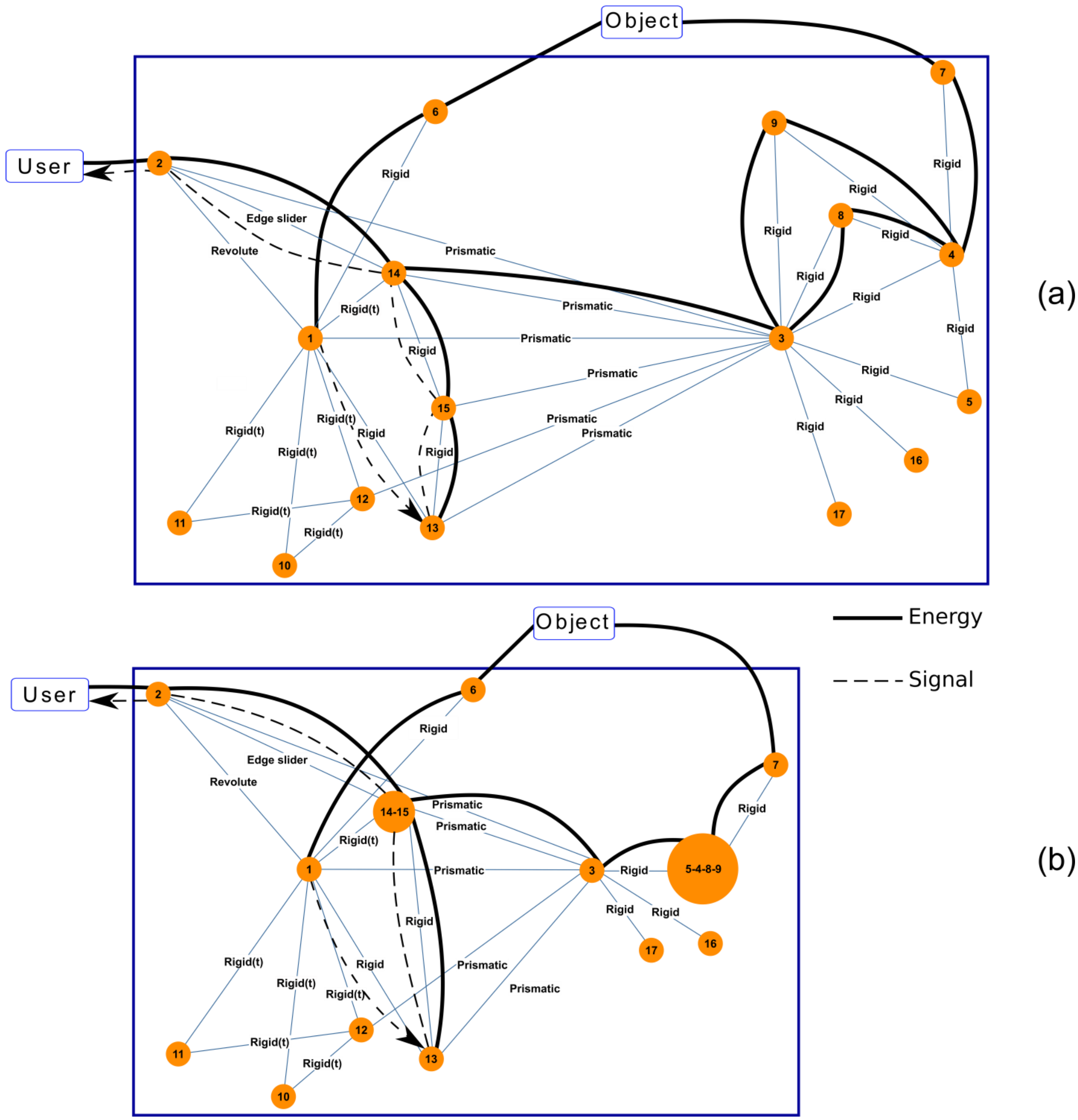


Figure 3-16 - Product's architecture showing Part-to-part kinematics relationships along with functional flows: (a) Initial architecture - (b) Minimized architecture

3.6.3 Final design

The generated minimal architecture has been used to design the components' geometries. A proprietary tool (Pegasus CAD Assistant [148]), was harnessed to semi-automatize the generation of the design spaces and the functional interfaces based on the kinematic relationships as shown in Figure 3-17.a. Based on these, the components have been designed by following two approaches including the one proposed in this paper and another one based on lattice structures. As an example, Figure 3-17.b presents a lattice structure developed for the tail stock (part number 4 in Table 3-3). A design in alignment with the required mechanical behavior of the part as well as the selected technique capabilities. On the other hand, the main body (part number 1 in Table 3-3) has been defined by using the proposed methodology. The final design results from a flow of integrated design intents, enabling to get an improved solution from a top-down manner.

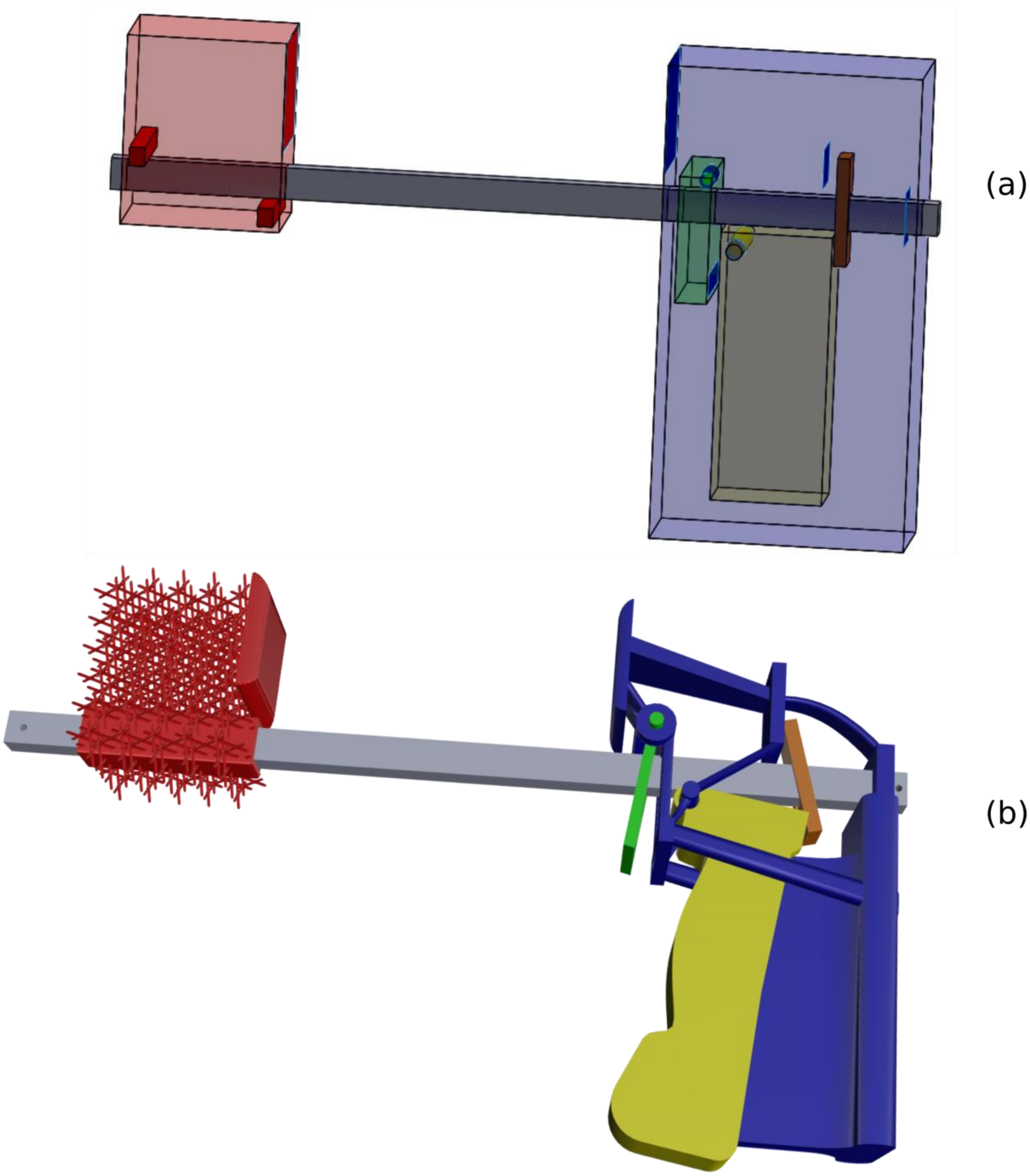


Figure 3-17 - (a) Design spaces definition and (b) emergence of the detailed geometry of the case study

3.7 Conclusion

In this chapter, the lack of a DFAM vision in 4DP has been addressed. A twofold proposal aimed at helping designers to take AM design freedoms and constraints into account has been made. First a methodology for part design in an AM context has been proposed, it leverages the shape complexity capability of AM to promote minimalist designs. The adopted strategy is to connect a part's functional surfaces with the bare minimum matter, based on the functional flows crossing it. By separating a 4DP item into an active and an inert structure, such approach – mainly dedicated at the inert structure – can improve the "4D" aspect, especially when shape changing materials are involved. Indeed as less matter is to be moved, the actuation capability of the 4DP item can be improved.

Furthermore, cases where 4DP reaches the state where it benefits mechanical assemblies have been envisioned. This aspect of the proposal follows the same minimalist vision. It considers assembly-related AM freedoms such as assembly-free mechanisms, part consolidation or multimaterial printing. Worth highlighting is that the proposed framework takes a proactive strategy by first setting an AM context. It typically selects how a product is to be manufactured (by which AM machines and in which materials) in order to minimize its architecture before it proceeds to detail design stages.

No particular assumption was made on SMs, which make the proposal versatile enough to benefit DFAM in context that are not related to 4DP.

Chapter 4 Design with Smart Materials (DwSM) 1: A design oriented view of smart materials

4.1 Introduction

The desire to make structures more efficient is the main driving force behind research in the field of materials. The performance sought is almost always the optimization of one or more structural properties (strength, density, conductivity etc.) of materials, which has led, for example, to the emergence of composite materials or functionally graded (FGM) materials. However with the discovery of piezoelectricity in 1880 and the SME in 1932 [54], the desired materials' performance is no longer solely structural but also functional. Thus, the need to provide materials with functional capacities has led to the emergence of the so-called SMs. Different definitions of SMs are found, but all agree that they are materials that are sensitive to a stimulus (or several stimuli [159, 160]) and able to alter their states as a response to the stimuli. There are for instance thermochromic material whose color change as a response to heat, electrostrictive materials which deform as a response to electric field, or magneto-rheological fluid whose viscosity is drastically increased upon exposure to a magnetic field.

Despite their interesting properties, there are relatively few products made of SMs that make their way out of (materials) laboratories. Even for SMA, which are the most studied and best characterized SMs, there are many applications that do not pass the stage of real industrialization; this is for instance the case of the Boeing Variable Geometry Chevron [161] using SMA pads which has not yet flown. Various reasons may explain this situation. SMs exhibit non-linear behavior and time-dependent properties. Properties such as Young's modulus, yield strength and conductivity can change significantly during product use or as a consequence of changes in the environment (temperature, humidity, etc.); this makes their uses more complex by a non-expert. Moreover, the technological maturity of these materials also hinders their adoption. Conventional materials are completely characterized and standardized: their behaviors and lifetimes can be predicted accurately. Such a level of reliability (and *technical readiness level*) is, however, not (yet) reached in the case of SMs in general. This gap often leads to conduct several validation tests and possibly to carry out many design iterations to develop a SM based product. Another set of (less tangible) limitations hinder a thorough adoption of SMs, these are related to design (as the activity). As SMs provide a functionality they cannot be handled in the design activity as it is for conventional materials. While many research efforts have been targeted at alleviating physical issues related to SMs adoption (syntheses, chemistry, characterization, manufacturing), a little has been done to help designers considering them. These stakeholders, which are likely to be non-expert of these materials, are the ones more inclined to find original industrial applications of SMs.

A field's expert is not necessarily a good designer, and it cannot be asserted neither that a good designer can effectively design a product considering a field he or she barely knows. As such, the endeavor to ease the design process for any project involving SMs, entails making the knowledge[20] on SMs available in a way accessible and understandable by designers. Such knowledge would serve the purpose of instilling the basic behaviors and capabilities of SMs.
Once designers are familiar with the different kinds of SMs, they should be able to elaborate their design solutions. This requires modeling the behavior of SMs, so that these can be easily assigned to spatial regions and accurately simulated. SMs, especially those exhibiting deformation as a response, do not usually work by their own. Homogeneous parts made of a single SM do exhibit the basic capability offered by the material; combined with other either smart or conventional materials, they yield more elaborate capabilities. The hypothetical hydrogel actuators proposed by Westbrook and Qi [162] are a good illustration of this claim. As shown in Figure 4-1, depending on how hydrogel is arranged with another inert material, the behavior is totally different. For this reason, we posit that on top of modeling the behavior of the SMs themselves, modeling their distributions that allow specific changes must be included in the design with SMs pipeline. Nevertheless, in addition to be able to use generic/previous distributions of SMs, in order to achieve a prescribed functionality, designers should be able to derive/tune/optimize their own distributions to realize a specific functionality. Finally, all these contributions (knowledge on SMs, models of SMs, models of distributions and simulation) should be gathered in some kind of procedural design methodology consistent with the fact that SMs are actually *functional* materials.

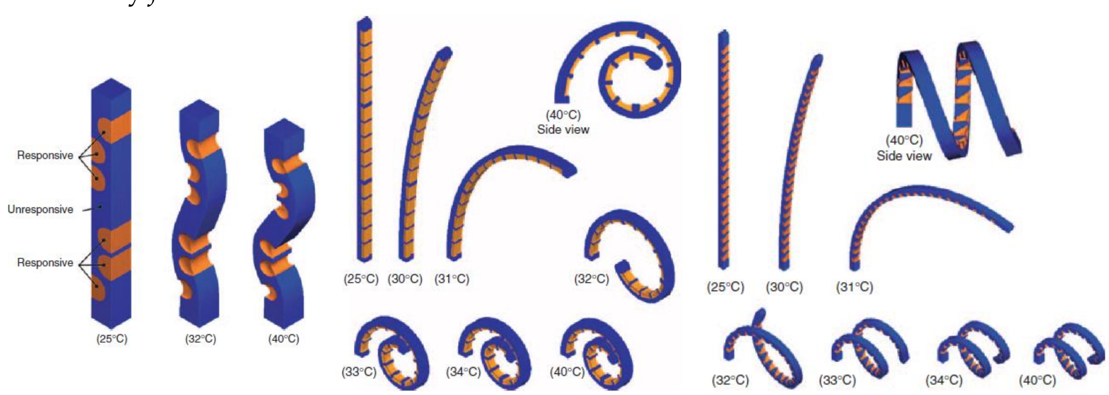


Figure 4-1 - Different arrangements of heat responsive hydrogel leading totally different funtions (adapted from [162])

[20] Throughout this chapter and unless stated otherwise, the word *knowledge* is not to be understood in the sense of ontology or know-how regarding a field or a product design (as it is for knowledge based systems). Rather *knowledge* is to be considered as information or more explicitly as the state or fact of knowing (as it could be in a handbook).

Given how essential SMs are to 4DP, there is a need to put forth a Design with Smart Materials (DwSM) ecosystem addressing the aforementioned design requirements (knowledge on SMs, models of SMs, models of distributions, simulation). This chapter is concerned with the knowledge aspect of SMs. It is intended to facilitate the consideration of SMs by designers, somewhat regardless of their background and as such the contribution would benefit designers beyond the scope of 4DP. More specifically the aim of this chapter is to address the lack of design knowledge on SMs, by:

- Simply letting designers know about SMs, in a way more explicit than "when the material is subject to stimulus X it provides the response Y",
- Letting designers select SMs for their applications, at the conceptual design phase,
- Let designers and material experts communicate in such a way that the former creativities can lead to new SMs discoveries or syntheses, and limitations on the materials expressed by the experts are well understood by the designers.

In this chapter, a proposal is first made about how SMs can be described for design activities, ways of determining SMs candidates for an application are proposed in the third section, finally a web application embodying this chapter's contributions is presented.

4.2 Proposal of how to describe SMs for design activities

Engineering designers, or more generally designers, do possess varying level of SMs knowledge. However they have a common background of the design activity and design tools. The goal of this research is to provide a design-oriented point of view on SMs. More specifically we aim at providing a generic description of the materials, also we endeavor to use functional representations and others abstracting techniques to makes the knowledge about SMs accessible to designers. A similar approach was taken by Nagel et al. [163] for biological systems. The so derived knowledge would serve the purpose of introducing the designers to the SMs' capabilities and also the purpose of providing all the information that are likely to ease the conceptual design phase of a SMs-based project and/or let designers make informed decisions in this phase.

4.2.1 Smart materials generic analysis

The background information on SMs provided in the literature review has shown the diversity in the behaviors of SMs. Nevertheless, they can be scrutinized from a unified point of view. In order to propose a way, or ways of making their design-related knowledge available, a generic analysis of SM is first conducted. This generic analysis entails: stimulus, response, behavior and functionality.

4.2.1.1 The stimulus

Important to the envisioned application is the stimulus the material is sensitive to, as this will somehow influence the application's architecture. Many stimuli are used to trigger a response in

SMs. As a matter of fact, each SM does have a *natural stimulus* that it is conventionally sensitive to, but the sensitivity of the material can be extended to other stimuli either by engineering the material or by using a stimulus-converter material (e.g. photovoltaic material to convert light into electricity, magnetocaloric material to convert a magnetic field into heat, any resistive material to be used as heater powered by electricity, etc.). Therefore for a SMs it is important to know its natural stimulus and others alternative stimuli that may be used (or that has been used) to trigger its behavior. Two characteristics are of interest to characterize the stimulus. These include exposure and its value.

Exposure.

This characteristic basically entails how the material must/should be exposed to the stimulus so that response is triggered. Two kinds of **exposure modes** can be distinguished: exogenous and endogenous. For the exogenous mode, the stimulus is applied from outside the material onto its boundary (e.g. triboluminescent materials) or part of it, while endogenous exposure is made from inside the material and is usually more efficient, this is the case for instance for electrochromic materials in which the electric current is provided internally to trigger a chemical reaction. By nature, some SMs respond to stimuli that are applied to them exogenously through a medium, however their structure or the shape they are given can be somewhat altered in such a way that the stimulus can be applied internally (as shown in [73]). This is the case when resistive wires are embedded into the material to provide Joule heating, as shown in Figure 4-2, or magnetic nanoparticules embedded in a polymer for magnetic heating [164].

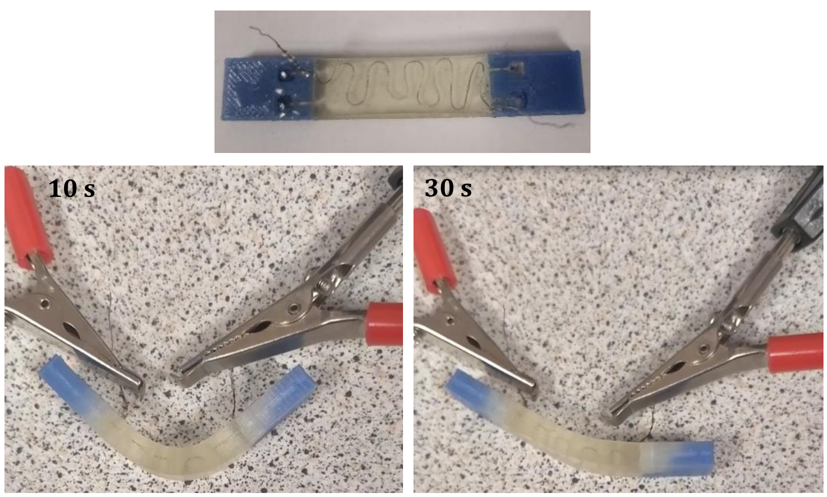


Figure 4-2 - Shape memory polymer activated internally by Joule heating. The thermochromic sections at the side are also activated.

Furthermore, application of the stimulus may be made remotely or it may require an actual medium for it to be applied. For instance photostrictive materials [165] or more generally light-activated SMs are inherently activated remotely as they respond to light (which does not require a medium to propagate), while thermochromic material for instance are, by nature, activated by heat which must be provided by a medium (usually water or a gas). Again for each SM there could be a natural **reaching mode** whichis related to the natural stimulus of the material. For instance SMA is naturally sensitive to heat and as such it naturally requires a contact with a medium for the stimulus to reach it. In return, magnetostrictive materials, as they are triggered by a magnetic field, can be naturally triggered remotely by the stimulus. Nevertheless as aforementioned, a SM may be altered to be responsive to a different stimulus and hence made

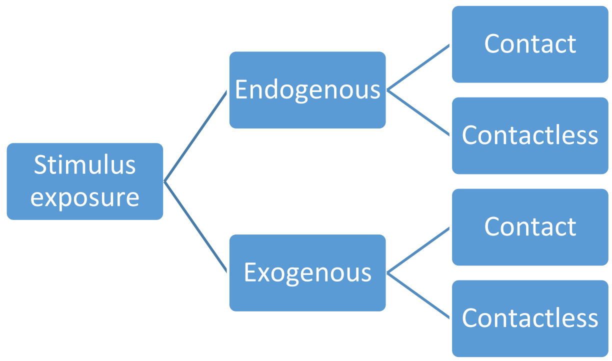


Figure 4-3 - Stimulus exposure typology

capable of a different reaching mode.

Value (or range of value) of the stimulus

While it is important to know how is the stimulus to be applied to the material, crucial to the project is also how much stimulus must be applied. What value of the stimulus is required? Can the actual value be anything around that value?

Applying the stimulus to the material may not necessarily trigger a response, or a noticeable response. Some SMs are sensitive to a stimulus as soon as this latter value is different from zero. This is the case for instance for photovoltaic material or piezoelectric material. The produced response may not be of a useful magnitude depending on the application made of the material. Other SMs can only sense stimulus whose value is beyond a certain value. Typically this is the case of SMPs for which there is a specific temperature by which shape recovery starts. For some others SMs (such as liquid crystal thermochromic materials) stimulus triggers a response only when it is within a certain range. These situations are illustrated in Figure 4-4.

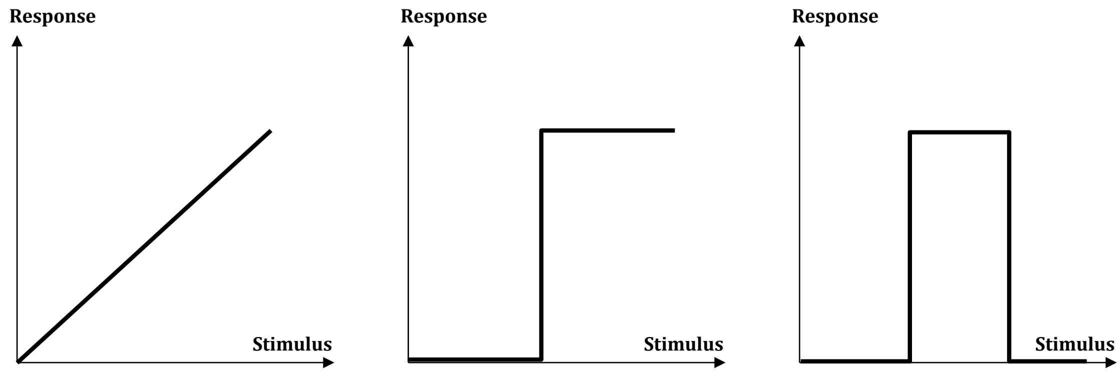


Figure 4-4 - The stimulus value

Regarding stimulus, SMs may then characterized by: a main stimulus, possible alternative stimuli, the way the material ought to be exposed to the stimulus and the required value of the stimulus for a response to be expected.

4.2.1.2 The response

Various responses can be produced by SMs and in many order of magnitude. Looking at the different groups of SMs presented in chapter 2, SMs may readily be characterized by the nature of response they produce. The produced response may be mechanical, thermal, optical, or electrical. Thinking of them in term of response's nature can be seen as a high-level approach in selecting them for an application and it expands the design space of the applications that can be made of them.

Furthermore, the types of responses provided by SMs can also be split in two categories: measurable responses and non-measurable responses. Typically all the materials in the shape changers, converters/sensors and state changers group do produce measurable response. In the optical sensors group, those materials emitting light can also be considered as exhibiting a measurable response: the emitted light can be quantified by its intensity and its wavelength. The only materials with non-measurable response are the optical sensors which change color, that is, the chromogenic materials.

Finally for materials with measurable response, the range of achievable values along with the conditions for getting these values is essential information for a designer. Without any alteration and in a homogenous form, how much response does the material produce? This is basically a quantitative indication of the produced change. Typically for shape changing materials this is the developed strain once the material is subjected to the stimulus. For light emitting materials, this could be the wavelength and/or the intensity of the emitted light.

In a nutshell a SM's response may be characterized by their nature, whether the response is measurable or not and, in case the response is measurable, the range of values achievable by the material.

4.2.1.3 *The behavior*

The material's behavior links the stimulus to the material's response.

History

One characteristics that is of interest in the material behavior is how the response varies according to the stimulus. This point has been somewhat addressed in the paragraph discussing stimulus's value. One may need to know whether the material respond continuously to the stimulus, in other words whether the response is a monotone function of the stimulus. Furthermore of importance is whether the stimulus need to be maintained for a response to be produced. The possible situations found in SMs are shown in Figure 4-5. For instance, regarding the direct piezoelectric effect, a dead load (i.e. a constant value of the stimulus) doesn't produce a sustained voltage, the load has to be dynamic for a voltage to be generated and maintained. A quite different relationship between stimulus and response is observed in the same material when considering the reverse effect, that is, strain developed in response to voltage: a constant voltage does produce a strain that is sustained and as soon as the voltage is turned off, the material returns to its initial shape. In others materials such as mechanochromic materials or electrochromic materials, the stimulus doesn't need to be maintained for the material to stay in its excited state: when the stimulus is turned off, the response is maintained, a characteristic which, depending on the application, may be seen as energy-efficient.

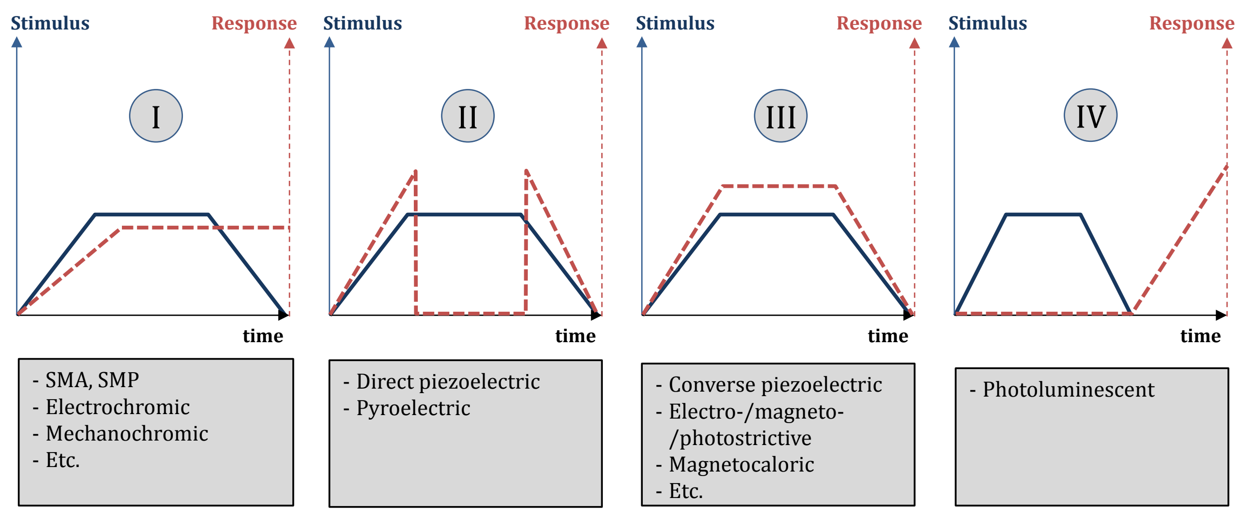


Figure 4-5 – Possible types of relationships between response and stimulus

Reversibility

Once a material is triggered at a point where it changes state. Does removing the stimulus or applying another stimulus (another kind or another value of the same kind) brings the material back to its initial state without any other intervention? Roughly is the material behavior reversible? The answer to that question is not necessarily dictated by the relationships between stimulus and response shown in Figure 4-5: while reversibility is found in type II and type III materials, in type I and IV materials, it depends on the material. Bringing back the material to its initial state, may not be possible (e.g. conventional SMP) or may be possible by reversing the stimulus value (e.g. electrochromic material) or by applying another stimulus (e.g. heating some mechanochromic materials which has been deformed brings their original color back). Depending on the application, reversibility may be a requirement (e.g. in actuators). Some materials whose behaviors are naturally non reversible can be engineered to be reversible, this is the case for instance for SMP [58]. In the same vein others materials which are conventionally reversible may be chemically tuned to be irreversible (e.g. thermochromic materials in some medicines packaging, medicines that must stay below a certain temperature to be usable).

Speed

How fast is the response's change once the stimulus is applied or removed? Some SMs respond as soon as the stimulus is applied, others some time to exhibit the expected response.

Fatigue

In case the material's behavior is reversible, can it be triggered indefinitely? In most materials there is some functional fatigue which limits the number of cycles that can be achieved without any capability's loss. Even in the case of materials whose behaviors are semi-reversible (such as conventional SMP) there is a functional fatigue.

4.2.1.4 Functionality

As stated by Burman et al [103], SMs are actually functional materials. An object has a primary function and other secondary functions which form a breakdown of the primary function. Hirtz, et al [143] have classified the basic functions a product can fulfill in eight group including: branch, channel, connect, control magnitude, convert, provision, signal and support. Furthermore, in addition to fulfil functions, a product is also characterized by the functional flows it processes. These are, at their lowest level of specificity material, energy and signal [68].

As functions providers SMs can also be classified from a functions basis point of view. Based on the groups presented in Figure 2-5, one can easily state that functions provided by SMs can be clustered within the functions: sense, actuate, convert and dissipate. However, for a thorough function-wise characterization of SMs, an approach could simply consist in collecting all the basic functions they have fulfilled and flows they have processed in the applications that have been made of them so far. In such way a vision of SMs purely from a functionality perspective can be provided to designers, a vision which would facilitate the generation of concepts based on SM.

This functional aspect of SMs can be captured in two different manners:

1. Material analysis: looking at the basic behavior of some SMs, on can easily state what basic functions they are likely to fulfil and what flows they are likely to process. For instance, electrochromic materials can fulfil the functions: indicate, display, track, convert etc. They can process the flows energy and signal. A functional representation of electrochromic material, based on the material analysis, may be the one shown in Figure 4-6.a.
2. Applications' knowledge[21] capturing: by analyzing how a SM has been used in an application, and more specifically which functions it has fulfilled, one can also easily capture its functional aspect. This aspect may be different from the one dictated by the material's basic behavior in that some kind of reasoning (one could say ingenuity) may have occurred before the material has been selected to fulfill a function or the material capability may have been somehow tweaked or enhanced to perform the desired functionality. Looking again at electrochromic materials, used for the B-787's windows (cf. Figure 4-8), one can easily find another functional representation of the material, a representation quite different from the basic one. Indeed in that application the material could have been chosen to fulfil the functions: control, attenuate, reduce, protect, shield. It processes the flow energy in form of light (or electromagnetic wave). Another functional representation of the material can be as shown in Figure 4-6.b.

The more such functional representations of a SMs are available, the easier these can be used in industrial applications.

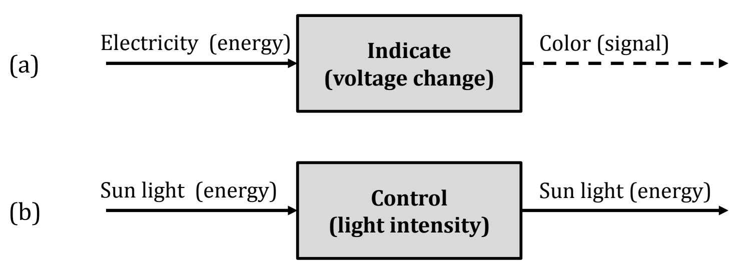


Figure 4-6 - A functional representation of electrochromic materials based on (a) material basic behavior, (b) material use in an application

Furthermore, the field (e.g. medicine as for minimally invasive surgery, defense, aircraft, etc.) is another way of looking at SMs from a functionality perspective. While some materials such as

[21] *Knowledge* in this context can be understood as *know-how.*

magnetorheological materials are more confined into automotive, building industries others SMs such as SMPs or hydrogels have potentials in medicine.

4.2.1.5 General material properties

As materials, SMs do possess others general properties that could make them suitable for an application or not. These include and are not limited to: type of material (e.g. polymer, metal, etc.), cost, availability, manufacturing processes. For this latter, in a 4DP context, it is of high interest to know whether the material can be processed with AM or not. As shown in the literature review the range of SMs commercially available in a form that can be processed by AM is rather limited: only thermochromic materials (in filament form for FDM) and SMPs (in resin form for SLA and filament form for FDM) are today commercially available. The others SMs that have been printed, require specific material preparations. Nevertheless, allowing designers to consider SMs is definitely a way of pushing printable SMs from laboratories to the market.

4.2.2 Smart material description

Based on the previously conducted generic analysis, we proposed a data-structure for describing SMs and which is both essential for understanding the materials, especially for non-experts, and for determining them as potential candidates in applications. The fields making up this data-structure are clustered in five groups (as shown in Figure 4-7); each corresponding to the five aspects of SMs discussed in the previous section.

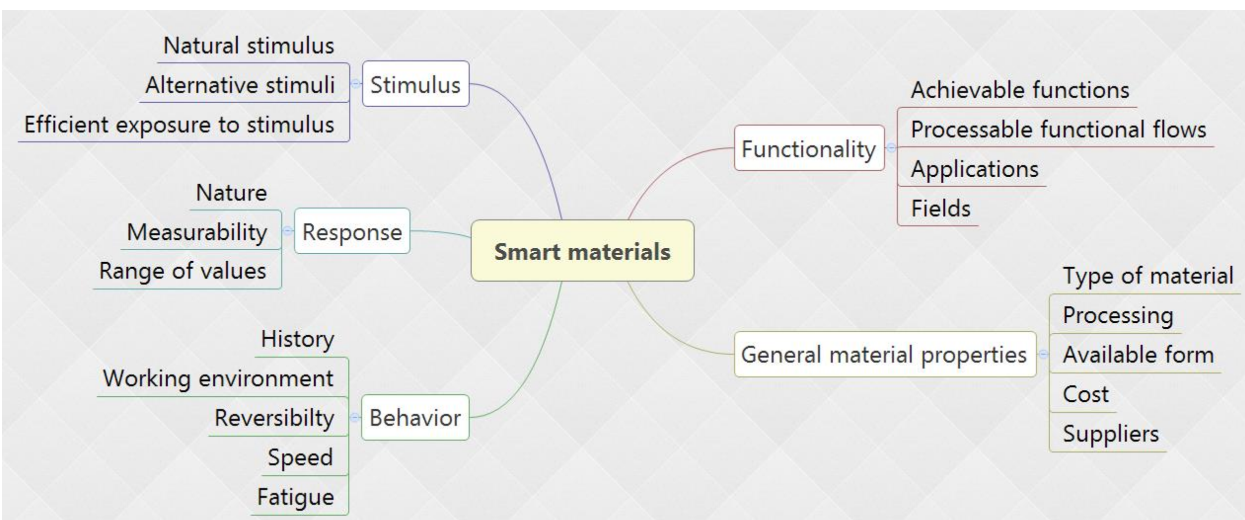


Figure 4-7 - The proposed data structure for smart materials description

This data-structure typically capture all the design-related information on a SM. As such describing any SM with these fields, in addition to a bit of explanation on how they work, would be sufficient to let designers know about them and consider them for innovative applications.

4.2.3 Proposal of ways of making the knowledge available

A generic analysis of SMs has been conducted from a design perspective and a data structure describing them has been derived. How can the so highlighted specificities of SMs be made available in a form that is easily accessible to designer? We have proposed three ways for making the design oriented knowledge on SMs readily accessible. These include text information, animation and interactive simulation. Essentially, all the data from the proposed data-structure can be made available in text form. Animation and interactive simulation are mainly for capturing the dynamic aspect of a SM.

Text information

This description form includes a qualitative description of the material and all the data in the proposed data structure. A template for providing this text information is provided in appendix A.

Animation

For conventional materials, text information providing a few material properties is sufficient to capture all that a designer needs to gage the suitability of the material. For SMs such static information may not be enough. Furthermore even a qualitative description (as proposed in the text information form) may not be enough to instill a detailed understanding of the material specificity. For these reasons, we proposed to describe SMs in the form of short animation as well. Basically such animation shows a sample of the SM or a simple application made of it and shows how the material does actually behave upon exposure to the stimulus.

Interactive simulation

Knowledge is better taught or instilled when it can be made somehow tangible. Furthermore, there is no a better way to learn about a system's behavior than interacting with it. In regards to SMs, the best way to provide this, would be through physical experiments. However the costs of these materials may – in some cases – hinder such experiments, or the experiments may not be easily feasible. Another alternative to strengthen the knowledge acquired (through either text or animation or both) on SMs may be through interactive simulation where designers can virtually "tinker with" components made of these materials, a distribution of the materials, the stimulus, etc. and observe how these components behave. While this way of acquiring knowledge cannot be credited to be the best, it is nevertheless a good surrogate for real experiments, and it has yielded significant benefits in teaching physical concepts [166].

4.3 Identification of SMs for design: how should it be performed to support SM-based concepts generation?

An important step in the journey towards prompting designers and engineers to consider SMs (and ultimately 4DP) has been made by summarizing the design aspects of SMs. More can nevertheless be done to promote SMs use by designers and that is related to the design process itself, especially the conceptual design phase. SMs' identification[22] for concept generation should be facilitated, so that designers have hints of where they could start generating a SM-based concept from. The goal is to generate a shortlist of SM that may suit application needs, based on criteria such as responsiveness (stimulus and response), functionality, environment, etc.

Figure 4-8 - Aircraft windows: (a) conventional design - (b) electrochromic material based design on B-787 Dreamliner

Let's first recall that the use of SMs in a design can have a tremendous beneficial impact on a product's final architecture. See for instance the Boeing 787 Dreamliner windows. To fulfill the "block light" function, aircraft windows are conventionally equipped with a sliding closing (as shown in Figure 4-8.a). Now the 787 windows have been designed differently by taking advantage of electrochromic material. Boeing designers came up with a simpler architecture and most importantly a lighter solution. The function is now fulfilled with a coating made of electrochromic material whose opacity can be controlled by a voltage. Passengers simply use buttons to control that voltage (cf. Figure 4-8.b). This saves number of components in the window and considering the 787-8 for instance with its 72 windows this is a non-negligible weight saving. How could a designer come up with such innovative solutions? We propose two

[22] Material identification is different from material selection in that it is made in the conceptual design stage when there is not a geometry yet. The goal in material identification, being to find potential material candidates for the envisioned applications. For further details between material identification and material selection the reader is advised to refer to: 167. Deng, Y.M. and K.L. Edwards, *The role of materials identification and selection in engineering design.* Materials & Design, 2007. **28**(1): p. 131-139.

approaches for easing or facilitating SMs based concept generation. Both are related to SMs identification and are explained in the following subsections. In both strategies, all the SMs are assumed to be stored in a database using the proposed data-structure.

4.3.1 Explicit smart materials identification

In this approach, we assume that the designer has already chose to use SMs for the concept. To keep the problem open, the material search is simply made by specifying a set of desired characteristics based on the data structure of SMs proposed in section 4.2. For the envisioned application, the designer may require a material based on stimulus, response, reversibility, or working environment, etc. Basically any of the characteristics defined in the data structure may be used. The more criteria are specified the more suitable for the application are the generated SMs candidates likely to be. In the same time, too much specified criteria are a way of restricting the number of candidates. Therefore some kind of compromise should be made on specifying the criteria. Two strategies can be adopted about how a shortlist of SMs candidates are generated.

The basic strategy entails generating first independent lists of materials meeting the chosen criteria one by one and then intersecting these lists to find materials meeting all the criteria.

While straightforward and pretty fast, this first approach has the drawback of being too restrictive in that a candidate material meeting all the criteria except one would not be shortlisted. Furthermore, depending on the requirements some SMs in the generated shortlist may be more suitable than others, a distinction that cannot be seen in such a shortlist. An alternative strategy is one that is based on scores. In this strategy, the designer specifies for each of the chosen criteria a rating on a 0-5 scale, gaging how important is the criterion to the project. Based on all the ratings a weight is computed for each criterion. Then each of the database materials is evaluated on each criterion. The material's evaluation is made by giving it a grade for each criterion, a grade (on a common scale) gaging how much it meets the criterion. Using the computed weights a final grade is assigned to the material and the selected materials are ranked according to that final grade. A number limit may be set in order to state the number of materials that must be retained in the shortlist. With this strategy more candidates can be selected and it is guaranteed to identify best materials candidates for the envisioned product.

4.3.2 Functional structure based smart materials identification

When designing a new product, an efficient way of not overlooking innovative solutions is by designing with functions, or more explicitly by detailing the basic functions the product must fulfill for its main functionality to be fulfilled. This helps for gaining "a detailed understanding at the beginning of the design project of what the product-to-be is to do" [158]. This is conventionally done by describing the product functional structure (FS) or performing its *function decomposition*. Basically this is a breakdown of its main function into basic functions, in addition these functions are connected by flows (which, at their lowest level of specification, are energy, signal and material [68]). Example of such FS is shown in Figure 3-5. The FS is then used to generate concepts in such a way that all of the required functions are fulfilled by the concepts. Recall that SMs are sometimes referred to as *functional materials*. This is simply because in the applications that made use of them, they basically fulfill some of the functions in the applications' FS.

The basic idea behind SMs identification based on FS is that SMs candidates can be determined simply by scanning through the product's FS and by recognizing function/flow combinations. This is where the description of SMs in term of functionality (subsection 4.2.1.4, page 96) finds its best utility. The procedure to identify SMs candidate for a concept is outlined in Figure 4-9. From the product main functionality, the product's FS is first defined. This definition is done using the same base for functions and flows as the one used to describe the SMs in the database. Doing so is a way of ensuring consistency in how the knowledge on SMs is stored and how it is expected to be retrieved. The FS is then submitted to a search engine that is connected to the SMs database and which scans through the FS to recognize patterns of SMs' in the form: *input flow – function –output flow*. To somehow make the identified set of SMs candidate, specific to the envisioned application, requirements directed by the design problem may be specified to the search engine. For instance, the designer may require the SMs to be 3D printable, to work in a wet environment or to be biocompatible. Some of the returned SMs candidates may not at first seem trivial in fulfilling the recognized functions; in such case consulting the material's description and particularly the applications made of it can help in understanding how to use the material for the recognized pattern.

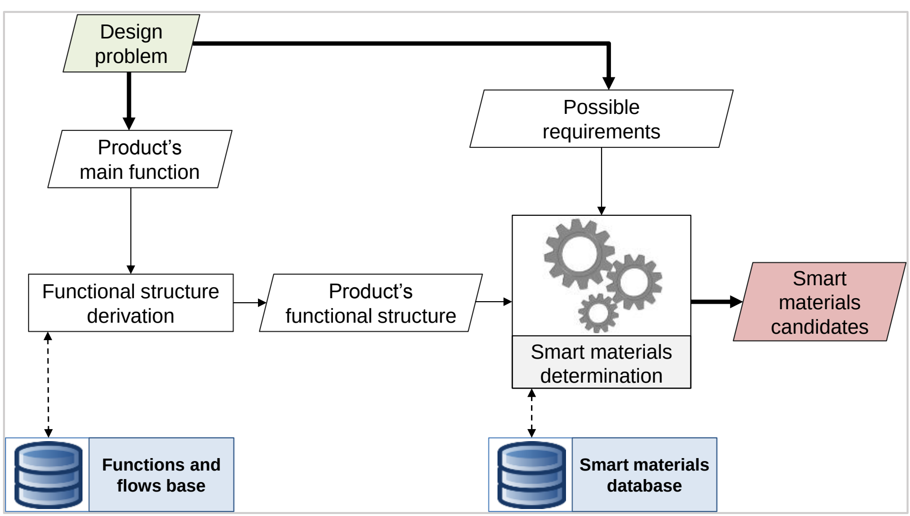


Figure 4-9 - Smart materials determination based on functional structure

The more functional representations of SMs (as described in subsection 4.2.1.4) are available the higher are the chances of identifying SMs that may fulfill functions included in the product's FS.

4.4 Embodiment: *smarterials.app*, a web application supporting SMs based designs

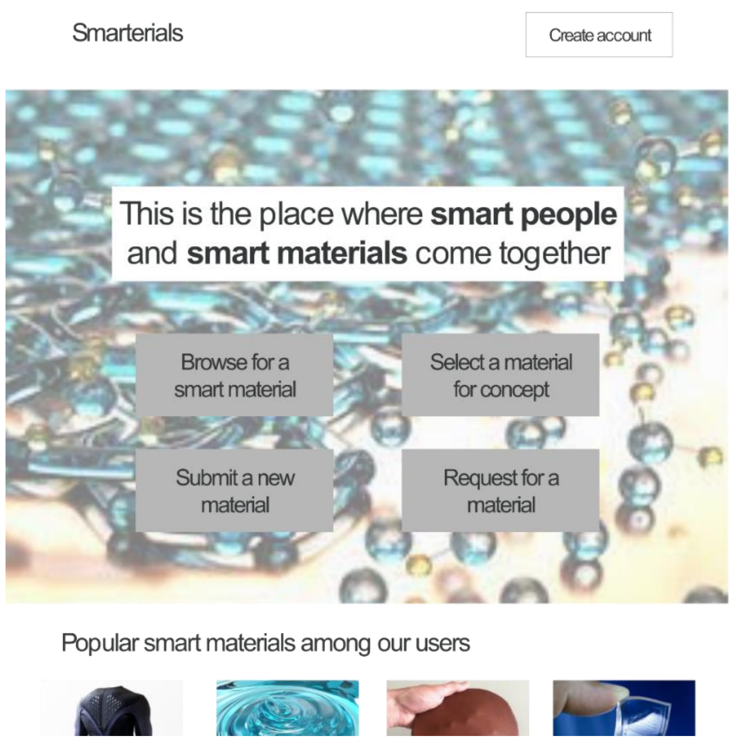


Figure 4-10 - smarterials.app: a web application for smart materials

The contributions proposed in this chapter for enabling designers to consider SMs, has been materialized through a web application: smarterials.app[23].

This application aims at bridging the gap between SMs laboratories and design offices. More specifically it is a living database on SMs to let designers know them and to use them in their applications. As shown in Figure 4-10, it has four use modes:

1. *Browsing the smart materials*: main mode for discovery, learning of SMs. Basically, in this mode, designers (supposedly SMs novices) can understand in detail the behavior of SMs, and see applications. The materials are here described in the three form proposed in section 4.2.3.
2. *Selecting smart materials for a concept*: mode for identifying SMs candidates at the beginning of a design project.

[23] At the time of the thesis printing, the web application is still in prototype stage

3. *Submitting a new smart material*: to enrich the database, it is assumed that materials experts can fill a form to add a new SM; the material datasheet will then be validated by the managers of the site before publication.
4. *Request for a material*: It is assumed that some designers will be able to come up with the idea of a SM that does not exist by describing their capabilities and potential use in an application. Material experts can then consult these queries and orient their researches accordingly.

For the *Browsing the smart materials* mode, there are several views:

- *Group*, here materials are gathered within groups reflecting their "smartness". Clicking on one of the groups takes the users to a page where the materials of this group are displayed. The materials may then be selected to consult their data.
- *Stimulus* > *Response*, like the wheel shown in Figure 1-7 (page 11). Clicking on one of the materials will lead directly to its data.
- *Stimulus*. In this view, all the stimuli that SMs are sensitive to are displayed. Clicking on one of the stimuli then leads to a page showing all materials sensitive to that stimulus. The choice of a stimulus basically leads to all materials sensitive to this stimulus. On that page, each stimulus is presented by an icon, at the bottom of which there is the stimulus name.
- *Response*. Similarly to *stimulus* mode, the choice of a response leads to all the materials having this response. Responses are classified according to their nature: electrical, magnetic, optical, thermal, mechanical, chemical.

Below is an example of how a material is presented.

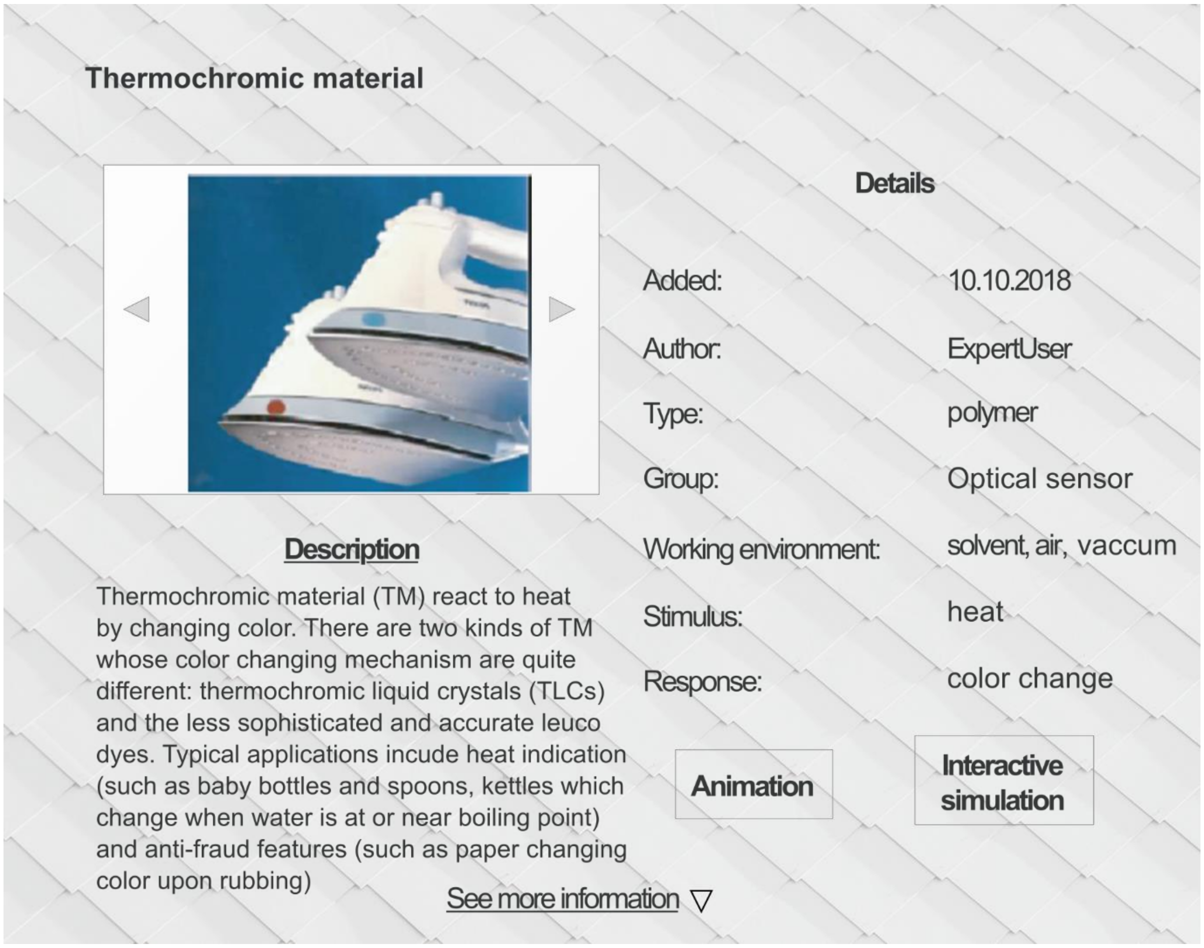


Figure 4-11 – Thermochromic material as presented in the application

Basic information is provided on the material. The user can scroll left and right some images showing the material. A short text explaining the material behavior is provided and user can choose to extend this view to consult all the information. Two other buttons allow the user to see the animation illustrating the material behavior and the simulation that allows him/her to experience what the material is capable.

4.5 Conclusion

In this chapter a contribution has been made to bridge the gap between SMs experts and designers. SMs have been scrutinized from a design perspective (rather than the usual material and manufacturing processes perspective). The goal was to establish a vision on SMs that can easily help designers at understanding the behavior (capabilities and limitations) of SMs. Ultimately the pursued goal was to foster consideration of SMs based products, a requirement for a 4DP way out of laboratories. For this latter goal a proposal has been made regarding SMs identification at conceptual design stage. Basically, the generation of a shortlist of SMs candidates that can suit an application. A website prototype (still on construction) has been proposed to materialize this design oriented vision of SMs.

Chapter 5 Design with smart materials (DwSM) 2: Voxel-based modeling and simulation of shape changing smart materials

5.1 Introduction

Since its discovery in 1987 (under the stereolithography apparatus patent [168]) additive manufacturing has evolved from a prototyping process to a fully established manufacturing process. Mainly praised is its shape complexity characteristic, indeed thanks to this capability shapes that are infeasible with conventional (subtractive) manufacturing processes are now manufacturable. In addition to shape complexity, other characteristics are among the 3D printing revolution engines: hierarchical complexity (features size at almost any length scale can be realized within the same part), functional complexity (mechanisms – with sometimes embedded electronics – can be manufactured without any assembly operations as shown in Chapter 3), and material complexity (parts with any material distribution and properties are now feasible). This latter capability – such as reviewed in [123] – is best illustrated with the PolyJet [53] AM technique. This technique works by selectively depositing tiny droplets of UV curable resins, by smoothing them in thin layers and by curing these layers. Up to 3 base resins can be mixed into any ratio to generate materials with a large range of properties including color, transparency, shore hardness, and many others. The obtained mixtures are the so-called *digital materials*. Parts with almost any material distribution (and thus multiple properties) can then be printed. Figure 5-1 (a) shows an illustration of a multi-material part made by the PolyJet technique. The material complexity allowed by AM has been further demonstrated by Katsumi et al. [169] who developed a 3D printing machine for depositing metal. Their machine has been used to manufacture a functionally graded material whose properties range from a metal (with low meting temperature) to a polymer as shown in Figure 5-1 (b).

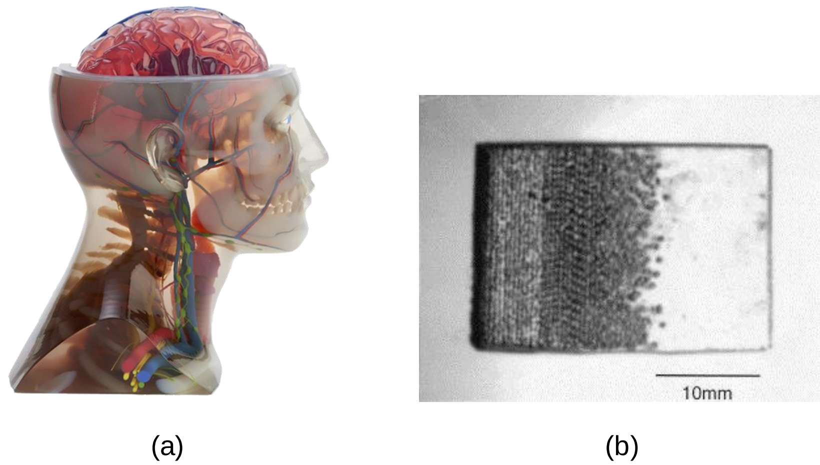


Figure 5-1 - Additive manufacturing's material complexity demonstrated by (a) a PolyJet printed model of human head [53], and (b) a functionally graded material made of metal and polymer [169]

In addition to the widely praised shape complexity allowed by AM, material complexity is expanding further the design space now available to designers, making creativity and imagination the main barriers. When the kinds of materials involved are taken into consideration the design freedom is more enlarged. In addition, the design space allowed by AM is being expanded further thanks to the interaction AM – SMs, which has been coined as 4D Printing [20]. Here SMs are materials whose state changes upon exposure to a specific stimulus. These materials owe their smartness to both what they are sensitive to and how do they respond to the stimuli. Examples include thermochromic materials, which change color under heat, magnetostrictive materials which deform upon exposure to a magnetic field or electrorheological fluid whose viscosity change with electricity. The characterization of their smartness can also be extended to whether their behaviors are reversible or not as explained in Chapter 4. The aforementioned material complexity of AM has been a main catalyst of what can be called the "4D revolution" making the AM-SMs interaction an attractive research topic; indeed despite its infancy, many review papers have already been published on the topic [26, 170-172]. What is sought through the use of SMs as raw materials in AM is basically to imbue structures with a smart behavior, in such a way that the material is/becomes the mechanism [173], and a passive source of energy (available in the environment or supplied internally) is what moves the mechanism[24] to produce the desired/designed behavior. Questions that may then arise include: can one single SM be sufficient to produce a desired behavior? If no, what other materials should be combined to it? How can SMs be 'mixed' to produce a behavior? Etc.

[24] The word mechanism here is not necessary to be understood as a machine or a mechanical device, but rather as 'the agency or means by which an effect is produced' (https://www.thefreedictionary.com/mechanism)

Answers to these questions may be found by analyzing the following examples. The helical part presented in [28, 99] is made of an inert polymer material and many other shape memory polymers (SMPs), which differ by their glass transition temperature (Tg), a specific temperature at which shape recovery is triggered. In this part, depicted in Figure 5-2(a), the material distribution is such that the part behavior is sequential: only the hinges are made of SMP, in such a way that their glass transition temperatures increase outwards; this material distribution is such that, at a temperature higher than all the Tg, the hinges shape recoveries (from the deformed straight shape to the permanent bent shape) occur sequentially, ensuring thus a successful shape recovery of the whole part. Another example, shown in Figure 5-2(b), is a part printed in our laboratory with SMP and a thermochromic material. Using the environment's medium (water) as heat provider, the material distribution is such that the thermochromic material turns totally white when the shape recovery of the SMP sections is complete, and it turns back to blue when cold indicating that the SMP material is rigid again. One more example whose material distribution is finer, more intricate and less intuitive than the previously described, is the one presented in [111], and depicted in Figure 5-2(c). This hypothetical part combines heat-responsive hydrogel and photo-sensible fibers. When the fibers' material is uniformly distributed in the gel, heat and light all have the effect of uniformly contracting (no bending) the gel, but when the fibers are used and the composite is not fixed on a surface, it contracts like an accordion under the effect of heat and bends when illuminated. These examples have prompted us to posit the idea that a 4D printed item owes its functionality mainly to the specific material distribution that it is made of; in other words one material distribution equates to one concept. Material distribution is then of high importance when it comes to design the material-is-the-mechanism like structures. This still holds even when SMs are not involved: a specific distribution of the same (conventional) material with void can yield unconventional behavior, which is well demonstrated by the so-called metamaterials [30, 174]. Such SMs-based examples support the idea that SMs combined with other materials lead to smart behaviors more complex than when taken alone. In a nutshell, considering the case shown in Figure 5-2(c), designing the right distribution may be a challenging task, unless being SM experts. Designers, which are more likely to find innovative 4DP-based concepts, may not be enough equipped to embrace this new design freedom.

In view of the above, it would be relevant to be able to compute materials distributions for simulating smart behaviors embedded into a physical part. Such efforts are needed in order to design smart products able to shift from one state to another and vice-versa via a stimulus provided internally or externally. This research issue requires efforts in a threefold manner:

- *Distributions reuse*: using a predefined distribution (whose behavior leads to the desired state change) and apply it to one of the states;
- *3D painting*: an explorative approach consisting in patterning freely the materials and simulating the so obtained distribution until the outcome meets the desired change;

- *Distribution computation*: in a topology optimization-like [175] manner, computing the appropriate material distribution.

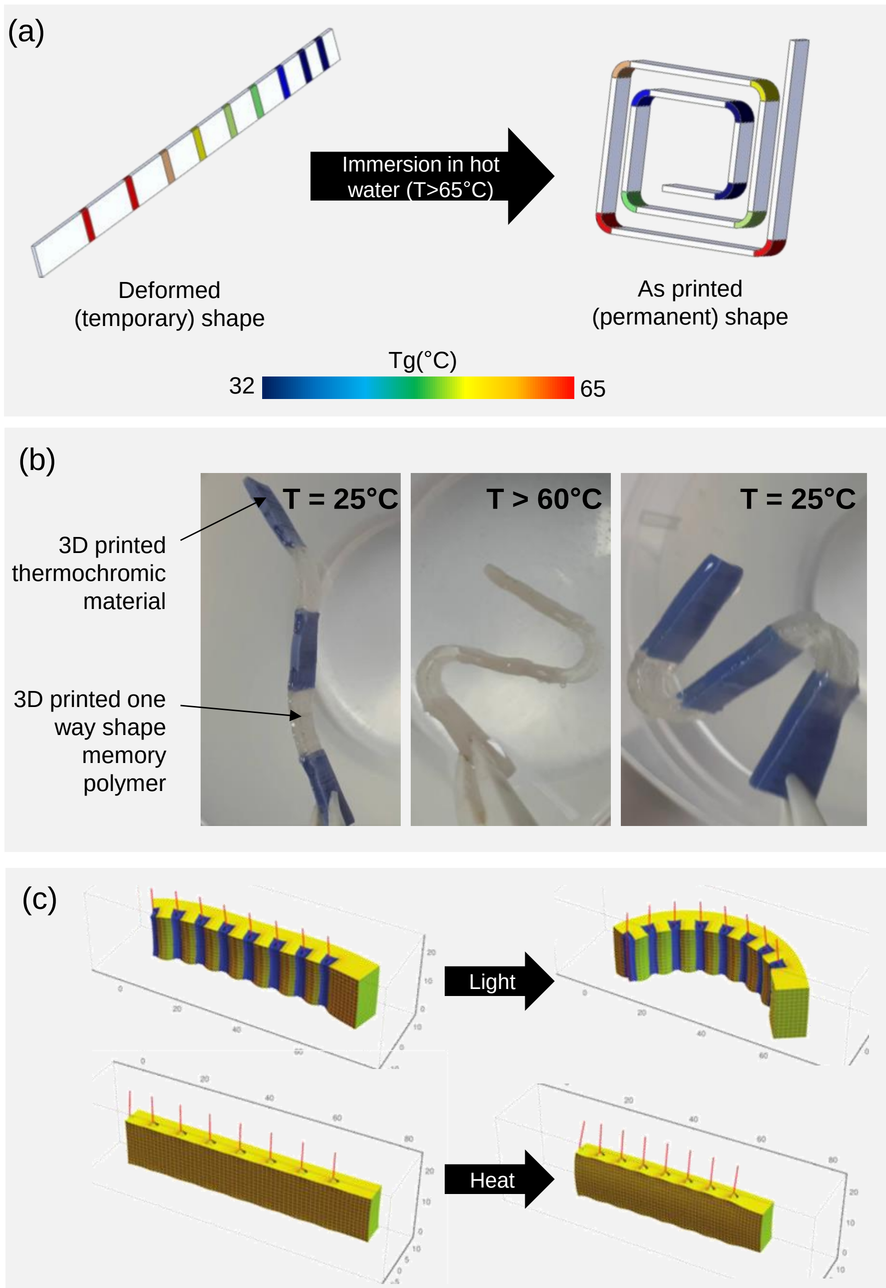


Figure 5-2 - Functional smart material distributions: (a) shape memory polymers distribution triggering a sequential behavior (adapted from [28]) – (b) 3D printed distribution of thermochromic polymer and shape memory polymer – (c) Hypothetical distribution combining heat-responsive hydrogel and photo-sensible fibers(adapted from [111])

Here the attention is focused on the last two solutions, especially for the case of SMs whose response induces a change of shape. As the existing approaches for determining SMs distribution are rather *ad hoc*, this research work aims to provide a methodological approach to this problem along with a supporting computational tool in the early phases of the product design process. The chapter is organized as follows: in section 2 the building blocks of our proposed approach are delineated and validated, section 3 presents an implementation of the proposed SMs modeling and simulation framework. A fourth section is dedicated at material distributions computation with the proposed modeling scheme. Finally conclusions are drawn on the proposal.

5.2 Matter modeling framework using voxels [176]

The proposed modeling framework is intent to be used in the conceptual design phase. It is targeted at rapidly knowing how a material distribution would behave. As explained in the introduction section, regarding SMs, one material distribution generally equates to one concept. The explorative *3D painting* approach to determine a distribution – that is, the ability given to designers to pattern materials in any arrangement in order to test their distributions' behaviors – makes it paramount to work on a framework which is quite fast (not too computationally costly). Moreover, this need for rapid iteration should not be at the cost of accuracy, even though the focus is mainly on a qualitative answer of how a given distribution would behave or what distribution would yield a prescribed behavior. For such modeling framework to be as physically realistic as possible and easily usable, it is required to:

- *Reproduce actual behavior of matter* – i.e. any deformation must be physically plausible.
- *Be volumetric*, as shape is involved – The actual three-dimensional shape of any modeled distribution should be reproduced.
- *Be sensitive* – Its behavior should be driven by changes in the environment. It must depend on variable measuring how much stimulus is sensed, so that behaviors are triggered accordingly.
- *Capture the actual behavior of the modeled SM* – Again, while the focus is not on accuracy, the proposed models for SMs should be based on their existing constitutive equations.

5.2.1 Continuum mechanics modeling setup for conventional matter

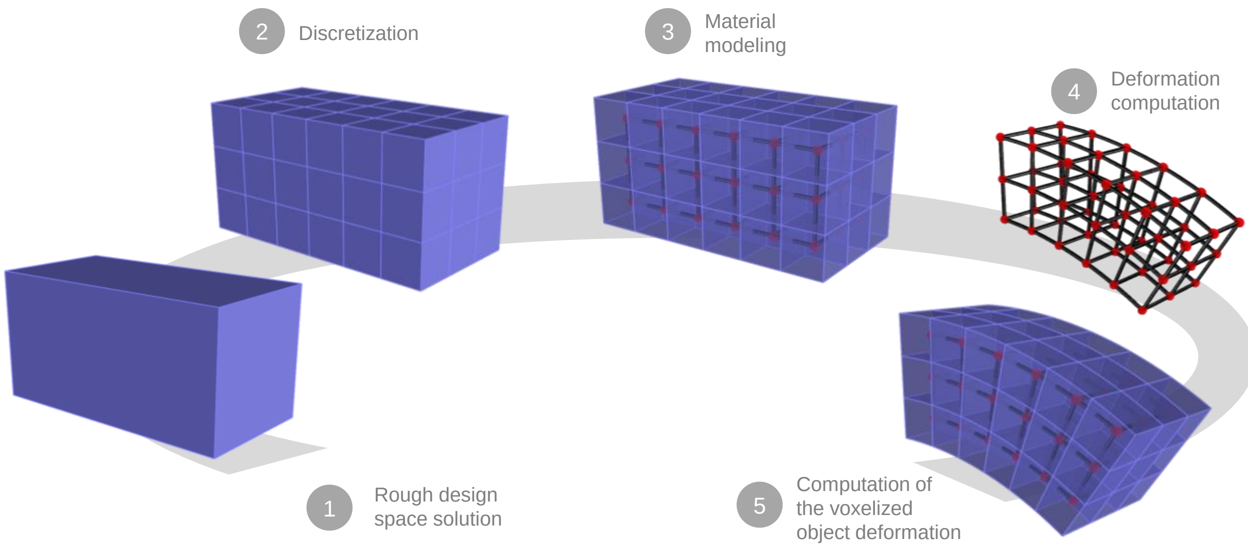


Figure 5-3 - Continuum mechanics modeling setup

As shown in Figure 5-3, the proposed approach for modeling conventional material behavior is organized in five main steps: (1) definition of rough design space, (2) discretization, (3) material modeling, (4) deformation computation and (5) Computation of the voxelized object deformation. These steps are described in the following subsections. Such approach assumes that material properties in a single voxel are homogeneous, i.e. a voxel is made of a single homogeneous material.

5.2.1.1 Discretization

Here an approach similar to mass-spring modeling has been considered to simulate the mechanical behavior of matter. First of all, the geometry to be simulated is first discretized – regardless of its (possible or intended) material distribution – into equally sized cubes: the voxels. Such representation and discretization of matter, despite being – depending of the chosen voxel size – at the cost of the accuracy of the represented geometry, allows for a finer control over the material distribution. In addition, chunking a shape into voxels does make the process of specifying a material distribution more intuitive compared to the use of spatial field functions [177] or others explicitly defined material functions [178]. As a shape is physically involved, spatial reasoning helps the cognitive aspect of the design process.

Voxels are connected (from their centers) not by springs but by three-dimensional beams. These beams form a 3D lattice frame, which acts as a backbone (or a control structure) of the whole shape. As they are extending from center to center, the beams are then initially of a voxel size. The frame is what "holds" the matter together and that governs the deformation of the whole geometry.

The idea of using a 3D lattice frame as a control structure of the whole shape is somewhat inspired by skeleton driven animation or more generally *skinning* [179]. Skinning (in computer graphics) is a set of techniques for manipulating a shape.

5.2.1.2 *Material modeling*

Each voxel is assumed to be homogeneous and made of a single linear and isotropic material. Thus, the material properties required to fully characterize its mechanical behavior are limited to Young modulus (E) and shear modulus (G). As explained in section 5.2.2, for SMs, other material properties are added to account for their stimulus-responsive behavior.

As it is the frame deformation, which drives the object deformation, voxels materials properties should be mapped to the beams material properties. To account for this, we have used an inheritance scheme: beams materials properties are inherited from the pairs of voxels they are connecting. In case where two voxels are made of the same material, the beam material properties are the same but when two voxels are of dissimilar materials, composite values for the material properties are used, as described by the formula:

$$E_c = \frac{2E_1E_2}{E_1 + E_2}, \qquad \text{and } G_c = \frac{2G_1G_2}{G_1 + G_2} \tag{5.1}$$

5.2.1.3 *Deformation computation*

Computation of the skeleton frame deformation (Step 4 of Figure 5-3)

The beams forming the whole frame are modelled as 3D Euler-Bernoulli beams which resist axial, bending and twisting actions. Let l denote, the voxel size. The cross-section properties of the beam (assumed to be along the X axis) are approximated as follows:

- Beam moments of inertia about the neutral (x) axis:

$$I_{yy} = I_{zz} = I = \frac{b \cdot h^3}{12} = \frac{l^4}{12} \tag{5.2}$$

- Beam moment of inertia characterizing torsional rigidity:

$$J_{xx} = J = \frac{bh(b^2 + h^2)}{12} = \frac{l^4}{6} \tag{5.3}$$

- Cross section area: $A = l^2$

The direct stiffness method [180] is used to compute the frame's degrees of freedoms (DOFs) and subsequently its deformed shape. Each node (again, which is a voxel's center) has six DOFs and the stiffness matrix for a beam oriented into the positive x direction is expressed (in its local coordinate system) as follows:

$$\overline{K_e} = \begin{pmatrix} R_a & 0 & 0 & 0 & 0 & 0 & -R_a & 0 & 0 & 0 & 0 & 0 \\ 0 & R_{z3} & 0 & 0 & 0 & R_{z2} & 0 & -R_{z3} & 0 & 0 & 0 & R_{z2} \\ 0 & 0 & R_{y3} & 0 & -R_{y2} & 0 & 0 & 0 & -R_{y3} & 0 & -R_{y2} & 0 \\ 0 & 0 & 0 & R_x & 0 & 0 & 0 & 0 & 0 & -R_x & 0 & 0 \\ 0 & 0 & -R_{y2} & 0 & 2 \cdot R_y & 0 & 0 & 0 & R_{y2} & 0 & R_y & 0 \\ 0 & R_{z2} & 0 & 0 & 0 & 2 \cdot R_z & 0 & -R_{z2} & 0 & 0 & 0 & R_z \\ -R_a & 0 & 0 & 0 & 0 & 0 & R_a & 0 & 0 & 0 & 0 & 0 \\ 0 & -R_{z3} & 0 & 0 & 0 & -R_{z2} & 0 & R_{z3} & 0 & 0 & 0 & -R_{z2} \\ 0 & 0 & -R_{y3} & 0 & R_{y2} & 0 & 0 & 0 & R_{y3} & 0 & R_{y2} & 0 \\ 0 & 0 & 0 & -R_x & 0 & 0 & 0 & 0 & 0 & R_x & 0 & 0 \\ 0 & 0 & -R_{y2} & 0 & R_y & 0 & 0 & 0 & R_{y2} & 0 & 2 \cdot R_y & 0 \\ 0 & R_{z2} & 0 & 0 & 0 & R_z & 0 & -R_{z2} & 0 & 0 & 0 & 2 \cdot R_z \end{pmatrix} \tag{5.4}$$

Where:

$$\begin{cases} R_a = \dfrac{EA}{L}, R_x = \dfrac{GJ}{L} \\ R_y = \dfrac{2EI_{yy}}{L}, \quad R_{y2} = \dfrac{6EI_{yy}}{L^2}, \quad R_{y3} = \dfrac{12EI_{yy}}{L^3} \\ R_z = \dfrac{2EI_{zz}}{L}, \quad R_{z2} = \dfrac{6EI_{zz}}{L^2}, \quad R_{z3} = \dfrac{12EI_{zz}}{L^3} \end{cases} \tag{5.5}$$

As the beams are located on a regular grid, each of them can be assumed to be oriented either into the positive x direction, y direction or z direction. The transformation matrix that is used to express their stiffness matrix in the global coordinate system (GCS) can therefore be easily pre-computed depending on their direction.

The nodes' DOFs, expressed in GCS, are represented by a vector:

$$U_i = [x_i \quad y_i \quad z_i \quad \theta_{xi} \quad \theta_{yi} \quad \theta_{zi}] \tag{5.6}$$

The whole system of equation is then formulated as:

$$KU = F \tag{5.7}$$

Where K is the global stiffness matrix, $U = [U_i \quad \ldots \quad U_n]^T$ (n: number of voxels) and F a $6n$-vector containing the boundary conditions (including forces and moments and prescribed displacements and rotations).

Once the DOFs are computed, they are used to compute the beam-deformed shape and ultimately the object deformed shape, as described in the following paragraph.

Computation of the voxelized object deformation (Step 5 of Figure 5-3)

The proposed methodology for computing the voxelized object, takes advantage of a well-established technique used in the computer graphics area: skinning; fall under the umbrella of this term all the techniques bringing 3D characters to life. Skinning [179] is the process of controlling deformations of a given object using a set of deformation primitives, which are transformations associated with bones of an animation skeleton.

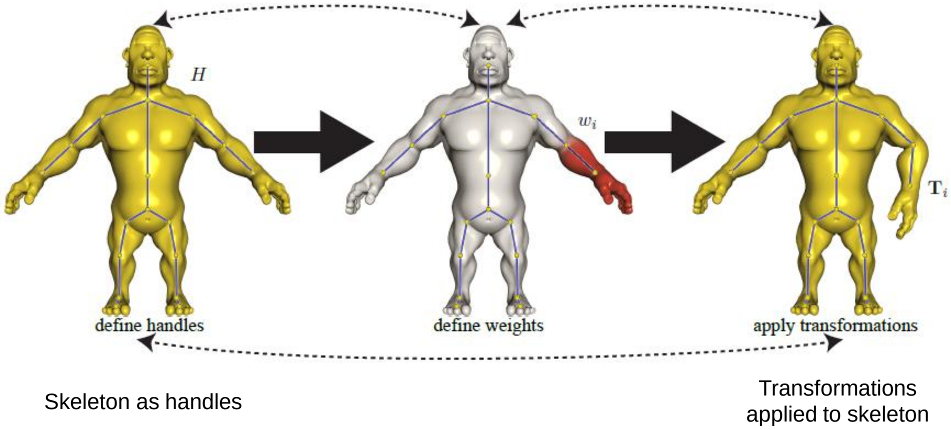


Figure 5-4 - The skinning process (adapted from [179])

Roughly speaking, the overall skinning process (as shown in Figure 5-4) can be described as: (1) skeleton extraction from the character geometry, the skeleton is then embedded within the geometry. A skeleton is composed of bones and joints. (2) Each vertex of the character is assigned a set of weights (each corresponding to a bone) quantizing how much that vertex is affected by transformations applied to the bones. (3) Applications of transformation (which are relative rotations) to the bones to animate the character.

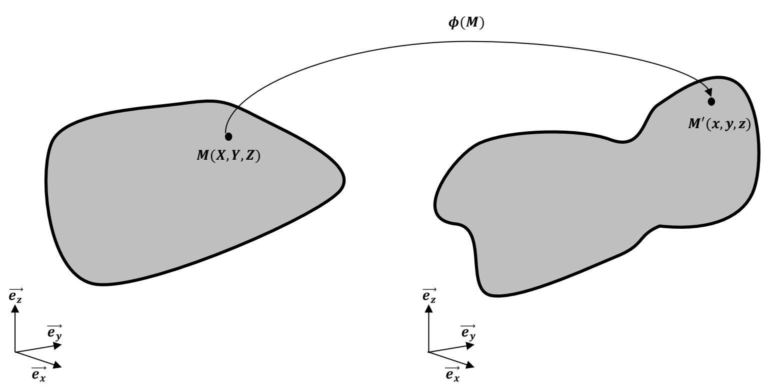


Figure 5-5 - The deformation map

In our case, the frame acts as the skeleton and the DOFs of the nodes act as the transformations moving and deforming the beams (i.e. the bones). While, in the case of skinning, simple rotation matrices are enough to describe how the bones move, in our case there is the need to find a more complex mathematical representation of the bones motions. Indeed, these latter do not have rigid body motion only: they can translate, rotate, bend, shrink, twist, etc. It is known that the deformation of any deformable object can be described by a *deformation map*, that is, a function which maps any point of the object in its initial state, to the same material point in the deformed state, as illustrated in Figure 5-5. This holds particularly for beams, when one needs to find its 3D deformed shape. With the deformation map associated to each beam, a step towards controlling the voxelized object's deformation with the frame's deformation can be achieved.

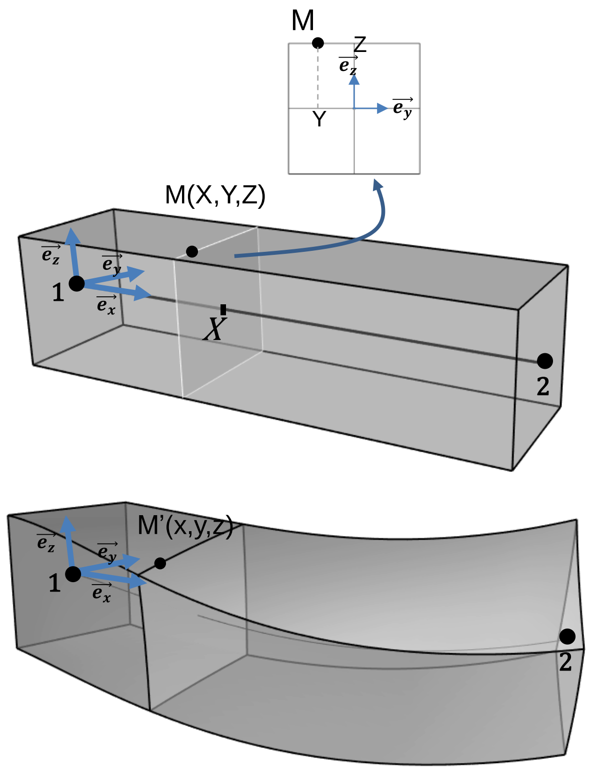


Figure 5-6 - Beam's deformation map

Let's consider a beam oriented into the positive x direction as shown in Figure 5-6, with its centerline extending form node 1 to node 2. M(X,Y,Z) is an arbitrary point of the beam in the initial state. In the deformed state, this point is located at M'(x,y,z). All the aforementioned coordinates are expressed in the beam local coordinate system as depicted in Figure 5-6. It can be shown that [181]:

$$M'(x,y,z) = \phi(M) = X\overrightarrow{e_x} + \begin{bmatrix} u_x(X) \\ u_y(X) \\ u_z(X) \end{bmatrix} + \Lambda(X)\begin{bmatrix} 0 \\ Y \\ Z \end{bmatrix} \quad (5.8)$$

Where $u_i(X)$ is the translational DOF along the i–axis at the position X. $\Lambda(X) = f\left(\theta_x(X), \theta_y(X), \theta_z(X)\right)$ (with $\theta_i(X)$ being the rotational DOF around the i–axis at the position X) is a tensor that characterized the rotation in space of a cross section to which M belongs. More explicitly $\Lambda(X)$ is expressed as:

$$\Lambda(X) = R_z(\theta_z(X)) \cdot R_y\left(\theta_y(X)\right) \cdot R_x(\theta_x(X)) \tag{5.9}$$

Where R_i being the matrix of a rotation about the i–axis.

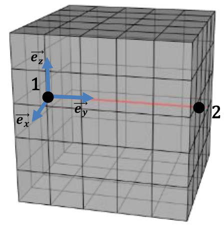
With the frame's deformation computation, the values of the DOFs are only known at the nodes 1 and 2, so we used shape functions to extrapolate their values at any location along the beam (to reduce clutter the dependency on X has been omitted):

$$\begin{gathered}
\begin{bmatrix} u_x \\ u_y \\ u_z \\ \theta_x \end{bmatrix} = \begin{bmatrix} N_1 & 0 & 0 & 0 & 0 & 0 & N_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & N_3 & 0 & 0 & 0 & -N_4 & 0 & N_5 & 0 & 0 & 0 & -N_6 \\ 0 & 0 & N_3 & 0 & N_4 & 0 & 0 & 0 & N_5 & 0 & N_6 & 0 \\ 0 & 0 & 0 & N_1 & 0 & 0 & 0 & 0 & 0 & N_2 & 0 & 0 \end{bmatrix} U \\
\theta_y = -\frac{du_z}{dX} \\
\theta_z = \frac{du_y}{dX}
\end{gathered} \tag{5.10}$$

Where: $U = [u_{x1} \quad u_{y1} \quad u_{z1} \quad \theta_{x1} \quad \theta_{y1} \quad \theta_{z1} \quad u_{x2} \quad u_{y2} \quad u_{z2} \quad \theta_{x2} \quad \theta_{y2} \quad \theta_{z2}]^T$ and:

$$\begin{cases} N_1(X) = -\frac{1}{L}(X - X_2) \\ N_2(X) = \frac{1}{L}(X - X_1) \\ N_3(X) = 1 - \frac{3\bar{x}^2}{L^2} + \frac{2\bar{x}^3}{L^3} \\ N_4(X) = \bar{x}\left(-1 + \frac{2\bar{x}}{L} - \frac{\bar{x}^2}{L}\right), \quad \bar{x} = X - X_1 \\ N_5(X) = \frac{\bar{x}^2}{L^2}\left(3 - \frac{2\bar{x}}{L}\right) \\ N_6(X) = \frac{\bar{x}^2}{L}\left(1 - \frac{\bar{x}}{L}\right) \end{cases} \tag{5.11}$$

Equations (5.8 – 5.11) are all written in local coordinate system (LCS). On implementing them, they have been adapted to handle points coordinates in GCS and yield points in deformed state M' coordinates in GCS as well; an independence to the beam orientation has also been implemented. On a computational aspect, morphing a parallelepiped beam according to the deformation of the underlying centerline was made by first meshing the beam surface and then moving the mesh's vertices by using the associated deformation map. Examples of how the beam deforms according to the end nodes DOFs are shown in Figure 5-7.



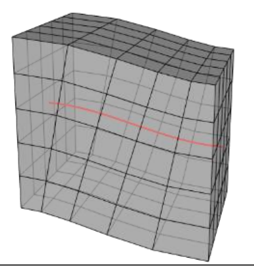
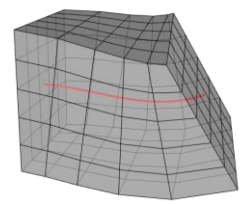
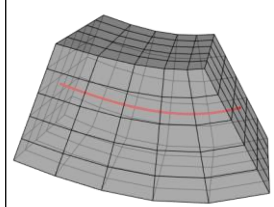
$U_1 = [0,0,0,0,0,0]$ $U_2 = [0,1,-2,0,0,0]$	$U_1 = [0,0,0,0,0,0]$ $U_2 = [0,2,0,0.5,0.2,0]$	$U_1 = [1,-2,1,-0.4,0,0]$ $U_2 = [0,2,0,0.5,0,0.1]$
		

Figure 5-7 - Beam's deformation

With each beam of the frame associated to a deformation map, there is one more step towards deforming the whole object. This is where skinning [179] has been harnessed to the proposed modeling framework. In our case, morphing the voxelized object according to the underlying skeleton frame is made through five steps:

1. **Voxels meshing –** All the voxels' surfaces are meshed. With a voxel size around 1mm, a mesh density of 5-10 faces along each direction, which is high enough for an accurate mesh deformation.
2. **Extraction of the vertices set –** All the voxels' vertices are extracted and stored in a list without duplicates.
3. **Weights computations –** The vertices should move according to which beams they are (likely to be) influenced by. Therefore, we first define an influence zone for each beam, a zone which is the space occupied by the two voxels that the beam is connecting; any vertex belonging to this space is then influenced by the beam deformation. A vertex at the border between many influence zones is considered to belong to all these influence zones. Using these assumptions, all the beams influencing any vertex can be found. We consider each vertex to be equally influenced by its influencers, which yield the weights: $\omega_i = \frac{1}{N}$ for all the beams, where N is the number of beams influencing that vertex.
4. **Vertices motions –** Each vertex is then moved by using a weighted average deformation map (which is a blend of the influencing beams' deformation maps).
5. **Voxels shape update –** Finally each voxel shape is updated by using the new position of its vertices.

On a computational aspect, as moving any vertex is independent of the others locations, the process for deforming the voxelized object is friendly to parallelization, and hence speed.

5.2.1.4 Modeling scheme validation

Homogeneous structures simulations compared with Finite Element Analysis

While the proposed model of continuum mechanics modeling scheme is used as a tool for conceptual design (to rapidly know how a distribution behaves), we found it worth gaging its accuracy compared to finite element method (FEM) simulations. Here two cases have been used to evaluate the modeling scheme:

- A cantilevered thick beam (50mm×10mm×10mm) made of a single material (E = 20GPa, G =7.69 GPa - structural steel) loaded at its free end with a 800N force.
- A thin squared plate (30mm×30mm×2mm) also made of a homogeneous material distribution (E=1000MPa, G=385MPa), fixed on the sides and loaded on a little square (3mm×3mm) at its center with a pressure of 16.5MPa.

For these two cases, the maximum displacement was used as a measure for comparison. For the beam a voxel size of 2mm was chosen, leading to a voxelized object of 25×5×5 voxels. The same voxel size was used for the plate which is then made of 15×15×2 voxels. The deformed shapes of the two cases are shown in Figure 5-8. The results of the simulation are outlined in Table 5.1.

Table 5.1 - Maximum displacement (mm) for the two cases

Case	Proposed voxel-based model	Finite Element Analysis
Beam	**1.86**	2.03
Thin plate	**3.7**	3.6

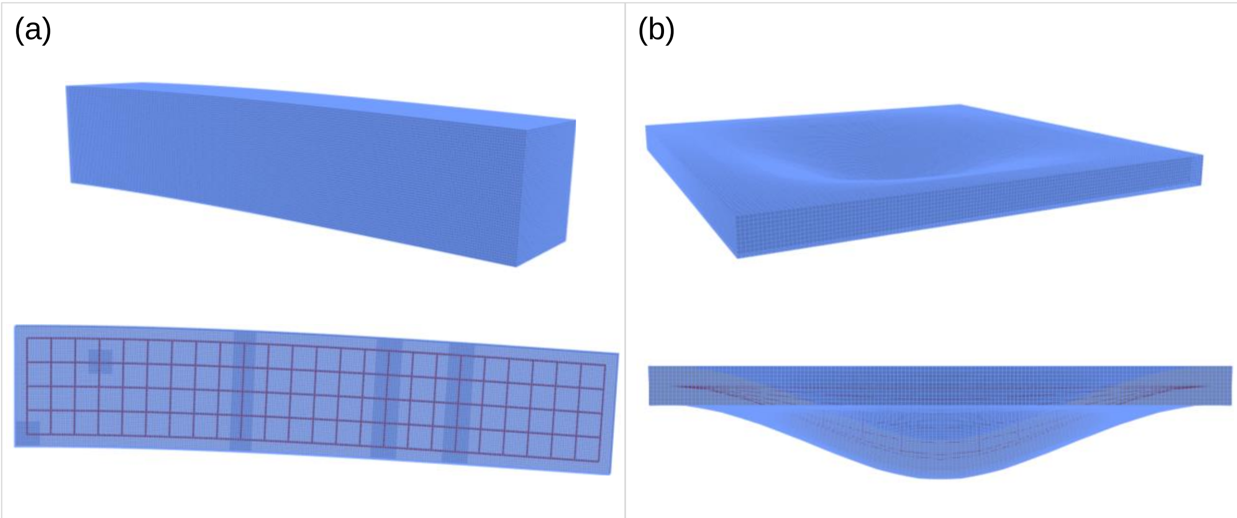


Figure 5-8 - Two simulation cases with our modeling scheme: (a) cantilevered beam loaded at its free end, and (b) thin plate loaded fixed on the sides and at its center

For these two cases, the deformations are physically realistic and maximum displacements are within the ranges of the results obtained from finite element analysis (FEA) with an extremely fine mesh. This discrepancy from the results yielded by a FEA may have multiple causes. The two most plausible are: loads, boundary conditions (BCs) locations and voxel size (discretization) which are not independent. For the cantilevered beam case simulated in a FEA software, the force was applied as a force per unit area on the beam free end surface, and a fixed constraint (all DOFs set to zero) was set on the fixed end surface. In the proposed voxel-based modeling scheme, the force was equally distributed over the (25) voxels centers located at the free end, while the voxels centers located at the other end were fixed. The distance between where the beam is actually fixed and where the load is actually applied is shorter than in the real case simulated in the FEA software, therefore the beam actually simulated with our modeling scheme is stiffer than the actual one hence a lower maximum displacement. Furthermore, our modeling scheme does only support point loads (and moments) applied at the underlying frame's nodes; this is not the type of load which has been used in the FEA. Finally, as the voxel size decreases, BCs and loads get closer to their actual locations and their distributions get more accurate. In the beam case, we used a voxel size of 2mm which means BCs and loads locations are 1mm off their actual locations inwards the beam.

Again, the proposed modeling scheme is not meant to be as accurate as established methods like FEM but is more aimed to provide qualitative evaluation of materials distributions in conceptual design.

Qualitative evaluation for heterogeneous structures simulation

The capability of our modeling scheme to handle multimaterial simulation has also be somewhat gaged. We used a cantilevered beam with increasing stiffness along the width, the material distribution is such that five materials with Young moduli (all expressed in GPa) 0.08, 0.1, 0.8, 10 and 20 were arranged along the beam width as shown in Figure 5-9.a. The beam is loaded at its free end with a 800N force. As one could expect stiffer sections would deform less since they are more load resistant; our model is able to reproduce this behavior as shown in Figure 5-9.b.

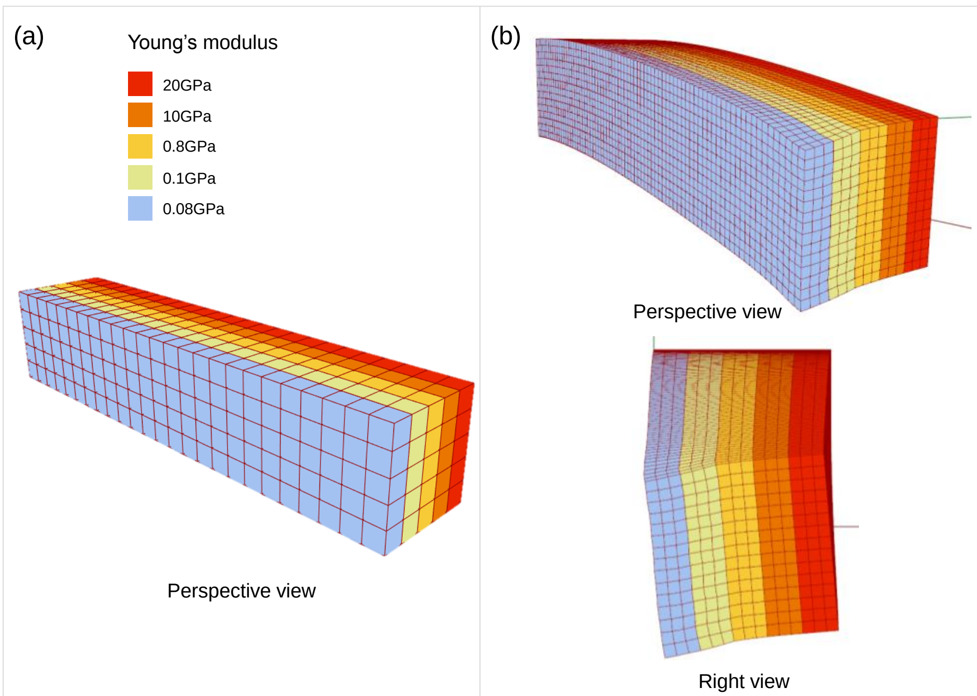


Figure 5-9 - Multimaterial beam with varying materials width wise

Another multimaterial beam case has been simulated. We used a cantilevered beam with in the middle a material ways softer than the material of the remaining of the beam. A load oriented upwards was applied to its free end. As one could expect, the beam bends at the soft section (see Figure 5-10)

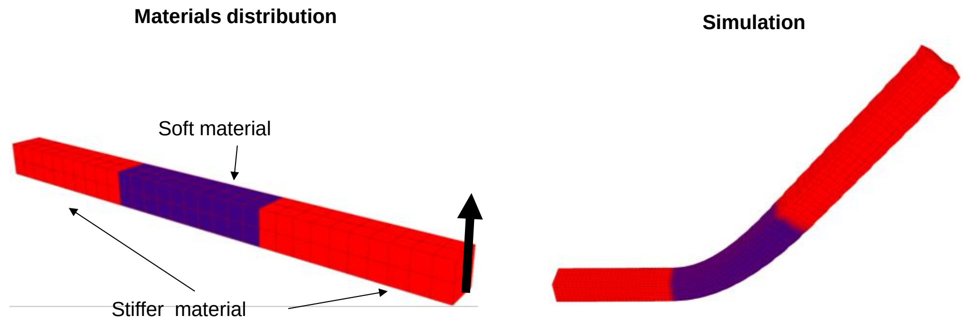


Figure 5-10 - Cantilevered beam with a soft and hard materials distribution

5.2.2 Modeling the stimulus responsive behavior of smart materials

5.2.2.1 Description of shape changing materials and parameters to be considered

Within the group of shape changing materials (SCMs), it is worth distinguishing two subgroups [182]: *programmable* SCMs (p-SCMs) and *non-programmable* SCMs (np-SCM). In np-SCMs the way the material can change shape is predefined during fabrication and the shape change is limited to dimensions change (shrinking or expansion isotropically or not). p-SCMs change shape according to a pathway that can be altered regardless of how they were manufactured. In other words, after manufacturing they can be trained to shift shape between almost any shapes. These materials are typically shape memory materials [104, 182]. Basically, they are formed into one permanent shape, and can be thermomechanically trained (or *programmed*) to assume one (or several) temporary shape(s) from which the permanent shape can be recovered. As such achieving a specific shape change with p-SCMs is rather a thermomechanical training issue than a material spatial arrangement determination issue. That is why this work is focused on smart materials distribution with np-SCMs, which are described in the following paragraphs. The descriptions serve the purpose of briefly introducing the reader to them and most importantly they aim at deriving equations governing the materials' responses for our modeling scheme. First of all, we derive the stiffness equations for a generic member made of a np-SCM.

For conventional (inert) materials, the beams' DOFs are governed by the member stiffness equations:

$$\bar{K}\bar{u} = \bar{f}_M \tag{5.12}$$

Where $\bar{f}_M$ is the vector containing all the (external) mechanical forces and moments applied to the beam (at its nodes). Equation (5.12) basically means that the only way for the beams to deform is by the mechanical forces and moments applied at their nodes. In our modelling scheme, the action of the smart materials will be modeled by introducing initial force effects, in a way similar to how thermal forces are modeled:

$$\bar{K}\bar{u} = \bar{f}_M + \bar{f}(\boldsymbol{S}) \tag{5.13}$$

$\boldsymbol{S}$ denotes the stimulus. For simplicity in understanding we will consider a planar bar member. In an unloaded state and upon exposure to the stimulus, its length is free to change from L to $L + \Delta L$, where ΔL is a function of the stimulus and the material properties:

$$\Delta L = L \times g(\boldsymbol{\alpha}, \boldsymbol{S}) \tag{5.14}$$

$\boldsymbol{\alpha}$ denotes a vector containing all the SMs properties related to its stimulus responsive behavior. The strain due to the stimulus can then be expressed as:

$$\epsilon_S = \frac{\Delta L}{L} = g(\boldsymbol{\alpha}, \boldsymbol{S}) \tag{5.15}$$

Now let's assume that the bar is also subjected to an (axial) force F causing the stress $\sigma = \frac{F}{A}$ (with A being the bar's cross section area), which induces the strain $\epsilon_M = \frac{\sigma}{E}$. The total strain in the bar is then:

$$\epsilon = \frac{\bar{u}_{x_j} - \bar{u}_{x_i}}{L} = \epsilon_M + \epsilon_S = \frac{\sigma}{E} + g(\boldsymbol{\alpha}, \boldsymbol{S}) \tag{5.16}$$

Which can be rewritten as follows:

$$\frac{EA}{L}\left(\bar{u}_{x_j} - \bar{u}_{x_i}\right) = \underbrace{\sigma A}_{\substack{mechanical \\ axial\ force}} + \underbrace{EAg(\boldsymbol{\alpha}, \boldsymbol{S})}_{\substack{internal\ force \\ induced\ by\ the\ stimulus}} = F \tag{5.17}$$

Where F denotes the total internal force. The joint forces are:

$$\begin{bmatrix} \bar{f}_{x_i} & \bar{f}_{y_i} & \bar{f}_{x_j} & \bar{f}_{y_j} \end{bmatrix} = \underbrace{\begin{bmatrix} \bar{f}_{Mx_i} & \bar{f}_{My_i} & \bar{f}_{Mx_j} & \bar{f}_{My_j} \end{bmatrix}}_{\bar{f}_M} + \underbrace{EAg(\boldsymbol{\alpha}, \boldsymbol{S}) \cdot \begin{bmatrix} -1 & 0 & 1 & 0 \end{bmatrix}}_{\bar{f}_S} \tag{5.18}$$

The member stiffness equations are:

$$\frac{EA}{L}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \bar{u}_{x_i} \\ \bar{u}_{y_i} \\ \bar{u}_{x_j} \\ \bar{u}_{y_j} \end{bmatrix} = \bar{f}_M + \bar{f}_S \tag{5.19}$$

Regarding the beam elements used in our modeling scheme, the internal force due to the stimulus will be expressed as:

$$\bar{f}_S = EAg(\boldsymbol{\alpha}, \boldsymbol{S})\begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T \tag{5.20}$$

What will differentiate the various modeled SMs will be the expression of $g(\boldsymbol{\alpha}, \boldsymbol{S})$ and the conditions of application of the related force.

Piezoelectric material

Of interest in the scope of this paper is the reverse piezoelectric effect by which a voltage (or equivalently an electric field) generates strain. An inherent electrical property of these materials is what is called the polling direction, usually referred to as the 3-direction; it is the direction along which most of the electric dipoles within the material are oriented. The other two orthogonal directions are denoted 1 and 2. At constant stress, strain generated by an electric field is defined by the equation [183]:

$$\epsilon_j = d_{ij} E_i \tag{5.21}$$

Where:

- E_i, is the electric field in direction $i \in [\![1,3]\!]$,
- ϵ_j, is the generated strain in direction $j \in [\![1,6]\!]$, with the convention 4: 1-2, 5: 1-3, 6: 2-3 for the shear strains,
- d_{ij}, are piezoelectric strain coefficients.

Commonly used piezoelectric coefficients for actuation are d_{33} (strain along the polling direction induced by an electric field along that same direction) and d_{31}(strain along directions perpendicular to the polling direction by electric field's component along that same direction). Function $g(\boldsymbol{\alpha}, \boldsymbol{S})$ as introduced in equation 14 is then expressed as:

$$g(\boldsymbol{\alpha}, \boldsymbol{S}) = d_{3j} E_3 \tag{5.22}$$

In our modelling scheme piezoelectric material properties will be represented by the coefficients d_{33} and d_{31},they will also be characterized by a polling direction (x, y or z). The internal force due to the stimulus will depend on the beams orientation: for beams along E_3, d_{33}will be used for beams in perpendicular directions d_{31} will be used. This setup assumes then that only situations where the electric field is along the material polling direction can be simulated. The highest strains are in fact obtained in this situation.

Electrostrictive material

Dielectric materials are materials that do not conduct electricity, nevertheless they are responsive to electric field by (among others) exhibiting *electrostriction*. These materials are made of electric domains which are randomly oriented within the material. When a sample is subjected to an electric field, the electric domains get polarized along the electric field. As the opposite sides of these domains are then charged with opposite charges they attract each other, thus they shrink in the field direction and the elongate in perpendicular directions according to the material Poisson's ratio. The effect is a second order one, that is, the resulting deformation is proportional to the square of the electric field; particularly reversing the field does not change the sign of the strain. The so described mechanism is to be distinguished from what is usually referred to as electrostriction in dielectric polymers [184] and which is discarded from the scope of this work as explained in section 5.2.2 introduction.

In a stress free sample of the material, three electrostriction coefficients [185] can be defined to relate the induced deformations to the polarization:

$$\begin{bmatrix}\epsilon_1\\\epsilon_2\\\epsilon_3\\\epsilon_4\\\epsilon_5\\\epsilon_6\end{bmatrix}=\begin{bmatrix}Q_{11}&Q_{12}&Q_{12}&0&0&0\\Q_{12}&Q_{11}&Q_{12}&0&0&0\\Q_{12}&Q_{12}&Q_{11}&0&0&0\\0&0&0&Q_{44}&0&0\\0&0&0&0&Q_{44}&0\\0&0&0&0&0&Q_{44}\end{bmatrix}\begin{bmatrix}P_1^2\\P_1^2\\P_1^2\\P_2P_3\\P_3P_1\\P_1P_2\end{bmatrix}\tag{5.23}$$

Where $P = [P_1 \ \ P_2 \ \ P_3]$is the polarization vector. In case of induced polarization (which is the case when the material is subjected to an electric field), there is a single polarization direction, the one in the direction of the applied field. This direction is denoted 1, which zeros P_2 and P_3 from equation (

$$KU = F \tag{5.7}$$

). The polarization is related to the electric field by: $P_1 = \epsilon E_1$, where ϵ is the static dielectric constant of the material. Equation (

$$KU = F \tag{5.7}$$

) can then be rewritten as:

$$\begin{aligned}\epsilon_1 &= Q_{11}\epsilon^2 E_1^2 = M_{11}E_1^2\\ \epsilon_2 &= Q_{12}\epsilon^2 E_1^2 = M_{12}E_1^2\\ \epsilon_3 &= Q_{12}\epsilon^2 E_1^2 = M_{12}E_1^2\end{aligned}\tag{5.24}$$

Function $g(\boldsymbol{\alpha}, \boldsymbol{S})$ will then be written as:

$$g(\boldsymbol{\alpha}, \boldsymbol{S}) = M_{1j}E_1^2 \tag{5.25}$$

Electrostrictive materials properties will then be represented by the coefficients M_{11} and M_{12}. The material polarization direction will be defined as the applied field's direction E_1. For beams along E_1, M_{11} will be used and for those in transverse directions M_{12} will be used.

Magnetostrictive materials

Any ferromagnetic (e.g. nickel, iron etc.), ferromagnetic (e.g. iron II,III oxide) and antiferromagnetic (e.g. chromium, nickel oxide, etc.) material exhibits a phenomenon called magnetostriction. Once subjected to a magnetic field they exhibit a slight change in dimension. Roughly speaking this is due to rotation of magnetic dipoles within the material as they align with the applied magnetic field. There is a positive magnetostriction where the material elongates along the applied field, and a negative magnetostriction in which the material shrinks. For instance when exposed to a strong magnetic field iron can elongate by 0.002 %, while nickel contracts by 0.007%. Some of these materials are termed as "giant magneostrictive materials" in reference to the higher strains they can produce. This is the case of Terfenol-D (up to 0.1%) or NiMnGa alloys (up to 9%). There are also dimensions' changes in the directions perpendicular to the applied field. The effect is measured by the developed strain: $\lambda = \frac{\Delta L}{L} = f(H)$. H being the applied magnetic field. Similarly to electrostriction, it is a second order effect: reversing the applied magnetic field doesn't change the developed strain. Magnetostrictive materials are usually characterized [186] by their strain at magnetization saturation λ_s (which is the maximum strain – or minimum strain in case of negative magnetostriction – that can be developed by the material) and the saturation magnetic field H_s. In the region before saturation, the dependency of λ to H is quadratic.

In our modeling scheme, we will only consider the strain developed along the applied field (as it is the most significant). The material's magnetostrictive properties will be λ_s and H_s. In addition the region before saturation will be approximated by a linear law:

$$g(\boldsymbol{\alpha}, \boldsymbol{S}) = \lambda = \begin{cases} \frac{\lambda_s}{H_s}|H|, & |H| < H_s \\ \lambda_s, & |H| \geq H_s \end{cases} \tag{5.26}$$

Only beams along the applied field will be subjected to the internal force resulting from magnetostriction.

Photostrictive materials

Photostrictive materials are materials whose dimensions change when exposed to light, a change which is different from and more important than the one associated with heat induced by the light. Photostriction is found in four main types of materials [165] including ferroelectric materials, polar and non-polar semiconductors, and organic polymers. Some photostrictive materials shrink while others expand. The mechanism responsible of the phenomenon is quite different depending on the material: in ferroelectric material photostriction is due to a combination of photovoltaic and the reverse piezoelectric effect, whereas in organic polymers the phenomenon is due to photoisomerization (light induced change in molecule structure). The effect is usually quantified with a single measure of strain, usually denoted $\frac{\Delta L}{L}$ and referred to as photostriction coefficient, which is an indication that the behavior is isotropic. While in ferroelectric, photostriction coefficient of 0.45% is deemed as a giant photostrictive response, in nematic elastomers photostriction can be up to 400% [66]. The literature on these materials is populated with experimental data showing the developed strain versus light's wavelength [165], exposure time to light [66] and light's intensity [187] but there are no close form relationships between the electrostriction coefficient and these characteristics of the stimulus. In addition there is a dependence on light penetration depth. In our modeling scheme we elected to restrain the dependency of photostriction to light's intensity (as the easiest controllable parameter), the effect is modeled as:

$$\frac{\Delta L}{L} = kI \tag{5.27}$$

Where, I is light's intensity and k, a material property.

In addition a parameter for light penetration depth is introduced, this will tell the number of voxels (thus the number of beams) in the material thickness that are reached by light.

Hydrogel

Hydrogels – which only work in wet conditions – are able to absorb or repel water (in a way similar to a sponge, except that they can retain the absorbed water in such a way that even pressure on it, may not release the water), and thus they can drastically change volume. Depending on their chemical composition they can be responsive to heat (as in most encountered hydrogels), light, electricity, solution properties (pH, salinity, concentration of a specific constituent, etc.). The exhibited shape change is an isotropic either shrinkage or expansion, depending on the chemical composition. In the case of heat as stimulus, there is lower threshold by which the dimension's change begins (usually referred to as lower critical solution temperature - LCST). Away from the critical temperature, the change stops, as the material reaches an equilibrium state. The material behavior is usually tracked by a volumetric swelling ratio (VSR), whose definition varies according to authors. In [162], the following definition of VSR was used:

$$\nu_s = \frac{V_0}{V_s} \tag{5.28}$$

Where V_0 is the material's volume in dry state, and V_s the current material's volume in swollen state. As such: $0 < \nu_s \leq 1$. With this definition, the higher is ν_s, the lower is the material's volume. In the case of shrinkage of the material with rising temperature, VSR's dependency on temperature is expressed [162] as:

$$\nu_s(T) = \nu_s^{min} + \left(\nu_s^{max} - \nu_s^{min}\right)\left[1 + \exp\left(\frac{LCST - T}{k}\right)\right]^{-1} \tag{5.29}$$

Where T is the temperature, k is a constant controlling how gradual the transitional behavior around the LCST is, ν_s^{min} and ν_s^{max} are the limits of the swelling ratio in fully swollen and collapsed (dry) state respectively. As the dimension change is isotropic (strain resulting from the volume change is the same in all the directions), function $g(\boldsymbol{\alpha}, \boldsymbol{S})$ can be expressed as:

$$g(\boldsymbol{\alpha}, \boldsymbol{S}) = \left[\nu_s(T)\right]^{-\frac{1}{3}} - 1 \tag{5.30}$$

Any beam in our modeling scheme made of hydrogel will then be subjected to the internal force resulting from temperature-driven volume change.

I.1.1 Stimulus modeling

The stimuli triggering the aforementioned SMs are: heat, light, electric field or equivalently voltage, and magnetic field. These can clearly be separated in scalar stimuli and vector stimuli. In our modeling scheme a stimulus is considered as an environment's variable that is sensed by each voxel (and thus each beam) the same way, that is, the value of the stimulus is considered to be the same for all the voxels. While such assumption is valid for electric or magnetic field (considering no electromagnetic shield is to be modeled), for heat and light it is questionable. Indeed heat propagates (from hot regions to colder ones) and light gets absorbed as it propagates through a medium. As the proposed modeling scheme is meant to be used in conceptual design (where the focus is more on functionality than accuracy), we elected not to take these phenomena into account. Nevertheless the framework may be extended to model all the stimuli field in the simulated object more accurately.

5.2.3 Validation with predefined distributions

In order to ascertain the accuracy of the proposed modeling framework for SMs modeling, a few existing material distributions have been simulated. Namely the printed smart valve from [23] and the hypothetical actuators from [162]. All these examples are based on heat responsive hydrogel.

5.2.3.1 Smart hydrogel valve

Bakarich et al. [23] have demonstrated 4D printing with a smart valve. Basically the printed valve is able to regulate water flow according to this latter's temperature. The SM responsible of this behavior is a thermally responsive poly (N-isopropylacrylamide) hydrogel commonly referred to as PNIPAAm. Its LCST (cf. subsection 3.2.1) is between 32°C and 35°C. The material exhibits a large decrease in water content as the temperature is around LCST. The valve, as depicted in Figure 5-11 and Figure 5-14.a, has been printed with 2 materials: an epoxy based adhesive (Emax 904 Gel-SC) for the inert sections and hydrogel for the active sections. As water flows through the central tubing (from the top) and warms the actuating hydrogel strips, these shrink to close the outlet, thus blocking the water flow.

Materials' properties were used as measured in [23, 188] and are summarized in Table 5.2.

Table 5.2 - Material properties used for the smart valve

	E (MPa)	G (MPa)	v_s^{min}	v_s^{max}	LCST (°C)
Emax	2.7	0.96			
Hydrogel	1	0.35	0.98	0.4	33.5

The valve has been modeled with a voxel's size of 1mm. Voxels in the first row from the top were all fixed. Results of the simulation for an increasing temperature are shown in Figure 5-11.

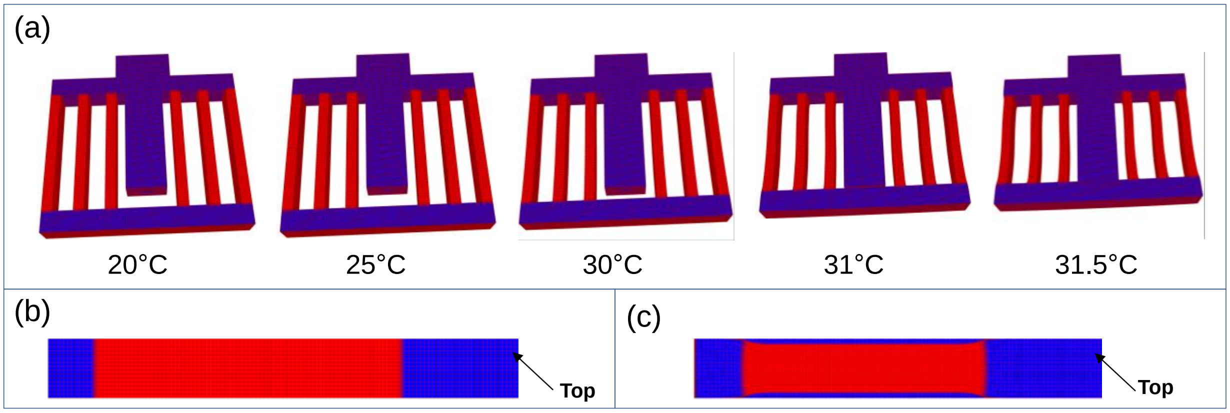


Figure 5-11 – (a) Results of the simulation of the smart valve at various temperature – (b) Side view at 20°C – (c) Side view at 31.5°C

5.2.3.2 Hydrogel actuator

In the previous example, the hydrogel sections work mostly in homogeneous configurations (the strips) and as such the motion they are responsible of are limited to one dimensional motions. This is a typical case in hydrogel applications. Using FEM based simulations Westbrook and Qi [162] designed hydrogel actuators that leverage heterogeneities to more complex shape changes. One of their theoretical actuators has (partially) been modeled and simulated with our voxel-based framework. It is the in which hydrogel shrinking is converted into bending. Such motion has been realized by patterning the hydrogel (red) into another non-responsive hydrogel (blue) as shown in Figure 5-12. Materials' properties were used from their study (some of them were estimated). The simulated actuator is simulated with the left end (see Figure 5-12) fixed.

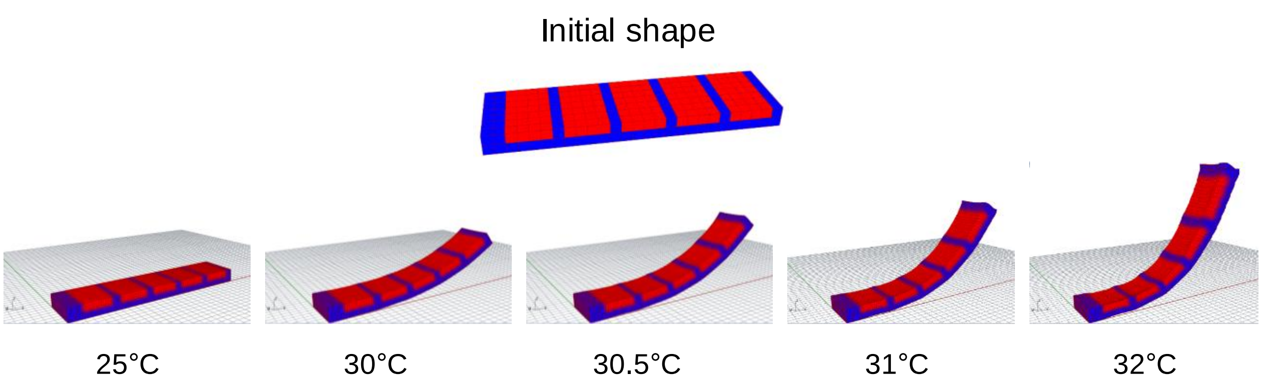


Figure 5-12 - Hydrogel actuator as temperature increases

The hydrogel (red) sections do shrink in the three dimensions as expected and the generated eigenstrain clearly induces a bending motion. Nevertheless there is a discrepancy between the way the actuator bends in our model and theirs. In both models the actuator bends upwards. In our modeling scheme, as the temperature increases sections near the fixed end bends downwards (without a curvature change). This bending motion is progressively reversed as one moves away from that end. This downward bending could be explained as an accommodation to the fixed end. In order to ascertain the actual behavior the actuator should be printed.

5.3 Implementation: VoxSmart

The proposed modeling scheme for SMs simulation has been made tangible by a computational design tool. The framework has been implemented in the Rhinoceros® [189] (RH) add-on Grasshopper® (GH). RH is a CAD explicit modeling software alowing a seamless design of complex shapes. GH is a graphical algorithm editor (without the need of any script) that allow form generation (in RH) and virtually any computation. A graphical algorithm is typically a collection of components (running each a computation) connected by wires which are the data flowing through them. What makes the GH computation engine virtually infinitely expandable is the possibility to develop plugins for specific tasks (e.g. design, simulation, even manufacturing control). There is a rapidly growing GH community of users (namely designers) and plugins developers. The shape complexity allowed by RH and GH has prompted us to develop a GH plugin for materializing our SMs modeling scheme: VoxSmart; the plugin has been scripted *ab initio* in C#. It includes six categories of components: Voxel Edition, Material Edition, Boundary Conditions Definition, Stimulus Definition, Simulation and Distribution Computation.

The Voxel Edition category gather components that are used to construct the voxel model of the object (which can be imported from Rhinoceros or generated in GH) to be simulated. A voxel model can be constructed by specifying an origin and voxels' counts along x, y and z or by voxelizing an input geometry (as illustrated in Figure 5-13); in both cases a voxel size (which can be seen as a resolution) must be specified. A voxel object can also be edited by adding/removing voxels and extruding one of the object's faces along any of the positive or negative x, y and z directions. In the Material Edition category, there are components for creating a conventional material (with its properties E and G), components for creating SMs and components for assigning these materials to specific regions within the voxelized object. The Stimulus Definition category gathers components for defining stimuli including: heat, electric field magnetic field, and light.

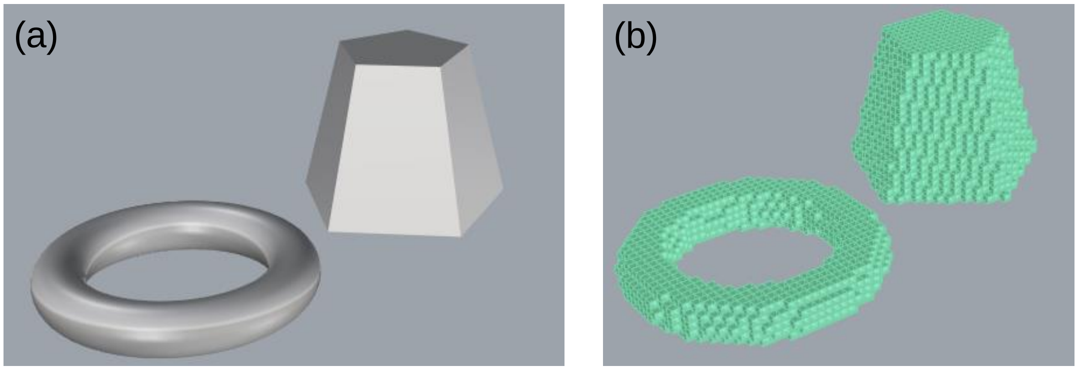


Figure 5-13 - Voxelization: (a) Initial shapes - (b) Voxelized shapes with VoxSmart.

The typical workflow for a VoxSmart definition is shown Figure 5-14. Groups of components have been highlighted (purple background) for the sake of explanation. The definition is the one that has been used to simulate the smart hydrogel valve introduced in subsection 5.2.3.1 (page 128). First the object's geometry is defined (Figure 5-14.a) with native GH components, then the geometry is voxelized (Figure 5-14.b). To avoid any simulation error related to voxel without any material, both components for creating a voxel model require as input a material that is initially assigned to all the voxel. Subsequent materials assignments to a voxel simply overwrite the initially assigned material. In a third step SMs are assigned (Figure 5-14.c) to regions of the voxelized object; these regions are specified as others geometries that can be defined within GH or in RH. Then boundary conditions are applied to the model. Finally, after specifying the stimulus the SM is sensitive to, the model is simulated.

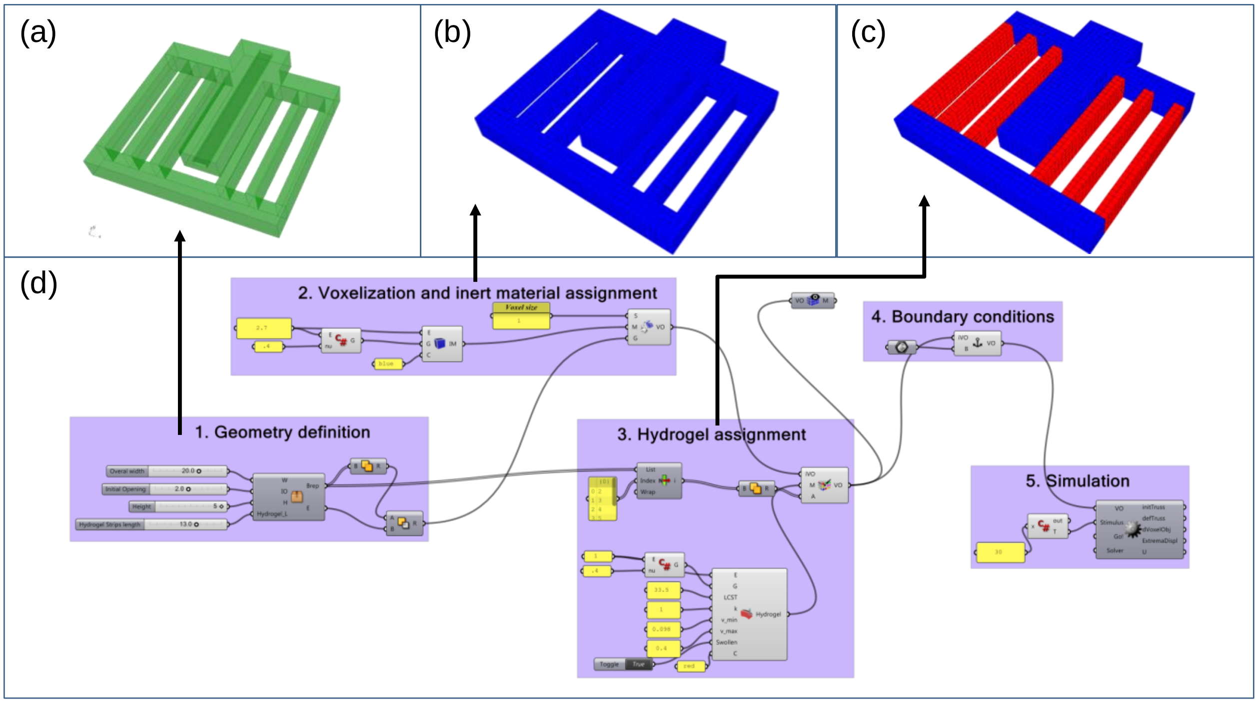


Figure 5-14 - Typical VoxSmart workflow: (a) geometry definition – (b) Voxelized geometry with a homogeneous (inert) material distribution – (c) Voxelized model with a heterogeneous material distribution including the hydrogel actuating sections – (d) The whole modeling and simulation Grasshopper definition.

A few components of VoxSmart are described in Appendix B.

5.4 Distributions computation

With the voxel-based SMs simulation engine in place, a step towards empowering designers to rapidly simulate a SM-based object has been taken. This encompasses the explorative approach of designing with SMs, the approach we termed as *3D painting* where the possibility is given to pattern any material distribution in a geometry and get how such geometry would behave. However, when a specific shape change is needed for an application, finding a right distribution achieving it may not be intuitive especially when one has limited knowledge of SMs and what strain mismatch between two dissimilar materials can lead to. Some kind of automation may then ease the design problem by at least providing a starting point, and thus by save multiple iterations time. This is the purpose of this section.

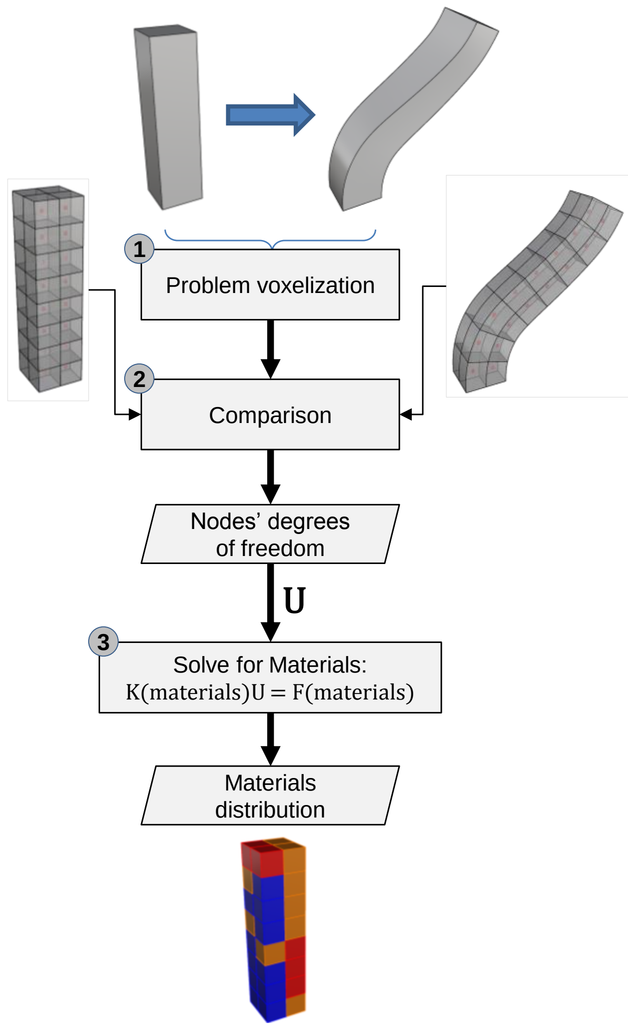


Figure 5-15 - Methodology for materials distribution computation

5.4.1 Problem formulation

Roughly speaking the problem of computing a distribution may be formulated as how can the SMs be spatially mixed (with the granularity allowed by the voxel-based model) to an inert (conventional) material in a source shape, so that this latter – upon exposure to the stimulus – deforms into a target shape?

More specifically the input of the problem are:

1. A predefined source shape S.
2. A predefined target shape T. This shape must be topologically equivalent to S. To ensure such equivalence, T should ideally be obtained by a combination of topology preserving transformations applied to S.
3. An inert conventional material that S is originally totally made of.

4. A finite number of different np-SCMs of the same type (e.g. piezoelectric materials with different d_{33} coefficients).
5. A stimulus state which is the stimulus the specified SMs are sensitive to. "State" here refers to how the stimulus field has to be at the moment the object is expected to be of shape T.

The solution to the problem yields a spatial arrangement of the SMs within shape S. Referring to our modeling scheme this will be a voxel distribution of the different materials making up the whole shape.

5.4.2 Method for computing a distribution

The solution to the problem described above is found through 3 steps which are delineated in the following paragraphs.

5.4.2.1 Problem voxelization

First of all the source shape is voxelized with a chosen resolution. In addition to the generated voxels (which are all in the form of a simple box mesh), two sets of geometrical entities are also to generate:

- The underlying frame's nodes: these are voxels' centers in the (non-deformed) shape S. These will be used to compute the nodes displacements.
- For each voxel, a set of two unit lines that are initially aligned with the y and z direction. The voxel's center along with these two lines define a plane that will be used to record the rotation DOFs (cf. Figure 5-16).

The so derived voxelized source shape S is then morphed into the desired target shape yielding a voxelized target shape T in which individual meshes (the voxels) have been deformed and the sets of points and lines have been moved to different locations. The lines are also morphed into curves.

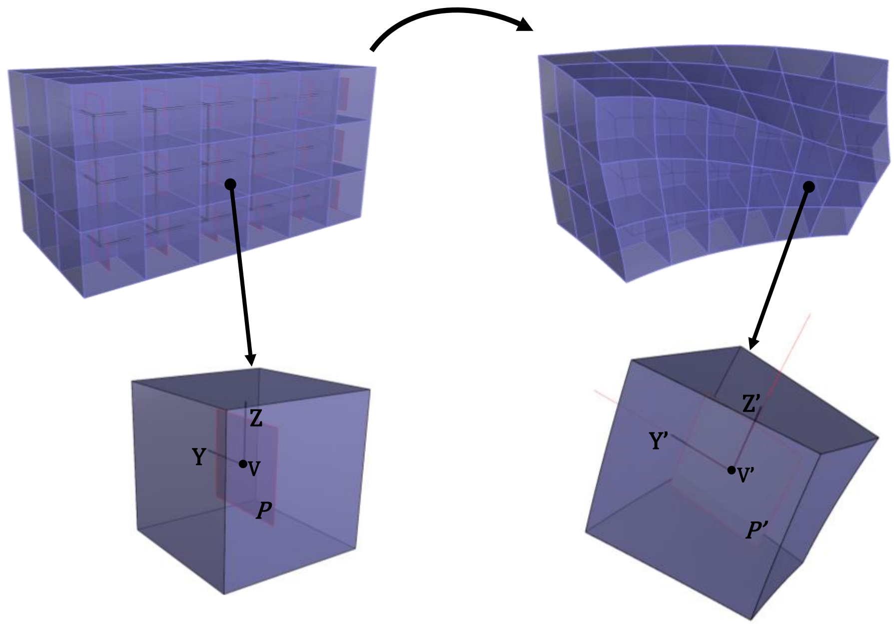


Figure 5-16 - Rotational DOFs' tracking between source and target shapes.

5.4.2.2 Comparison

A comparison is made between the voxelized source shape and the target one in order to get the underlying frame nodes' DOFs (the **U** vector as introduced in equation 5.6). The required displacements are readily computed by finding the vectors translating the voxels' centers. Getting the nodes rotational DOFs is made by planes comparison. An initial plane P is generated at the center of a voxel (denoted V) using this latter and the unit lines (aligned along y and z) introduced in the problem voxelization. These lines will be denoted Y and Z. In the deformed state the voxel center is moved to V' and Y and Z are morphed into curves. Let Y' and Z' denote the tangent to these curves at V' (cf. Figure 5-16). V', Y' and Z' are used to generate the deformed plane P'. P and P' are then moved so that they intersect. Using quaternions operations, the rotations about x, y, and z that lead from P to P' are computed and these are taken as the required rotational DOFs.

At the end of this stage, all the frame's DOFs required for the shape change S → T are known and are stored in a vector $\boldsymbol{U_{target}} = [u_{x_1}, u_{y_1}, u_{z_1}, \theta_{x_1}, \theta_{y_1}, \theta_{z_1}, u_{x_2}, u_{y_2}, \cdots]$.

5.4.2.3 Material distribution computation

The distribution is to be derived as a solution to an inverse problem. In the forward scheme, we go from a material distribution making up the initial shape, stimulus and possibly loads are applied and then the global stiffness equation is solved to get the deformation. In this problem what is sought is somehow the opposite: the deformation ($\boldsymbol{U_{target}}$) is given as known quantities (based on source and target shape) and given a stimulus, we compute the material properties of each voxel.

More specifically, the goal is to find a material distribution that minimizes the difference between the DOFs $\boldsymbol{U}_{\boldsymbol{target}}$ and the DOFs $\boldsymbol{u}$ computed (for the same voxelized object) with that distribution. Again, in our problem formulation any voxel's material is chosen from a set of materials including one conventional material and a finite number of other SMs of the same type. As such a material distribution can be represented as an array of integers indicating which materials are the voxels made of. This is illustrated in Figure 5-17 with a set of two materials.

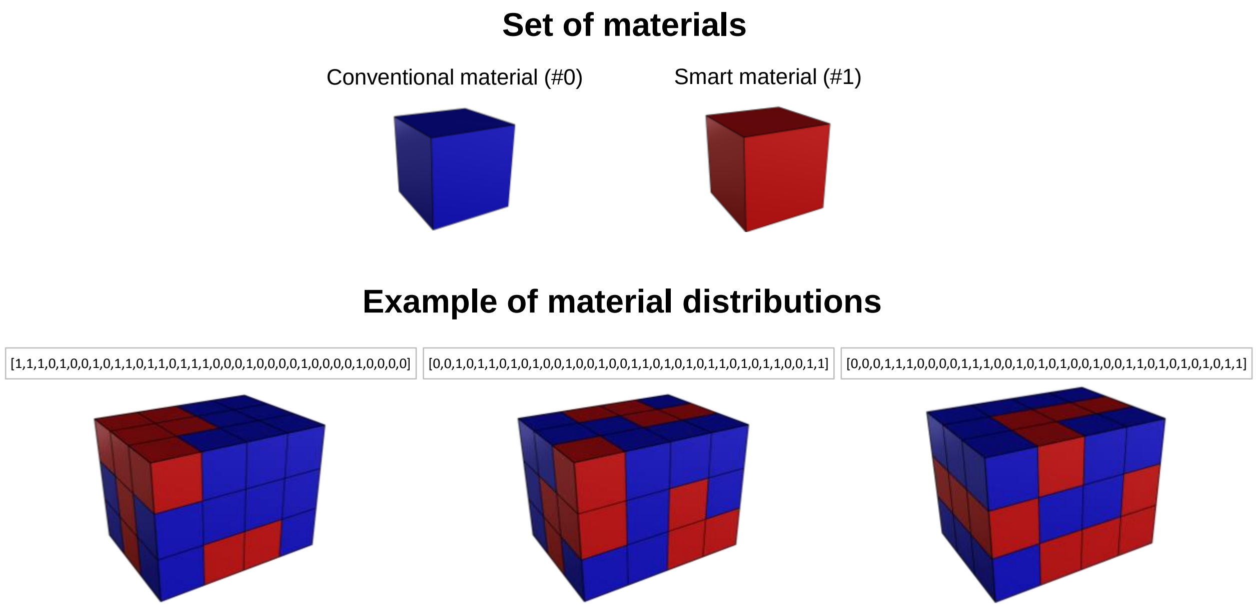


Figure 5-17 - Illustration of material distribution representation for a 4 x 3 x 3 voxels objet. The smart material count is limited to one.

In such setting, the material properties are not allowed to vary continuously; the problem is actually an integer-constrained optimization problem. Besides the objective (which is a scalar measure of the difference between desired DOFs and the computed ones) is not a linear function of the material distribution. These conditions preclude any gradient-based optimization methods from solving the problem efficiently. We then elected to use a stochastic method, namely genetic algorithm (GA) to solve the problem. GA is indeed efficient at solving such nonlinear integer-constrained problems (as demonstrated for instance in [190]).

Using the GA terminology, an individual (or a genome) is a material distribution (as shown in Figure 5-17) whose genes are the entries of the array representation. As fitness function the squared norm of the vector formed by the difference between $\boldsymbol{U}_{\boldsymbol{target}}$ and $\boldsymbol{u}(individual)$: $\boldsymbol{fitness} = \left\|\boldsymbol{U}_{\boldsymbol{target}} - \boldsymbol{u}(individual)\right\|^2$, has been used. Population size is between 100 and 200 individuals.

On a computation aspect, the power of the Matlab [191] GA toolbox has been harnessed to solve the problem. A semi-automatic interoperability between VoxSmart and Matlab has been created. Basically a VoxSmart component has been created to handle the input problem: source shape, target shape, set of materials, boundary conditions and stimulus state. The component then computes $\boldsymbol{U_{target}}$ and stores it, along with the other input, in matrix form. All the constructed matrices are finally packed in a .mat file which is subsequently loaded in Matlab. A script (shown in Appendix C) has then been written in Matlab to handle the input problem and run the optimization problem with the built-in GA toolbox.

5.4.3 Illustrations

5.4.3.1 Verification case

The accuracy of the proposed scheme to find a distribution has first been gaged. Basically DOFs computed for a known distribution have been fed into the algorithm as $\boldsymbol{U_{target}}$. The case is the one shown in section 5.2.3.1, for the hydrogel actuator. The actuator's distribution was made of a conventional material and hydrogel. The number of generations was limited to 150 and for each generation crossover rate was set to 0.95 and elites count (number of best individuals of a generation that survive till the next generation) was set to 10 (which is a pretty good figure for 100 individuals generations). Only two candidates materials (conventional and hydrogel) were given as input to the algorithm.

The results for the fitness function over the 150 generations are shown in Figure 5-18. The deformation resulting from the optimal distribution along with the one resulting from the original distribution are shown in Figure 5-19.

The fittest found individual scores 9.5 which is pretty higher than the theoretical best fitness: 0. Nevertheless, on the one hand (the square root of) this residual is to be distributed over the 2258 DOFs making up the whole problem, which may not be significant. On the other hand, deformation computed for the found optimum is close to the desired deformation as shown in Figure 5-19. This is an indication that the problem of material distribution computation may not be one with a unique solution. A finding which can be ascertained by the fact that the problem: Find K and F, such that: $KU = F$ doesn't have a unique solution (consider for instance the simple case: $K \times u = F$, where K, u and F are numbers).

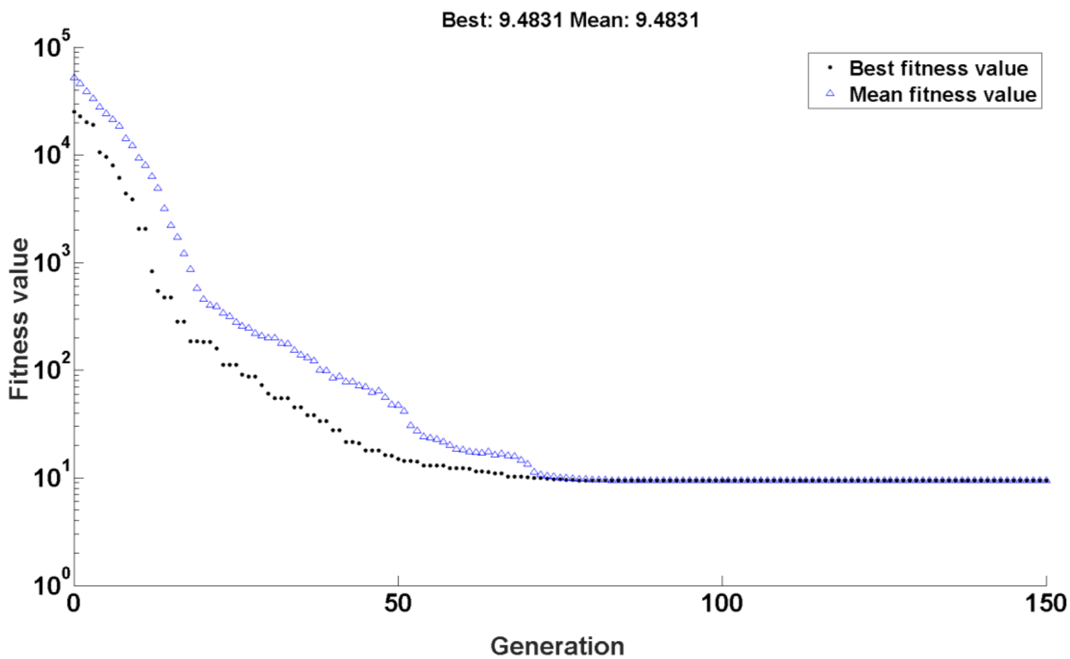


Figure 5-18 - Fitness plotting over the generations

It can be stated that the GA method yields pretty reasonable solutions to the material distribution computation problem.

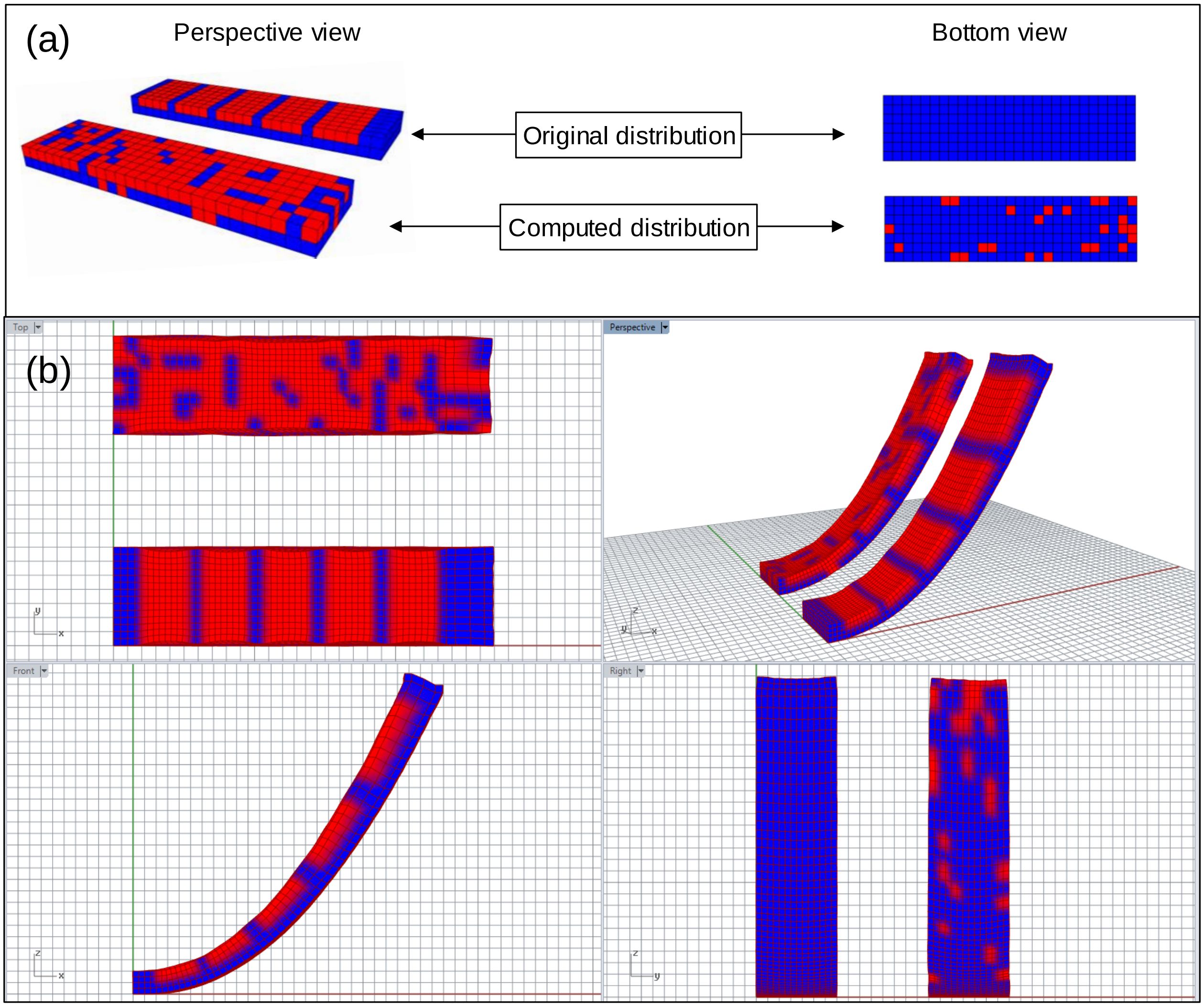


Figure 5-19 - (a) Original and computed distributions - (b) Rhinoceros® viewports of the deformations as computed by VoxSmart

5.4.3.2 Use case

Material distribution computation has been illustrated with an aerospace use case, namely an adaptive compliant wing.

In order to prevent a whole wing from stalling at the same time, wings are usually slightly twisted (a feature usually referred to as wing twist). These wings are twisted from root (near the fuselage) to tip. In most case this twist is downward from root to tip. In such configuration, angle of incidence at the tip is always lower than the one at the root, thus tip – where most of the control surfaces (especially those responsible of pitch) are located – stalls quite later than root allowing the pilot to adapt the pitch angle before the plane totally stalls. Wing twist is conventionally a fixed feature. Flight phases such as take-off are where stalling is most likely to occur, while in cruise phases the probability of such event is pretty lower. Therefore, not all the lift that can be generated by a wing is achieved with a fixed twist wing. With a wing that can be twisted at will (e.g. at take-off) and let straight at cruise for instance, there could be a higher lift at cruise and hence less energy consumption. Such adaptive compliant wings are conventionally manufactured with an underlying actuating truss which morphs the wing's skin. An alternative that could be made possible by 4DP is a bulk wing made of light conventional and smart materials in such a way that *the material is the mechanism* [173].

We elected to consider the case of a single spar wing. The wing span is of 200mm, typical of a micro unmanned aerial vehicle (MUAV). The problem has been formulated with as source shape the straight wing and target shape the twisted wing as presented in Figure 5-20. The spar crosses all the vertical sections' centroids, and the so defined axis is used as the twist axis.

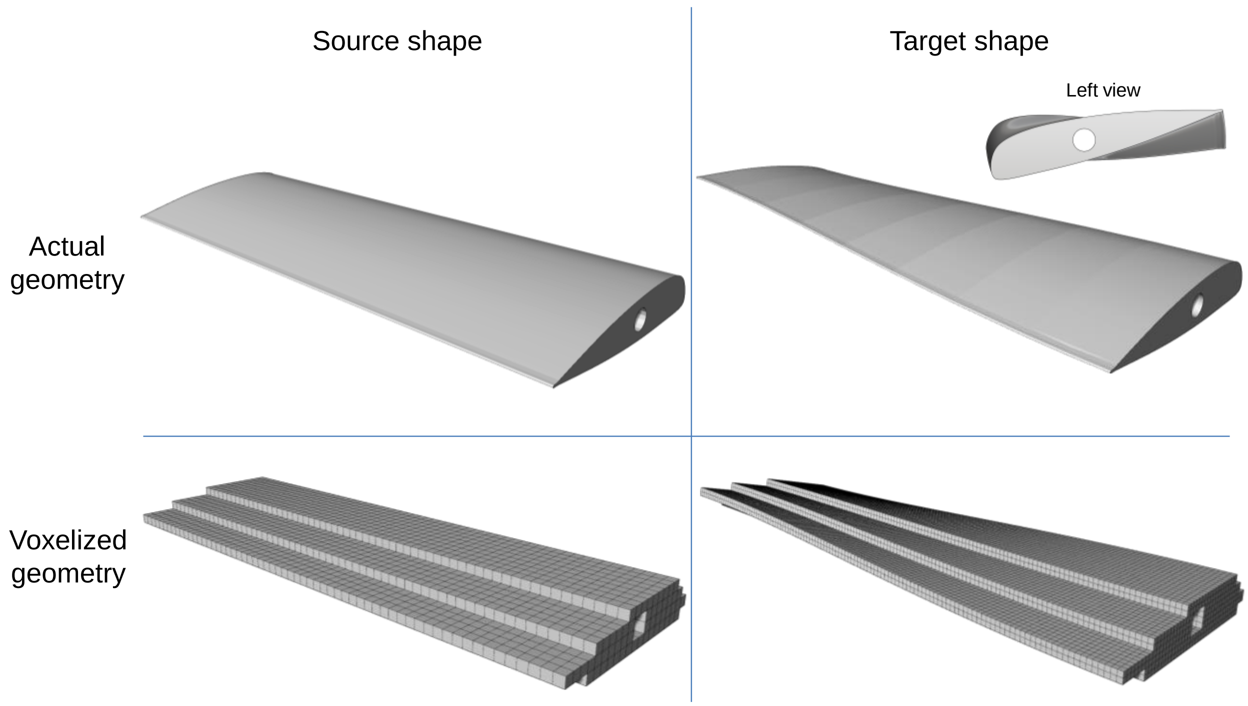


Figure 5-20 - Wing twist problem formulation

As SMs we considered polymeric magnetostrictive materials. These are obtained in composite form [192] with magnetostrictive fillers dispersed in a polymeric matrix. A carbonyl iron/silicone [193] composite has been demonstrate to exhibit a strain of almost 10% at saturation.

We then consider a set of three materials including a hard silicone (as the conventional material) and two hypothetical magnetostrictive composite material; the properties are outlined in

Table 5.3.

Table 5.3 - Materials properties for the twist wing case

	E (MPa)	G (MPa)	λ_s (%)
Silicone	30	10.07	
Magnetostrictive composite 1	30	10.07	10
Magnetostrictive composite 2	20	6.7	30

Figure 5-20 shows the source and target shape both in actual geometry and voxelized geometry. The target shape is such that the twist angle is of 15° at the wing tip.

With these settings, the return distribution is shown in Figure 5-21.a. All the magnetostrictive materials were considered to be at saturation. The deformed wing with the determined distribution is shown in Figure 5-21.b. With this distribution, the actual twist angle at tip is 12°. While the overall twisted configuration is achieved by this MD, the undulations caused by the local deformations are likely to reduce the airworthiness of the plane. Nevertheless this MD could be used as a starting point to a detailed design of the wing. In addition in the MD computation problem, constraints may be set to enforce homogeneous regions, and thus to reduce the local deformations.

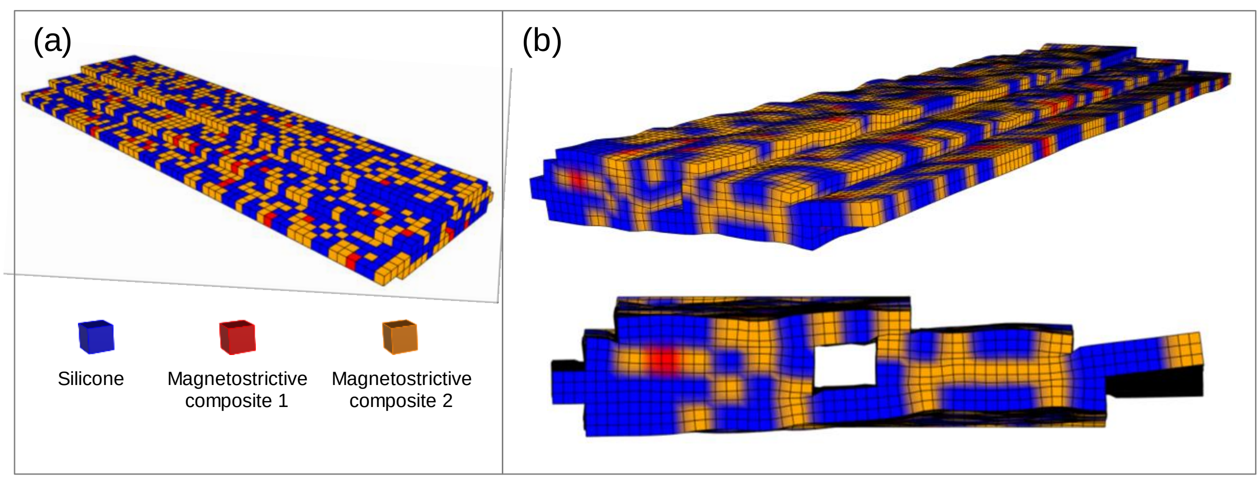


Figure 5-21- (a) Determined distribution – (b) Perspective and side view of the deformed wing when the magnetostrictive materials reach saturation

5.5 Conclusion

In this chapter a contribution has been made to SMs modeling and simulation for conceptual design. A voxel-based modeling framework has been put forth to model and simulate the behavior of both conventional and (non-programmable) shape changing SMs. With this modeling framework, the possibility is given to designers to rapidly test a given distribution of SMs and check how it behaves upon exposure to stimulus before proceeding into detail design. In this endeavor a Grasshopper® add-on, VoxSmart, has been developed to embody the theoretical modeling framework.

A few simulations were run with VoxSmart in order to somehow validate the proposed modeling scheme, both as regards conventional and SMs behaviors.

In addition to the possibility of a seamless modeling and simulation of any material distribution (forward scheme), we proposed – based on the modeling scheme – a methodology for distribution computation, using a source and a target shape (backward scheme). Such generated distribution could be a starting point for a finer design.

Simulation run with VoxSmart were quite fast and in agreement with physics. Worth highlighting nevertheless is that it is not meant to be a surrogate to established methods such as FEM; rather it is a complimentary design tool (for conceptual design) that precedes design efforts which can be invested in FEM.

Chapter 6 Proposals of other manufacturing routes to 4D Printing

Most of the 4DP studies presented in the literature rely on high end AM machines such as the Stratasys© Connex machines. The required huge investment for such machine is likely to hinder a broader exploration of the technology. This situation is not peculiar to 4DP, indeed first AM machines were expensive machines and were confined to a few research laboratories and companies. Over the course of the development of new processes, techniques and machines, AM got democratized, in companies and through the Maker Movement [194]. That movement is favored by and increasing number of FabLabs [195] and 3D printing services companies (e.g. Shapeways) worldwide. An increasing number of low cost machines and open source projects (such as RepRap [196]) have also been part of the so-called *3Democratization*.

The journey to 4Democratization is still a long way to go. A number of requirements must be met:

- Low cost machines capable of handling smart materials
- Smart materials: more off the shelf SMs should be made available in forms that can be 3D printed. Furthermore the possibility to somewhat tailor the material properties without being an expert would also contribute to a larger adoption.
- Customization: the possibility to somehow tweak the machines handling SMs to achieve specific capabilities.

In this section a contribution is made in that regard. First a machine for printing SMs is proposed, and then a semi-automatic alternative route for 4D printing is put forth.

6.1 Liquid Deposition Modeling (LDM) machine

In the endeavor to come up with a low cost machine that is easily customizable and that allow freedom on the type of materials, we elected to use an extrusion based technique. It is the one sometimes referred to as bioprinting [45] in the literature, as it has been used for tissues engineering through 3D printing. To avoid the medical connotation and to be in line with the widely used extrusion-based technique fused deposition modeling (FDM), we use the term *Liquid Deposition Modeling* (LDM).

LDM works by using materials in resin form, the material is mounted on a print head, and it is then deposited line-wise according to the part's cross-section being printed. Crucial to the success of a layer deposition is the curing method, which should occur while the material is being deposited or right after it has been deposited. The chosen method depends on the resin itself and particularly its viscosity: the lower the viscosity of the material the faster must be the curing method in order to prevent the resin from spilling too much before it cures. Methods include:

- Evaporation: an air flow, that may be combined with platform heating, is used to dry and cure the resin;
- Chemical reaction: an additive is deposited on the resin's layer to trigger its polymerization;
- UV curing: in a way similar to SLA, the resin is exposed to an UV light to photopolymerize. Obviously this requires the resin to be photopolymerizable.

The UV curing method is the most straightforward and the fastest one. Therefore we have elected to use it for our machine. This choice has had an influence on the range of materials that the machine can process.

It is one thing to be able to deposit and cure a material in resin form, but it is quite a different challenge to program the control chain leading from a part CAD file to the machine controls. Controlling the machine requires moving axes, for depositing the material where it has to be, stopping the deposition, turning on/off the curing UV light. All these controls must be expressed in the form of a G-code after the CAD file has been sliced.

The following subsections explain how these challenges have been overcame.

6.1.1 Hardware platform

6.1.1.1 Machine base

The necessity to easily move axes and the need to have a highly customizable machine have led us to choose a CNC machine as the base of the whole machine. Indeed, these machines are well known and established for their axes control capability. They are cheap (for as low as 100€ a fair CNC machine can be purchased) and they can easily be tweaked.

A standard three-axis CNC machine from ZenToolWorks was selected; the chosen machine is shown in Figure 6-1.

Figure 6-1 - The chosen CNC machine

This machine has a limited footprint and allows for a 304×178×127 printing zone, which is quite large both for proves of concept and functional parts. The resolution is of 0.025mm in XY.

6.1.1.2 Components around and on the machine

Deposition system

For the material deposition system a pressure based system for fluid dispensing was chosen. Such systems are usually used for dispensing precise and repetitive amounts of a fluid (e.g. glue). The essential components of the system are:

1. A syringe which contains the fluid to be dispensed. In most cases it is mounted with a needle for the deposition to be accurate, but in others applications, especially when the fluid is very thick, it may be used without a needle. The fluid is either moved out or retained in the syringe by an airflow applied from the top and which is supplied by a controller.
2. A controller: this component has an inlet for pressurized air and an outlet from where airflow at a desired pressure is sent to the syringe. The inward airflow is permanent with a nearly constant pressure, while the outward airflow can be blocked, controlled in term of pressure, and reversed (Venturri effect for avoiding drops formation from the needle when deposition is stopped).
3. A commander. This is an interface that sends signals to controller in order to tell when the fluid is to be deposited and when not. Commonly such interfaces are in form of a pedal or a manual trigger. Some systems allow for automatic commands by an input/output port. Such a system was chosen for our machine, as the system is used for 3D printing, which required a G-Code to be interpreted.

The basic workflow for the system is shown in Figure 6-2.

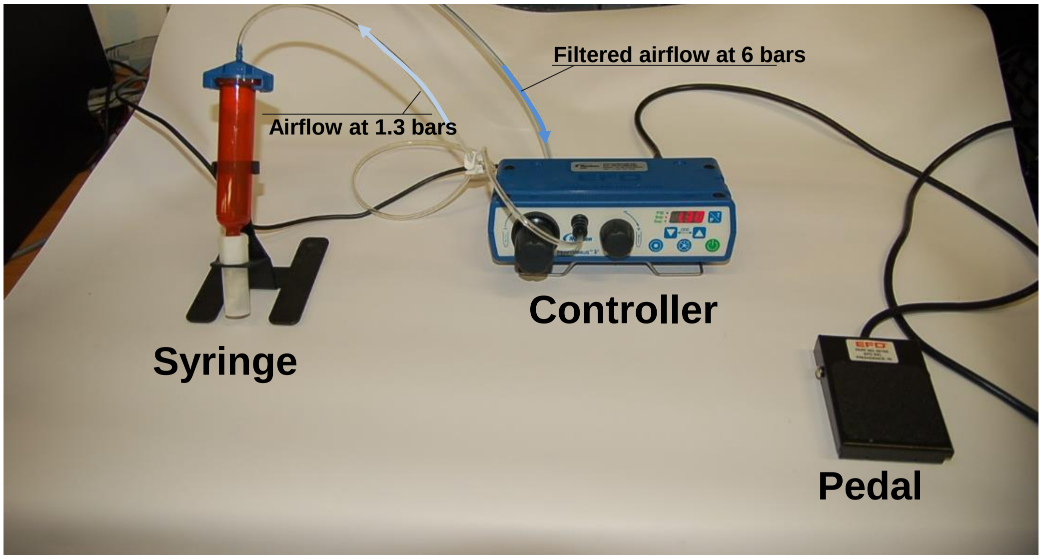


Figure 6-2 - The dispensing system workflow

The Perfomus V (Nordson, USA) precision dispensing system was chosen. This system allows the deposition of accurate, repeatable amounts of virtually any assembly fluid - including adhesives, epoxies, lubricants, paints, and grease. The outlet airflow pressure – from the controller – can be chosen between 0 and 7 bars. It has an input/output DIN port that can be used to send commands from a breakout board.

The syringe is mounted on the CNC machine. We designed a printing head that was firstly intended for mounting three syringes to deposit three different materials as shown in Figure 6-3. However, the designed printing head was finally used for only one syringe.

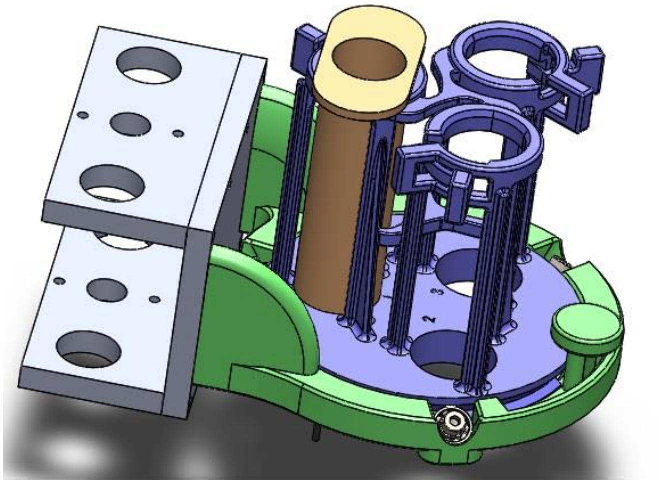


Figure 6-3 - The designed machine printing head; it was initially meant to be used for three materials deposition.

UV curing

As the chosen curing method is UV curing, an UV lamp was also made. The lamp is made of six UV LEDs connected in series (cf. Figure 6-4). The LEDs have a radiant flux of at least 1W and emit a wavelength between 390nm and 395nm. A metal sheet was formed into the form shown in Figure 6-4. and the LEDs were bolted on it. To prevent the LEDs from melting due to the light-induced heat, a layer of thermal paste was applied between them and the metal. This paste improves heat dissipation from the LEDs through the metal sheet.

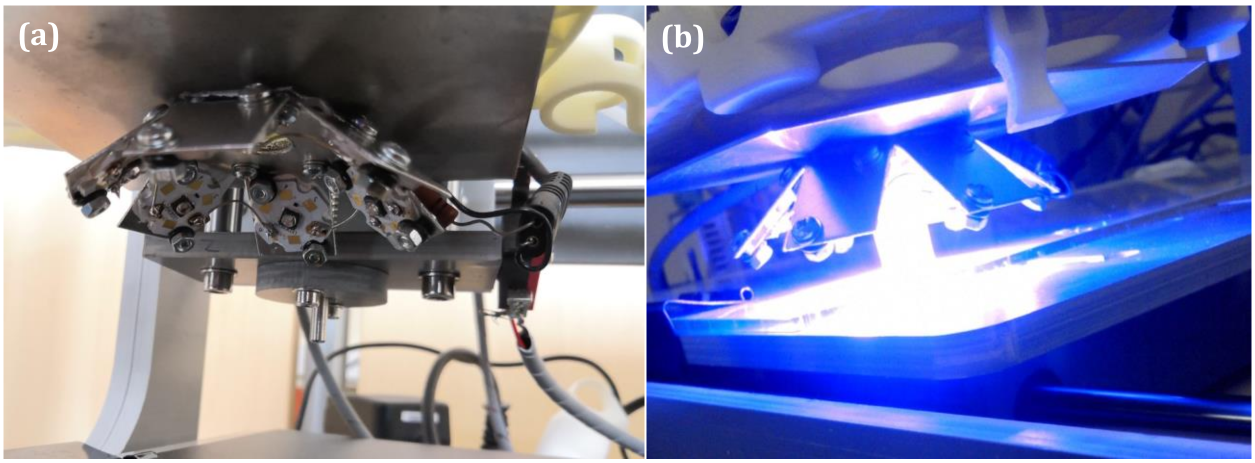


Figure 6-4 - The UV curing system. (a) It is made of 6 UV LEDs bolted on a metal sheet in such a way that they all focus on a common point. (b) The lamp as it is during printing.

Machine calibration

By default the CNC machine comes with limit switches that are used to set the zero (home) and limit positions on each axis. Setting home for the X and Y axes can be done once and for all with the limit switches. However for the Z axis, home must be set right at the location where the needle touches the printing bed. As many different needles (with varying lengths) could be used on a syringe and the syringe is to be often moved or replaced, there is the need to set the right Z axis home using the needle tip. A setting that must be done at the beginning of each printing. To solve this issue we used an anti-vandal pushbutton as a switch for homing on the Z axis. That pushbutton was secured on the print bed using a holder (as shown in Figure 6-5), accesses were provided for the wires to be connected to the breakout board. For this method to be as most accurate as possible, the height from platform at which the needle truly presses the button must be measured. This can be done by moving the Z axis, from the control software, until the needle touches the platform and moving it downwards the button until the signal from this latter is received. The difference between the two positions as shown in the control software yields the required height.

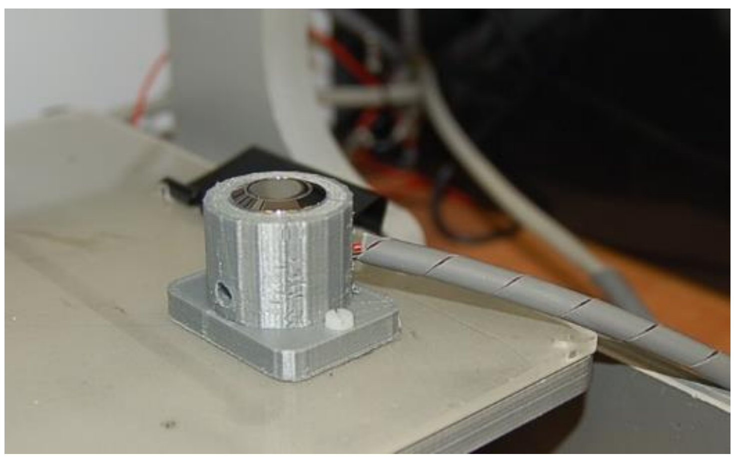


Figure 6-5 - Probe used for accurate Z zeroing

Breakout board

The CNC machine was delivered with a control package including, among others, a Mach3 Breakout Board. This board allows for control of up to 5 axis stepper motors. In addition it has an on board spindle on/off control relay and 5 input ports, to accept the signal from end stops and emergency stops. These latter were also used for the Z calibration pushbutton. The spindle on/off relay was used as the commander to the deposition system's controller.

6.1.1.3 Materials

As material for the machine we used UV curable resins purchased from ABChimie (France). The resins' properties are shown in Table 6.1.

Table 6.1 - Materials used with the LDM machine

	ABchimie 225UV	ABchimie 15K-UV	ABchimie 42K-UV
Nature	Polyester acrylate	Polyester acrylate	Urethane acrylate
Color	Transparent	Transparent	Transparent (light yellow coloration)
Curing thickness	0-5 mm	0-5 mm	0-5 mm
Viscosity (at 20°) in Pa.s	16	15	42
Cured harness	D40	D60	D30

These resins have a good adhesion to many substrates; in the cured state they are soft. They are quite viscous (as a comparison honey's viscosity is in the range 2-10 Pa.s) which make them suitable for our LDM machine. In layers as thick as a few millimeters they cure upon exposure to UV light within a second. They were used in our machine for their shape memory effect.

6.1.2 Software

The software component of the designed machine entails G-code generation and machine controls with that G-code.

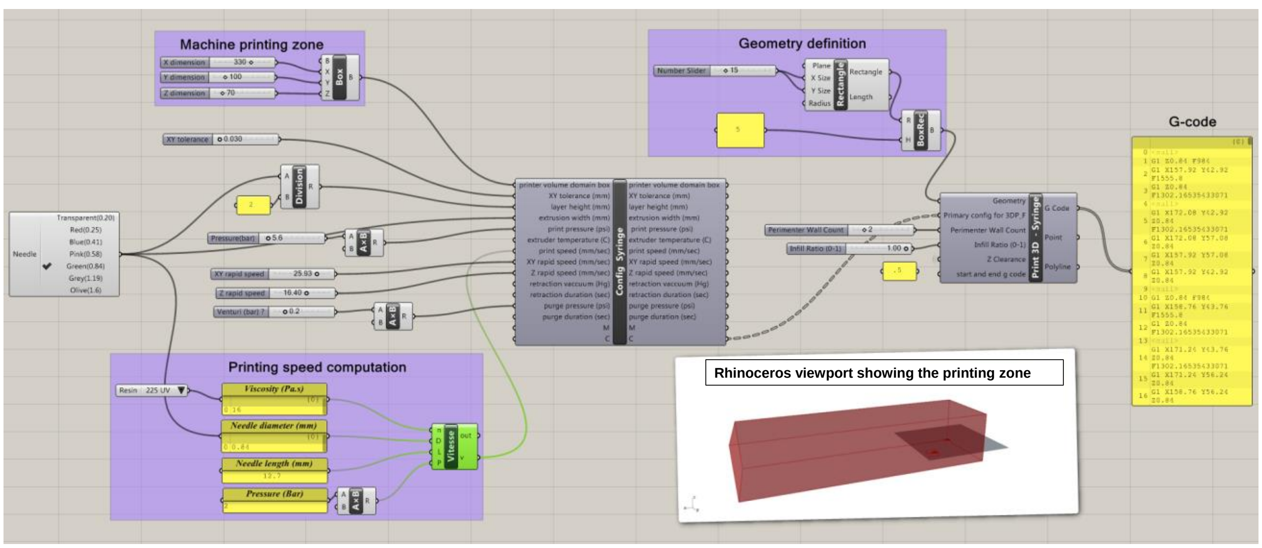


Figure 6-6 G-code generation from the Grasshopper© add-on Xylinus

In the endeavor to facilitate – in the future – the printing of material distributions generated from VoxSmart (see section 5.3 at page 130) in GH, we elected to use a GH based G-code generator. The Xylinus [197] GH add-on has been chosen for that purpose. This add-on can generate G-code for several AM techniques including FDM, DLP, ink-jet and syringe-based printing. We then used the components dedicated at this latter technique. The workflow to generate the G-code is quite simple (only two Xylinius components are required), but a number of others input are required, namely geometry to be printed and settings for the machine. These settings include, inter alia, printing volume domain box, layer height, printing pressure, printing speed, wall count and filling ratio. A GH definition of the G-code generation is shown in Figure 6-6.

Regarding printing height, the *half of the nozzle diameter* rule of thumb has been used. In order to ensure an accurate deposition (no gaps in the deposited lines or no over-extrusion) the printing speed has been set to the speed of the resin at the needle's tip. Only straight needles were used and the resin viscosity makes its flow laminar in the needle. The flow is due to the difference in pressure between the top of the needle (where the pressure is the one delivered by the controller, up to 7 bars) and the needle's tip at atmospheric pressure. In such condition the flow follows a Hagen-Poiseuille law. The resin's speed at the tip can then be derived from the Hagen-Poiseulle law fiving the flow rate:

$$v = \left(\frac{D}{2}\right)^2 \times \frac{\Delta P}{8\eta L} \tag{6.31}$$

Where:

- D is the needle diameter,
- ΔP is the pressure difference,
- η is the resin dynamic viscosity
- L is the needle's length.

This formula was implemented in the GH definition for the G-code generation (see the *Printing speed computation* group in Figure 6-6).

The so generated G-code has been somewhat tweaked to suit our LDM machine's needs. As such the G-code only provides commands for the printing head motions but no control over the dispensing system controller nor over the UV curing light. We elected to keep the UV light on during printing. The G-code was only tweaked for the dispensing system controller. This latter is plugged to the spindle relay output of the breakout board. So the G-code commands M04 (*spindle on*, that is, *deposition*) and M05 (*spindle off*, that is, *no deposition*) have to be inserted. Some of the lines of the initial G-code are for travel motions while others correspond to printing. The difference between these two states is the federate (the motion speed). This difference has been used to insert the M04 and M05 command at the right lines. Technically a short Matlab script was written to read the code generated from Xylinus and to modify it accordingly.

The so modified G-code is then saved in a .tap format and loaded into the Mach3 software from which commands are sent to the machine.

The whole workflow can be seen in Figure 6-7.

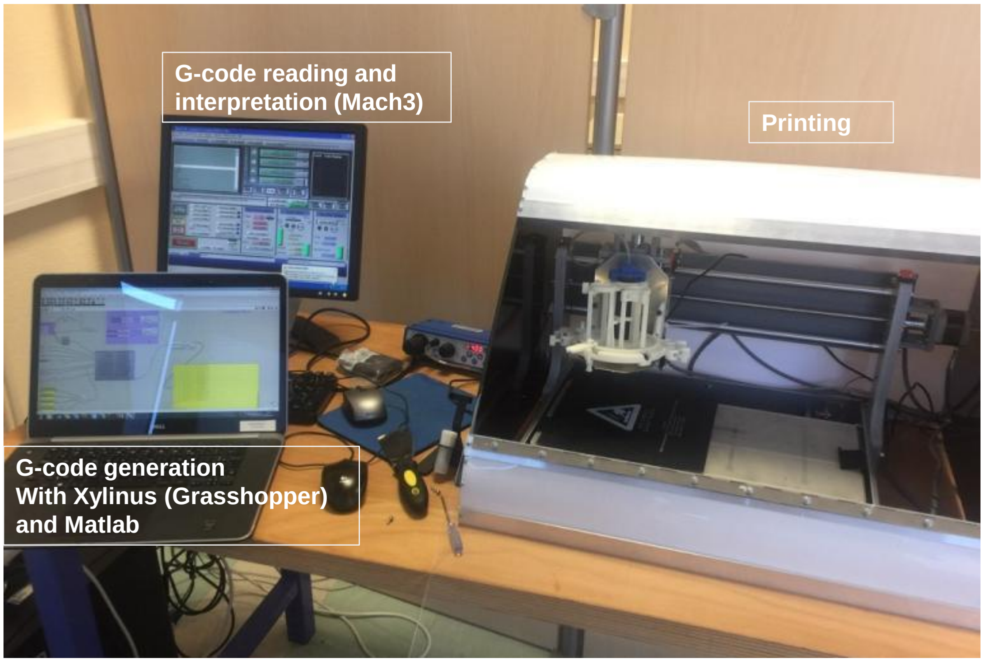


Figure 6-7 - The developed LDM machine workflow from CAD file to printing

The Mach3 software that can control the breakout board can only work on a desktop computer running Windows XP as operating system. This requires thus the G-code to be transferred to another computer connected to the breakout board.

6.2 Future evolutions of the proposed LDM machine

6.2.1 Software

Despite being operational, the machine's use is not straightforward. Especially because of the required data transfer to a computer running Windows XP. This burden is imposed by the breakout board delivered with the CNC machine. A near future evolution would consist in controlling the machine with an Arduino breakout board. Such card can seamlessly be used on a PC and there is also a GH add-on Firefly [198] that can send commands to an Arduino card right from GH.

6.2.2 Hardware

The machine can currently process one material at a time, which means that only homogeneous parts can be printed. However, as explained in 0, 4DP should be explored with a multimaterial approach. Even though the current syringe holder has been designed to hold three syringes (meant to rotate for material change during manufacturing), it cannot really be used for multimaterial printing. Indeed the lamp at the bottom of the print head prevents such motion. Furthermore, there is no guarantee that the needles, when depositing, would always have their tips at the same location which may be a cause of inaccuracies. A better option would consist in having a single needle fueled by different barrels. This option can be realized by the print head shown in Figure 6-8. At least there should three different materials: one for an inert material, one for a smart material and third one for support structures. This explains why there is three inlets for the proposed print head.

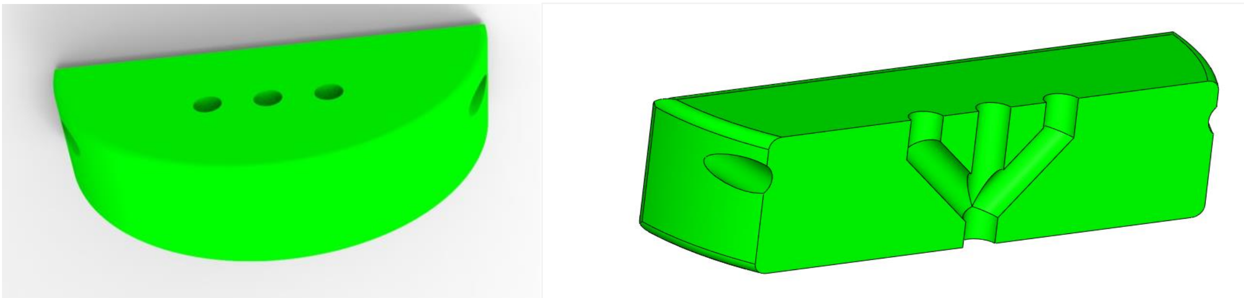


Figure 6-8 – Perspective view and section of a print head for multimaterial deposition

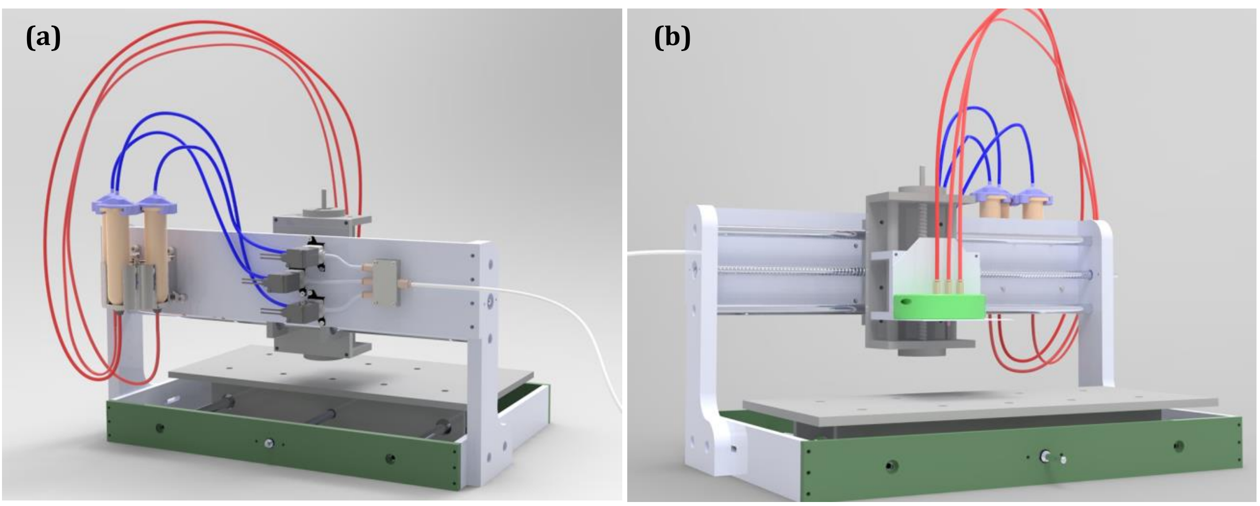


Figure 6-9 - A future version of the LDM machine for multimaterial printing: (a) back view showing three syringes all converging to the printing head. (b) front view showing the printing head (green) mounted with a single needle.

The whole new version of the machine is shown in Figure 6-9.

6.2.2.1 Materials

Materials processed by the machine are currently limited to SMP sensitive to heat. The raw material in resin form allow for more customization. Given a photocurable resin which in cured form behaves like a conventional material, composites resins can be prepared by adding fillers depending on the desired functionality. Such route for customization can work, provided the fillers stay in suspension in the resin, do not clog the needle and do not scatter the UV light. For instance carbon nanotubes may be added to such resin to make it sensitive to light for light heating, or magnetostrictive fillers may also be used to print magnetostrictive composites [192].

6.3 A semi-automatic approach

A route to 4D printing which combines multimaterial FDM and manual processing has been proposed as well. It is route also based on SMs in resin form. The approach is for printing parts made of an active structure and inert. It requires an FDM machine that can print with at least two materials with one which is easily removable. Basically the easily removable material is used to form a mold that surrounds the inert structure printed with the other material. That mold is used latter on to process the active material in resin form. The mold is finally removed.

We used this approach with an Ultimaker 3 Extended FDM machine. This machine is a dual extruder one which can print parts with two materials. As easily removable material we used the Ultimaker water soluble PVA filament and as inert material a PLA filament was used. The whole procedure (shown in Figure 6-10) is as follows:

1. CAD model: the part CAD model is an assembly of components making up the inert structure and the mold structure. Inert structure must be connected to the molds in such a way that the resin can flows from the mold into the inert structure. This can be ensured with notches in the inert structure as shown in Figure 6-10.a. The notches allow for bonding between the inert structure and the active structure.
2. Printing: the so designed assembly is then printed with the FDM machine (Figure 6-10.b)
3. Resin processing: the resin is poured into the mold in 1mm layer and cured. The process is repeated until the mold is totally filled. (Figure 6-10.c).
4. Mold removal. The whole part (inert structure, cured active structure and mold) is immersed in water until the mold is totally dissolved. (Figure 6-10.d).

The so printed part in Figure 6-10 is made of a thermochromic material (as the inert structure) and SMP made of the ABchimie 225UV resin.

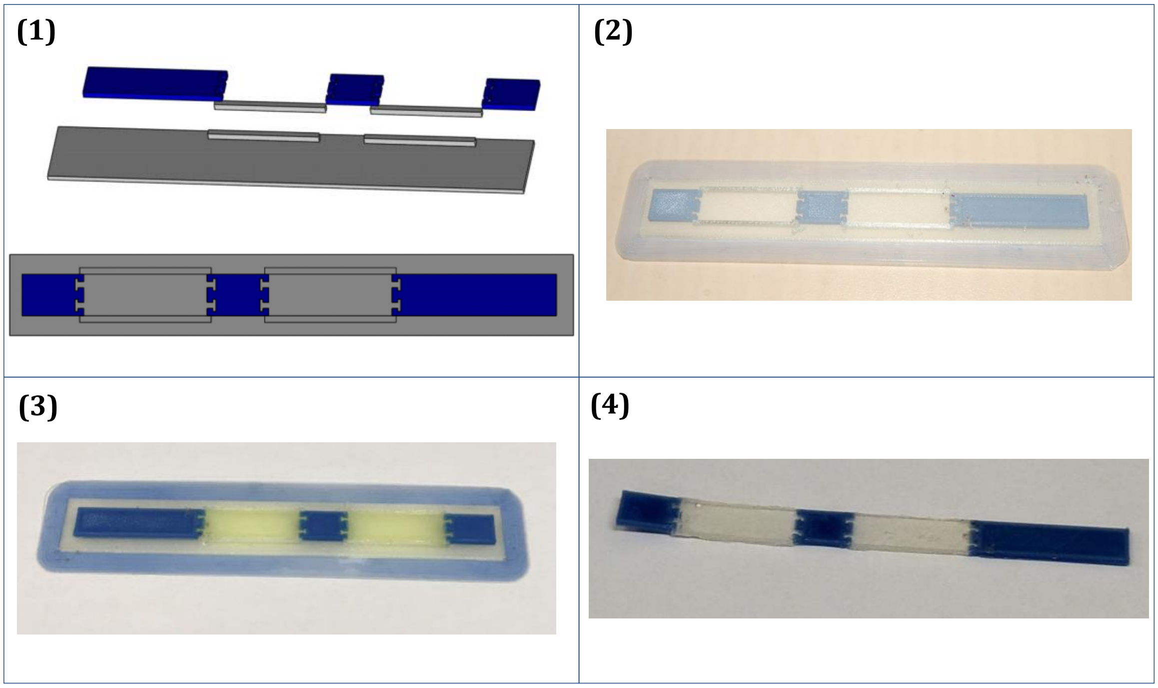


Figure 6-10 - Steps of the semi-automatic approach

Chapter 7 Conclusion and recommendations for future work

4DP has been mainly scrutinized from a manufacturing and material perspective. So, as highlighted in the literature review, there was a lack of design tools and methodologies to help designers considering this breakthrough in manufacturing. To the best of our knowledge, this thesis is the first one looking at 4DP purely from a design perspective. The goal the PhD project was to put forth a methodological framework to Design for 4DP.

This last chapter summarizes the contributions made to achieve the aforementioned goal and it stresses out work that still need to be done for a broader 4DP establishment among designers and thus in the industry.

7.1 Contributions

A 4DP product is inherently a 3DP product and as such designing such product cannot be made regardless of what AM can and cannot do. To account for this, a DFAM approach has been proposed. An approach for the design of not just single components but also products, that is, assembly of several components. From a product concept, it aims at providing a minimal architecture of a product based on the available AM techniques' capabilities; in addition it generates a manufacturing plan that directs detail design of the product. A minimal architecture is one in which components are consolidated up to what is allowed by the selected AM techniques (e.g. components' merging, assembly-free mechanisms, multimaterial printing, etc.). In addition to the generation of the minimal architecture the approach also provides a methodology for part design with a minimalist vision, that is, which leverage the shape complexity capability of AM to use the bare minimum matter. The methodology is based on functional flows. This contribution is meant to benefit:

- Designers considering AM of mechanical assemblies,
- Designers considering 4DP, in that in can be used to design the inert structure of the product.

What makes the essence of 4DP is the SMs used as "ink" for 3DP. The functional aspect of SMs requires designers to be aware of how they work rather than just how much load (be it mechanical or not) they can withstand (as it is for conventional materials). Another contribution of the thesis has been made in that regard. Noticing that SMs were not given consideration from a design perspective, we provided a design-oriented view of SMs by putting forth a data structure on SMs that capture all the information designers may need to consider them. Building on this, a proposal has been made to help the identification of potential SMs candidates for envisioned applications. As such this contribution is meant to promote SMs in industrial application and it also meant to be a first step in a design project considering 4DP. A web application (still in prototype state) has been proposed to foster a worldwide SMs adoption among designers.

It is one thing to understand how SMs work, but it is quite a different issue to predict how they work when they are arranged in a specific pattern with others conventional materials and SMs. We highlighted how valuable multimaterial printing of SMs is of high importance to 4DP, but also the lack of design tools for predicting (especially in conceptual design phase) how such heterogeneous objects would behave upon exposure to stimuli. The thesis has also contributed to DF4DP in that sense. A theoretical model of matter simulation, allowing a seamless modeling and simulation of heterogeneous objects, has been proposed. These objects are made of material distributions including both conventional and smart materials. Material distribution specification is made easy through voxel-based modeling. In the DF4DP toolbox this model is meant to rapidly simulate how a distribution of SMs would behave and as such it will benefit the conceptual design stage of 4DP products. Furthermore, recognizing that finding the right distribution – producing a desired shape change – is not an intuitive task (unless highly experimented in heterogeneous strain), we proposed a methodology for computing distributions based on a source and a target shape. These two proposals (distribution simulation and distribution computation) have been materialized by a computational design tool, a GH plugin (VoxSmart). It is hoped that this tools would prompt designers to explore the design space around SMs and thus 4DP.

7.2 Future work

This DF4DP spark is hoped to be built on. A number of other directions can be taken to expand both DF4DP and 4DP.

Regarding 4DP, an interaction that is still unexplored is the one between SMs and lattices structures [199]. Indeed such intricate structures are likely to improve the performance of SMs which currently are limited by shapes we are used to. Furthermore the possibility to embed electronics components into 3D printed part can also be harnessed to make SMs smarter. For instance these can be made sensitive to sound, or wireless signal such as Wi-Fi. Finally 4DP is currently mostly focused on shape changing SMs, a situation fully encapsulated by the sentence: "The types of stimulus-responsive materials capable of change in physical properties can be classified into shape-change material and shape memory material."[200]. As shown in the literature review, given the 30 types of SMs there are at least 250 feasible ways – AM technique and SM combinations – of exploring 4DP.

In regard to DF4DP, a broader view can be taken to tackle the design problem. A view that considers transformation not at the material scale but at product scale. Such approach would basically sets how a product should transform (be it mechanically or not) to change from a source state to a target state, by generating a backbone of the product consistent with the desired change. This vision is wholly depicted in meta-framework shown in Figure 7-1 .

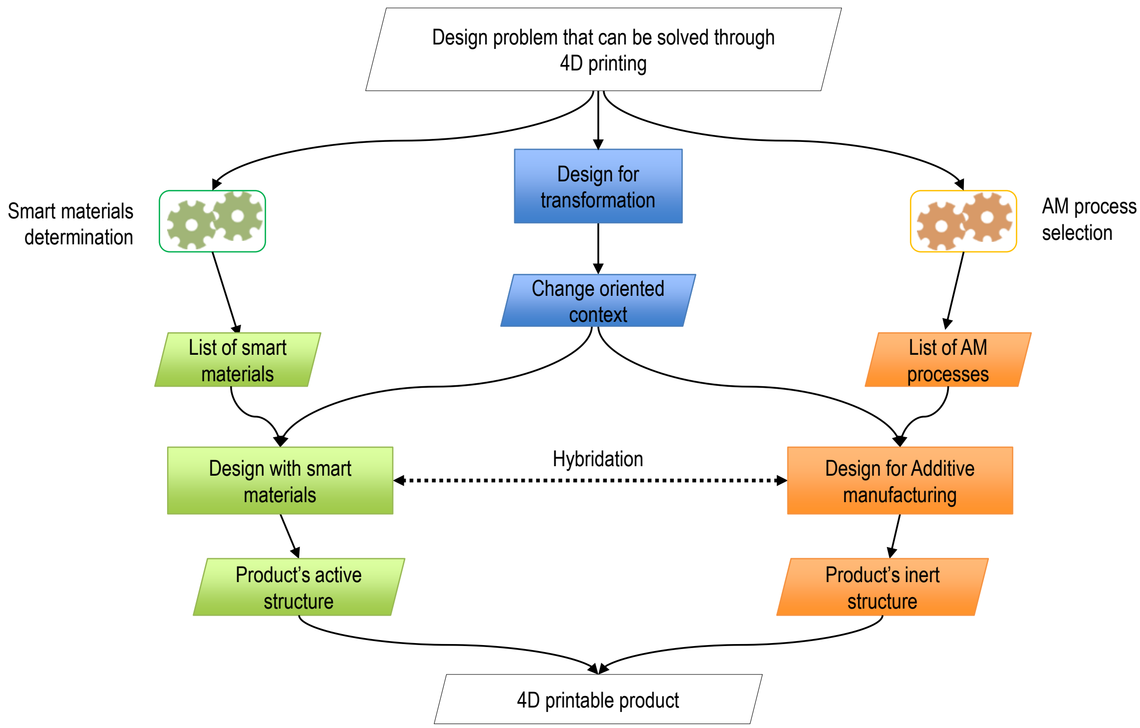


Figure 7-1 - A future vision of Design For 4D Printing [56]

A design for transformation scheme methodology would first be used to design a context – or a backbone – that is consistent with the desired change and that directs (and somehow constrains) downstream stages of the design process. This change oriented context would then be used to design the active and inert parts of the product using a Design with SMs (DwSM) approach and a DFAM scheme.

The proposal regarding a design related view of SMs is about to be expanded through a more theoretical approach, which is currently addressed by a recently funded PIA ISITE BFC project called HERMES[25] (spatiotemporal semantics and logical knowledge description of mecHanical

[25] contract ANR-15-IDEX-0003

objEcts in the era of 4D pRinting and programmable Matter for nExt-generation of CAD systemS). The HERMES project aims at elaborating (i) a strong foundational theory enough suitable for covering the semantic and logical description of dynamical phenomena knowledge at various scales (i.e. territory/building, mechanical assembly, material, etc.), (ii) a multi-layer ontology for semantic and logical reasoning, on which (iii) computational mechanisms will be developed in order to deliver dynamical CAD models ready for 4D printing.

Besides, regarding SMs distributions, gathering them by functionality in libraries of distributions could ease the process of designing for 4DP. In a way similar to how standard parts' components such as bolts, nuts, or technical pair are available in some CAD software, libraries of SMs distributions with their tuneable parameters can be implemented into CAD software.

More specifically and regarding our modelling scheme for SMs in 0, in spite of the interesting results, our proposal still has room for improvement. The necessity to anchor at least one voxel hinders the simulation of free objects. Besides, the way stimuli, especially the scalar ones, are modeled typically ruled out the possibility to simulate deformations that could be induced by non-uniform stimuli fields. Finally in the current setting, voxels making up an object must be of the same size. An adaptive voxelization with a variable voxel size according to regions of interest, could further reduce computation time and allow for bigger objects to be simulated. In addition to the aforementioned limitations, future work can also include effects such as collision, friction and gravity. Furthermore as regards materials, shape memory materials could also be modeled; the exploration of what a distribution including SMs of different types (e.g. one sensitive to heat and another sensitive to light) is another way of extending the modeling scheme. Regarding distribution computation, the stimulus itself could also be optimized (along with the materials) to achieve the desired target shape, provided that the stimulus is not a design constraint. In the same vein, the way material distribution is computed will be improved: currently the exploration is made voxel-wise, however a more efficient approach could be to explore the design space group of voxels-wise, for instance a constraint can be set so that materials must be the same within a 3D Manhattan distance of 2, 3, etc. voxels from specific set points. Other constraints on materials may also be imposed, such as a conventional material at desired regions.

Research work publications

1. Peer-reviewed international journals

Sossou, G., Demoly F., Montavon G. and Gomes S. (2018). "An additive manufacturing oriented design approach to mechanical assemblies." Journal of Computational Design and Engineering 5(1): 3-18. https://doi.org/10.1016/j.jcde.2017.11.005

Sossou G., Demoly F., Qi J.H., Belkebir H., Montavon G., Gomes S. (2019). "Design for 4D printing: A voxel-based modeling and simulation of smart materials." Materials & Design, 175, 107798. doi: https://doi.org/10.1016/j.matdes.2019.107798

Sossou G., Demoly F., Qi J.H., Belkebir H., Montavon G., Gomes S., Design for 4D printing: Modeling and Computation of Smart Materials Distributions. Materials & Design, Under review, 2019.

2. Peer-reviewed international conferences

Sossou, G., F. Demoly, G. Montavon and S. Gomes (2018). "Design for 4D printing: rapidly exploring the design space around smart materials." Procedia CIRP 70: 120-125. doi: https://doi.org/10.1016/j.procir.2018.02.032

Sossou, Germain, Frédéric Demoly, Ghislain Montavon and Samuel Gomes. “Towards A Top-Down Design Methodology For 4d Printing.” 21st International Conference on Engineering Design, 2017.

Sossou, Germain, Frédéric Demoly, Ghislain Montavon and Samuel Gomes. “Towards an approach to additive manufacturing oriented design.” 11th International Symposium on Tools and Methods of Competitive Engineering. 2016

3. Peer-reviewed national symposium

Germain Sossou, Frédéric Demoly, Ghislain Montavon, Samuel Gomes. “Vers une méthodologie de conception proactive pour la fabrication additive.” 15e Colloque National AIP-Priméca, 2017.

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Appendix A: Text information template for smart material description

Material name: [text]

Qualitative description of the behavior *(Description of the behavior of the material)***:** [text]

Type *(the condition or material form in which the material is conventionally available)***:** [polymer, metal, ceramics, fluid-like]

Group *(the smart material category):* [shape changers, converters, optical sensors, state changers]

Working environment *(the environments or media in which the material can be used)***:** [air, solvent, vacuum, any] – many are possible in case *any* is selected, all the others are automatically selected

Stimulus *(what the material is sensitive to)***:**

- **Main stimulus** *(the stimulus to which the material is originally sensitive to):* [light, heat, electric field, magnetic field, chemical concentration, pressure]
- **Possible alternative stimuli** *(others stimuli that the material may be sensitive to):* [light, heat, electric field, magnetic field, chemical concentration, pressure]

Response: [color, light, heat, deformation, stress, electric field, magnetic field, stiffness/viscosity]

Quantitative description:

Exposure to stimulus for response to be effective *(any specific information about how should/must the material be exposed to the stimulus so that the response is triggered)***:**

- Stimulus location: [Endogenous, exogenous]
- Explanation: [text]

Cycling *(is the behavior reversible? Are there limitations?)***:**

- Reversible: [yes, no]
- Limitations: [text]

Forms *(in which form(s) is the material available?)***:** [resin, powder, sheet, predetermined (solid) shape]

Suppliers (names and links to website**):**

- Supplier name: [text]
- Website: [link]

The one filling the form should be able to add as much suppliers as wanted. These will then be displayed to the users in a table form.

"Processability" ***(****how is the material usually processed? Has it been 3D printed? Can it be 3D printed?****)*****:**

- Conventional processing method: [molding, forming, machining, others]
- 3D printability: [yes/no]
- (If 3D printable) 3D printing techniques and references
  - 3D printing technique: [a list of the 3DP techniques will be provided]
  - Reference: [links]

  The one filling the form should be able to add as much 3DP techniques as wanted. These will then be displayed to the users in a table form.

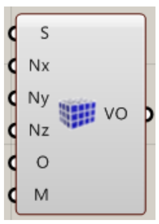
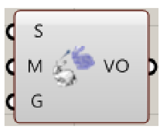
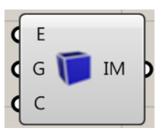
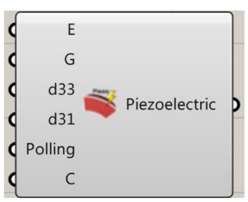
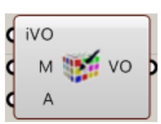
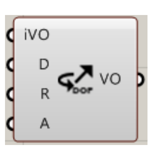
List of functions that can be fulfilled or that has been fulfilled by the material: [text] – this will not really be a text but rather a *tag*. The one filling the form could add up to 5 functions, and as he or she is typing, there should be autocompletion: a menu appears below the field containing (basic functions) database entries that match the partial input. Data for these functions are provided in the excel file.

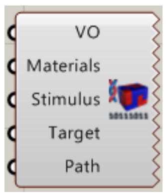
Examples of applications:

- Application name: [short text]
- Description: [text + possible image]
- Reference: [link]

The one filling the form can add as much applications as wanted. To users, these will be presented by name. And clicking the name will lead to the application's description page

Appendix B: Main VoxSmart's components

	Component		Description	Input	Output
Voxel Edition	Cubic object		Generates a voxel object in the form of a regular 3D grid	• S: voxel size • N*i*: number of voxel along the *i* direction • O: origin, this is the position of the voxel with the lowest coordinates values M: material	VO: a voxel object
	Voxelizer		Voxelizes an object of any shape	• S: voxel size • M: material • G: geometry to be voxelized in a Brep form	VO: a voxel object
Materials	Inert material		Generates an inert material object	• E: Young modulus • G: shear modulus • C: color	IM: an inert material object
	Piezoelectric material		Generates a piezoelectric material object	• E: Young modulus • G: shear modulus • d33 and d11: piezoelectric coefficients • Polling: polling direction • C: color	Piezoelectric: a piezoelectric material object
	Material painter		Assigns materials to specific regions	• iVO: a voxel object • M: list of material object • A: list of regions of the voxel object	VO: a voxel object
Boundary conditions	DOFs		Assigns prescribed degrees of freedom (displacement or rotation) to voxels within specific regions	• iVO: a voxel object • D: Prescribed displacement in the form of a vector • R [optional]: Prescribed rotation in the form of a vector • A: list of regions of the voxel object	VO: a voxel object

	Fixing		Fixes voxels within a region. All the degrees of freedom of these voxels are set to zero.	• iVO: a voxel object • B: A region	VO: a voxel object
Distribution computation	Distribution		Handles the distribution computation problem and packs all the input in a file that is read by Matlab	• VO: voxel object in the initial state • Materials • Stimulus • Target: the prescribed DOFs • Path: full path to Matlab file in which all the data are stored.	

Appendix C: Matlab script for the genetic algorithm

```
clc
clear;
%% Loading
load('file.mat'); % data sent from VoxSmart
%% Handling the input
%----- Materials -----
Materials = cell(size(MaterialsInput,1),1);
Materials{1} = Material(MaterialsInput(1,1), MaterialsInput(1,2));
for i = 2:size(MaterialsInput,1)
    Materials{i}      =      FHydrogel(MaterialsInput(i,1),      MaterialsInput(i,2),
MaterialsInput(i,3));
end

%----- Voxels -----
VoxelLinks = cell(size(VoxLinks,1),1);
for i = 1:size(VoxLinks,1)
    lks = VoxLinks(i,:);
    VoxelLinks{i} = lks(lks>0);
    clear('lks');
end

%----- Links -----
Links = cell(size(LkVoxelsOrient,1),1);
for i = 1:size(LkVoxelsOrient,1)
    Links{i} = Link(VoxSize, LkVoxelsOrient(i,3), Materials{1}, LkVoxelsOrient(i,1),
LkVoxelsOrient(i,2));
end


%% Testing
%SF = SmartForce([1 1 0 0 0 1], Materials, Links, VoxelLinks, Stimulus);
%Kdistrib = GlobalStiffnessDistrib([1 1 0 0 0 1], Materials, Links, VoxelLinks, K,
NodeTag);
%% running the GA
%----- Bounds on our Vector of Indices -----
lb = zeros(1, size(VoxLinks,1));
ub = (size(MaterialsInput,1)-1) * ones(1, size(VoxLinks,1));

%----- Constrain All the Variables to be Integers -----
intCon = 1:size(VoxLinks,1);

%----- Set Options for Optimization -----
options = gaoptimset('CrossoverFrac',0.85,'PopulationSize',100,...
    'StallGen',125,'Generations',150,'EliteCount',10,...
    'PlotFcns',@gaplotbestf);

%----- Run the Genetic Algorithm -----
[distribOpt,fVal] = ga(@(x)Fitness1(x, Materials, Links, VoxelLinks, Stimulus, Target,
NodeTag, K_inert),...
     size(VoxLinks,1),[],[],[],[],lb,ub,[],intCon,options);
```