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Knowledge formalization and recommendation in computational design synthesis for 4D printing

Saoussen Dimassi

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Version provisoire

THÈSE DE DOCTORAT DE L'ÉTABLISSEMENT UNIVERSITÉ BOURGOGNE FRANCHE-COMTÉ
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Knowledge Formalization and Recommendation in Computational Design Synthesis for 4D Printing

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par

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Ingénieure en Mécatronique

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À Maman, À Papa !

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Abstract

Coined in 2013, 4D printing is considered as a promising technology that combines additive manufacturing (AM) processes and smart materials (SMs). Through this technology, objects can change over time in terms of functionalities, shape, or properties under the effect of energy stimulation. Although AM processes allow shape, hierarchical, functional, and material complexities to the 3D objects, the conjunction with SMs provides much more freedom in designing adaptive/transformational structures. Over the last decade, a growing body of research with *ad hoc* proofs-of-concept have been proposed at the physical level (i.e., by using different AM processes with commercial or customized 3D printers and tuned SMs). Despite the numerous endeavors, 4D printing requires more research efforts in design and engineering to define complex structures aligned with new usage scenarios. Considering that product architects and designers are neither AM experts nor materials experts, this innovative technology requires the development of new models, approaches, methodologies, and tools in design. The main objective of this PhD – falling under the domain of design for 4D printing – is to address 4D printing knowledge formalization and reuse, especially in computational design synthesis. First, a framework is proposed to build an ontology from both a top-down approach (based on multi-dimensional theories and basic formal ontology) and a bottom-up approach (based on research experiments). Then, an ontology – formalizing and representing the knowledge in 4D printing (with its main pillars: AM processes, SMs, stimuli, and transformation functions) is developed. It constitutes a relevant knowledge base for various purposes in design for 4D printing, such as material-process selection, transformation sequence planning, and materials distribution recommendation, to name a few. Built on this the second contribution is focused on the multi-representation of a 4D printed object at the computational design synthesis stage because it plays a crucial role (i.e., functional, behavioral, structural) in the design for 4D printing. This multi-representation is then further described as a sub-ontology to be integrated into the domain ontology respecting different rules and constraints. Finally, a recommendation method is proposed - allowing quickly identifying the material distribution in 4D printed objects with comparison to experiments from the literature. The latter constitute the instances for the ontology and a semantic base (composed of words) to feed a vector space model in order to propose a specific material distribution. Case studies have been introduced and a dedicated application has been developed in the Rhinoceros3D/Grasshopper environment to demonstrate the applicability and the relevance of the proposal.

Keywords: 4D printing, design for 4D printing, additive manufacturing, smart materials, ontology, recommendation method, formalization, vector space model.

Résumé

Créée en 2013, l'impression 4D est considérée comme une technologie prometteuse qui combine les procédés de fabrication additive (FA) et les matériaux intelligents (MI). Grâce à cette technologie, les objets peuvent évoluer dans le temps en termes de fonctionnalités, de forme ou de propriétés sous l'effet d'une stimulation énergétique. Bien que les processus de FA permettent des complexités de forme, d'usage de matériaux, etc. aux objets 3D, la conjonction avec les MI offre davantage de liberté dans la conception de structures transformables. Au cours de la dernière décennie, un nombre croissant de recherches avec des preuves de concept *ad hoc* a été proposé au niveau physique (c'est-à-dire en utilisant différents processus de FA avec des imprimantes 3D commerciales ou personnalisées et des MI). Malgré les nombreux efforts, l'impression 4D nécessite beaucoup plus d'efforts de recherche en conception et en ingénierie pour définir des structures complexes s'alignant avec les nouveaux scénarios d'utilisation. Considérant que les architectes et les concepteurs de produits ne sont ni des experts en FA ni des experts en MI, cette technologie innovante nécessite le développement de nouveaux modèles, approches, méthodologies et outils de conception. L'objectif principal de cette thèse est d'aborder des problématiques de recherche sur la formalisation et la réutilisation des connaissances en impression 4D, notamment en synthèse de conception computationnelle sous le domaine de la conception pour l'impression 4D. D'abord, un framework est proposé pour construire une ontologie à partir d'une approche descendante (basée sur les théories multi-dimensionnelles et d'une ontologie basique formelle) et d'une approche ascendante (construite à partir d'expériences dans la littérature). Cette ontologie formalise et représente les connaissances en impression 4D (intégrant les procédés de FA, les MI, les stimuli et les fonctions de transformation). Elle constitue une base de connaissances pertinente dans le contexte de conception pour l'impression 4D, plus particulièrement en ce qui concerne la sélection des matériaux actifs, la planification des procédés de FA et les séquences de transformation, et la recommandation de distribution de matériaux. En se basant sur cette ontologie, la deuxième contribution concerne la multi-représentation des objets imprimés en 4D en phase de synthèse de conception computationnelle car elle joue un rôle important (i.e. fonctionnel, comportemental, structurel) dans la conception pour l'impression 4D. Cette multi-représentation est ensuite décrite comme une sous-ontologie à intégrer dans l'ontologie du domaine en respectant différentes contraintes. Enfin, une méthode de recommandation permettant d'identifier rapidement la distribution des matériaux dans les objets imprimés en 4D est proposée - en faisant des comparaisons avec une base sémantique composée des expériences issues de la littérature. Ces expériences constituent les instances de l'ontologie et la base qui alimente un modèle spatial vectoriel afin de proposer une distribution de matériaux spécifique. Des

études de cas ont été proposées et une application dédiée a été développée dans l'environnement Rhinoceros3D/Grasshopper pour illustrer l'applicabilité et la pertinence des contributions.

Mots clés : impression 4D, conception pour l'impression 4D, fabrication additive, matériaux intelligents, ontologie, méthode de recommandation, formalisation, modèle spatial vectoriel.

تلقطُ شذورَ العلمِ حيثُ وجدتها... و سلها و لا يخجلكَ أنك تسألُ
إذا كنتَ في إعطائكِ المالَ فاضلاً... فإنك في إعطائكِ العلمِ أفضلُ

Fragment of an Arabic Poem

Translation:

**Pick up the fragments of knowledge wherever
you find them... and ask it, and do not be
ashamed that you are asking**

**If you are virtuous in giving your money, then
in giving your knowledge you are more so.**

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Glossary

Term	Definition
4D printing	A single-material or multi-material printing of a device or object that can change in shape/properties/performance triggered by an energy stimulation.
System	A collection of interacting or interconnected pieces that function in accordance with a set of rules in order to produce a coherent whole.
Product development phase	The step-by-step procedure of all the actions needed to take a product from its initial concept to its market presence.
Design activity	The product architect or the product designer endows form and ensures functionality of a given product.
Product life cycle	The length of time from a product first being conceived, then manufacturing, introduced to consumers until it is removed from the market.
Computer aided design	The use of computers (or workstations) to aid in the creation, modification, analysis, or optimization of a design.
Design for X	It is an approach of concurrent engineering putting the disposed resources together into best use; X is a variable that can be additive manufacturing, assembly, ergonomics, 4D printing, etc. Its objective is raising productability and efficiency and improving quality.
Rhinoceros 3D	It is a freeform surface modeler CAD software that uses parametric modeling for customized design.
Grasshopper plugin	It a visual programming environment that runs within the Rhinoceros 3D computer-aided design application and supports users' developments.
UML diagram	An UML (Unified Modeling Language) diagram is a visual representation of a system, together with its major actors, roles, actions and artifacts or classes, with the goal of improving understanding, altering, maintaining or documenting information about the system.

Reverse engineering	A method or procedure used to deduce how a previously constructed object, process, system, or piece of software executes a task with little or no knowledge of how it does so.
Mereotopology	First-order theory, embodying mereological and topological concepts, of the relations among wholes, parts, parts of parts, and the boundaries between parts.
Ontology	The branch of philosophy that studies concepts such as existence, being, becoming, and reality.
Word embedding	A term used for the representation of words for text analysis, typically in the form of a real-valued vector that encodes the meaning of the word such that the words that are closer in the vector space are expected to be similar in meaning.

List of acronyms

Acronym	Definition
AM	Additive Manufacturing
SMs	Smart Materials
SM	Smart Material
MI	Matériaux Intelligents
FA	Fabrication Additive
CDS	Computational Design Synthesis
DFX	Design for X
CAD	Computer-Aided Design
IoT	Internet of Things
ASTM	American Society for Testing and Materials
API	Application Programming Interface
FFF	Fused Filament Fabrication
DIW	Direct Ink Writing
SLA	Stereolithography
DLP	Digital Light Processing
SMP	Shape Memory Polymer
SME	Shape Memory Effect

BFO	Basic Formal Ontology
VSM	Vector Space Model
DbA	Design by analogy
HERMES	spatiotemporal semantics and logical knowledge description of mechanical objects in the era of 4D printing and programmable matter for next-generation of CAD systems
OWL	Ontology Web Language
DL	Description Logic
SPARQL	SPARQL Protocol And RDF Query Language
SHACL	Shape Constraint Language
NIST	National Institute of Standards and Technologies
EMMO	European Materials Modeling Ontology
SWRL	Semantic Web Reasoning Language
SQWRL	Semantic Queries Web Reasoning Language
ML	Machine Learning
DFAM	Design for Additive Manufacturing
MD	Material Distribution

List of symbols

Symbol	Definition
\sqsubseteq	The entity is defined as a subclass of a later definition
\forall	Universal restriction
$\cap, \cup, \bar{}$	Intersection, union, and complement of concepts
\exists	Existential restriction
$= 1$	The entity defined within it has only one concept
\leq_c	Concept subsumption
\cap_C	Concept intersection
ρ_R	Axiom signature (Object Property)
sC	Concept set
sT	Datatype set
sR	Role set
sA	Attribute set
sI	Instance set
sV	Datavalue set

Chapter 1 Introduction and research context

“On the outskirts, everything looks the same. It is very far, at the end of every worry, that we find clarity”

Michèle Mailhot, Le Fou de la reine

“L’axiome doit être simple. Doit-il être clair? Pas nécessairement. Simplicité et clarté, c’est deux »

Victor Hugo

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1.1 Introduction

Manufacturing makes progress – in the same way that any other scientific or technological domain does – when it shows the accumulation of knowledge. History has shown that manufacturing has never stopped moving forward, from crafting stones three million years ago to the discovery of making papers in 105 BJC until nowadays. It can be observed how extensive the contemporary manufacturing milestones are, from handmade crafts to conventional technologies (i.e., turning, milling, etc.), additive manufacturing, and finally, 4D printing. However, this PhD thesis is not about analyzing the history of manufacturing and humankind evolutions but is still valuable to know these evolutions concisely throughout time. 4D printing stands here as a ‘new episode’ of manufacturing, giving way to trendy and innovative smart products – promoted by the unique capabilities of smart materials (i.e., materials responsive to energy stimulation) and additive manufacturing processes. This chapter introduces an overview of the manufacturing industries and product/system capabilities evolutions in the two following sections. The fourth section presents 4D printing technology in brief. The general context of this thesis and its related motivations and objectives are announced respectively in the fifth and sixth sections. Finally, the last section establishes the main thesis structure.

1.2 Evolution of the manufacturing processes

Humans were constantly on the lookout for methods to improve their ability to create goods to satisfy their survival requirements. From the stone age until now, tremendous progress is noticed. The above-mentioned requirements have grown exponentially (i.e., from survival to economic, competitive, entrepreneurial, scientific challenges, financial, research, discovery, etc.). This progress can be traced in these primitive ages upon pre-history¹:

- *The stone age*: Lasted around 3,4 million years and came to an end 120 000 years ago; the stone was frequently used to manufacture tools with an edge, a point (**weapons**), or a percussive surface, known as **stone tools**;
- *The Neolithic age*: Lasted some 20.000 to 10.000 years ago BJC; this era was marked by the emergence of farming, agriculture, **pottery**, and the **use of fire**;
- *The bronze age*: 3300 years BJC; this period was characterized by the **use of bronze**, **proto-writing**² and other features of urban civilization;
- *The iron age*: 1200 years BJC; in this prehistoric period, the iron or steel manufacture has progressed to the point that **iron tools** and **weaponry** have mostly replaced their bronze counterparts. It was also the beginning of the invention of the city.

¹ Britannica.com/technology/history-of-technology/Technology-in-the-ancient-world

² Proto-writing is a symbol system consists of the use of visible marks communicating a specific information.

At the end of these periods, human has already known **coating** (i.e., covering that is applied to the surface of an object), **moulding** (shaping strip of wood as a decorative architectural feature), **forming**, **cutting**, and **joining** (i.e., attaching an arrowhead to wooden arrow shaft using resin or other materials). Although in 45 BJC, a Greek inventor named Hero of Alexandria designed the world's first steam turbine: the movement of steam through the device caused the sphere to revolve, demonstrating the potential for using steam as means of propulsion. But it did not contribute to speeding up production. The dispositive stood up 17 centuries later – just as the world's first aeolipile presented the physical transformation of steam into rotary motion – until it was exhibited at the end of 17th century to harness its power into manufacturing.

- *Early, high, and late middle ages* (14 centuries) & *The Viking age* (from 15th to 17th century): In this historical period, humans have known an enormous multiplication in materials' usage and, in technological and military innovations: i.e., windmill, distilled spirits, astrolabe, a rotation system for planting crop, advanced building technologies, cannon, gunpowder, etc. In this era, scientific progress was tremendous and breath-taking, but how we manufacture goods did not globally change from the previous ages. Until this era, all the manufacturing processes were handcrafted, hand-operated and not mechanized yet – even though some wheels and lathes have marked the ancient Egyptian civilization – unless the **chemical properties change** can be added and noticed as a particular way of manufacturing tissues.
- *The industrial revolution* (18th and 19th centuries) has brought up the proper **mechanization** of manufacturing processes. Steam engines have made steam power available and contributed thoroughly to this revolution. Different domains leveraged profit from this invention and were economically and technologically boosted up in that era, such as textile machinery, iron industry, cement production, gas lighting, and glassmaking. In the wake of these changes, the world has known several other manufacturing processes like for example **rolling** in 1783 (the process of passing metal stock between one or more pairs of rollers to lower the thickness, make the thickness uniform, and/or impart a desired mechanical feature to the metal stock) and **puddling** in 1784 (the process of producing bar iron i.e., the molten crude iron was stirred in a reverberatory furnace resulting in wrought iron). In a significant advance, two **metal shaping** processes have marked the last two centuries of the manufacturing industry: **turning** in 1752 and **milling** in 1816. The process of turning consists of cutting away undesired material; it is a type of machining known as material removal. It is used to make rotating components by removing the unwanted material during this process. A turning machine or lathe, a workpiece, a fixture, and a cutting tool, are required for the turning process. As for milling, the material is cut by moving the cutter forward into the workpiece. Milling is one of the most common types of machining. A wide range of activities and machinery are used in milling, ranging from small individual pieces to massive, heavy-duty gang milling operations on a wide variety of sizes. This period has also emphasized **assembly lines** (i.e., a manufacturing process in which parts of such a product are added

from workstation to another as the semi-finished assembly moves and it respects a precise sequence until the final assembly occurs) and **mass production** (i.e., which is sometimes referred to as flow production, series production, or serial manufacturing; it is ultimately the manufacturing of large quantities of standardized products).

- *20th and 21st centuries* are marked by the discoveries of electronics and the internet, which has contributed to the emergence and full reign of automation technology where machines are capable of operating on their own. This reliable innovation resulted mainly in three major manufacturing technologies. First, the **computer numerical control (CNC)** was invented in 1930, which consists of the fact that a computer can control machining equipment (such as drills, lathes, mills, and lately 3D printers) to automate manufacturing. By following a coded program and commands - and without the involvement of a physical operator – a CNC machine may precisely process a given piece of material (metal, plastic, wood, ceramic, or composite) to fulfil such criteria. Second, **computer-aided manufacturing (CAM)** was invented in 1952, which automates a manufacturing process via software and computer-controlled gear. Toolpath generation software instructs a machine on manufacturing a product by producing toolpaths. Third, **Additive manufacturing (AM)** was invented in 1984 [1] and consisted of fabricating a three-dimensional product from a **computer-aided design (CAD) model** or a three-dimensional digital model. It is also known as "3D printing". It refers to a range of procedures in which material is deposited, connected, or solidified under computer control to make a three-dimensional object, with the material being placed together (such as polymers, metals, composites, etc. being fused) in different forms (i.e., liquids, filaments, powders, pellets, etc.), in a layer-by-layer fashion.
- *Industry 4.0* or the fourth industrial revolution results from increased interconnectedness and intelligent automation. The convergence of technologies such as artificial intelligence, gene editing, sophisticated robotics, and blurring borders between the physical, digital, and biological worlds are all part of this period of industrial transformation. As a result of the ongoing automation of traditional manufacturing and industrial practices, as well as the use of modern smart technology, large-scale machine-to-machine communication (M2M), and the internet of things (IoT), fundamental shifts in how the global production and supply network operates are taking place.

Referring to all the technologies listed above as rudimentary steps in manufacturing industry, it can be seen that any technology starts from scratch, proofs-of-concept, and *ad hoc* experiments until it arrives at such level of maturity³ (case of the steam engine) and formalization. At least this would provide a deeper valuing of the significant milestones that 4D printing has reached.

³ A level of maturity is a well-defined evolutionary plateau that establishes a level of capacity for improving such a process/system/product.

1.3 Evolution of products/systems capabilities

Regarding the evolution of manufacturing processes over time – as explained briefly in the previous section –, the product delivered by these multiple technologies differs from an era to another: a weapon from the stone age is indeed much less sophisticated than a gun of the middle ages which is in its turn less refined of any other contemporary product. The manufacturing industry has been progressively forced to increase product/system capabilities and compact its lifecycles by ensuring a certain level of flexibility and efficiency as competitive edges, especially in the product development phases where design activities and decisions have a significant impact on downstream processes (i.e., manufacturing, assembly, etc.) [2].

The above has been successfully achieved by considering the capture and integration of lifecycle constraints and knowledge (e.g., design for X (DFX) spectrum approaches and advanced CAD) in mechanical product design to deliver lifecycle friendly products. Over the last decades, efforts have been made towards integrating a wide range of manufacturing technologies and lifecycle purposes in product design. As such, several methods and tools falling under the concept of DFX [3] have been proposed. DFX aims to concurrently consider lifecycle purposes like assembly, manufacturing, recycling, product design, etc., and delivering lifecycle friendly designed definitions (see mechanical product box in Figure 1). Integrating other disciplines such as electronics in the mechanical product design has permitted the mechatronic product's achievement, which ensures system control and signal processing (see mechatronic product box in Figure 1). Furthermore, the integration of computing capabilities in the era of the IoT has delivered connected objects such as smartphones, to cite a few (see connected objects box in Figure 1) [4].

Figure 1 shows that such kinds of systems have generated interesting and fruitful results in theories, models, approaches, and tools with a high level of maturity (from Levels 4 to 5). One promising and emerging trend consists in augmenting systems/products responsiveness and smartness once manufactured regarding user needs and then increasing their lifetime by providing appropriate usage and configuration in a specific use context and environment (see the blue box in Figure 1) [5][6]. Over the last decade, many smart products/systems have emerged likewise products/systems that are capable of adapting to their environment, changing in terms of form or properties, self-assemble, repairing themselves and being able to sense their environment and react accordingly in a programmable manner, to name a few. Thus, innovative additive manufacturing technologies - that adds time as a dimension of transformability - has required to deeply revise the current well-established design and engineering approaches so as to deliver dynamic product definitions at various levels of description (i.e., design, product geometry, functional material, manufacturing, transformation logic, etc.) [7].

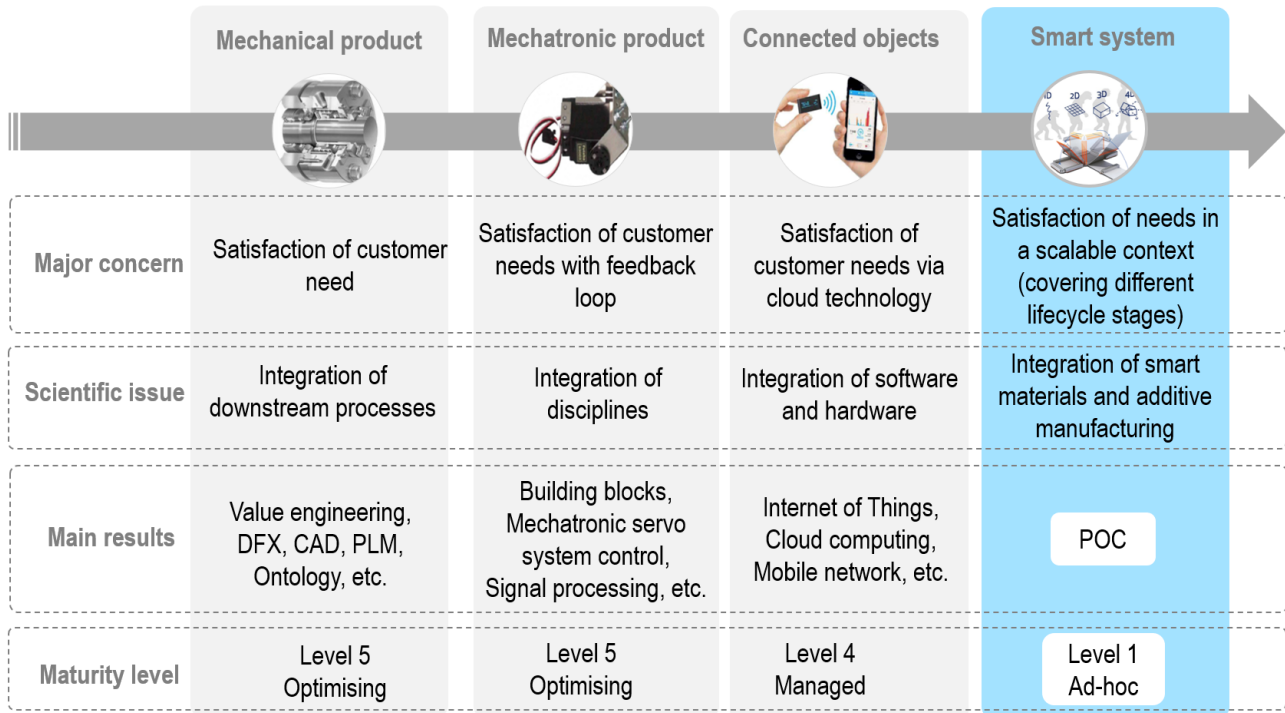


Figure 1. Evolution of product types and related scientific challenges, results, and maturity levels [8]

It remains essential to be mentioned that the transformability concept of objects dates from antiquity, i.e., from the Egyptian civilization, as shown in Figure 2. Nowadays, 4D printing is seeking the conjunction of multiple concepts and advancements to assure a smart transformable product that can adapt to such environment/stimuli, layerally manufactured, numerically designed with a controlled machine and processes. Such initiatives remain *ad hoc* from a maturity level point of view and deserve to be intensively explored in the upcoming years [9].

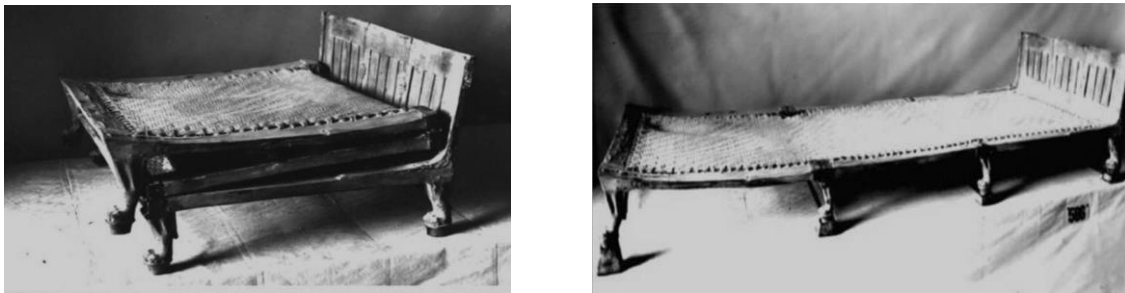


Figure 2. Sophisticated folding bed of Pharaoh Tutankhamun⁴

To ensure the full adoption of 4D printing in industry and academia, it becomes vital to address design for 4D printing issues in terms of elaborating knowledge models, methods, and tools. The above rationale is emphasized by current 4D printing practices, related proofs-of-concept and *ad hoc* experiments showing

⁴ Scienceinfo.net/sophisticated-folding-bed-of-pharaoh-tutankhamun.html

scattered and disparate knowledge due to the multiple involved expertise. But before addressing these issues, let's understand this technology in the next section.

1.4 4D printing

The main pillars of 4D printing technology are AM processes/techniques, SMs, and stimuli; although the following sub-sections will present AM, SMs, and 4D printing in general to introduce the technology.

1.4.1 Additive manufacturing

Since the beginning of the 1980s, rapid prototyping – which is also known as three-dimensional (3D) printing or AM – has received growing attention from academia and industry (about 150.000 scientific papers), mostly federating a broad spectrum of scientific domains [1][10][11]. Thanks to the ingenuity of three French scientists: Jean-Claude André, Alain Le Méhauté and Olivier de Witte, layers of materials are added to a CAD model to create complex 3D solid parts, as presented in the generic and general process for this technology in Figure 3. The above is done without additional resources or specific equipment for parts, reducing geometric complexity and the limits of topology optimization imposed by traditional production. As opposed to more traditional production processes, AM has the potential to transform the manufacturing business. Although no other standard manufacturing technology can match its capacity to create intricate forms and geometries. According to various criteria, there are several classes for AM technology. AM processes are frequently categorized based on the raw material used and the baseline technique used as input [12]. By comparing the capabilities and limits of various processes, these categories aid in the selection of a suitable process. The American Society for Testing and Materials (ASTM) classified the AM processes into seven categories [13]. The latter are VAT polymerization, material jetting, material extrusion, sheet lamination, binder jetting, direct energy deposition and powder bed fusion as shown in Figure 4 for such an example of metal as raw material.

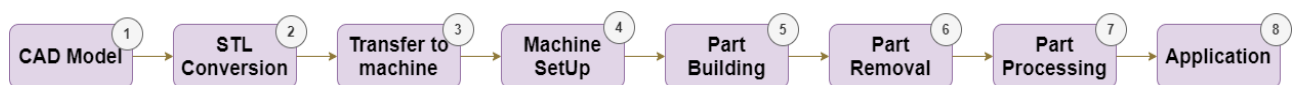


Figure 3. Generic process of AM technology

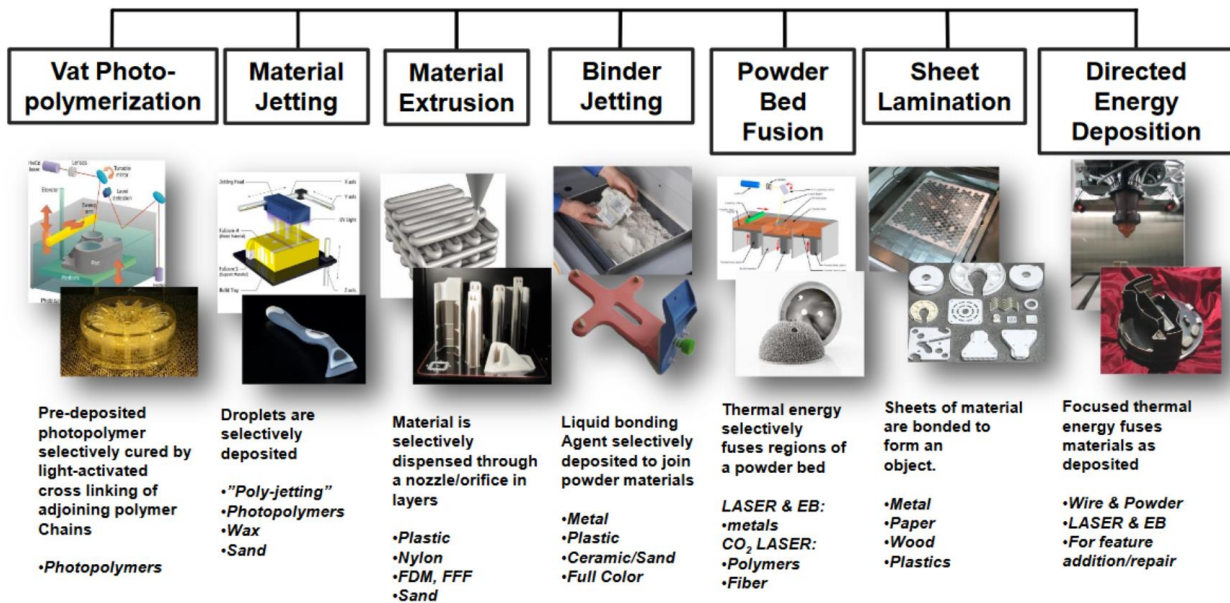


Figure 4. Seven AM processes according to ASTM committee F42 on AM. source: Boeing/ASTM⁵

1.4.2 Smart materials

Nature appears to possess an aptitude for adaptability, transformation, self-organization, and self-healing that should be harnessed in the design of materials [14]. A SM – also known as an intelligent, active, programmable, or stimuli-responsive material – is a type of material whose characteristics may be considerably altered in a controlled manner by external stimuli, such as stress, moisture, electric or magnetic fields, light, temperature, pH, etc. Researchers working on this issue have made considerable progress in the last three decades and found applications in a wide range of fields, such as medicine, artificial muscles, sensors, actuators, and deployable structures, to name a few [15].

1.4.3 Brief scope about 4D printing

Beyond the engineering opportunities and challenges offered by AM, two emerging and interrelated paradigms have been derived, namely 4D printing and bio-printing [16]. Both technologies aim to integrate transformation capabilities into additively manufactured parts using stimuli-reactive matter. The main interest in this thesis is strictly about 4D printing in which the ability to evolve is imbued and appended to static objects. As such, many definitions can be found in literature:

- “The initial configuration is created by 3D printing, and then the programmed action of the shape memory fibers creates time dependence of the configuration – the four-dimension (4D) aspect” [7];

⁵ <https://insights.globalspec.com/article/7447/factors-to-consider-when-3d-printing-or-additive-manufacturing-metal-parts>

- *“... 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” [17];*
- *“... 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 AM techniques...” [18];*
- *“... 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 ...” [19].*

By combining several transformation primitives, such as bending in Figure 5, it is possible to create a variety of responsive transformations, including 1D linear transformation, 2D surface expansion and contraction, 2.5D texture change, and 3D folding, to name a few [20][21]. To achieve a curving transformation, spores were applied across the entire substrate; as for an angular transformation, they were applied in lines on top of the substrate. In the latter case, a stiffer material can be attached to substrate regions without spore actuators to stabilize the structure and enhance the effect of a sharp fold. Here, new advances across design, science and engineering fields have opened an opportunity to program SMs [22]. By relating AM techniques and SMs, 4D printing can play a crucial role in fabricating transformable, deployable and adaptive structures that carry out a predictable shift [7][23][24]. This challenging association provides a temporal dimension in which stimuli trigger transformation. Therefore, the development of 4D printing applications requires taking advantage of AM techniques capacity and multi-material printing ability [25–27]. With both capabilities, parts are subsequently designed and manufactured as alive objects able to shift into different physical states or geometric configurations concerning their trigger conditions [28]. Indeed, stimuli are required to activate changes such as structure, shape, properties, and functionalities at various levels.

Primitives



Transformations

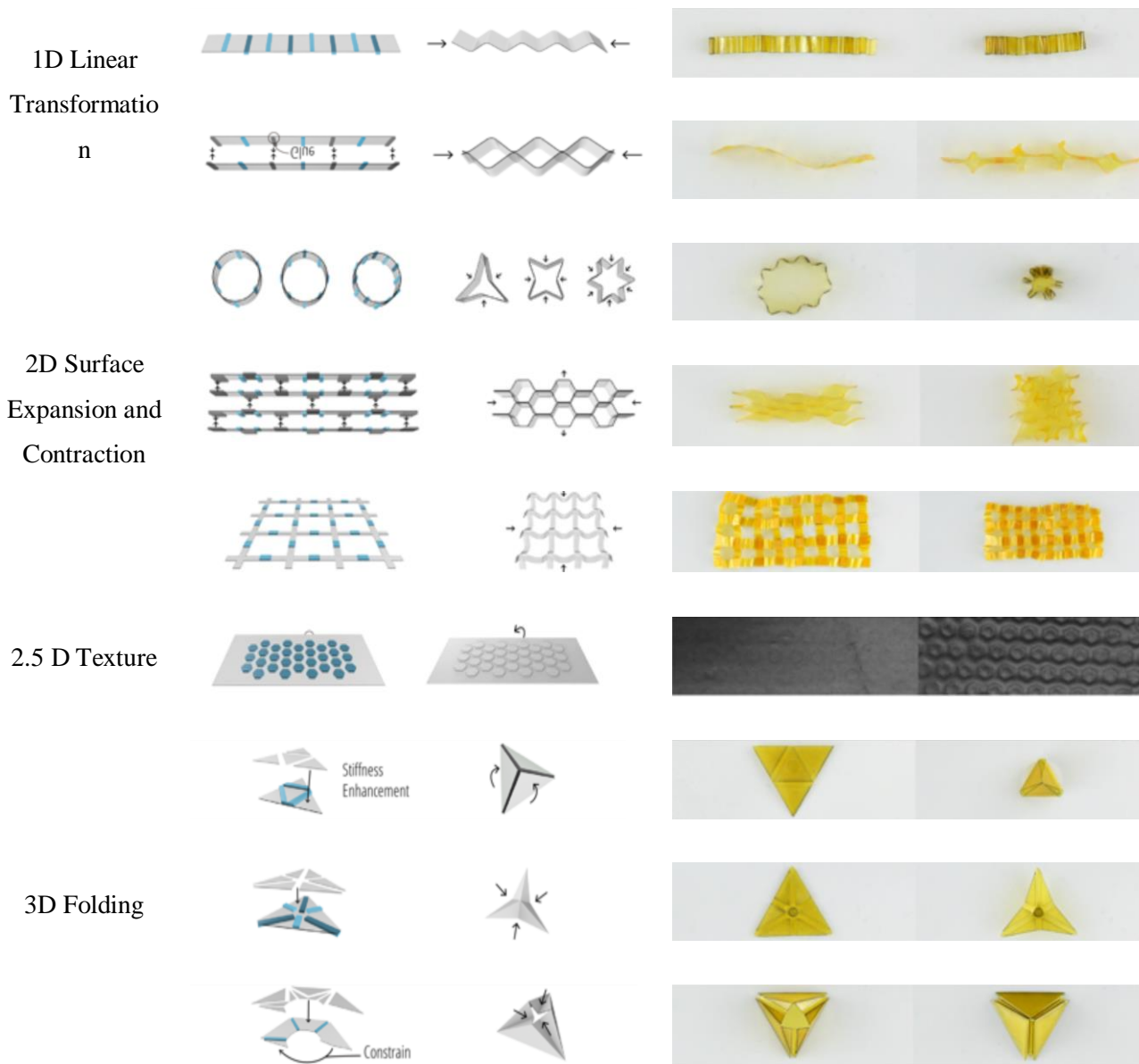


Figure 5. Examples of shape-changing primitives from 1D to 3D and its 4D printed prototypes [20]

As an illustrative example in Figure 6, BMW manufacturing company has tried to undertake this issue to build its latest prototype “Vision Next 100” with the “alive geometry concept by using dynamic capabilities of Rhinoceros3D CAD software with Grasshopper plugin (exhibiting algorithmic and parametric modelling via a visual programming representation) and 4D printing potential. This capability offers information storage, computation, and transformation in shape and/or material property.

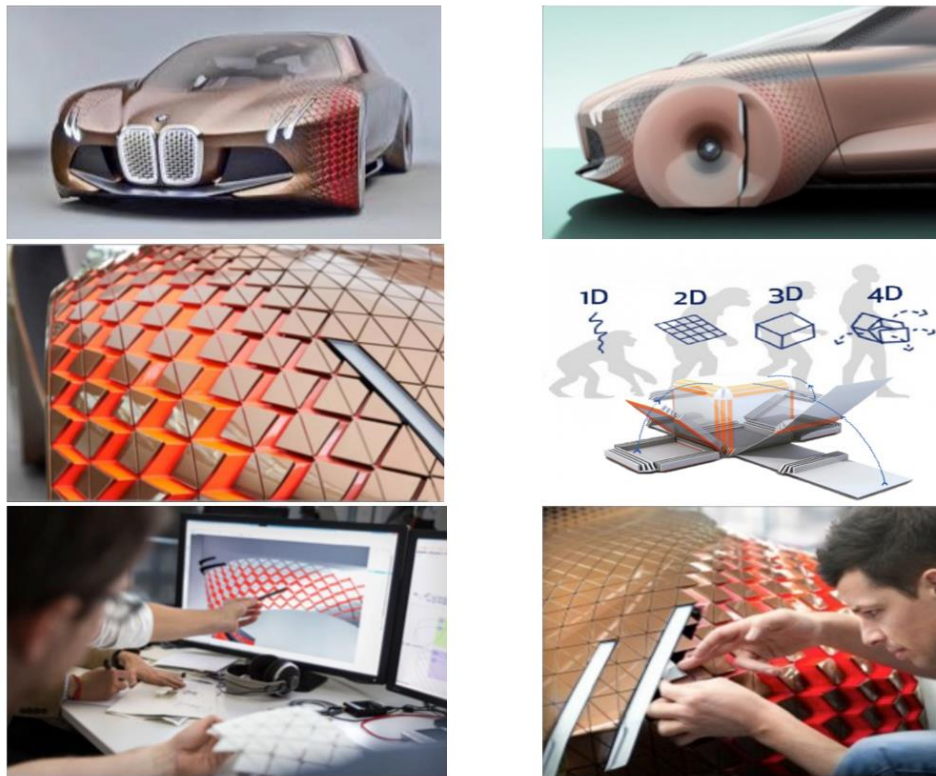


Figure 6. BMW prototype Vision Next 100 and their “alive geometry” concept developed by using Rhino3D/Grasshopper

Recently, this emerging technology has attracted researchers’ attention worldwide at the point of building a 4D printing Society⁶ in 2021. This scientific society brings both scientists and engineers from various backgrounds and disciplines and serves as a forum for discussions about the exploration, promotion, and commercialization of this technology. UTBM⁷ is among the members’ organizations with other universities like Georgia Institute of Technology, Deakin University, Concordia University, Singapore University of Technology and Design, etc.

⁶ <https://4dprintings.com/>

⁷ University of Technology Belfort-Montbéliard

1.5 General research context

Nowadays, the concept of 4D printing technology is seen as an emerging and innovative way to build active/responsive and reversible mechanical structures by combining AM capabilities and SMs, therefore providing an additional dimension (i.e., time) to manufactured physical products/systems [23]. It addresses a change (i.e., configuration, shape and physical properties) of physical objects over time but with specific approaches, which need to be aligned and adopted from a semantic and logical point of view for further computational issues in the design of smart products/systems [29][30]. In other words, the definition of physical objects and their relationships over space and time requires a common-sense engineering approach, also called the transdisciplinary approach, that concerns and governs many disciplines in a top-down fashion [30]. As illustrated in Figure 7, 4D printing is considered as an emerging research domain (currently located at the innovation trigger level of the 2018 Hype cycle [31]) that is still in its infancy phase and based upon the interaction of AM and SMs to build active/living objects with external stimuli (e.g., temperature, pH, light, electricity, mechanical force, magnetic force, etc.).

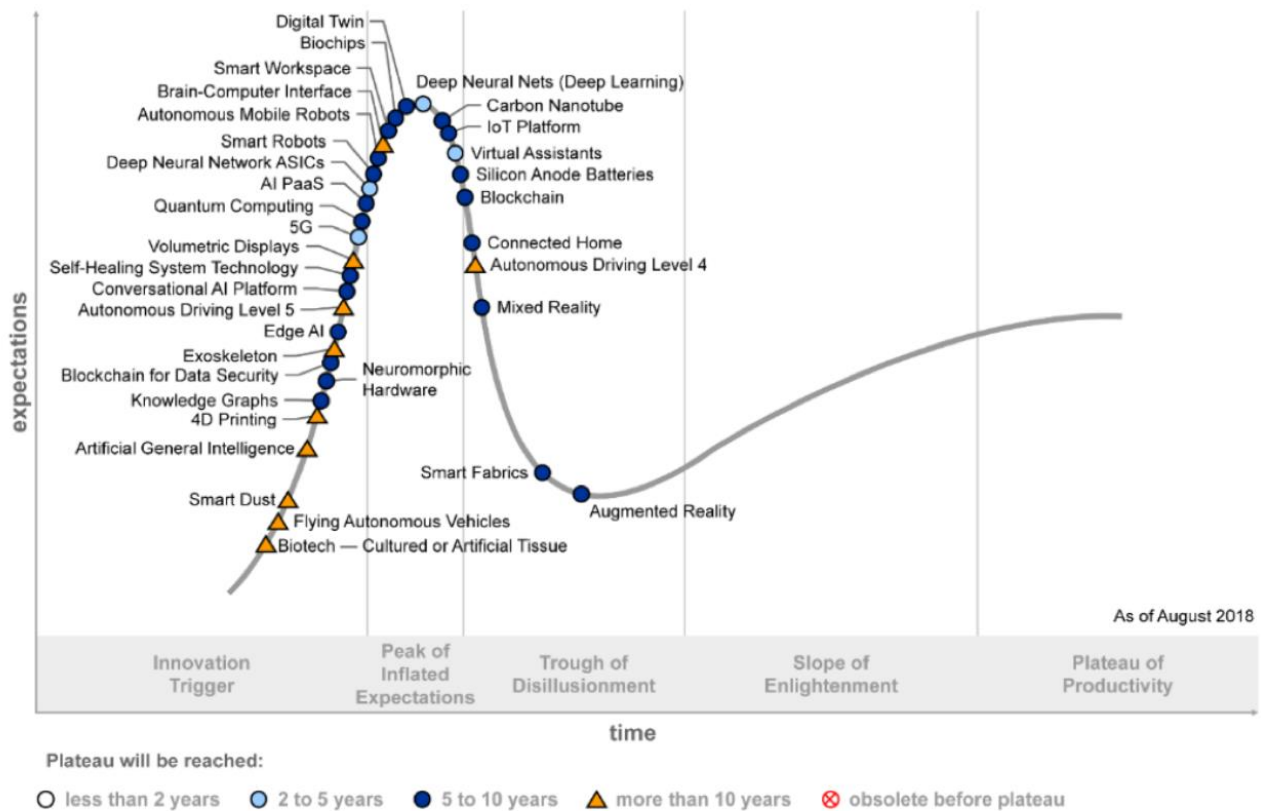


Figure 7. Hype cycle for emerging technologies 2018 [31]

One crucial challenge consists of tackling the lack of support to the designer to ensure shape/material programmability in the design stages and physical capabilities in fabrication [32]. Consequently, new design models, methods and tools are needed to fully utilize complex dynamics, multi-material programmability, self-assembly and self-reconfiguration behaviors, and domain-specific knowledge. Programmable products/systems can evolve in different contexts (e.g., state transformation, kinematic, form, etc.) to provide an appropriate service to the final user. In such a way, the fact of designing and manufacturing them will require engineering and manufacturing research efforts at different levels, such as product/system level (mechanical structure to intelligent systems), process level (traditional manufacturing to additive manufacturing) and material level (standard material to smart ones). As for programmable material, matter can change its physical properties (e.g., shape, density, optical properties, etc.) in a planned manner based on autonomous sensing. Such promising concepts tackle a common issue at different hierarchical levels (i.e., physical object, material, etc.).

Indeed, 4D printing is identified as promising manufacturing technology and a cross-disciplinary research field to deliver the next generation of dynamic products [16][24][33]. This PhD proposal is part of a research project – called **HERMES** (spatiotemporal semantics and logical knowledge description of mecHanical objEcts in the era of 4D pRinting and programmable Matter for nExt-generation of CAD systemS) – funded by the PIA ISITE-BFC program at the level of the University Bourgogne Franche-Comté. It mainly focuses on developing theories, models, and approaches to designing smart products/systems using 4D printing technology and programmable materials. This PhD tends to cover the scientific objectives of the HERMES project elicited in the next section. It is prepared at the ICB UMR 6303 CNRS laboratory, more precisely at the COMM (Design, Optimization, and Mechanical Modeling) department in cooperation with the LIB EA 7534 (French abbreviation for Laboratoire d’Informatique de Bourgogne) laboratory.

1.6 Motivations & Objectives

Based on the research context mentioned above, this PhD aims to exploit the potential of 4D printing and programmable matter to make the technology more mature and push further our knowledge about it so that designers and product architects can leverage profit from it. 4D printing is at the engineering, manufacturing, material science, and information technology interface [17][34]. Henceforth, such technological triggers provide an extra dimension (temporal dimension) to the traditional static three-dimensional products/systems’ definitions and require new theory, model, and approach to rationalize their engineering and manufacturing processes from knowledge and computational point of view. This technology encompasses limitations and problems on mainly two axes (i.e., scientific and engineering) as mentioned below:

Scientific problems related to 4D printing technology and the use of the products manufactured by it:

- Transformation, deformation, and evolution

The transformability of 4D printed products needs an accurately defined programmability of smart materials. All the proposed *ad hoc* case studies present an inaccurate actuation and insufficient control of the varying phases of deformation/transformation/evolution. Also, the latter has poor velocity and undefined parameters to be controlled with. Thus, the transformation process is soft, but it should not block the 4D printing technology in the long term [28][35][36].

- Control of the deformation inside and outside the laboratory

Most current demonstrations are considered as proofs-of-concept. These lab-made prototypes are far from being manufactured in industries since they do not fulfil precise specifications. For instance, what will happen to the product if the stimulation intensity does not match up perfectly with what is planned/expected? Will it be a loss of material and time since there is not any know-how to recover back a wrongly triggered product? Assuring that the structure's active region is suitably exposed to the stimuli, but the passive region was not shielded correctly from it or was not correctly connected to the active region. The most important is that this passive region is manufactured with a material partly sensitive to that stimuli: this stands as a gap to gid too [8][37][38].

- Materials' programmability and characteristics

The more a product/structure is deformable, the less rigid and resistive to cyclic loads and repetitive triggers. This can impact the experiment's repeatability and reversibility. The vast majority of materials are incapable of returning to their initial state on their own; they necessitate a sophisticated pre-programming to perform a charge/discharge cycle [39–41]. Nonetheless, electroactive materials seem to be a promising road to perform repeatable processes [42].

Engineering problems related to 4D printing:

- Formalization (database or knowledge base)

The design of a part/structure intended to be manufactured with AM processes and to transform on its own after being triggered by an adequate stimulus create a problem of solutions' imagination and suggestion for beginners (e.g., engineering students and product designers who are not initiated to 4D printing). For example, the relations between materials-stimuli-AM processes are not federated yet; the designer cannot rapidly arrange needed specifications and choices due to a lack of solid knowledge background [8][43].

- Design

Designing dynamic products requires changes in how they are conceived to improve the efficiency and usability of a 4D printed product and optimize its life cycle from the design phase to the use phase. Material experts, AM specialists, and product designers are primarily responsible for designing and manufacturing such a product. They are indeed not ready to embrace the new design freedom provided by 4D printing regarding

the lack of adequate tools and methodologies, which enlarges the gap between lab-made prototypes and their possible integration into the industry [6].

- Modeling and simulation

The capacity to create a virtual representation of the final product is essential to any design process. Current design tools cannot couple AM, material, and geometrical complexities. The question arises: how well can they mimic SMs' response to stimuli? The existing modeling tools were not designed to accommodate these newly developed technologies. One can state that there are insufficient tools for product designers and mechanical engineers to test and control their 4D printed products at early design phases [34].

- Benchmarking and normalization

The notion of standards, norms and benchmarks is commonly used in any other mature technologies and several design software. For example, suppose we want to introduce a screw for attaching a part to another. In that case, we are asked to choose the precise inside and outside diameters and even the tapping beforehand, according to an exact existing norm. But for 4D printing, we are far from that! Hence, a normalization/formalization/standardization is needed to bring the design for 4D printing closely and narrowly to facilitate design for 4D printing [44].

To fulfil some of these gaps, an essay needs to develop an interdisciplinary knowledge base facilitating the research about computational and design challenges – that endure in 4D printing – and increasing the smartness of systems at various physical levels. A relational database is strongly needed to give a global and close idea about the technology and inform which stakeholder affects the other so that the knowledge existing behind this innovative technology can be used and enriched. The related multi-perspective knowledge needs to be formalized and represented to be reused correctly in the product development phases. Therefore, it becomes vital to establish a concrete semantic and logical foundation on which several stakeholders from various research fields can refer to. Indeed, this crucial issue is currently tackled from multiple perspectives; still, a harmonization is needed to embrace 4D printing and programmable matter capabilities.

The main research objective is to formalize and represent 4D printing knowledge related to AM processes and techniques, SMs, stimuli, and transformation issues in such a context. Such critical knowledge must be appropriately described and computer interpretable along the product design stages so that product architects and designers will be aided to make the right decisions during the design process of alive and transformable objects. This thesis is mainly concerned with addressing the issues mentioned above, namely, developing a knowledge-based design environment that allows for and facilitates the design of 4D printed objects. Hence, the concrete objectives can be summarized as follows:

- (O₁) The description of dynamical phenomena knowledge semantically and logically at various scales and implementing a multi-layer ontology for semantic and logical reasoning. It focuses on establishing

a comprehensive overview and transdisciplinary theory of objects' descriptions and their relationships over time-based on first-order logic. This replies to the first scientific issue (i.e., transformation and deformation) and the first engineering issue (i.e., formalization with a database and/or a knowledge base).

- (**O₂**) The development of a specific add-on ensuring a multi-representation (i.e., graph, skeleton, structure, form, etc.) of 4D objects and their dynamic sequencing and integrating it in the active and multi-layer above mentioned ontology for semantic and logical reasoning, which fulfils partially the gap stated in the second engineering problem (i.e., design).
- (**O₃**) The development of a recommendation method based on specific knowledge for aiding the product designer in the computational design synthesis phase for material distribution choice. Also, an implementation of a laboratory prototype for this recommendation method within a CAD system for the definition of dynamic and semantic/logic enriched CAD models ready for 4D printing is envisioned with a dedicated application programming interface (API); this objective replies also to in the second engineering problem (i.e., design).

1.7 Thesis Structure

Figure 8 describes the architecture of the PhD dissertation and how the state of the art, research questions, and contributions are stated. After introducing the research context and the related objectives in this chapter, the structure of the thesis can be described as follows:

Chapter 2 conducts a literature review in-depth in the fields of 4D printing and ontology models for design, emphasizing product design and reasonings, on which motivation is highlighted.

Chapter 3 presents an ontology-based framework to ensure the semantic and logical description of transformable objects in the era of 4D printing. This ontology will be conceived as a strong knowledge base of the 4D printing technology.

Chapter 4 presents a multi-representation of the 4D printed objects respecting different transformations and formalizes this representation as part of the ontology.

Chapter 5 introduces recommendation method based semantic and case-based reasoning of the material distribution in such a 4D printed object.

Chapter 6 presents case studies and an implementations demonstrating and illustrating the contributions presented in this thesis.

Chapter 7 concludes the above research works and discusses the proposed contributions and the perspectives that can be considered a result of the proposed research work.

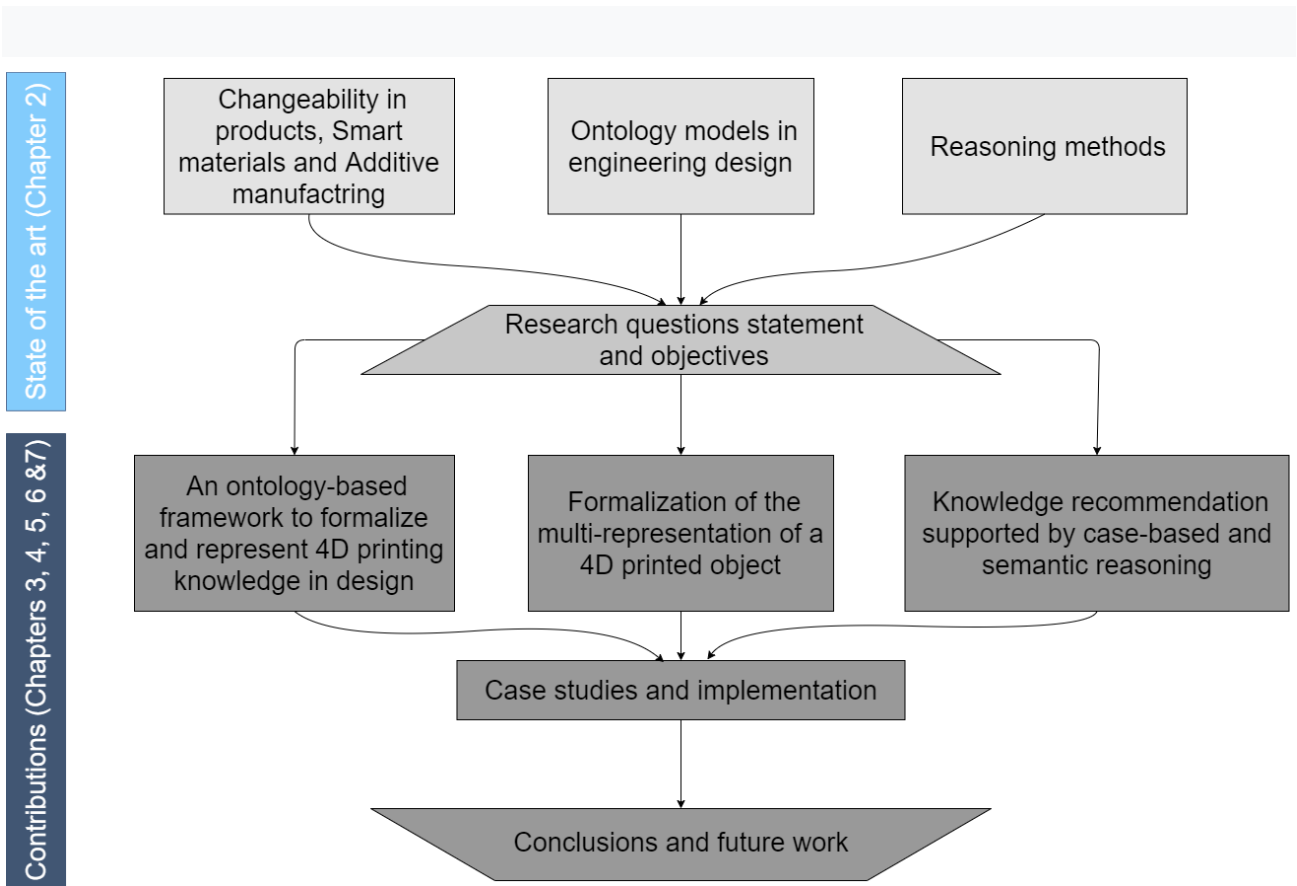


Figure 8. Structure of the PhD dissertation

Chapter 2 State of the art and research questions

“One can state, without exaggeration that the observation of and the search of similarities and differences are the basis of all human knowledge”

Alfred Nobel’s Saying

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2.1 Introduction

This chapter details significant published research works about 4D printing technology and other research studies related to the problem set out in the previous chapter, i.e., ontology engineering, research in design, and reasoning methods. So, section 2.2 undertakes the background on 4D printing and its main pillars (i.e., AM techniques, SMs, and stimuli). Section 2.3 highlights some crucial studies in research in engineering design in general and design for X in particular. Section 2.4 reports ontology models for design and delineates current challenges in these fields to be tackled in the specific context of this thesis. Then the final section (2.5) describes some reasoning methods (e.g., semantic reasoning and case-based reasoning). This state of the art allows us to define the scope of our contributions and, as a result, establish a scientific reference by which we may better place our research works.

2.2 4D Printing

Since the Ted X Talk⁸ of Skylar Tibbits in 2013 presenting his proof-of-concept of a self-bending structure in the MIT⁹ form as shown in Figure 9, the word 4D printing was coined, and researchers have rushed to investigate it more in detail. This breakthrough technology has received growing scientific interest with numerous proofs-of-concept demonstrating different transformations; it is a part of ongoing AM studies [45]. Indeed, the number of studies - conducted on this technology- have not stopped increasing: around 2000 scientific papers until now.



Figure 9. Self-Bending Structure in the MIT from [24]

Specifically, 4D printing refers to a technology coupling AM processes and SMs under the effect of an energy stimulation (e.g., electric current, heat, magnetic field, chemical solvent, to name a few), which can be external or internal stimuli [7][23][35][46]. It can be considered a disruptive manufacturing technology introducing a temporal dimension to objects and structures; see Figure 10. This fourth dimension (time) introduces transformability in the static objects and imbue them with the capacity of evolving. The latter increases the

⁸ https://www.ted.com/talks/skylar_tibbits_the_emergence_of_4d_printing

⁹ MIT : Massachusetts Institute of Technology

device's performance in shape-, properties-, functionalities-, and state-changing abilities [47]. As such, 4D printing offers greater design freedom and flexibility in printable geometry and greater cost efficiency because the latter capabilities allow expanding the design space [43]. This modern technology supports multiple transformation scenarios (i.e., while or after printing the part/structure, with internal or external stimulation, with single or multiple materials, to cite a few) between two objects' states (e.g., case of a deployable origami-based cube as shown in Figure 11) [8][38][45][48–50]. The following sub-sections will introduce deeper the main pillars of 4D printing, i.e., AM processes, SMs, and stimuli.

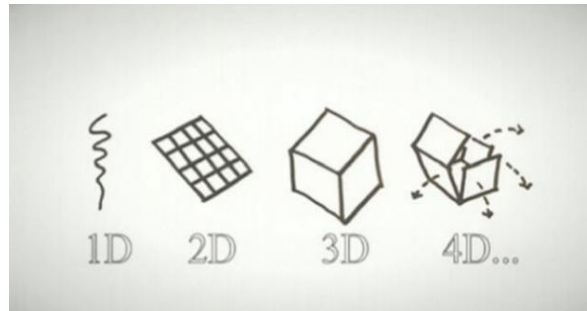


Figure 10. The general concept of dynamic object

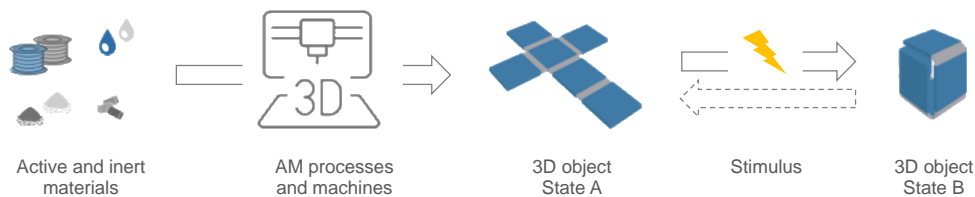


Figure 11. 4D printing paradigm illustrated through a shape-changing object (according to [8])

2.2.1 Additive manufacturing processes

It remained until the 80s when rapid prototyping or 3D printing was developed [1]. It was introduced in different domains like, for instance medical devices, pills, industrial arts, jewellery, automotive industry, robots, soft sensors and actuators, and space engineering [51][52]. ASTM categorizes AM in seven processes [13], but few techniques of these processes are applied in 4D printing (see Figure 12), ranging from material extrusion (fused filament fabrication (FFF) [7][40] and direct ink writing (DIW) [49][50]), photopolymerization (stereolithography (SLA) [53][54], digital light processing (DLP) [55][56]) to material jetting (drop-on-demand and PolyJet) [57], to name a few. These processes present single and multi-material printing capacities due to multi heads and multi tanks usage. Multi-material printing capability adds a plus-value to the 4D printing technology because it allows combining different materials characteristics which enhance 4D printing performance [58]. The following sub-sections describe some processes used in 4D printing technology, such as material jetting, extrusion-based processes, and photopolymerization.

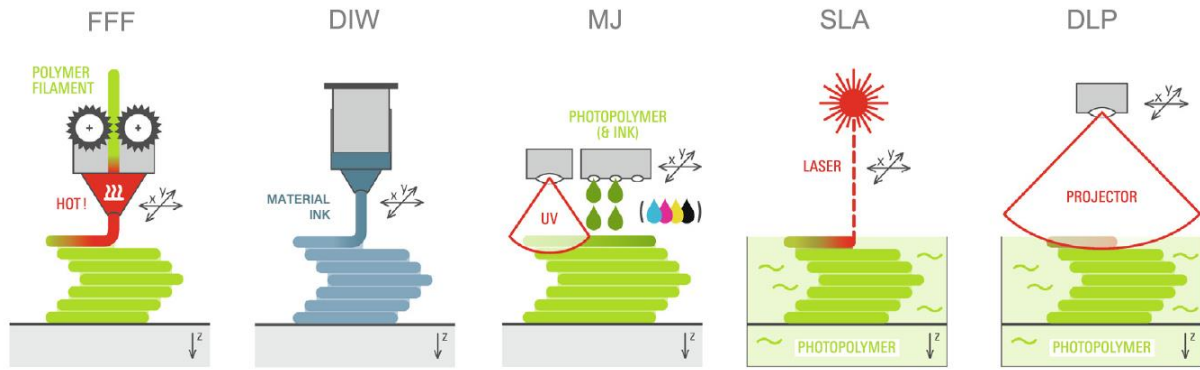


Figure 12 Some AM processes used in 4D printing technology [8]

2.2.1.1 Material Jetting

Material jetting, or in particular, inkjet 3D printing technique, is an established AM process that can create parts by depositing droplets of liquid photopolymers using piezo printing heads and curing the photopolymers using ultraviolet lamps. Inkjet 3D printers, such as PolyJet from Stratasys and MultiJet from 3DSystems, can selectively deposit multiple photocurable polymer resins simultaneously to fabricate multi-material parts. Sacrificial support materials are automatically generated and deposited with photopolymers to support overhanging structures [59]. While early 3D printers were limited to printing only primary wax material that was liquefied, more recent 3D printers (such as the Stratasys Objet Connex 260) are capable of printing with (photo-)polymers that have a variety of different material properties (e.g., color, stiffness, melting point) [60]. Solidification or photopolymerization are two methods for curing the deposited material. The droplets of a photocurable resin are first selectively placed on a bed, and then the resin is flashed with a UV light, causing it to cure instantaneously. After that, the procedure is repeated until all layers have been printed. The droplets are deposited from a print head that stretches over the whole length of the platform (line-wise deposition) [61].

2.2.1.2 Extrusion based processes (DIW/FFF)

The methods within this technique work by depositing material through an extrusion nozzle. The material (with the appropriate viscosity) is extruded during the printing process [62]. The nozzle scans a platform according to the printed part's cross-section; the deposited cross-section is immediately cured. Some key characteristics 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, the ability to generate support structures, and bonding between layers [63]. Extrusion-based methods are often utilized with polymer and, to a lesser degree, organic materials as building blocks for the process (such as food or living cells in tissue engineering solutions). The primary technique is FFF [64]. The raw material is fed in the form of a filament, which is driven through a heated nozzle to melt before being deposited on the object's surface. Polymers are the most often used materials; however, their qualities may be enhanced by filling the polymer with a specific filler that enhances a particular attribute [65]. DIW is a technique that includes the controlled

deposition of material [66]. This can be accomplished in various ways, including the extrusion of liquid ink, the ejection of material droplets onto a substrate, or the use of aerosol jetting [67].

2.2.1.3 Photopolymerization

The photopolymerization technique is the driving force behind the world's first 3D printing machine [68]. A platform is initially plunged for a short distance down into a vat of photocurable resin before being removed from the vat. When exposed to a particular light, a resin of this kind cures. It is then necessary to selectively expose the thin coating of resin on top of the platform to a light source (usually an ultraviolet light source) to create the part cross-section that has been previously created. This procedure is confined to polymers, although it may be reinforced by filling the resin with more polymer to achieve particular qualities such as hardness. Photopolymerization methods use single material deposition: SLA in which a laser spot is used to cure the resin and micro-stereolithography (μ SLA), which works in the same way as SLA but is only suitable for complex shaped parts with a size of less than a millimeter [69].

Also, processes conditions in general are extremely valuable for this technology, Figure 13 shows that it is possible with one material to control the transformation by adjusting the trajectory of the nozzle (stresses induced during the material deposition phase).

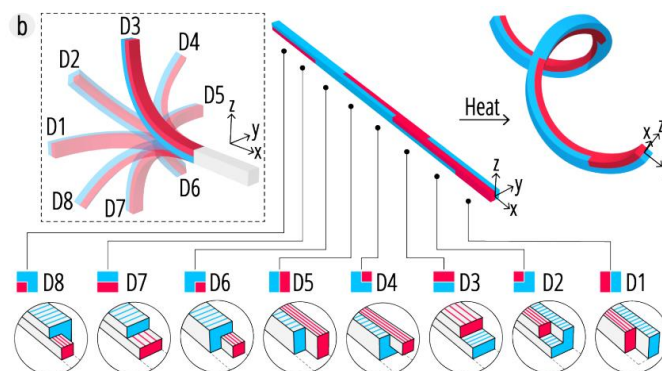


Figure 13. The usage of different material distributions in the same structure has resulted to a helixing transformation activated with heat, noting the fact that every distribution can lead the transformation function in a particular dimension [64]

2.2.2 Smart materials

Polymer scientists initially addressed this research domain by developing shape morphing structures and shape memory polymers (SMP) or artificial muscles [70–72]. Pioneer works to set up behavioral studies of the glass transition temperature, magnitude of stress and elasto-viscoplasticity deformation [41][73–77], whose applications are scattered in different domains [40][49][78–80]. These early efforts have coupled specific AM processes (e.g., DIW and material jetting) and SMs like for example, nanocomposites polymers and polymeric hydrogels, which has resulted in important applications like tissue engineering, biomedical applications, and jewellery to name a few [40][49][56][78–81]. Along with the cited works, some material embedding dynamic

behaviors were developed to fulfil transformation primitives such as bending, twisting, and folding – once exposed to different stimuli, i.e., solvent, light, magnetic and electric fields, etc. [82–84]. In addition, shape memory composites and pH-responsive materials like hydrogels were developed for self-folding transformation, which was presented in many experiments using origami hinges or multi-layered materials [85–90]. In the early last decade, pioneer research works have focused only on shape memory polymers. Still, nowadays, applications have included photostrictive, chromatic, electrically and magnetically responsive materials, to name a few [91]. Other research efforts have initiated programming materials by tuning constitutive laws [22][92].

SMs can be divided into shape-changer materials and programmable materials [93]. Some materials change in form after applying a stimulus and instantly after its removal, yield to their permanent forms or not: it depends on the shape memory effect (SME). As for programming shapes, some steps are required to make the material “remember the desired shape” [19] (see Figure 14). The SME can also be divided into a single and multi-way SME [93]. A significant problem with classical unidirectional SMEs is irreversibility [94]. A dual-SME material has one continuous form and one temporary form, while a triple-SME material has one continuous form and two temporary forms (see Figure 15). A multi-SME material is similarly shaped in one strict permanent form and the rest global number minus one temporary form [95][94]. The following sub-sections define some materials’ classes and present multi-material structures and digital materials.

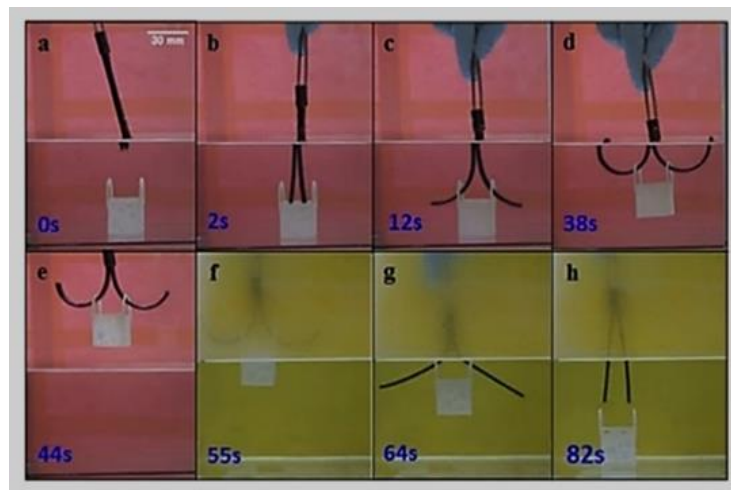


Figure 14. Smart hook. (a) The programmed hook. (b-c) The bending deformation of the structure under hot water with temperature of 30 °C. (d-e) A small box is lifted up from water. (f-h) Releasing the small box into another container. The water in the container is in 70 °C [96]

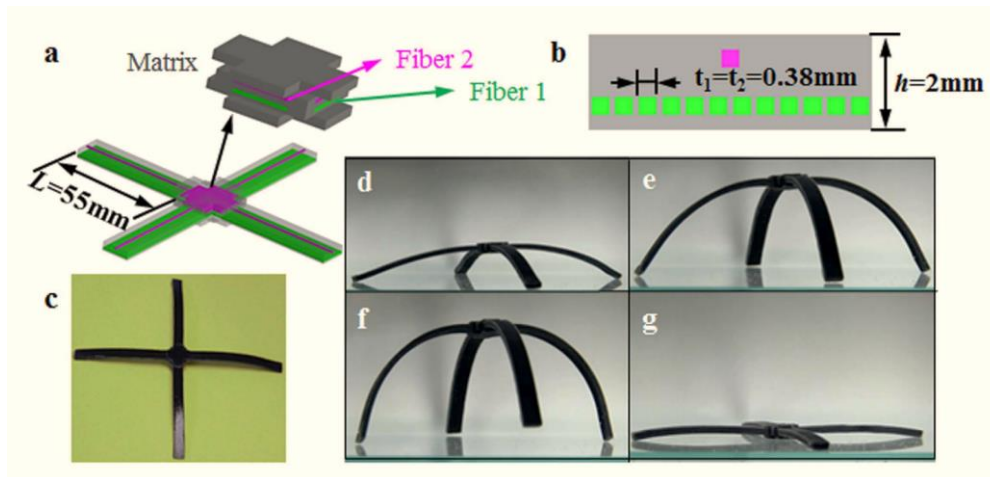


Figure 15. Self-assembling and disassembling trestle. (a) The design of the trestle. (b) The cross-section of the composite strip. (c) The shape of the structure after programming. (d–g) The deformation behavior of the structure in the recovery process [96]

4D printing has been coined to cover these efforts with AM technologies, particularly material jetting at first; it can create dynamic and flexible structures; this ability depends primarily on a suitable choice and mixture of SMs [7][17][23][24]. Most of the proposed works have addressed *ad hoc* experiments manufactured with multiple materials and triggered directly off the print bed, whether dipped in water (e.g., hydrophilic polymer material), or triggered with electricity. In the same context, different composite materials have been introduced to boost advances in 4D printing, like gels with photo-responsive fibers, thin composite, and polystyrene [14][50][93][94].

2.2.2.1 Classification

As stated above, SMs are materials that are handled to respond in a controllable and reversible way, modifying some of their properties as a result of external stimuli such as mechanical stress, temperature, moisture, electric or magnetic fields, light, temperature, pH, or chemical compounds among others. SMs are also defined as active materials and can be classified as follows:

- Optical sensors are materials whose response is optically perceivable. For example, thermochromic materials, triboluminescent materials, and switchable mirrors are all examples of this type of material class [95].
- State changers have many conditions that respond to external stimuli (such as resistance to an electrical current passage). Electro-/magneto-rheological fluids and shear thickening fluids are examples of these types of materials that can change in state.
- Flow changer materials like conductor (i.e., materials that allow electrons to flow freely from particle to particle), impedant (i.e., materials permitting to manage the flow of electricity in a circuit board) and insulator materials (i.e., material that does not transmit energy easily).

- Shape-changer materials - such as hydrogels and piezoelectric materials - merely vary in size unlike SMP that can alter their shape in response to the change in size [93]. This class is subdivided into the following categories:
 - Piezoelectric materials are those that generate sound waves. These materials are sensitive to electrical currents and atmospheric pressure. In certain ceramics, the direct piezoelectric effect occurs when the material is strained, resulting in voltage generation.
 - Electrostrictive materials: These materials are sensitive to electric fields in a way that is similar to that of piezoelectric materials. When exposed to an electric field, they create strain, but they do not have a "direct action", which means that pushing them does not generate voltage.
 - Magnetostrictive materials are the magnetic equivalents of electrostrictive materials. They essentially elongate in the direction of a magnetic field that is applied to them. They also have a "reverse" effect, i.e., deforming magnetostrictive material results in the generation of a magnetic field [77].
 - Photostrictive materials can perform non-thermal changes in the dimensions that occur when exposed to light (e.g., ferroelectrics, polar and non-polar semiconductors, as well as polymers) [76].

2.2.2.2 Multi-Material Structures

A single-material structure that is intended to be transformable is trivially made of a SM. Suppose it is manufactured of more than one material, in that case, it can be a mixture of different SMs or a combination of SMs and inert materials, it is indeed based on a specific material distribution, see Figure 16. The latter can result in different shape-shifting behaviors such as bending and twisting beyond linear expansion and contraction [99].

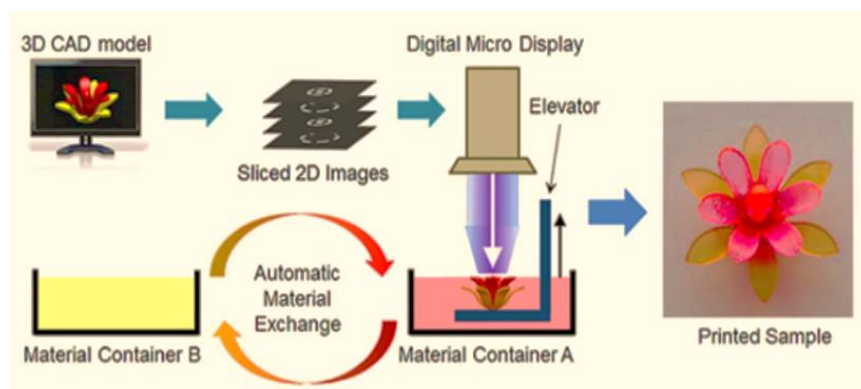


Figure 16. Multi-material fabrication using digital light processing (DLP) [99]

2.2.2.3 Digital Materials

The digital conceptualization can be expanded into material structures [100]. The voxel, identified as the basic and physical bit that occupies a 3D physical room in a voxel grid, allows us to switch from analogue components to digital materials [100-102]. A digital material is defined as a voxel [100][102]. Biological structures usually consist of basic building blocks that can be considered physical voxels like DNA¹¹ and proteins [100]. Physical voxel (printed voxel) can be defined similarly in 4D printing and related multi-material structures as building blocks for 4D printed object. The temporal arrangement of voxels performs a significant part in characterizing a 4D-printed structure [99].

2.2.3 Stimuli

A 4D-printed structure may change shape, properties, or functionality. This change occurs when the structure/part is subjected to an energy stimulation [36]. Owing to stimuli responsiveness of SMs, the literature has revealed a broad spectrum of stimuli such as temperature/heat, electric field, magnetic field, moisture, mechanical force, electric charge, light, pH and chemical substances, as illustrated in Figure 17 [7][103]–[106].

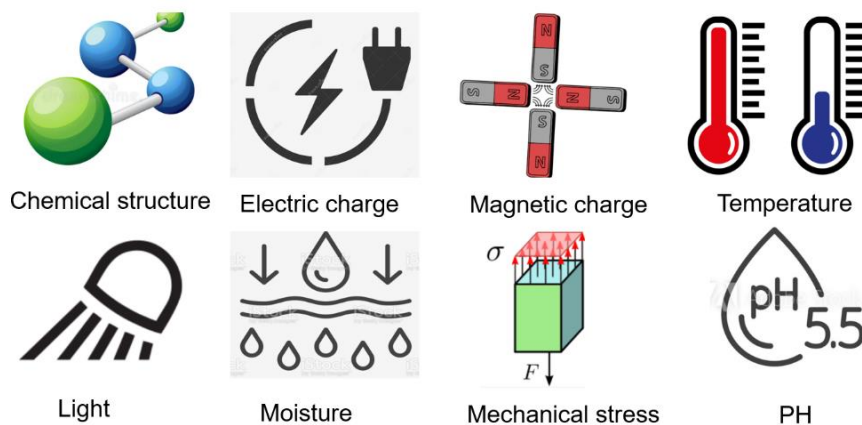


Figure 17. Illustration of the different stimuli

However, an interaction mechanism must be identified so the 3D printed smart structure can respond adequately to the stimulus. There are many types of 4D-printing mechanisms [107], basically hydromechanism and thermo-mechanism, and other composed mechanisms such as unconstrained hydro thermo mechanism, unconstrained pH mechanism, unconstrained thermo photo mechanism, and osmosis mechanism, as described in the following subsections:

2.2.3.1 Unconstrained-hydro mechanism

Here a smart printed structure consists of a hydrophilic active material and a rigid material (see Figure 18). Water is used as the external stimulus so that the structure can undergo shape-shifting underwater and return

¹¹DNA: Deoxyribo Nucleic Acid is the hereditary information material in humans and all other organisms.

to its original shape after drying. This mechanism is driven by various swelling ratios between active and rigid materials. SMs expansion generates a force that leads to shape change. Complex shape-shifting behaviors can be achieved when the SMs are arranged adequately with other rigid materials. The shape change's magnitude and direction depending on the two materials' spatial arrangements [23][24][99][87]. This mechanism is naturally reversible, so drying the smart structure can recover the original shape. However, a unique structure of stiff and elastic plastics can also force the shape-shifting conduct to be irreversible.

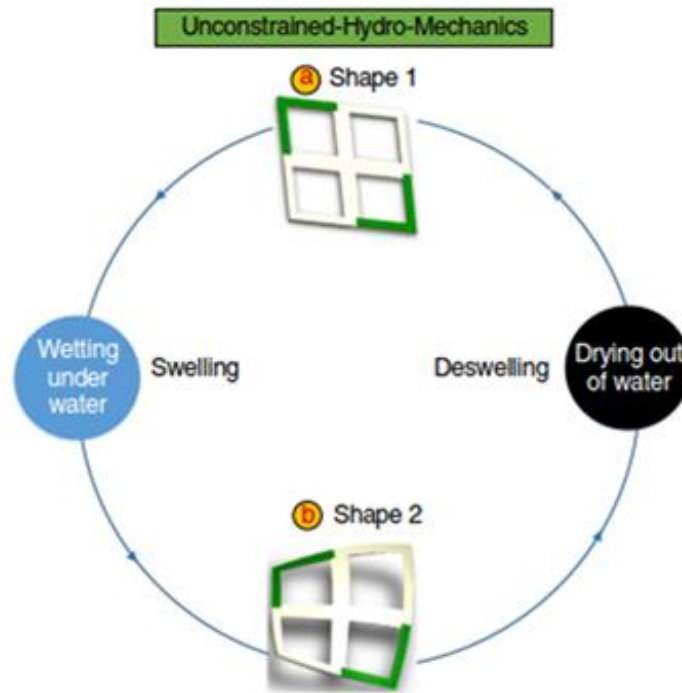


Figure 18. Unconstrained hydromechanism [26]

2.2.3.2 Constrained-thermo mechanism

In such a case, the printed structure is heated to the highest temperature (T_H), and the cycle begins in the following order at T_H . First, at T_H , the original structure is stretched with some strain depending on specific applications (see Figure 19). Then, the structure is cooled to the lowest temperature (T_L) while the strain remains unchanged. Next, the external stress is removed. After this step, the desired temporary shape is obtained. Finally, the structure can be reheated to T_H in loose stress to retrieve its initial form. Temperature is an external boost in this mechanism [7][17]. In some research works, water with various temperatures was used to transfer heat to the printed structure as a medium. The temperature is still the only stimulus in this cycle to trigger the shape-shifting behavior. This mechanism is applied in the sequential, multi-shape memory structure [108]. It is feasible to control the multi shape-shifting sequence in a polymeric matrix [109].

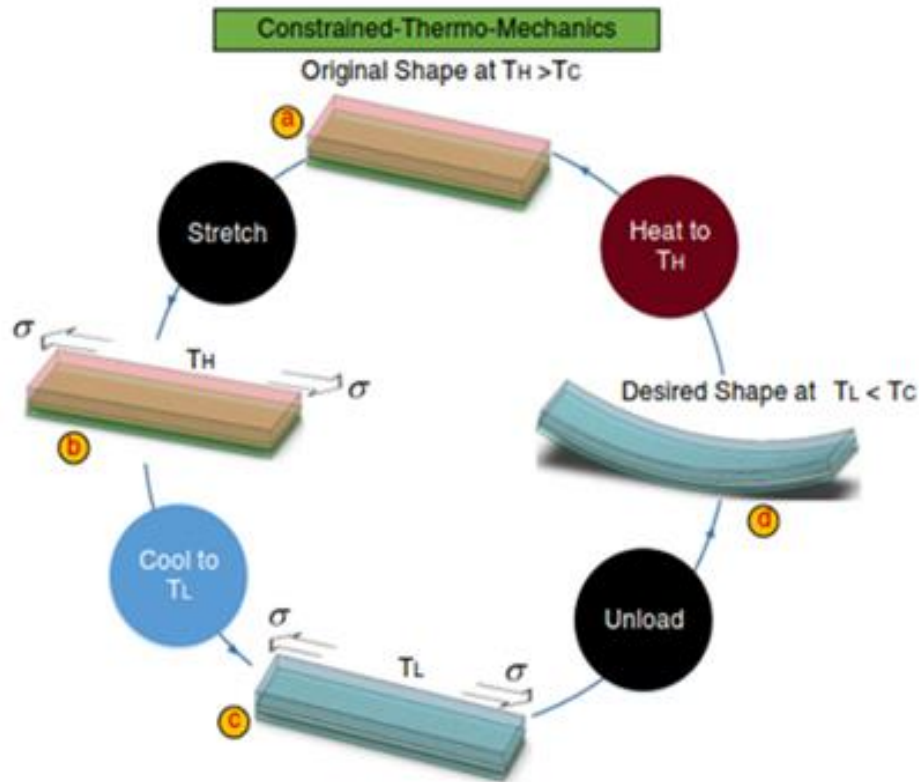


Figure 19. Constrained-thermo mechanism [26]

2.2.3.3 Unconstrained-thermo mechanism

Unlike the previous mechanisms, under constrained-thermo mechanism does not include the external load (see Figure 20). Only two temperatures are needed. One is higher than the active material involved in the structure, and the other is lower than the critical temperature. The printed structure is primarily heated to T_H . The cycle starts at T_H . And proceeds as follows: first, the original structure is cooled to T_L , where the desired shape is achieved at the end of this step. Then the structure can heat to T_H to restore its original shape. External stimulus is the temperature in this mechanism. There are plenty of types of shape-shifting behaviors in smart, lightweight, and thin composite structures, such as transformation from a planar sheet to floral 3D structures, periodic 3D structures, and adaptive metamaterials [110].

2.2.3.4 Other mechanisms

With the unconstrained-hydro-thermo mechanism (such as illustrated in Figure 21), the 4D printed structure undergoes two shape-shifting cycles [18]. It first swells in cold water, then hot water, without constraints. Swelling and deswelling procedures are safe, with limitations on external load [111].

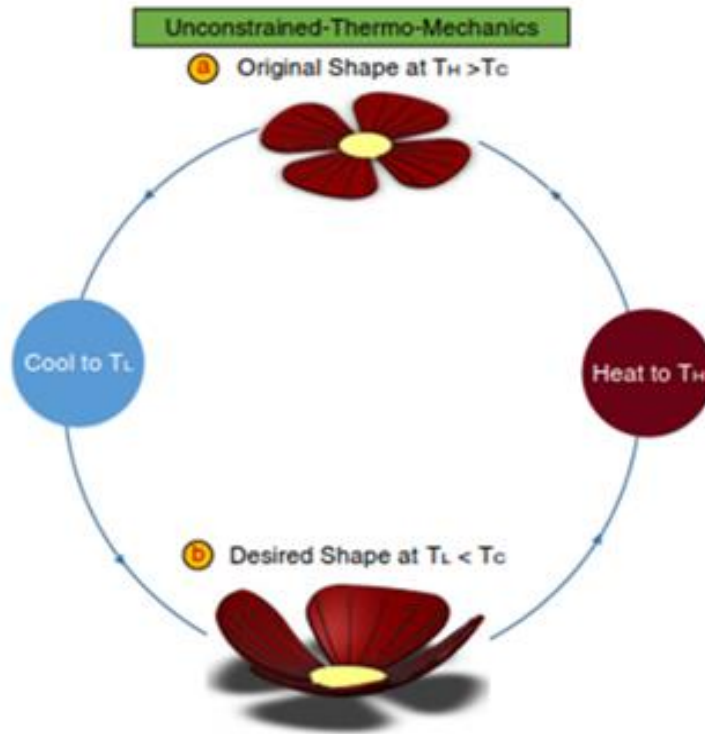


Figure 20. Unconstrained-thermo mechanism [26]

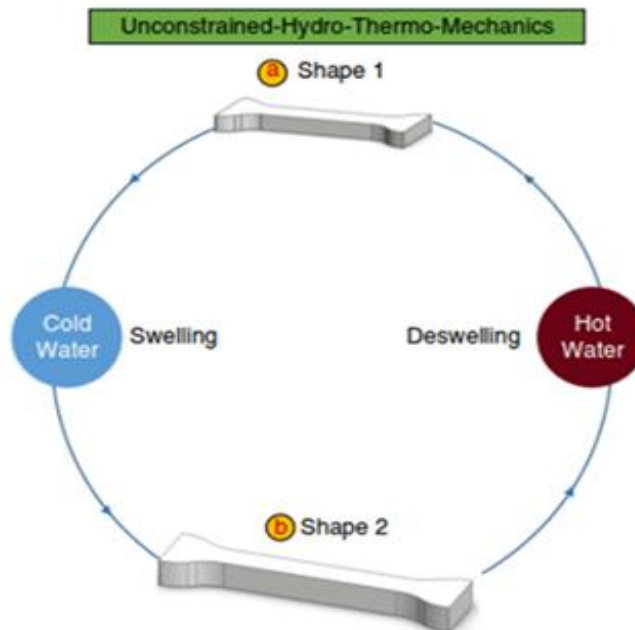


Figure 21. Unconstrained hydro-thermo mechanism [26]

Unconstrained pH mechanism is implemented with pH-responsive hydrogels able to swell linearly at a specific pH level and then shrink at another designed pH level [112]. This cycle is mainly conducted in an aqueous environment and is suitable for shaping hydrogels. Applying light, heat, or combining both stimuli on those

fibers could yield printed structures with different morphologies [113]. As for osmosis-mechanics, a bilayer lipid interface joins two aqueous droplets with different osmolarities. The droplet with the higher osmolarity swells and the droplet with the lower osmolarity shrinks until they reach the same osmolarity, allowing self-bending [114].

2.2.4 Classification of transformations

4D printing technology has shown a range of behaviors, and they are classified in the following sections. Every transformation can fulfil different dimensions: like for instance from 2D origami structure to 3D cube, or from 1D line to 3D spatial structure.

2.2.4.1 Bending

Bending characterizes the slender structural element's distortions, creating an angle less than 180° occurring within a perpendicular axis to the element's longitudinal axis. In our context, bending is a fundamental primitive of transformation. It may be buckling and creasing a linear belt with alternating sections of rigid and active materials [24]. In bio-printing, 2D-to-2D automatic bending is shown in Figure 22 [114]. A rectangular network could be bent into a circle. This change of shape is based on the osmolarity differences in the droplets. High osmolarity droplets swell, and, on the counter part, the droplets will shrink within a less osmolarity; until the gradient becomes zero. The 3D bending [50] can be illustrated in the bio-printed prosthesis fingered from thermoplastic elastomer (TPE), see Figure 22. Figure 23 has demonstrated a multi-bending behavior. The creation of a floral-like structure has been shown in a 2D-to-3D self-bending behave [113].

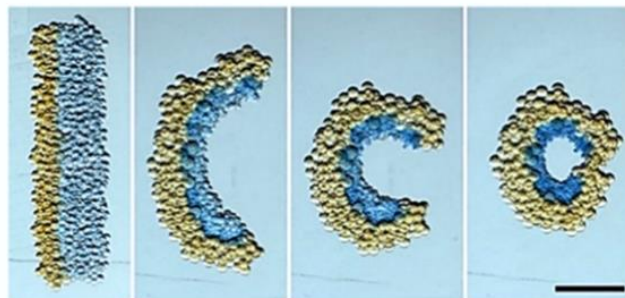


Figure 22. Self-bending in which a rectangular network transforms into a circle [114]

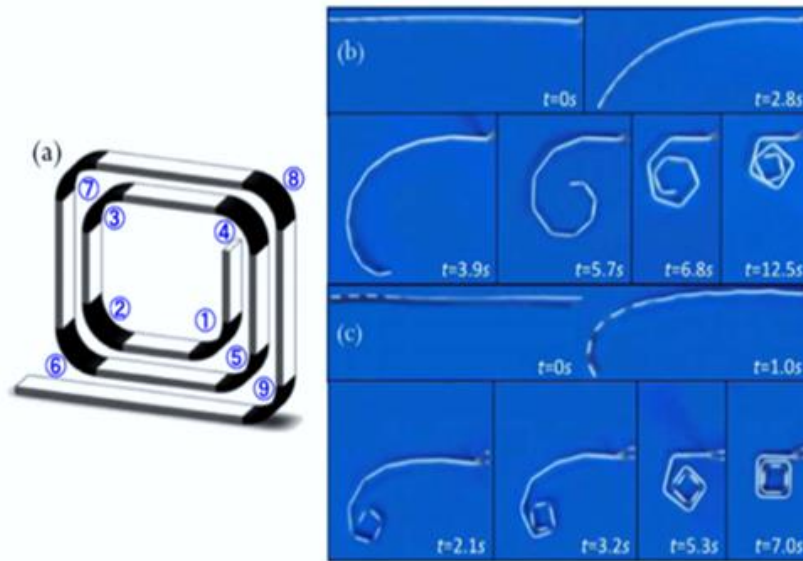


Figure 23. An example of multiple bending behaviors [115]

2.2.4.2. Folding

Folding primitive is bending with an exact angle equal to 90° . Figure 24 shows a folding cube manufactured with a SMP, manufactured with the FFF technique and triggered with temperature [24]. Researchers have demonstrated various programs for folding applications, such as a sequential actuation of hydrogel membranes into 3D folded architecture [116]. Also, a linear stretching structure (from 1D to 1D), a 2D folding and stretching structure and a 3D topographical surface change have been demonstrated [99]. Nevertheless, shape changes were demonstrated based on the self-folding mechanism from a 1D strand to a 3D crambin-protein structure [24].



Figure 24. Folding Cube from [24]

2.2.4.3 Comparison between folding and bending

There are nuanced differences between folding and bending, as shown in Figures 25 and 26. The curvature is global in bending, see Figure 25-d, but folding is localized just like in Figure 25-a and associated with sharp corners that occur in a narrow area [84][117]. Bending outcomes in a sequence of local rounding where surface topography can depict the local deviations of a flattened plane. Folding, plunging, and humping are typical features. These characteristics are usually presented in compressive load conditions and examined in quantity

[118-120]. They enable an approach based on the Maxwell stability criterion so that different types of these features can be initiated and developed.

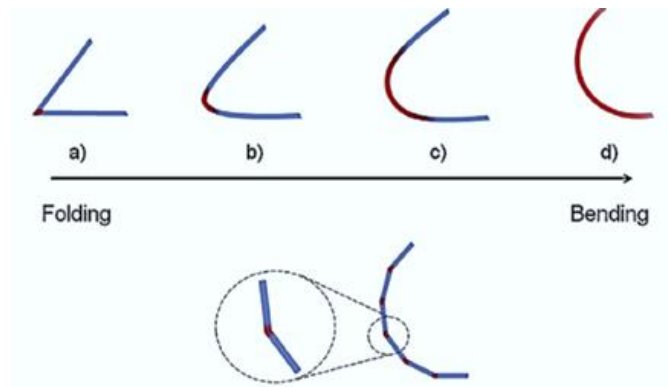


Figure 25. Illustration of angles' gradient measures from folding to bending [115]

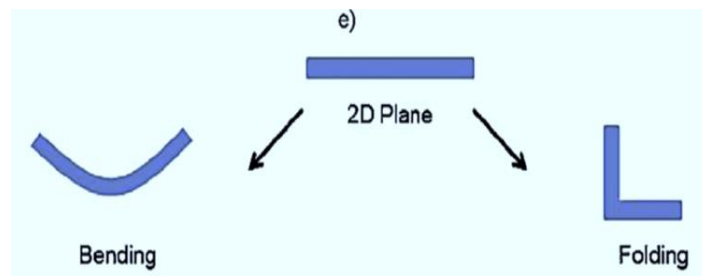


Figure 26. The difference between folding and bending [115]

2.2.4.4 Expansion/Contraction

A linear spread/contraction of 1D-to-1D through an AM process (FFF) was demonstrated in [18][109]. For example, the stimulus used in one of the mentioned experiences was water, and the 4D printed structure contains alternating layers of rigid disks and active hydrogels [99]. The hydrogel pieces become swollen if the stiff disks stay the same once the unit is placed in water. Another example explicates this linear shifting in Figure 27. It is manufactured with SMP and the FFF technique, includes the usual programmed steps of reversibility and is triggered with heat.

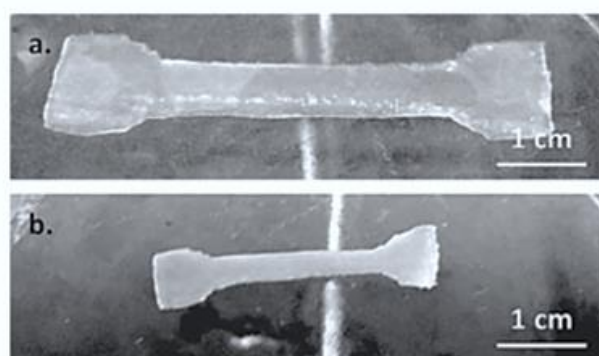


Figure 27. An example of expansion/contraction behavior [18]

2.2.4.5 Twisting/helixing/waving

It exists a demonstration about helical constructions of different spiral grades by pivoting a 2D plate and turning it into 3D forms [110] (see Figure 28). Fibers with certain corners cause distortion, and the ultimate bend angle can be altered. A demonstration is conducted about 2D-to-3D twisting [111]. The variances in the swelling ratios of active and rigid materials underwater caused this shape-shifting behavior. The 2D-to-3D bending, twisting, and mixture of both were also illustrated in [7] (see Figure 29). Figure 30 presents a waves-like structure triggered by hot water; it can also be classified under multi-bending behavior.

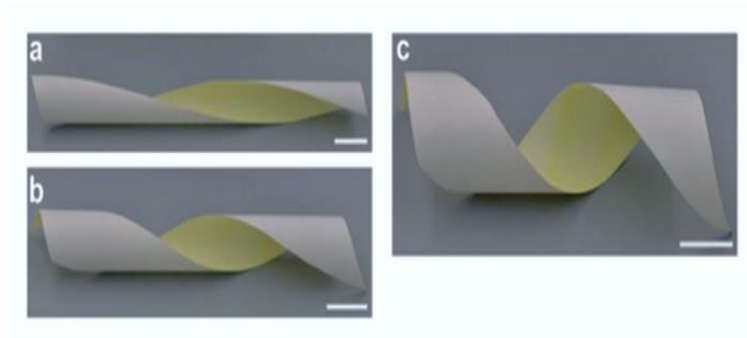


Figure 28. A example of helixing behavior [110]

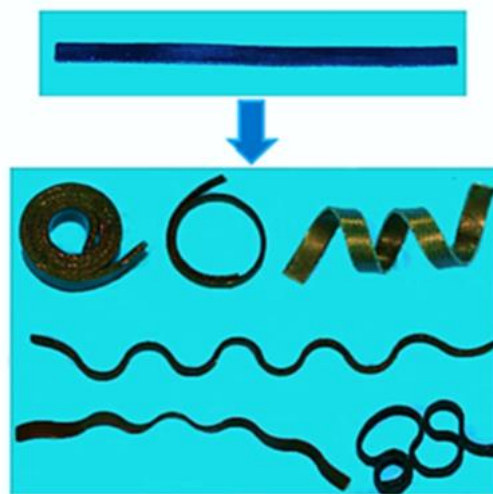


Figure 29. A example of bending, twisting, and waving behaviors [7]



Figure 30. An example of waving behavior [24]

2.2.4.6 Surface Curling

The famous article of Tibbits [24] presented a surface grid structure that produced a mathematical sine surface underwater with alternating upper and lower sections of expandable substances. This demonstrated a behavior shifting from 2D to 3D with a surface curling function, as shown in Figure 31. This shift is enabled by a stress mismatch from their various swelling properties underwater between rigid and active materials.

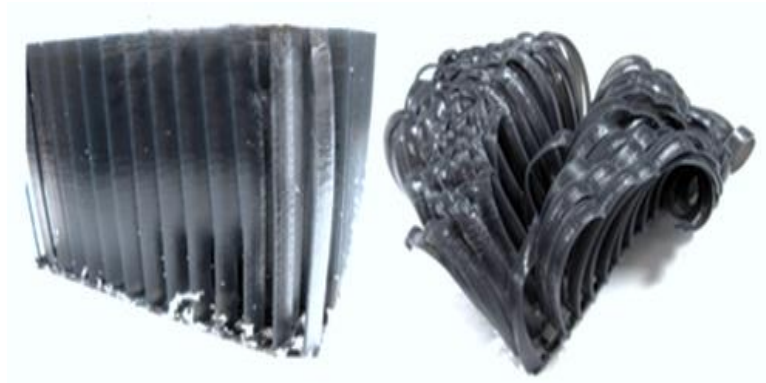


Figure 31. An example of a curling behavior [24]

2.2.4.7 Surface topographical change

Mountain and valley characteristics can be produced from concentrated environments in the existence of a suitable stimulus. This shows the change in surface topography from 2D-to-3D (see Figures 32 and 33). It is allowed by pressure misconduct between stiff and active materials from their various stretching characteristics submerged. 3D-to-3D linear growth and contraction behavior has been proved in this reference [18]. This surface topographical change is allowed through a linear loose hydrogel swelling or shrinking in warm and cool water. Global and local shrinking for 3D-to-3D shape-shifting behavior have been illustrated in [113].



Figure 32. An example for multiple curving behavior [24]



Figure 33. Surface topographical change behavior [24]

2.2.5 Attempts for simulation and computation

In addition to the research mentioned above about the experimental correlation between materials-stimuli-AM processes, other researchers have focused efforts on controlling and simulating some transformations resulting from 4D printing. The bending and the folding were controlled by using reverse engineering and monitoring some parameters like fiber length, hinge length and location, strain and temperature [17][105][121]. Also, kinematic studies of different bending configurations and folding patterns activated by several stimuli (e.g., thermal, chemical, optical, and magnetic) were conducted by Hernandez *et al.* [117]. Such studies and modeling, therefore, demand to be considered beforehand in the design process to control self-folding materials [34]. For instance, positive Gaussian curvature surfaces can be produced with concentrated rings. An orthogonal bilayer lattice structure can produce surfaces with negative Gaussian curvature or saddle-like surfaces. Then, combining these two print paths can yield a structure with varying Gaussian curvatures (see Figure 34). Analyzing 4D printing depends on suitable parametrical design [111], as shown in Figure 35. It seems essential to anticipate the form change after printing over time. This anticipation offers the theoretical designs required to prevent accidents between structural parts during self-assembly procedures and decreases the number of preliminary experiments.

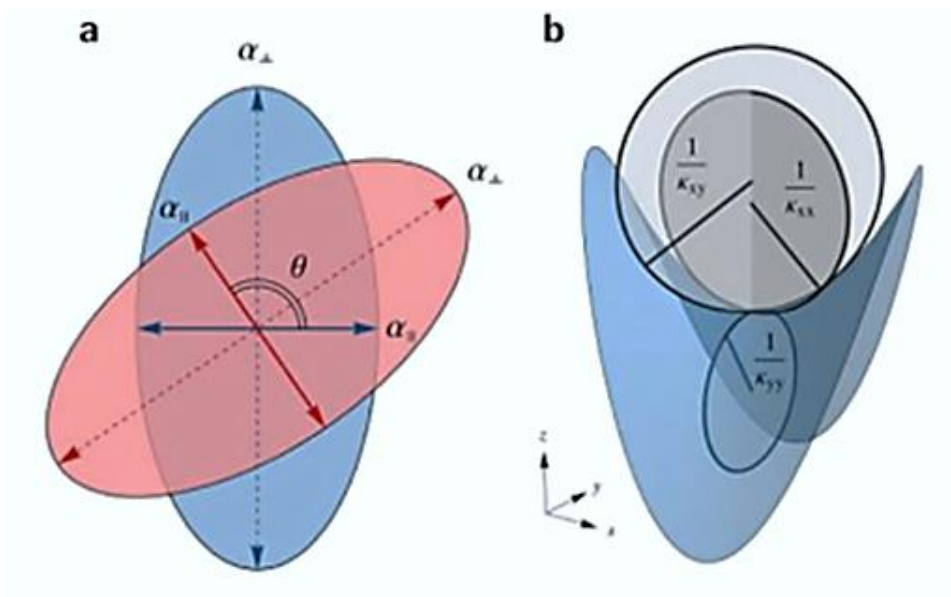


Figure 34. (a) print paths quantified by the angle Θ between the two layers, and (b) final desired shape quantified by curvature tensor K , mean curvature Gaussian H , and Gaussian curvature K . [111]

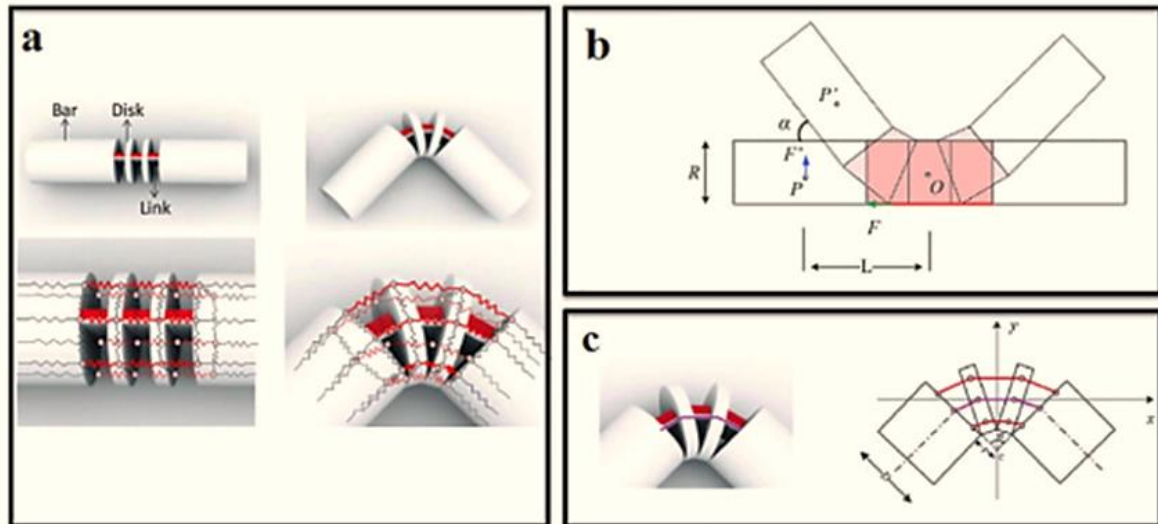


Figure 35. Parameters definition for the 4D-printed hinge with the spring-mass concept [111]

Evaluating and determining SMs distribution in the design of 4D printed structures is crucial. Thus, Sossou *et al.* [122][123] have predicted materials distribution in the part geometry to enhance shape/form morphing by allocating the materials with a voxel-based representation using a genetic algorithm. Therefore, the designer will receive a predictable recommendation while still in the preliminary design phase. In the Rhinoceros3D environment, a Grasshopper plugin called VoxSmart has been developed to realize the voxel-based SMs modeling and simulation [122][123]. The proposed tool can simulate in real time any heterogeneous object with any materials distribution, including SMs and inert materials (see Figure 36).

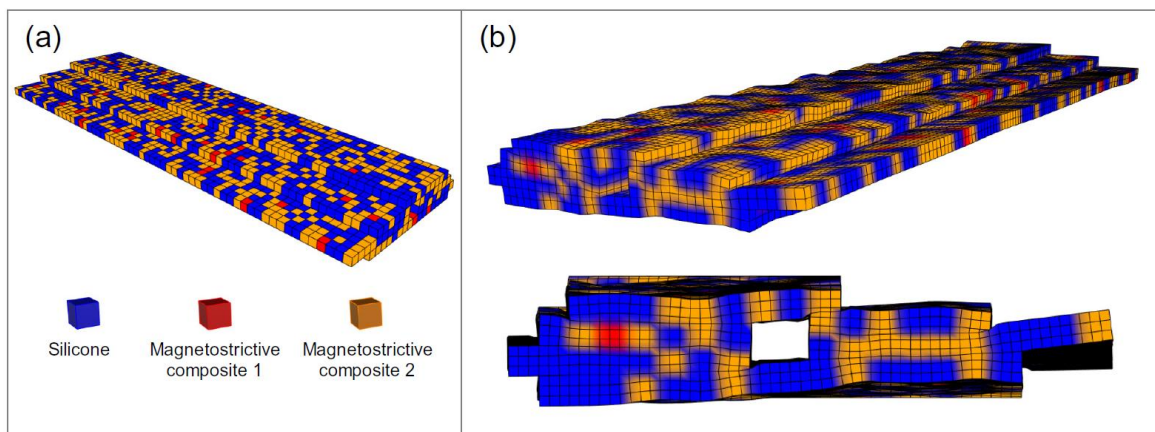


Figure 36. (a) Predicted distribution, (b) perspective and side view of the deformed wing when the magnetostrictive material reach saturation [122]

The interest of using knowledge and conceptual ideas of spontaneous self-organisations to obtain such a desired form was investigated in [124]. The authors have concluded that when it comes to 3D/4D printing, it

is necessary to adopt a powerful method to establish elements' arrangement (voxels) in various environments through SMs. Hence, voxels' arrangement in such a part can impact and guide its evolution, behavior, and motions [8][36].

In the same way, optimization approaches for 4D printing oriented design have been conducted: parametric optimization techniques were pointed out via Kriging meta-model and genetic algorithms to find the best combination of design variables to reduce weight and manufacturing costs for shape-changing printed parts using SMPs [125]. More recently, topology optimization was applied to obtain a soft actuator with an optimal structure to achieve a bending function [126]. Nevertheless, a Grasshopper example is introduced in Figure 37, including a transformation sequence: (a) substrate definition; (b) actuators definition; (c) simulating in high relative humidity; (d) simulating in low relative humidity to deliver dynamic CAD models ready for 4D printing [127].

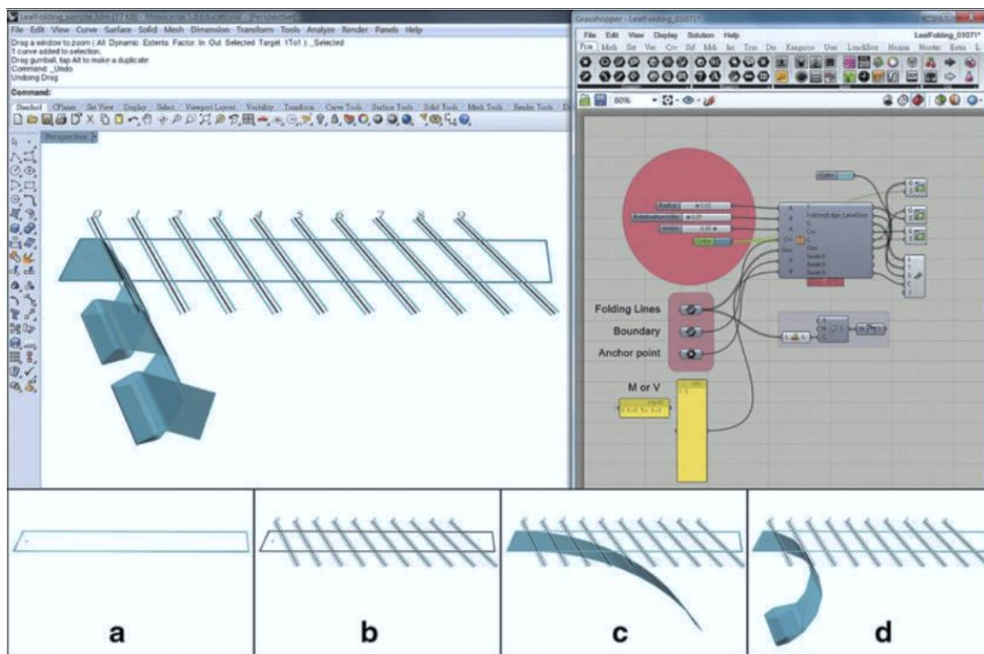


Figure 37. Dynamic 3D model built within programming logic of Rhinoceros3D/Grasshopper [127]

A fuzzy model and a discrete stiff finite element (FE) model to estimate the bending time of 3D printed porous polyelectrolyte hydrogel actuators in response to a given applied voltage was also developed in [39][42]. A distribution optimization of two materials (active and passive) based on an evolutionary algorithm and FE analysis was proposed in [37]; the model comprises identically sized voxel units. A genetic encoding has spatially split the functional composite structure. The 4D printability of electroactive materials was addressed in [128], and they have suggested that AM processes are limited to DIW, FFF, SLA, and selective laser sintering (SLS). Electroactive materials – used in the literature – were classified into five primary types: carbon-based composites, metal nanoparticles, polyelectrolyte hydrogels, conductive inks, and SMPs.

The optimum deformation angle (i.e., maximum) of a stimulus-responsive composite material (polylactic acid, PLA) strip onto the surface of a paper is determined; it is printed with the FFF technique and triggered by heat to deform and recover the initial shape. Different processing parameters – heating temperature, heating time, pitch, and printing speed – were used to investigate the material’s deformation angle and recovery angle [129]. Printing active composites (PACs) is a paradigm of 4D printing that involves directly printing SMP fibers in an elastomeric matrix to enable programmed shape-changing of the composites. The SMP fibers are used in the PAC system, which can fix a temporary shape and recover to its permanent form in reaction to temperature change. The bending angle Θ is used to characterize the performance of the hinge, and it is dependent on the hinge materials (matrix and fiber thermomechanical constitutive behaviors), geometric parameters (hinge length L and laminate/lamina arrangement), and programming parameters (ϵ_0 , T_H , and T_L), as illustrated in Figure 38.

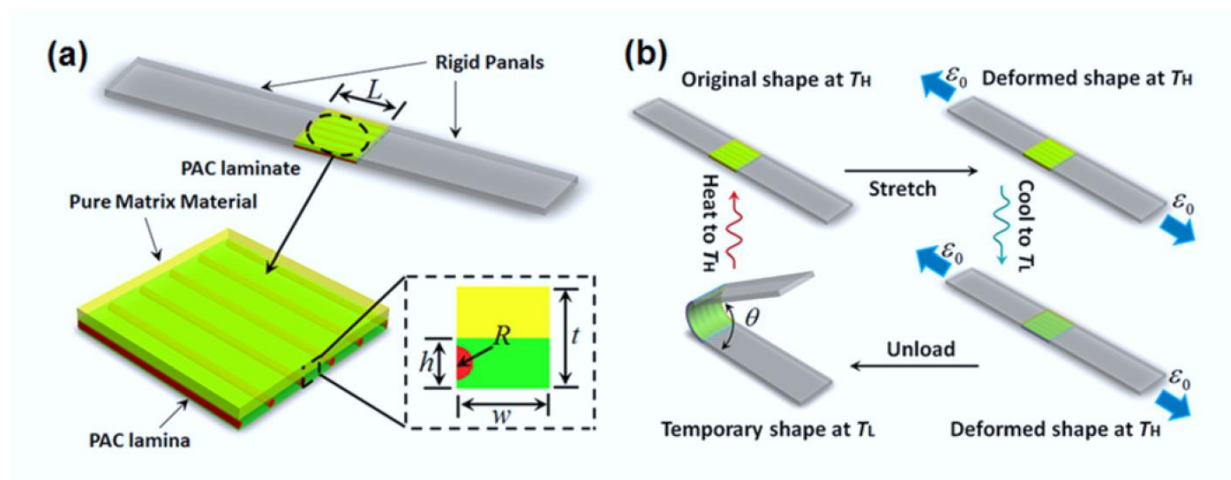


Figure 38. Schematics of a PAC hinge and the thermomechanical programming step, (a) geometric and mechanical properties of a PAC hinge, (b) thermomechanical programming steps to train a self-folding/unfolding PAC hinge [129]

Researchers have started qualitatively predicting such materials’ distribution mentioned above to increase the maturity of 4D printing technology. These distributions are influenced by the AM techniques and related machines capabilities and give considerable freedom in designing transformable structures. It may be gradient, uniform, bilayer, sandwich, etc. Multi-scale voxel-based modeling seems to be very important for enabling both material design (mechanical properties, micro and macro compositions) and design for 4D printing, (see Figure 39) [130].

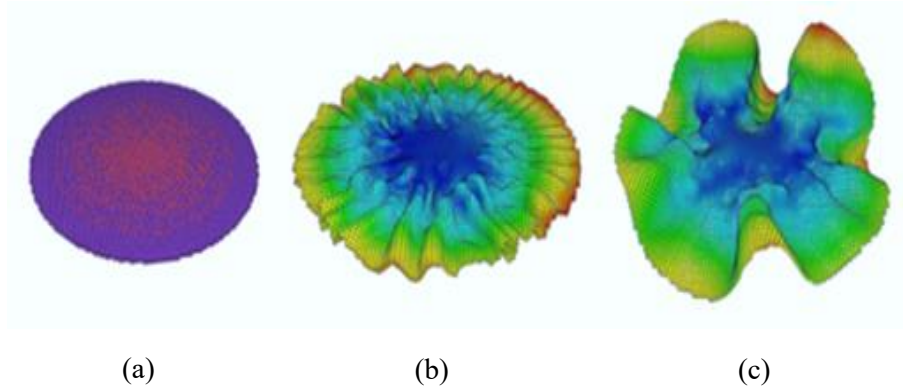


Figure 39. The simulation related to gradient distribution of material structure, (a) red indicates the rigid material and purple indicates the active material, and (b-c) the results of its immersion in water [130]

Multiple software are needed for streamlining the entire design process of 4D printed objects since an adapted software for 4D printing – that includes design, simulation, modeling, slicer, host/firmware, monitoring, and printing management – is still not concretely established yet [131]. In this context, proposing an appropriate design process and principles for 4D printing is fundamental to further modeling, simulation, and software development.

2.2.6 Applications

4D printing has shown promising capabilities as well as a broad range of possible applications; the following usages reveal the promising potential of this innovative technology:

- Self-assembly: The relocation of a 4D printed device through a tiny gap into a human body stands as a potential application of self-assembly at a micro-scale. At a macro scale, structures can be manufactured by specific AM machines and then triggered into bigger-sized systems (e.g., satellites, antennas, spacecraft), which ease the transportation of some large-scale systems [113]. A lesser size form can be first printed, and the other size(s) can be activated with the necessary performance at the target position. Printing a low-dimensional item is comparatively simple, quick, and cost-effective. In addition, it is more comfortable to store and transport lower-dimensional items. The inclusion of the 4th dimension may contribute here notably.
- Self-adaptability: Unlike textiles produced of elastic fibers, self-adaptive intelligent textile design can be adjusted to new dimensions without tensile charging. Multifunctional smart textiles can manage body moisture or temperature, monitor wounds, provide skin care, protect against harsh climates, or adapt clothing color [49].
- Time gain: Some structures [107] are adjustable to avoid the use of external electromechanical devices, 4D printing incorporates possibly sensors and actuators straight into a product. This reduces the

number of pieces in design, installation times, equipment and power expenses in addition to the amount of fault-prone machines commonly used in present electromechanical systems [24].

- Medical devices have been created, including self-deploying structures, actuators, hinges, grippers [104][132][133], and drug delivery systems (DDS) [134]. A thermo-responsive tracheal stent for bilateral bronchial involvement was published in [135], which resolved two problems of present tracheal stents. First, it better fits the arcade pattern and cartilaginous rings and provides a stable state that prevents migration. Second, the shrunk insertion form prevents injurious insertion. After being inserted into the body, the tracheal stent can expand to the permanent shape with a local temperature increase. Nevertheless, a 4D printed, thermo-responsive, SMP-based, cardiovascular stent was manufactured in [104]. Also, a high-response and reversibility skeletal muscle-like actuator was proposed in [18]. They put it in a smart valve and controlled water flow by opening the valve in cold water and closing the valve in hot water. This experiment demonstrates 4D smooth mechanical actuators.
- A pH-responsive hydrogel valve showing dynamic, reversible swelling and shrinking behavior was printed in [112]. It can regulate the flow rate at different pH levels. This structure can be a valuable platform for pH-responsive membranes [136] and photonic gels [72].
- Adaptive metamaterials enabled by 4D printing were reported in [110][35]. The lattice design could be reversibly reconfigured in both pieces of research where heat is an external stimulus. Metamaterials have adjustable lattices, and their mechanical properties depend on their geometric architecture rather than their chemical composition [35]. Adaptive metamaterials with adjustable band gaps are helpful to control elastic waves [110]. Adaptive metamaterials can change their stiffness depending on geometry modifications while maintaining steady mass [35].
- Soft robotics: A caterpillar lateral movement was presented in this reference [137]. These tests are appropriate for intelligent parts for new advanced systems. Active devices such as sensors, programmable structures, stent, and actuators [35][126][136][139]. A smart key-lock connector was created in [50]. The experiment was as such: before swelling, the walls are flat, and after swelling, convex and concave deformations occur in the wall, which reduces the cuboid's internal size and, finally, the interlocking. The key-lock connector can be used as a physical connection between body parts, such as tendons and muscles. It can also be used as a specific pick-and-place in gentle machines.
- An active origami box was demonstrated in [17]. Origami has recently drawn significant attention in solving engineering problems linked to packaging giant constructions into tiny quantities for transport and shipping [17]. An origami layout algorithm for the freeform surface was conducted by [140]. Furthermore, it was suggested and produced self-bending based bio-origami constructions that can be used in tissue engineering [87].

2.2.7 Synthesis

One can state that the essential elements shaping 4D printing technology are stimuli, geometry, AM processes and techniques, SMs, and transformation functions [26][141]. It allows the change in shape/property/functionality after being manufactured and triggered. It combines sciences with engineering technology indeed. To enhance its applications, multidisciplinary studies are needed because there are still obstacles to overcome in designing for 4D printing. Firstly, it depends on the quality and the efficiency of the used AM processes and techniques. When confronted with the multi-material setups and complicated printing structures utilized in 4D printing, common 3D printing abnormalities such as delamination between the printing layers and discontinuity of the printing material may be exacerbated. Second fold, the usefulness of 4D printing is constrained to exact working circumstances or to a fixed number of operations, both of which are undesirable. For example, SMPs are not reversible and need additional programming to be converted into other forms [36][38][43][115]. The study mentioned above of significant research works in 4D printing has highlighted a broad spectrum of knowledge over multiple domains and scales. This provides a large body of knowledge with spectacular results and leads to difficulties if they have to be integrated into a dedicated design process.

2.3 Research in design

Design problems are diverse in their complexity and diversity, occurring across all disciplines. Engineering design approaches and strategies continue to grow constantly [142–144]. Preliminary works have attempted several methodologies to define design activity in engineering. The product and its use activities can be seen as systems (activity system, function system, organ system and part system) or as models (function, behavior and structure) [145]. The design phases are generally: (i) planification and clarification (iii) conceptual design, (iv) embodiment design, (v) detail design and (vi) implementation (see Figure 40) [146][147].

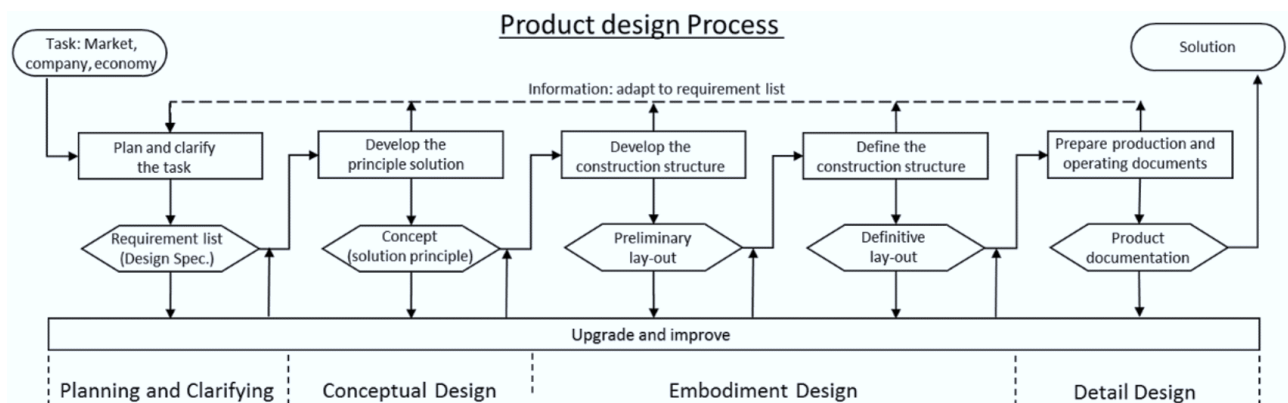


Figure 40 Traditional design process [148]

The embodiment design phase is currently expanded in computational design synthesis (CDS) [149]. CDS is a research area focusing on automating synthesis activities in design. The resulting methods may be fully or partially automated to reduce time-consuming engineering tasks and simply explore the creative abilities of computational systems. There is a fuzzy line between CDS and applied optimization [150]. Additional works highlight other notions that have affected research about engineering design, e.g., design for X methods (X stands for a downstream lifecycle phases) and knowledge-based design [151–153]. Many methods have introduced knowledge-based decision supports and feature-based modeling tools to provide planned solutions ready for particular lifecycle purposes to cite a few [3][150–152]. Lately, the emphasis has shifted from sequential to concurrent and integrated design, and more recently, towards generative design [157].

Design for X research-related field has perpetually growing approaches, methods, methodologies, solutions, and mechanisms [158–160]. Amongst these design mechanisms, design-by-analogy (DbA) is increasingly becoming an issue of interest in academia and industry [161]. DbA seeks to assist designers in identifying and developing examples related to case studies, scenarios, and experiences to solve design problems [162]. Although, designers could identify non-obvious similar solutions using a DbA mechanism, including in situations where the linkage between concepts is thin or from separate domains, which is the case for 4D printing. DbA is a powerful cognitive reasoning mechanism that can be categorized into four groups: analogy encoding, retrieval, mapping, and evaluation; and it can be supported by many machine learning (ML) techniques [163][164]. The DbA is classified into three models, namely symbolic, connectionist, and hybrid [165]. In this context, semantic reasoning based-rules and case-based reasoning for recommendation purposes are symbolic DbA mechanisms that fall under retrieval and analogy encoding purposes [166–168].

Indeed, product architects and designers still cannot take profits from the capabilities of this trendy technology, dissimilarly from conventional manufacturing processes and some AM techniques (e.g., SLS) that already have guidelines and rules for design and process planning nowadays [169–171]. Since 4D printing encompasses many scattered artifacts, and little is known about how these factors influence a 4D printed part, its future use requires a distinguished design process, specific process planning knowledge, adapted methodologies, and tools to cite a few. Knowledge capture and federation behind this technology seems crucial to let the designer and other involved actors leverage to profit from it under design for 4D printing [115]. The latter requires rethinking well-established models, methods, and tools to develop innovative devices with changing capacities. However, very little work is still done to support designers in considering this technology. It is essential to recommend appropriate knowledge such as material distribution, design rule, or any constraint to aid the designer in developing dynamic and multifunctional objects [172]. As defined in the previous section, this technology is interdisciplinary, complex to understand in design, and still in its infancy phase yet. Then developing design principles that are compatible with SMs' distribution patterns – since the transformation is based on stimulus-responsive materials usage in such a part/structure – and suggesting methods for using them are a crucial gap nowadays.

2.4 Ontology models for product/process/material design

With the introduction of the semantic web in the early 2000s in computer science, a broad spectrum of ontologies has been developed to describe concepts formally and explicitly within a specific knowledge domain. An ontology is a highly organized set of ideas that encompasses a given domain's processes, objects, characteristics, and the intricate relationships between those concepts in that domain [173]. Such knowledge bases – which present subjects, objects, processes, and ideas as entities or concepts and relationships as unary or binary predicates – are constructed with axioms, definitions, and theorems [174–176]. It also contains formal definitions and axioms that restrict understanding the words [177]. As a whole, an ontology can represent knowledge according to the triplet subject-predicate-object (e.g., square – subclass of – shape) as schematized in Figure 41.

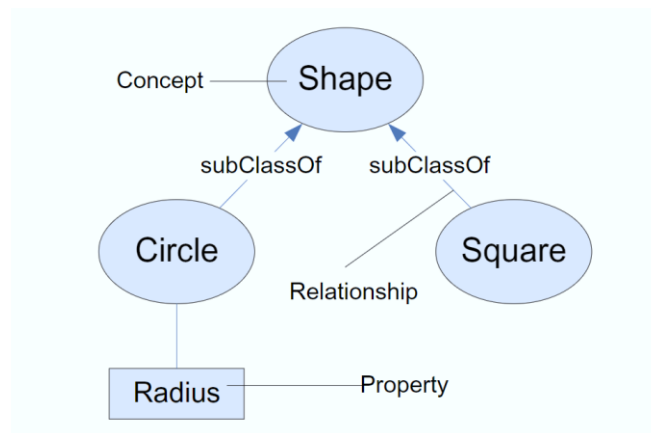


Figure 41 Simple example of an ontology [178]

The backbone of an ontology is composed of a concept hierarchy linked by a subtype relationship. Once built with axioms and constraints, the latter makes explicit domain assumptions and provides a common understanding of the knowledge domain. An ontology can then be informal or formal with a systematic and axiomatic development of logic for all forms and modes of existence [179][180]. In such a context, OWL (Ontology Web Language) and DL (Description Logics) rules provide a solid basis for machine interpretation. The formal ontology can further formalize the following descriptions: universal concept (denoted A box), the impossible concept, atomic concepts (denoted T box) and negations of atomic concepts, the intersection of concepts, value restrictions for concepts, universal and existential quantification restrictions. Axioms such as disjunctions and equivalences may be represented and instantiated concepts and roles assertions. A feature-based ontology captured semantic information for integrating CAD, and computer-aided process planning was created [181]. An ontology has been proposed to support a first-order process planning for sheet lamination technology [182]. For the same manufacturing process, an ontology embedding manufacturing rules for further automatic features recognition procedure was developed [183]. A design for AM ontology to represent a set of information on part design, AM processes, and capabilities to define design rules was proposed [184]. The

reasoning is then possible to evaluate design features against manufacturing constraints. Liang *et al.* [185] has created an informal generative ontology model for AM process planning in the same context. From a material perspective, properties of heterogeneous materials to the core product model were developed at the National Institute of Standards and Technologies (NIST) [185], which initially was a generic product model [186]. In addition, an ontology-based framework for selecting material in domain-oriented knowledge was presented and semantically retrieved and querying it [187]. Among the numerous published materials ontologies [188]–[190], a materials ontology at the European level called European Materials Modelling Ontology (EMMO) was developed, which covers materials, physics laws, and physical models [191]. EMMO is built upon an upper ontology called formal basis ontology (BFO) [192]. In this context, Hagedorn *et al.* [193] have demonstrated the use of BFO over-engineering domains in interoperation, investigation, and simultaneous capture of knowledge. Furthermore, the spatial-temporality and the dynamic phenomena of objects' transformations, in general, have been addressed by a multi-layer ontology covering multiple domains and dimensions [30].

In the engineering context, ontology formalization of design concepts and domain knowledge is perceived as an essential part of conceptual design after stating concept sketch and solution principles when the designer attempts to capture and represent different aspects of the product design at various stages [143]. But implementing ontologies is not about staying only at the level of capturing knowledge; it can be helpful in several aims, e.g., knowledge extraction, reasoning layers following, querying missing items, etc. For instance, extracted knowledge has a considerable interest as knowledge resulting from an ontology that respects multiple expertise and domains. Moreover, Brank *et al.* [194] have stated that evaluating the semantic relations in such an ontology and applying them for a specific application is among powerful ontology evaluation techniques. Lembo *et al.* [195] have implemented extractors for their ontology in the finance domain to react to user inquiries and prevent the complete and time-consuming of reading all ontological instances.

Additionally, an application of ontology views modeling and versioning on determining a building maintenance task was carried out in the geospatial domain [196]. Ontology management is an issue that interests many researchers, either extracting knowledge from an ontology; or reversely extracting data to enrich and deepen the ontology itself. For that reason, Astrova and Stantic [197] proposed a methodology for extracting data from HTML¹² forms to migrate them into an ontology after optimizing and normalizing them to make the web content understandable. Further usages were denoted by Siddharth *et al.* [198], e.g., an engineering knowledge graph was extracted from the USA¹³ patent database then formalized according to ontology implementation rules. It serves mainly for engineering design retrieval purposes by applying reasoning inference engines. In summary, we can see that many challenges in 4D printing and ontology-

¹² Hypertext Markup Language is a core technology for building Web pages

¹³ United States of America

oriented design have not been addressed yet. But also, Green *et al.* [199] have suggested that starting such a design process with an ontology can be a plus value and time gaining method since it overlaps all the formalized concepts and facilitates its management in such a process.

On the other hand, semantic technologies enable reasoning about knowledge from multiple heterogeneous information sources and disparate domains. After implementing ontologies or knowledge graphs, semantic reasoning rules are often established as reasoning layers to enhance knowledge interpretation or constraints retrieval [200]. For example, semantic rules supported a range of queries and design scenarios to define features accuracies (i.e., thread pitch angle, radial clearance, and hemisphere radius) for a thread machine model [201]. Also, semantic reasoning rules were established for constraints' subassembly identification in product design to identify geometric incoherence [202]. Different languages are proposed in the literature, to cite a few: semantic web reasoning language (SWRL) [203], semantic queries web reasoning language (SQWRL) [204], and shape constraints languages (SHACL) [203][204].

To specifically address a design problem, it is crucial to establish a classified and structured knowledge base that such software invokes in its libraries and queries it fluently. Hence a description of the dynamical phenomena at various scales is strongly needed to formalize the knowledge behind logical continuity over the design stages. Based on the study in this section highlighting the importance of ontologies in establishing a prior level in DFX, ontology development is required to formalize the previous knowledge behind such a paradigm. An essential step is bringing relevant knowledge to the designer to make the right decisions. It has been argued that a domain ontology describing, and formalizing 4D printing knowledge is still lacking. Thus, according to the promise of a large industrial market, it seems crucial to elaborate one supporting the spatiotemporal understanding of transformable parts/objects over time. The so-called design for 4D printing requires rethinking well-established models, methods, and tools to develop innovative devices with changing capacities over time.

2.5 Reasoning methods

In engineering design, comparative reasoning-based ML techniques to define new design solutions or concepts are referred to as incorporating artificial intelligence in the whole design process, a discipline with intensive research over the last decades. Jiang *et al.* [207] have integrated some ML methods into a design for additive manufacturing (DFAM) framework. This integration follows a principle suggested by Rosen *et al.* [208] about the process (e.g., print temperature, speed, etc.) – structure (e.g., geometric accuracy/surface roughness) – property (e.g., mechanical strength, strain stress behavior) relationship, which is suitable to DFAM. This influence of one stakeholder on another (e.g., geometric accuracy on mechanical strength and vice versa) is established by ML techniques in any required direction using the available AM data, i.e., deep neural networks were proposed for point data and convolutional neural networks for distributions and image data.

Furthermore, using a predefined large scale semantic network, Linsey *et al.* [209] introduced the WordTree approach for linguistically representing design difficulties. This method can assist designers in seeking potential analogies for idea generation by helping them to explore prospective analogies for design problems. In addition, a functional vector approach was suggested to describe design documents as vectors based on the word frequency of available verbs from the functional basis model, which was developed by Murphy *et al.* [210]. These works lend credence to the assertion that using reasoning techniques, e.g., ML, case-based reasoning, and many others like vector space models, can enhance and facilitate the engineering design phase by applying analogies and comparative tools.

Specifically, the vector space model (VSM) depicts documents and queries as vectors in a multidimensional space, the dimensions of which are the words used to construct an index to describe the documents (see Figure 42); this algebraic method serves to apply case-based reasoning approaches [211].

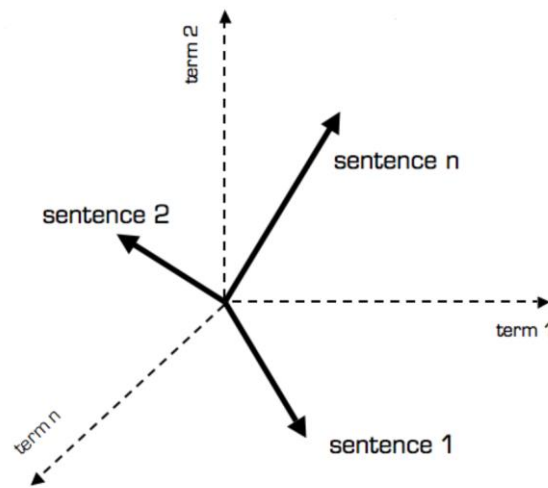


Figure 42 Example of sentences definition in VSM¹⁴

It is utilized in information retrieval, indexing, and relevance rankings, and it may be used effectively in the assessment of online search engines [212]. The VSM method may be broken down into multiple phases [213]. The document indexing step is the initial stage, during which content-bearing words are extracted from the document text [214]. The second step involves weighting the indexed keywords to improve the retrieval of documents relevant to the user [215]. The last step scores the document concerning the query based on a similarity metric [216]. The angle between the document vector and the query vector is determined using a standard similarity metric called the cosine measure [217]. The angle between two vectors is regarded as a measure of divergence between the vectors; the cosine angle is used to calculate the numeric similarity between the document vector and the query vector when represented in V -dimensional Euclidian space (V is the size), [218]. So, this method is an algebraic model representing a text or an object as a vector and distance measurements help to determine nearby concepts, objects, or solutions in the defined space [219].

¹⁴ <http://bitsearch.blogspot.com/2011/01/vector-space-model-for-scoring.html>

When designing and reasoning by analogy to case studies, an ontology may support a case-based reasoning approach for computer-aided tolerance specification for several purposes: similarity between part features, tolerance features, topological relations between parts, targets, and previous cases [220]. The above was implemented respecting three significant steps: (i) define prior cases as previous cases and each new tolerance specification issue as a target case, (ii) an ontology-based similarity measure may be used to get comparable prior instances for a target case, and (iii) process of reusing and revising tolerance cases. The above steps may be overlapped with the steps mentioned above of the VSM method.

2.6 Synthesis and key research questions

Reported research works have shown an extensive spectrum of knowledge in 4D printing, design, ontology, semantic reasoning, and case-based reasoning. It was conducted across many problematic areas and scales, leading to plenty of knowledge available with remarkable outcomes. However, there are various constraints when these findings are required to be incorporated into a comprehensive process that includes design, modeling, simulation, control, and manufacturing, which are vital requirements to underpin this technology's advancements. Hence the first requirement here is federating the knowledge related to 4D printing technology. Moreover, the 4D printed product carries a dynamic aspect as stated in the literature. This fact raises a second requirement about its representability in design. Establishing a knowledge base to a recently emerging technology or a domain of innovation always pursues many rules, from ontology to information extraction, computation theory, then automated reasoning. For that reason, establishing an ontology and using it, is a logical pursuit to evolve the formalized knowledge and to develop suitable approaches based on semantic and case-based reasoning. Still, using the ontology itself verifies and proves usability regarding the important elicited works above. The last section demonstrates that VSM is a valuable tool in semantic indexing solutions and a practical approach in comparative reasoning. Thus, recommending such knowledge according to 4D printing ontology concepts in the CDS phase seems critical for product architects and designers. Therefore, developing reasoning layers complementary to 4D printing domain ontology via building semantic rules and case-based rules to recommend a particular knowledge is crucial. For instance, the distribution (also called spatial arrangement) of smart and inert materials in such a part stands as a driving force that binds the different aspects of this technology. A good and well-defined materials' distribution will assure a specific transformation, enhance the performance and characteristics of the 4D printed part, to cite a few. Thus, researchers focus on designing and simulating the materials (smart and inert) distributions in such part/product/structure intended to be manufactured with 4D printing. Design methodologies are still poor and not decisive enough to recommend a precise and well-given distribution. Hence, aiding designers by suggesting materials distribution of a 4D printed object is crucial. Nonetheless, proposing any other knowledge (e.g., materials type, application of the stimulus, etc.) is also a key element in supporting and facilitating designers' tasks.

So, the key research questions for this PhD can be formulated as follows:

1. Given the interdisciplinary aspect of 4D printing, the dynamic aspect of a 4D printed object, and the lack of formalization for this knowledge, how to represent and formalize its related knowledge to be used in the different design phases?
2. How to represent and formalize CAD representations of a 4D printed object over CDS?
3. How to reason with the 4D printing knowledge to recommend contextual/specific knowledge useful for the product designer in the CDS phase?

To address these key research questions, three contributions are proposed. The main objective is to create knowledge, models, methods, and tools to assist the designer in CDS for 4D printing. The proposed research aims at:

- Developing a domain ontology, gathering, and formalizing the interdisciplinary, disparate, and scattered 4D printing knowledge for use in the CDS phase;
- Defining a multi-representation of a 4D printed object in the CDS phase;
- Building a recommendation system aiding the designer to select/determine the materials distribution according to the specific requirements in the CDS phase.

Chapter 3 An ontology-based framework to formalize and represent 4D printing knowledge in design

“The process of building or engineering ontologies for use in information systems remains an arcane art form, which must become a rigorous engineering discipline”

N. Guarino, 2002

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3.1 Introduction

The 4D printing paradigm has received intensive research efforts, whether in the AM or SMs development. Related research works have generated many *ad hoc* solutions with relevant disparate and scattered knowledge. This lack of common core knowledge is mainly due to the multiple involved expertise fabricating stimuli-responsive structures. The scientific issue of federating and reconciling knowledge is interesting, especially if this technology must be integrated into the product design process, falling under the field of design for 4D printing. It becomes crucial to formalize and represent knowledge relating to AM processes/techniques, SMs behaviors, stimuli, and transformation functions with various design objects to tackle this challenge. In such a context, this chapter aims at developing an ontology-based framework for the semantic and logical description of transformable parts/products/structures in the era of 4D printing for product-process design-related purposes. This framework – built upon a foundational ontology associated with BFO – introduces a domain ontology equipped with reasoning capabilities supported by DL for SMs selection and distribution, transformation sequence planning, and AM process planning purposes. This ontology stands as the first contribution of this PhD and relies on autonomous knowledge description of objects. Section 3.2 establishes the ontological framework with the underlying epistemic scientific hypotheses and the support of the BFO [192], along with the use of 4D printing knowledge in design. Built on this, Section 3.3 presents the proposed ontology for formalizing and representing 4D printing knowledge. The proposed ontology embeds reasoning capabilities supported by mereotopological relationships and DL in CDS for 4D printing purposes, presented in Section 3.4. Discussions and conclusions wrap up this chapter in the last section.

3.2 HERMES framework

The formalization and representation of 4D printing knowledge for design-related purposes require a dedicated framework built upon foundational hypotheses and theories beforehand. The objectives of such an ontological framework – presented in Figure 43 – are then twofold: (i) providing a domain ontology construction strategy and (ii) clarifying the ontology usage scenarios. Since 4D printing highlights objects transformation upon a time, it seems convenient to address three-dimensional [221] and four-dimensional [222] theories to describe transformable objects. The upper ontology BFO has been adopted for such representation issues to reconcile both mentioned visions through endurants and perdurants concepts (i.e., also known as occurrents, accidents or happenings, perdurants objects are those entities for which only a part exists if we look at them at any given snapshot in time) [192].

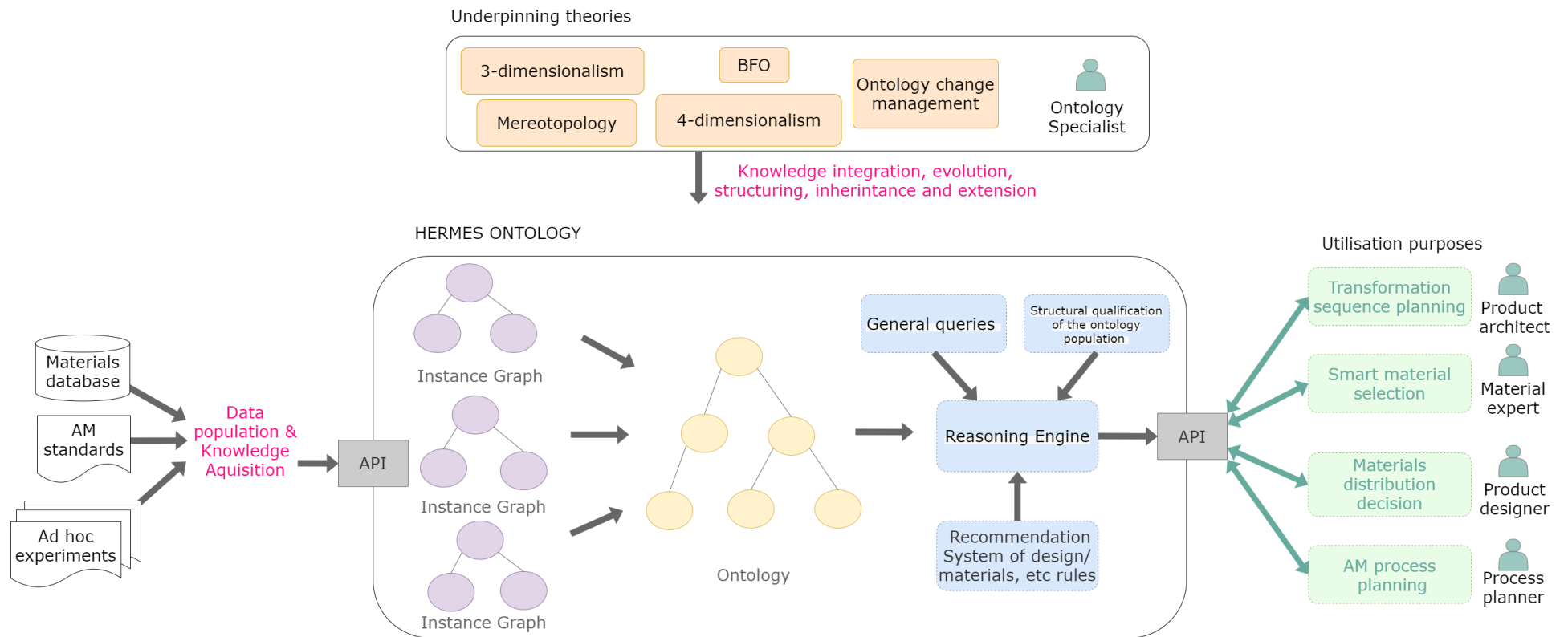


Figure 43. HERMES framework

In its actual shape, BFO is not suitable enough to cover the semantic articulation between the material objects, immaterial objects, and processes participating in design for the 4D printing process. In such a context, mereotopology is considered a complementary theory relating mereology (i.e., part-whole theory) and topology to introduce specific relationships and object properties between the classes mentioned above. Considering these underpinning theories enables knowledge integration and evolution (with ontology change management procedures) through the top-down construction over structuring, extension, and inheritance of the proposed domain ontology [196].

On the other hand, such critical 4D printing knowledge cannot be described from scratch. It is important to consider current information and data sources ranging from AM processes and techniques standards, materials databases, and proofs-of-concept from published research works. Such knowledge acquisition and data population will be part of the bottom-up construction of the domain ontology with view-specific ontology instances. Following such a coordinated construction strategy should clarify the design purposes and scope (i.e., description of dynamical phenomena knowledge, implementing a multi-layer ontology, and semantic and logical reasoning). 4D printing actually can be addressed in design via different points of view, such as system design, product/part design, and material design. In this contribution, the knowledge domain will be limited to product/part design, although each design scale merits to be investigated. The introduced artefacts provided by 4D printing issues can be considered an interdependent constraints network. The envisioned ontology – called HERMES (mecHanical objEcts of 4D pRinting and programmable Matter for nExt-generation of CAD systemS) – will enable multi-view decision support and knowledge-aided design regarding design for 4D printing. As an example, future usages can cover:

- transformation sequence planning;
- smart materials selection;
- smart material distribution;
- AM process planning;
- Etc.

These utilizations require dedicated APIs related to the involved stakeholders. As a result, this framework (shown in Figure 43) places the HERMES ontology under the supervision of the ontology specialist. Different actors (i.e., product architect, product designer, material expert, process planner) can formulate multiple rules-based reasonings and queries with different purposes in the design process. However, we are limited in this PhD to **the product designer in the CDS phase**.

3.3 HERMES ontology development

Respecting the framework presented in the previous section, this section builds the HERMES ontology development. For the sake of clarity, a labelling convention has been adopted as follows: the names of classes

are written in capitalized/lower case (i.e., *My_part*) with Arial font, the names of attributes and relationships use mixed Case notation (i.e., *isParentOf*) with courier font while names of instances are in italics (i.e., *Part1*) with times new roman font. Also, the word “class” is used in this PhD to name a “concept” in the ontology in an undifferentiated way.

3.3.1 Basic Formal Ontology

This section defines BFO classes [192]. BFO contains much more classes than those used in this PhD, although Figure 44 describes only the classes used to define HERMES ontology. Only the classes “*Generically_dependant_continuant*” and “*Role*” are described and not used for the sake of clarity and a better understanding of the other siblings’ classes. The subclasses of every top-class are not exhaustive, i.e., there is always the possibility of adding new subcategories.

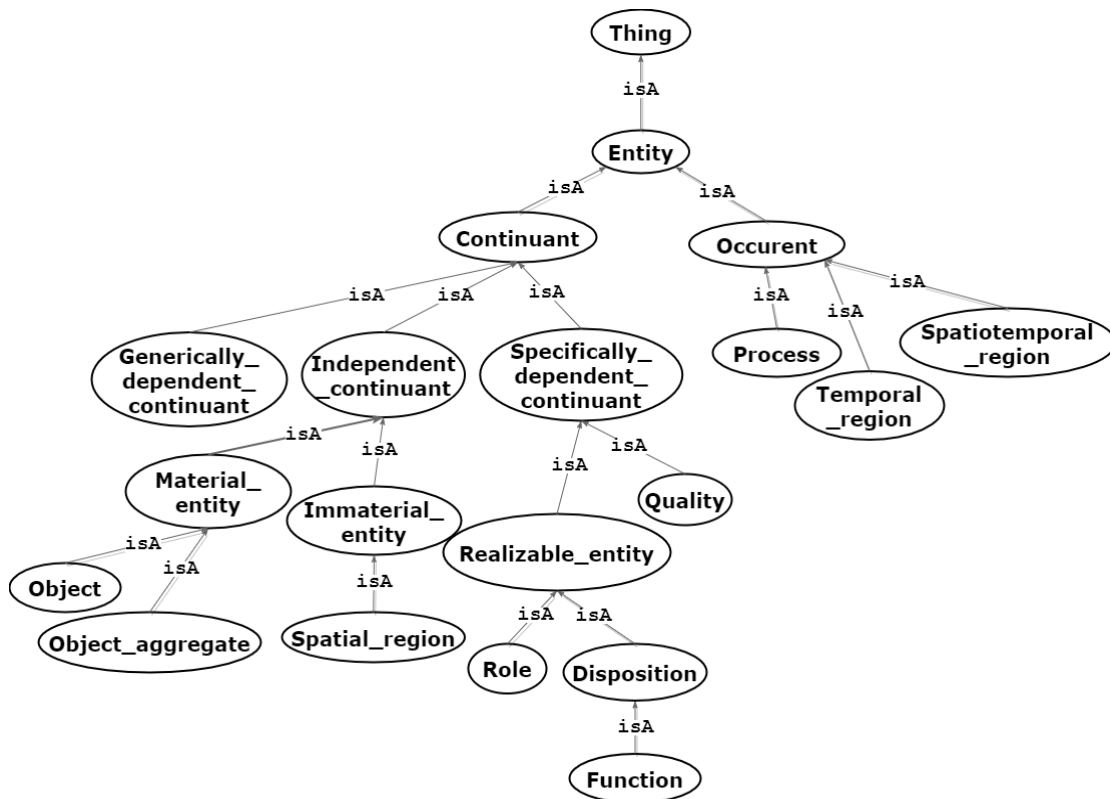


Figure 44. Main top-classes of the upper ontology BFO

- Entity is anything that exists, according to BFO definitions.
- Continuant is an entity that persists, endures, or continues to exist through time while maintaining its identity.
- *Generically_dependent_continuant* is an entity that commonly relies upon one or more entities, e.g. pdf file on a laptop, etc.
- *Independent_continuant* is an entity that doesn't depend on / rely upon any other entity, e.g. atom, etc.

- **Material_entity** is an independent continuant that has some portion of matter as proper or improper continuant part, e.g., human being, forest fire, sea wave, etc.
- **Object** e.g., organism, planet, etc.
- **Object_aggregate** is an entity always consisting of a plurality of objects as member parts at which it exists, e.g., car, restaurant, etc.
- **Immaterial_entity** is divided into two subgroups: boundaries and sites, which bound, or are demarked in relation, to material entities, and which can thus change location, shape, and size.
- **Spatial_region** is a continuant entity that is a continuant part of such a geometrical space.
- **Specifically_dependent_continuant** depends on some entity that is its bearer. Therefore is such that it cannot migrate from one bearer to another.
- **Quality** is a specific dependant continuant that, in contrast to roles, does not require any other process to be realized.
- **Realizable_entity** is a specific dependant continuant that inheres in some independent continuant that is not spatial region and is of a type of instance.
- **Role** is an entity that exists if and only if there is another single bearer entity of it, e.g., the role of student: receiving knowledge and using it.
- **Disposition** is a realizable entity that if it ceases to exist, then its bearer is physically changed, and its realization occurs when and because this bearer is in some particular physical circumstances.
- **Function** is a special kind of disposition. It is a realizable entity whose realization is its bearer's end-directed activity.
- **Occurrent** is an entity that unfolds itself when it is the instantaneous boundary of such an entity.
- **Process** is an occurrent entity with proper temporal parts and depends on some material entity.
- **Temporal region** is an occurrent entity that is part of the time as defined relative to some reference frame.
- **Spatiotemporal_region** is an occurrent entity that is part of space and time.

As the HERMES ontology has been developed by considering both top-down and bottom-up constructions strategies, the top-level classes of this domain ontology have been defined accordingly with BFO (see Figure 45). The latter opens a great perspective to gather and align multiple domain ontologies with the Industry Ontology Foundry (IOF) community and is suitable for applying 3- and 4-dimensional theories. The objective of formalizing and representing design for 4D printing knowledge requires mapping concepts (later called classes) and properties of the investigated domain and providing formal specifications to be computer-interpretable.

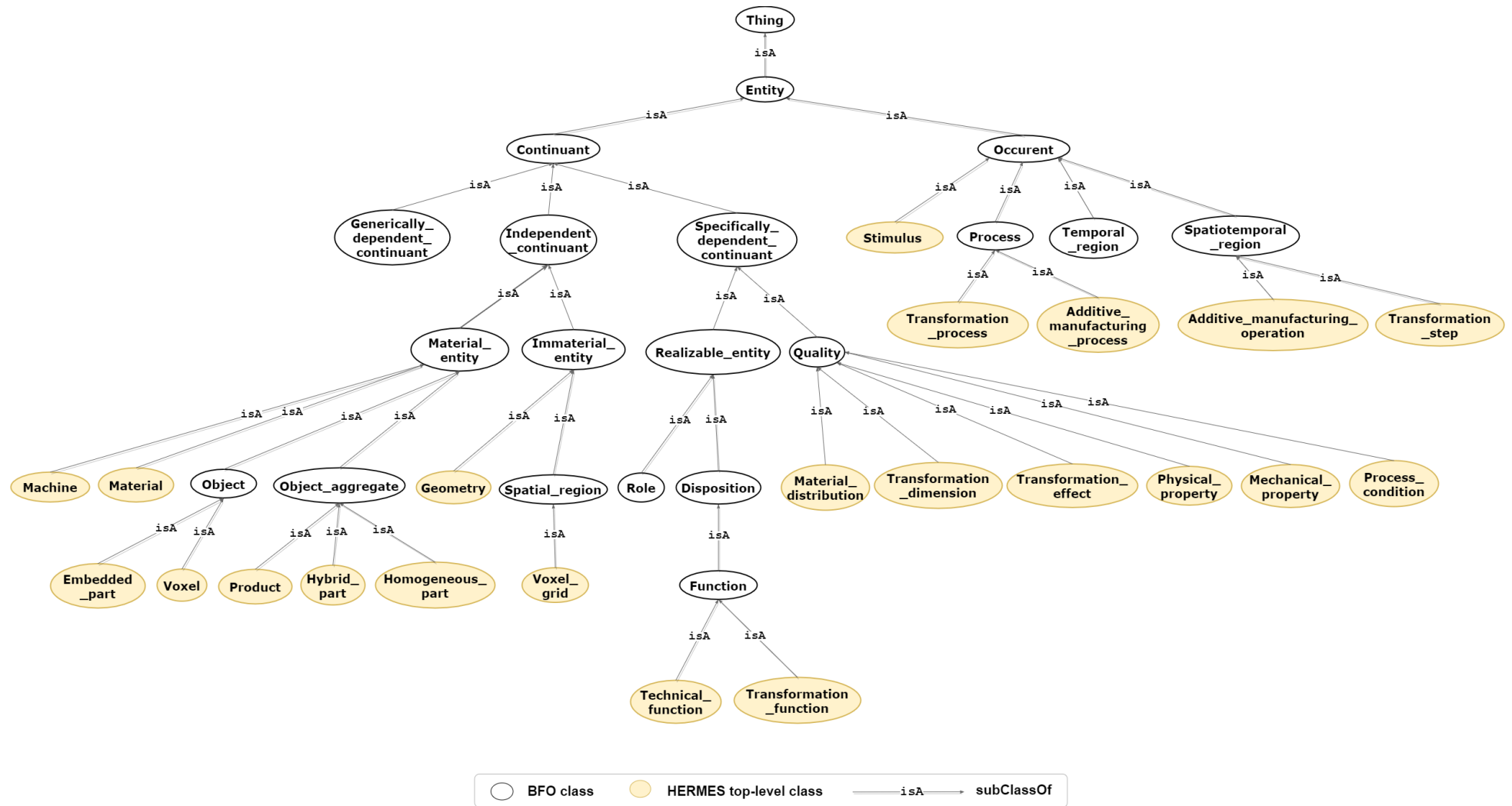


Figure 45. Top-level concepts of the HERMES ontology built from BFO

Grey circles denote BFO classes in Figure 45, yellow circles denote HERMES ontology top-classes, and arrows schematize the heritage-relationships between HERMES classes as subclasses of BFO classes with the object property `isA`. Some classes are registered as equivalent classes in BFO (they went up one level), this is explained by the fact that the classes in BFO have some limits in their definitions. For example:

- Stimulus is defined as a subclass of `Occurent` and an equivalent class to `Temporal_region`, `Process`, and `Spatiotemporal_region`; because it cannot be a `Region` or a `Process`, it is a trigger that occurs in laps of time, imposes a changeability in a specific form and carries an existing and natural property like heat for example.
- `Geometry` is defined as a subclass of `Immaterial_entity` and as an equivalent class to `Spatial_region`. Assuring the fact that `Immaterial_entity` presents two other subclasses: `Site` and `Boundary` but none of the three subclasses can define `Geometry` because it is the properties and relations of points, lines, surfaces, solids, and higher dimensional analogues. Hence, it englobes the three subclasses, and it seems more convenient to define it as `Immaterial_entity` simply.
- `Material` and `Machine` are defined as a subclasses of `Material_entity` and equivalent classes to `Object` and `Object_aggregate`; because it is possible to define them both as `Object` and `Object_aggregate` depending simply on the level of granularity that we are limited to in our definitions. And since `Object` and `Object_aggregate` are used at a part/product level, it seems convenient to level up `Material` and `Machine` classes to `Material_entity` to avoid any possible overlap.

For the sake of clarity, the upcoming subsections highlight the ontology model through several concerned views such as:

- Design and engineering view presents some changes in product models;
- Material view describes the main properties between materials, their characteristics, their distribution, and stimuli;
- AM process view presents relationships between object-process and object-machine to cite a few.
- Transformation process view models change in a 4D printed product/part/structure.

3.3.2 Design and engineering view

The integration of 4D printing knowledge in mechanical design requires changes in traditional product models. This technology mainly features shape, function and property transformations, and multi-material printing capabilities. It is crucial to rethink current established design and engineering models to support multi-perspective knowledge and rules over space and time. Therefore, this view – presented in Figure 46 – can be

considered as an integration driver to connect all 4D printing surrounding aspects. Designing a part/ structure for 4D printing highlights the need of providing an appropriate knowledge representation. According to BFO, a Material_entity can be either an Object or an Object_aggregate as presented in Figure 46, but not roughly; thus, it provides an exciting knowledge modeling strategy to represent objects with different points of view.

Grey circles denote BFO classes in Figure 46; yellow circles denote HERMES ontology classes, green circles represent the data properties of the classes (a data property is a characteristic of such a class presented in values or parameters that impact design, analytical, and computational processing), continued arrows schematize the heritage-relationships with the object property *isA*, and dashed arrows model the object properties between independent classes (how a class is related to other without a heritage relationship between them).

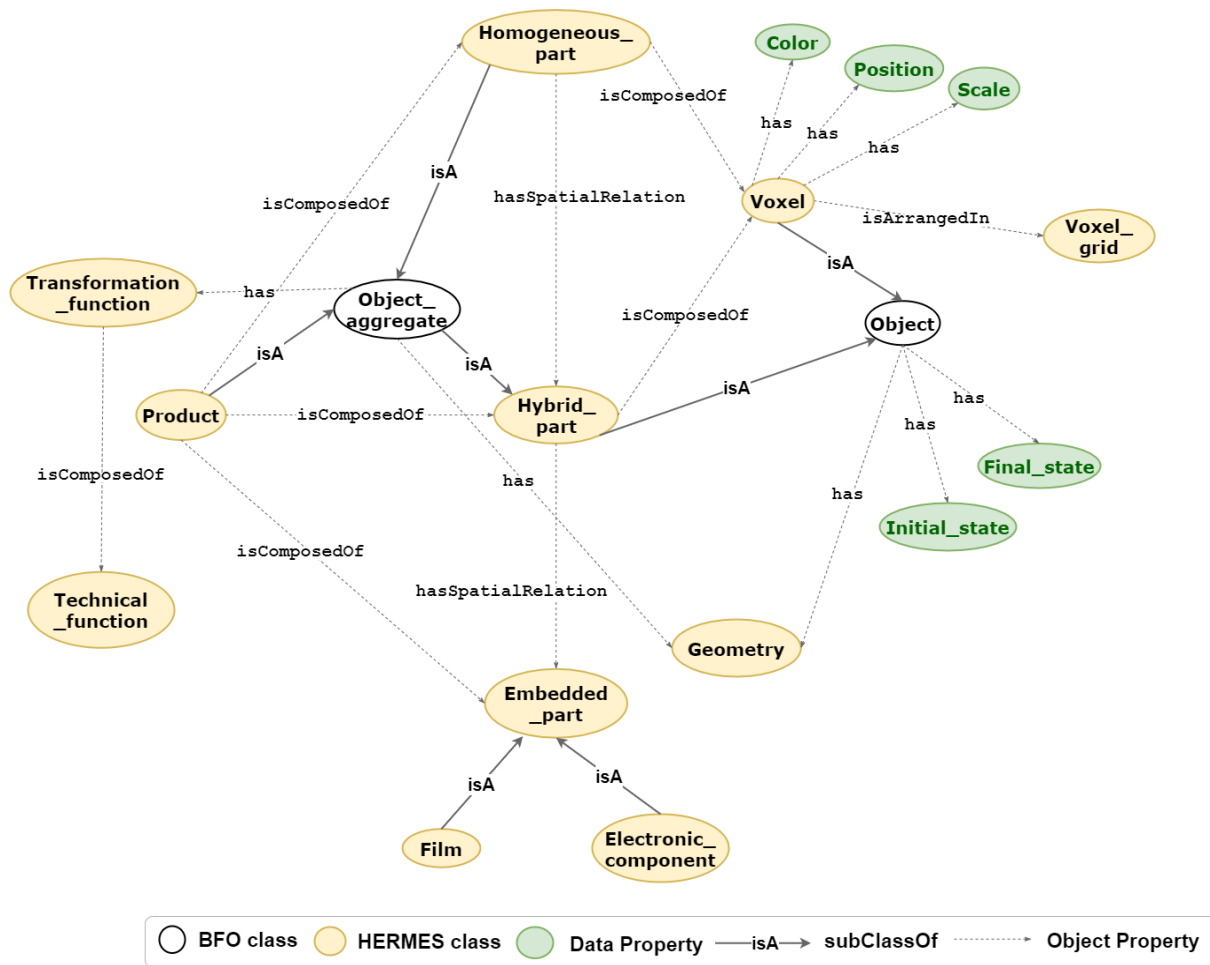


Figure 46. Design and engineering view with classes and object properties

For the actual purpose, an Object class can concern a 4D printed part with multiple states (e.g., manufacturing state denoted Initial_state, use state indicated Final_state) over space and time. But also, this class can be related to Embedded_part (e.g., electronics part, liquid crystal elastomer film, electrode, etc.), which is a separate manufactured part generally introduced during the AM process.

Homogeneous_part and Hybrid_part classes have been specified to address different compositions. Homogeneous_part is exclusively composed of a single material. The material typology – partially covered here – will be further defined in the material view. The Hybrid_part class – described a part of a Product composed of at least two Homogeneous_part(s), therefore providing multi-material modeling capacity. Both classes are composed of Voxel(s) (see Figure 47). Since 4D printing-related literature has shown the introduction of Embedded_part(s) to enhance transformability with dedicated SMs, it seems necessary to introduce it into the Product class.

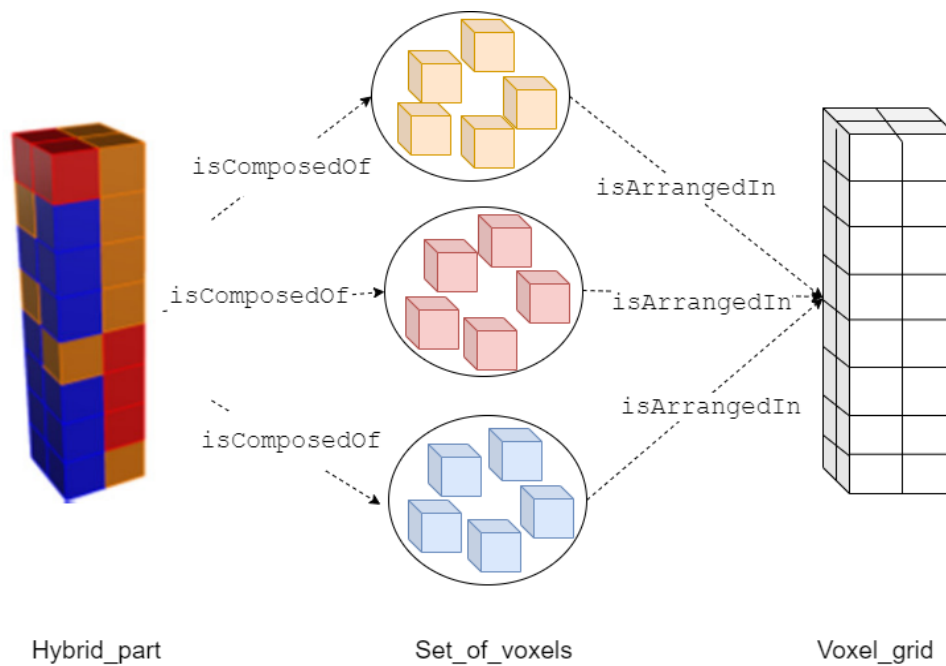


Figure 47 Illustration of Hybrid_part composition

Referring to mechanical design, Product has the disposition to gather material entities like embedded, homogeneous and hybrid parts through spatial and mereotopological relationships (i.e., isOverlappedBy (when a voxel is surrounded by a set of voxels), isTangentTo, etc.) (see Figure 48). The latter denotes multiple semantic descriptions ranging from topological relations to direction and distance relations and therefore provides suitable semantics for further qualitative spatial reasoning.

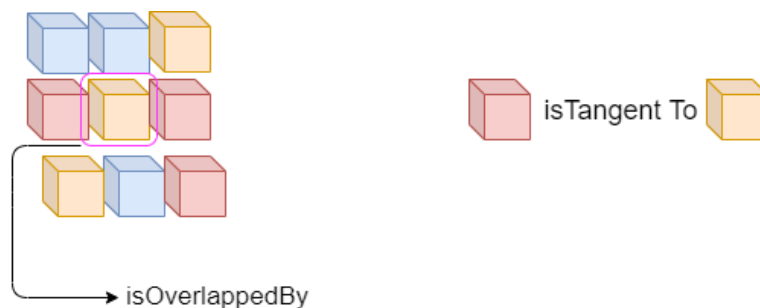


Figure 48 Illustration of some mereotopological relationships

When the identity of an entity varies, there is a particular evolution/transformation of this entity into a new one. It can be defined as the uniqueness of a part/product/structure, regardless of its attributes or values. It is the feature that distinguishes one 4D printed Product from all others. Identity is essential in conceptualizing and modeling a phenomenon [224][225]. This concept is very subjective because it depends on the criteria selected by the user to define the identity of an entity. In the same Object class, the Voxel class is described as a volume element arranged and spaced in a Voxel_grid (considered as a kind of Spatial_region in BFO), which bearers multiple data properties (e.g., color, position, and scale in terms of size in a grid), multiple mechanical properties, and multiple materials. It may be defined within a specific spatial resolution and appropriately subdivided with quadtree and/or octree related data structures for numerical analysis or ML-based reasoning purposes. Voxel can be an enabler for decomposing any 3D object in multiple sub-objects to allocate materials, simulate their behavior, or even increase AM printing capabilities. To meet 4D printing requirements in terms of multi-material and printing capabilities, such above-mentioned singular objects must be spatially organized in a Voxel_grid to build a 4D printed Product.

The Transformation_function enables the different states and related definitions of the 4D printed Object(s), geometrically 1D, 2D, or 3D. Hence, according to spatiotemporal modeling, an instance of the class Object carries out the identity of an object that evolves during space, time, and views. In addition, the Object_aggregate class plays the role of a set of objects. Thus, spatiotemporal modeling is a pretty heterogeneous domain that supports identifying generic characteristics for modeling entities over time. A spatiotemporal entity represents the real-world entities, which are mainly composed of an identity, descriptive properties, and spatial properties. While identity describes a fixed specification of the entity, alphanumeric and spatial properties can vary over time and thus represents its active part.

This view exhibits relationships with the other views semantically, whether in the association of Object(s) with Material(s), AM processes and related Machine(s), and Transformation_function. In such a context, the design/engineering view is strategically developed with dedicated classes from other views to articulate 4D printing-related knowledge.

3.3.3 AM process view

Design for 4D printing demands beforehand to consider existing AM processes knowledge. AM has already been covered by the taxonomies and standards of the ASTM Committee F42 and the ISO Technical Committee 261 - ISO/ASTM 52900 - Internal Organization for Standardization [12]. Additive_manufacturing_process class has many subclasses respecting different rules, such as the used raw material (solid, liquid, and powder) and the deposition technique, as detailed in Figure 49.

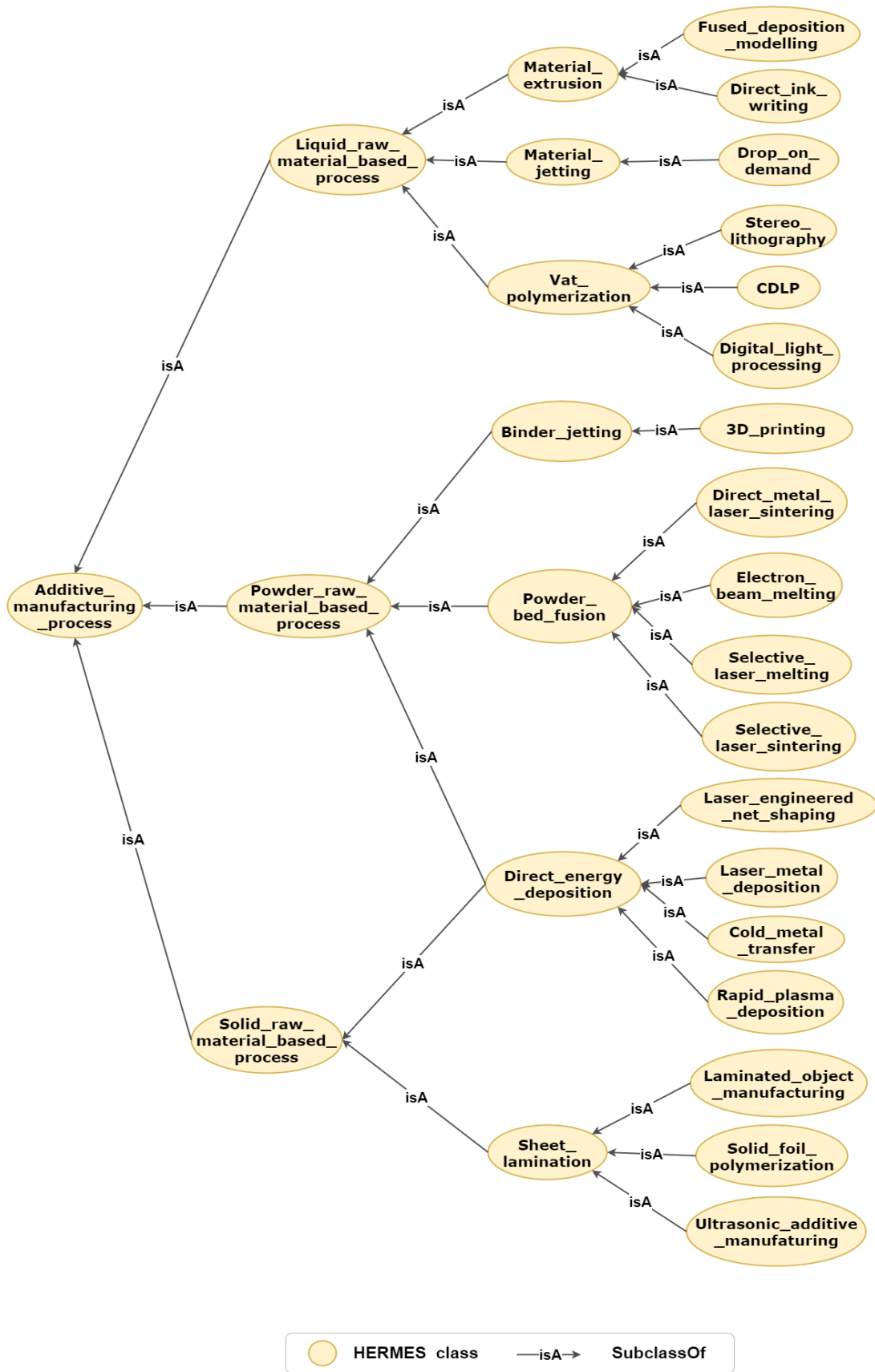


Figure 49. Part of the AM process view describing AM families and techniques taxonomy

This view aims to gather – through `Additive_manufacturing_process` class as a subclass of BFO `Process` class – AM technologies and techniques that could be linked to SMs printing method, Machine(s), and Process_condition(s), as illustrated in Figure 50. In addition, the `Machine` class – which is a subclass of the BFO `Material_entity` class – enables the elicitation of commercial multi-material printers and customized ones. `Process_condition` class specifies `Machine` control parameters aligning `Machine` capability and `Material` forming requirements. Among the AM parameters that affect the 4D printing process, one can cite the printing speed, printing path orientation, layer height, hot-end temperature, etc. A variation of these parameters can influence the object’s geometry quality, the mechanical behavior, or the target transformation. Figure 50 presents the view with top-level concepts relating to `Machine`, `Process_condition`, `AM_operation` and `Additive_manufacturing_process`.

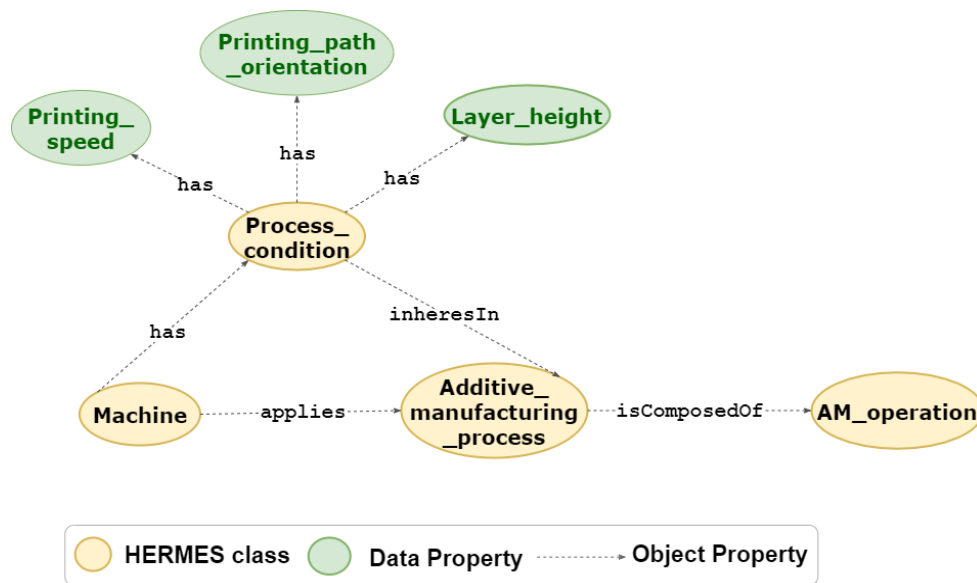


Figure 50. AM process view with top-level concepts

3.3.4 Material view

In addition to the previous views, material-related knowledge is also a pillar of the 4D printing paradigm. Material selection is always addressed to embody the desired mechanical properties; it is an additional step to define structure and shape. This importance is still valid with 4D printing technology. Nevertheless, in this actual context, the role of materials is augmented with technical functions or functionalities (i.e., active, structural, and sacrificial) to cover the transformation issue (this aspect will be discussed in the next section). Figure 51 on the next page presents the `Technical_function` class and its subclasses that can express the technical requirements of transformable systems. Beyond their traditional structural role, materials – covering `Metal`, `Alloy`, `Composite`, `Polymer`, and `Ceramic` – embody smart behaviors. This embodiment entails the consideration of SMs from the CDS stage to define 4D printed parts, which can be composed of a single material (i.e., `Homogeneous_part`) or multiple materials (i.e., `Hybrid_part`).

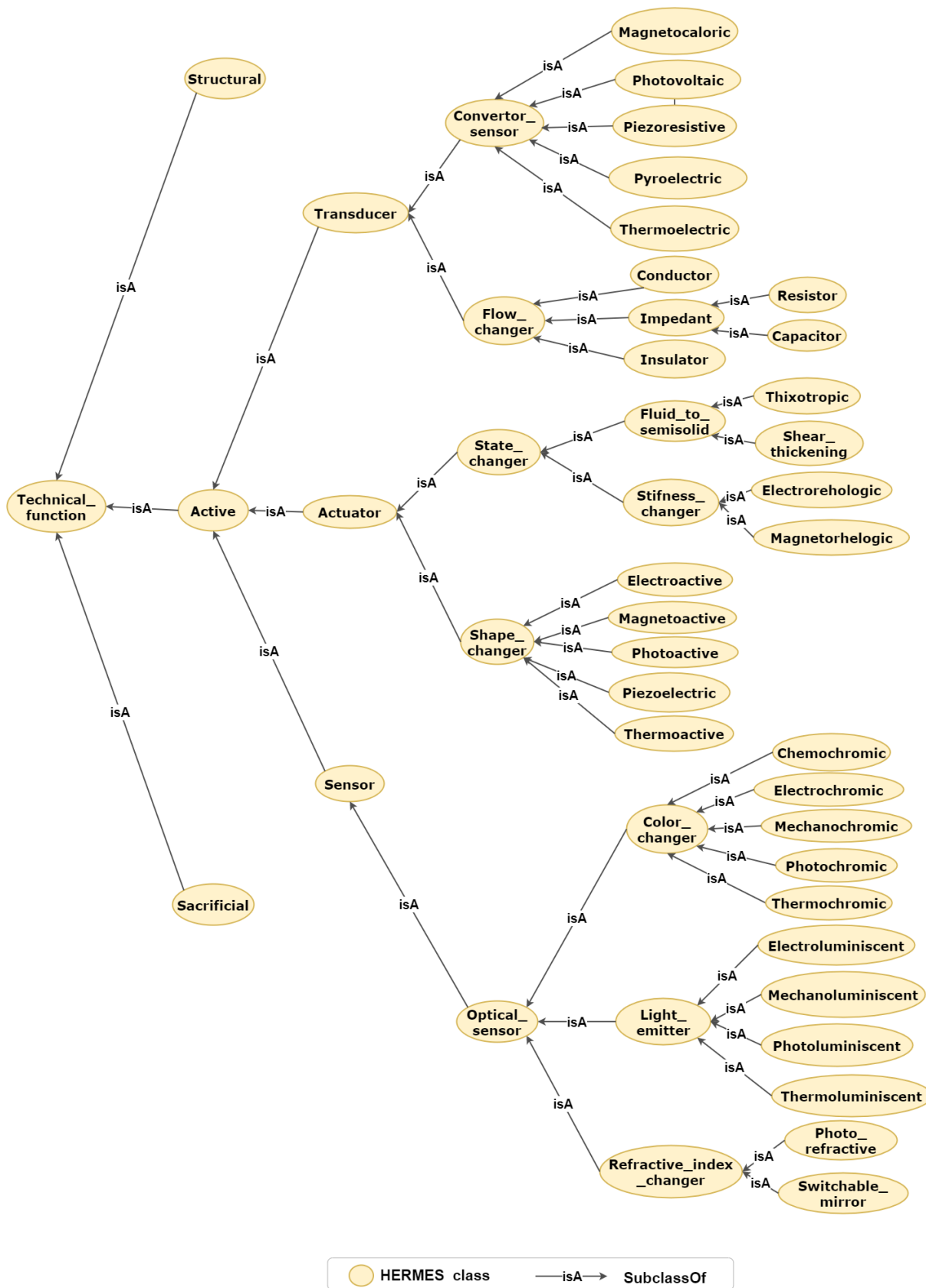


Figure 51. Part of the material view describing technical functions taxonomy

A Material can fulfil a Sacrificial function where the support structure is needed during AM process or a Structural one in a 4D printed object with no peculiar responsive characteristics to a stimulus. The complexity lies in the Active function, where the Material can act as Transducer, Sensor, and/or Actuator with a broad spectrum of stimuli. As subclasses of BFO Quality class, Mechanical_property, Material_distribution and Physical_property classes stand either as qualities of the Material or Quality of a Stimulus, whose semantic relations are described in Figure 52.

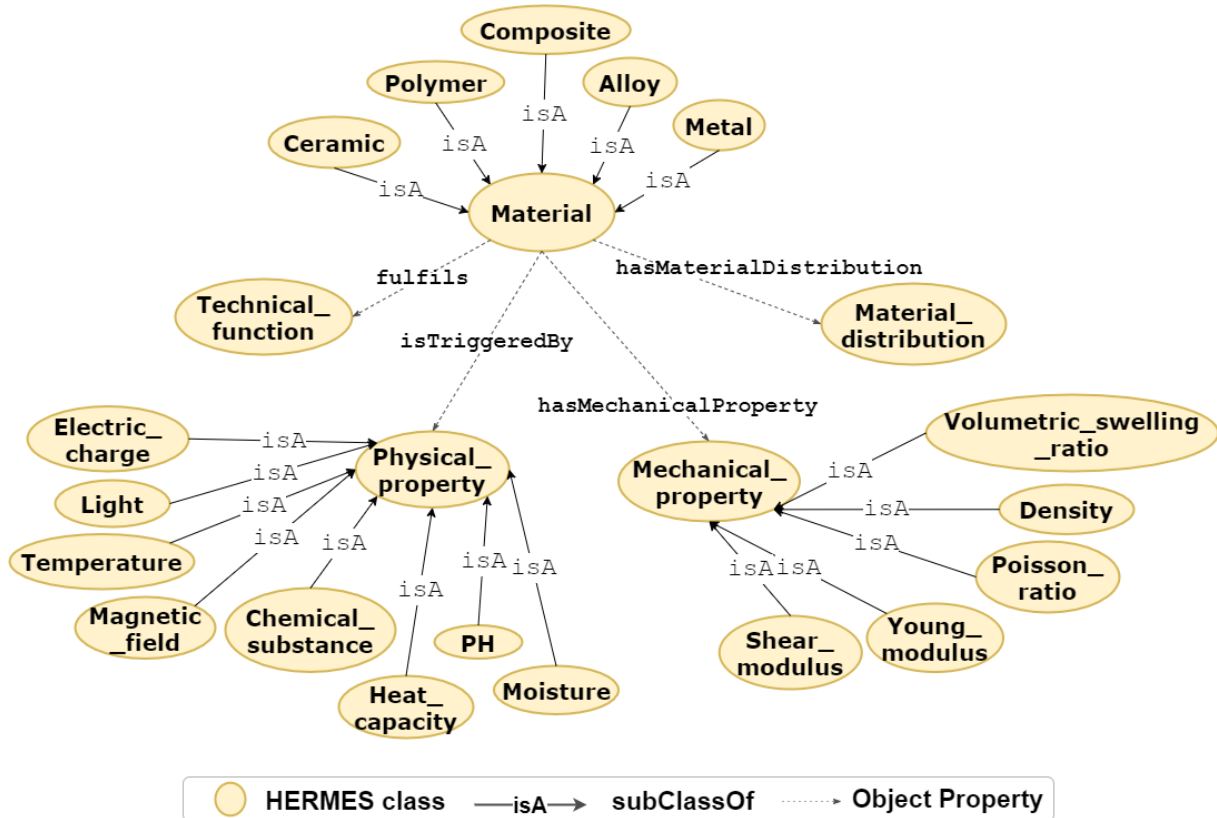


Figure 52. Material view with top-level concept

Material_distribution class exhibits spatial distribution patterns of smart (i.e., Active material) and inert (i.e., Structural material or Sacrificial material) materials (as illustrated in Figure 53) to carry out the desired transformation of an object and also to take advantage of the multi-material printing capabilities.

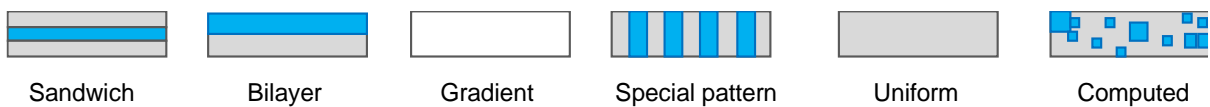


Figure 53. Materials distributions

Here the Material(s)_distribution(s) provide design freedom to distribute Mechanical_property change within the structure for a 3D shape/functionality/property transformation. Such Mechanical_property changes are intrinsically connected to stimulus and its underlying physical properties. Therefore, Physical_property class gathers the needed qualitative and quantitative characteristics that a Stimulus bears to trigger a Material and consequently a 4D printed structure/product/part. This view is semantically connected to the two previous views, as presented in Figure 54 below.

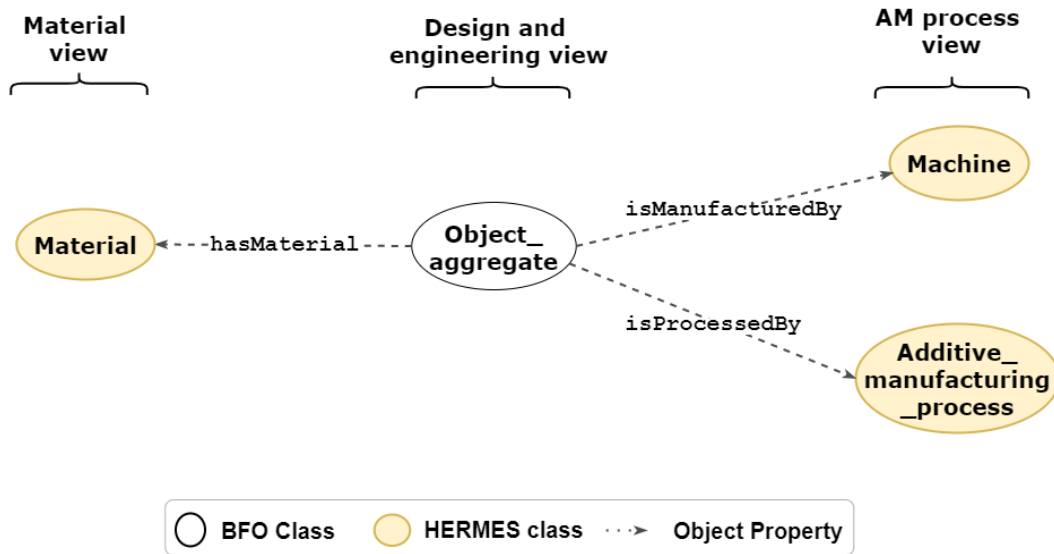


Figure 54. Semantic associations between material view, design and engineering view, and AM process view

3.3.5 Transformation process view

This view refers to the inherent temporal dimension from 4D printing. Current product design practices are focused on building static geometric definitions related to a specific physical state. The present objective needs to capture additional knowledge to describe transformable objects over time in terms of shape, functions, or property. Thus, designing dynamic products requires beforehand specifying functional requirements and Technical_function(s) as part of inherent Transformation_function in addition to traditional service and constraint functions that a system/product/part must fulfil. Figure 55 delineates the transformation process view featuring the essential transformation functions. One can first describe Expansion/Contraction, Twisting, Folding, Bending classes for shape transformations among such functions. Properties_changing is about changesets in color, swelling ratio, stress, or stiffness of such an object, and State_changing represents a material state change (i.e., either liquid or solid) shown in Figure 56. From these primitives, other behaviors can be elaborated, such as Waving, Helixing, Curling, Buckling, and Chemical_properties_change.

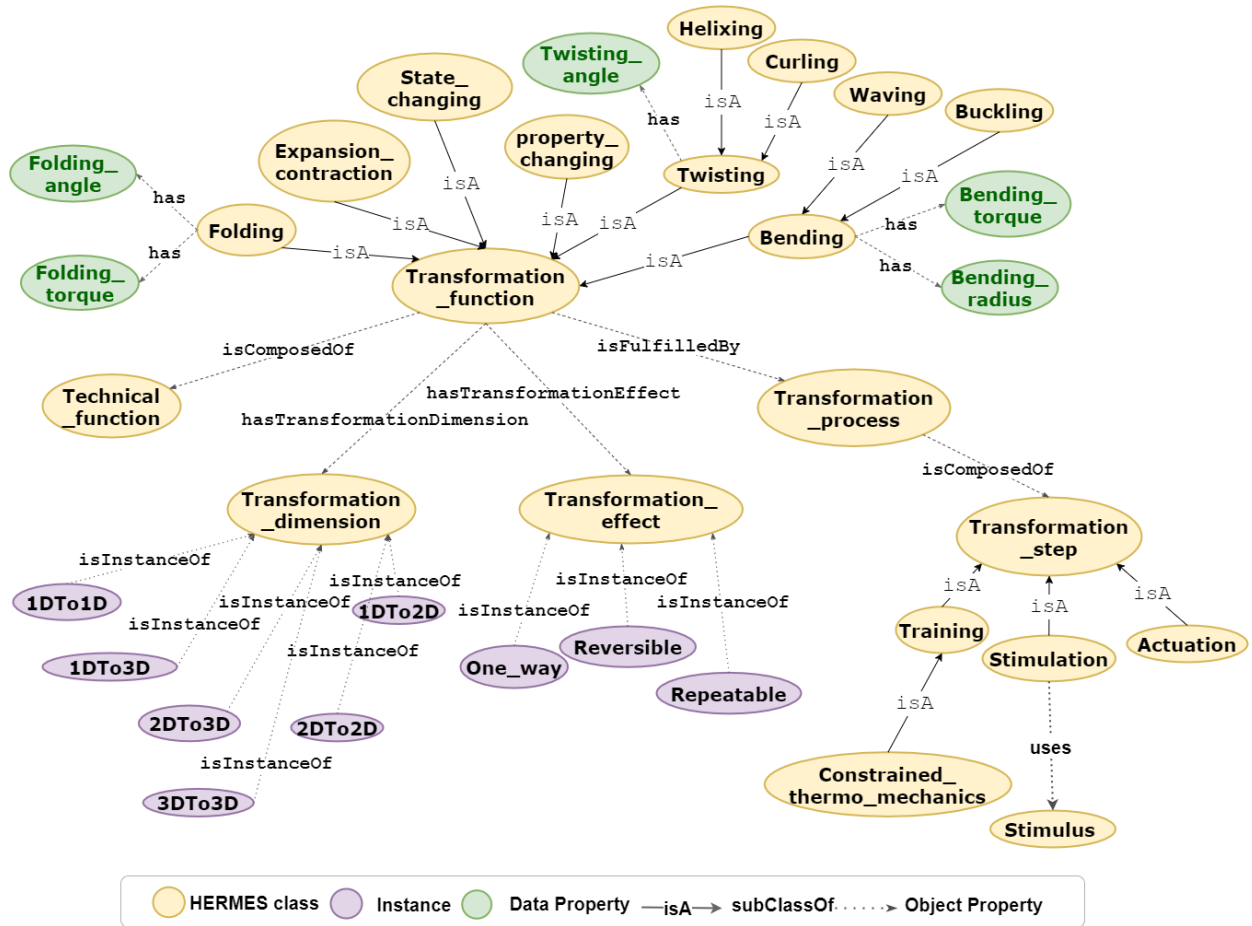


Figure 55. Transformation process view

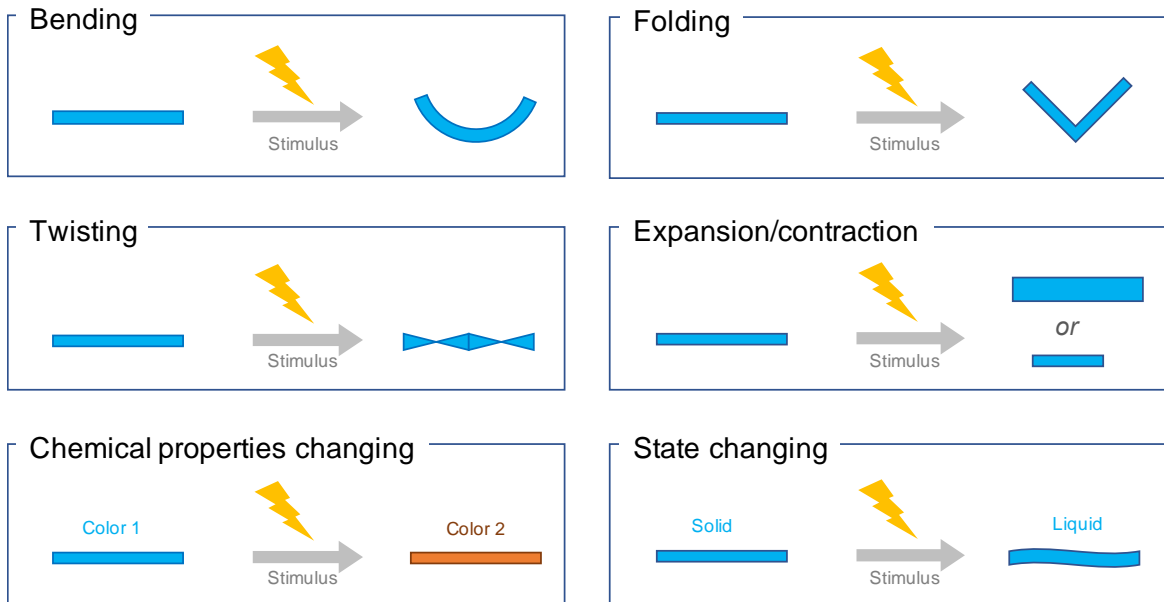


Figure 56. Basic transformation functions

Here, one can specify Transformation_function with Transformation_dimension and Transformation_effect classes to capture the dimensional nature of the transformation states (e.g., from 2D to 3D, 3D to 3D, etc.) and the cycle of transformability, especially the following instances: *One_way*, *Reversible* (i.e., two ways) and *Repeatable* (i.e. more than two ways), as shown in Figure 57. *One_way* is changing an original shape/property to a permanent shape/property after being triggered. As for *Reversible* and *Repeatable*, product /part/structure will switch between two states in a single cycle or several ones, respectively.

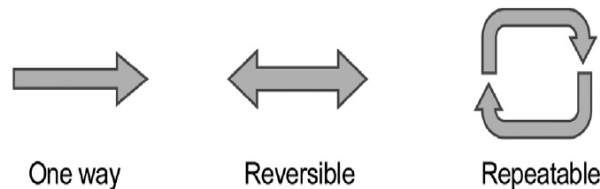


Figure 57 Transformation effects

In this transformation process view, a Transformation_function can be fulfilled by a Transformation_process (as a Process class in BFO) that is composed of a set of Transformation_step(s) (amongst Training, Stimulation, and Actuation classes). Transformation_step is presented as Process class in BFO. The latter class introduces a temporal logic order required to build the targeted shape, property, or functionality changes, as illustrated in the example in Figure 58.

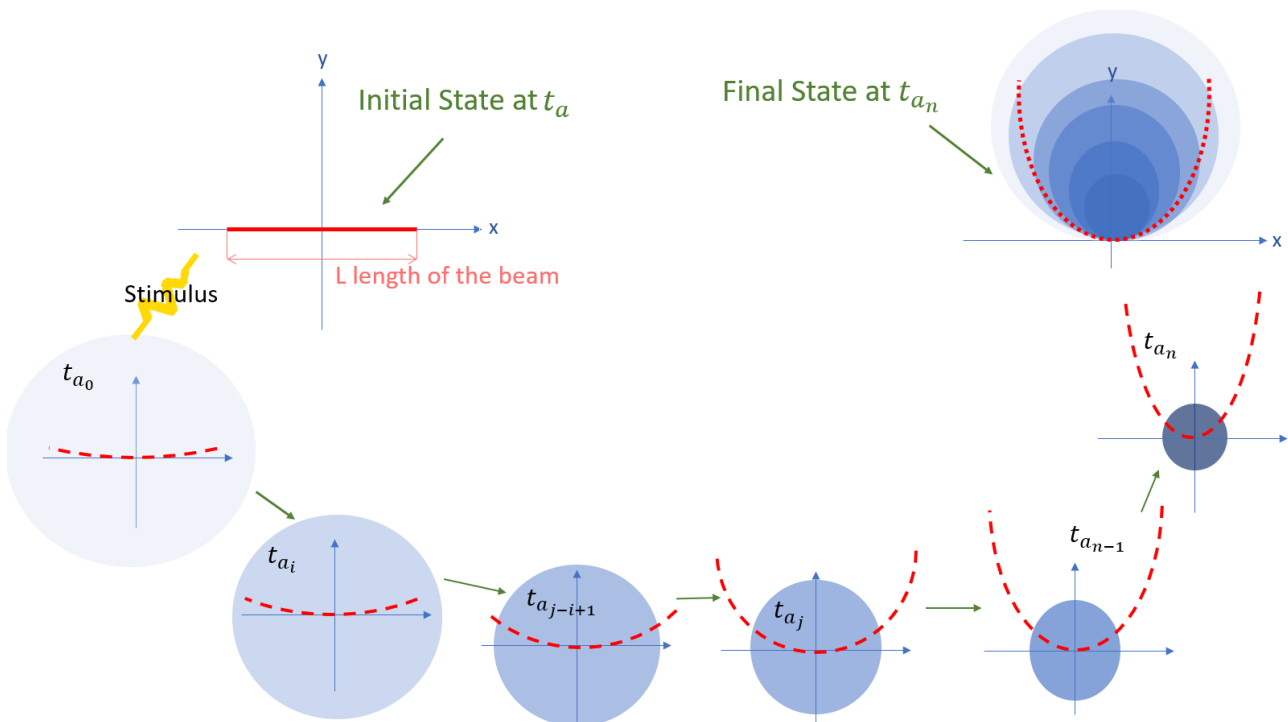


Figure 58 Illustration of a Transformation_process for a Bending transformation

The circles with gradient blue denote the intensity of the bending curvature and its location in the beam. It starts with a flattened beam as an initial state in a t_a , which denotes the starting time of the trigger and ends at a t_{an} the ending time of the Transformation_process. The t_{ai} are the timings of some intermediate states of the beam.

The Training step is presented here in one mechanism, Constrained-Thermo-Mechanics – but not roughly limited to –, in which the trigger is done sequentially. For example, such a step is about heating to the material's highest critical temperature, applying a strain to the structure, cooling while keeping the pressure. The desired shape is obtained, and the structure should be reheated to retrieve the initial shape. The Stimulation step applies one or several stimuli (as a subclass of Occurrent in BFO). Exposing SMs to a specific Stimulus will require the support of the Transformation_process – ensuring the allocation of appropriate Physical_property(ies) with the correct value at the right place and time respecting a specific duration – in order to achieve the Actuation towards the targeted shape. The Stimulus is selected according to the application’s requirements, which will also determine the kind of SMs used in the 4D printed structure.

Notably, the Stimulus class in this view is semantically associated with the material and design and engineering views, as shown in Figure 59. The whole HERMES ontology is presented in Figure 60.

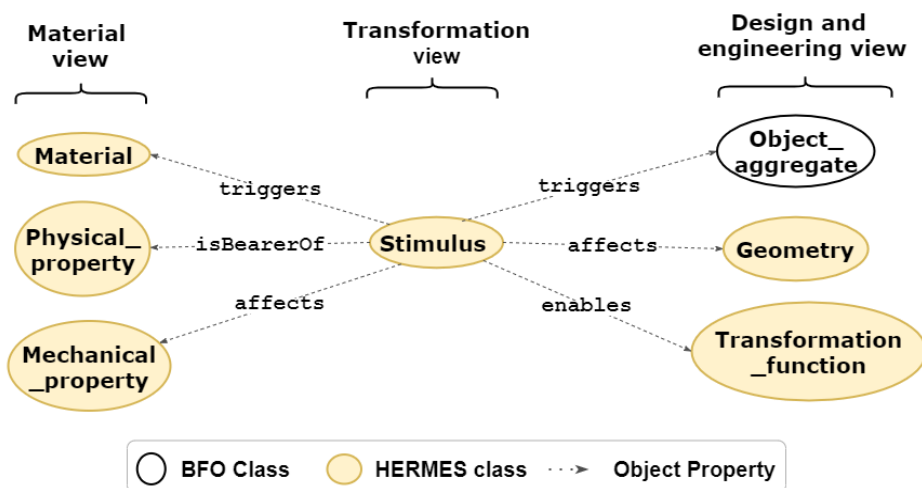


Figure 59. Semantic associations between material, transformation, and design and engineering views

3.4 Restricted Definitions for classes and relations

This section introduces some specifications and restrictions of the classes and properties in HERMES ontology, as explained in the following subsections: object properties and description logic.

3.4.1 Object properties

Object properties define the relations between classes and subclasses semantically. They are classified within various characteristics, to cite a few:

- *Functional*: This characteristic means that the property can have at most one value for any given individual. At most, there can be one outgoing relationship along with the property for that individual. If multiple individuals are specified as values for the property, these values will be inferred to denote the same object.
- *Inverse functional*: This characteristic means the inverse property of the selected property (explicitly declared or not) is functional. At most, there can be one incoming relationship along with the property for that individual. Note that if multiple individuals are specified as incoming values for the property, these values will be inferred to denote the same object.
- *Transitive*: This characteristic means that if the individual (e.g., x) is related to the individual (e.g., y), and the individual (y) is associated with the individual (e.g., z), then the individual (z) will be related to the individual (x).
- *Symmetric*: This characteristic means that the property is inverse, so if the individual (x) is related to the individual (y), then individual (y) must also be related to the individual (x) along with the same property.
- *Asymmetric*: This characteristic means that if the individual (x) is related to the individual (y), then the individual (y) is not related to the individual (x) along with the same property.
- *Reflexive*: This characteristic means a property is reflexive causes every single individual to be related to itself via that property.
- *Irreflexive*: This characteristic means an irreflexive property means that an individual cannot be related to itself via that property.

The object properties of the HERMES ontology are defined within these characteristics in the Table 1 below.

Table 1 Object properties' characteristics

Object Properties	Functional	Inverse Functional	Transitive	Symmetric	Asymmetric	Reflexive	Irreflexive
isA	X		X				
has	X				X		X
isComposedOf	X						
hasSpatialRelation	X		X	X			
isArrangedIn		X					X
applies	X			X			
inheritsIn	X				X		
fulfils			X			X	
hasMaterialDistribution	X		X			X	
isTriggeredBy		X			X		
hasMechanicalProperty	X				X		

Object Properties	Functional	Inverse Functional	Transitive	Symmetric	Asymmetric	Reflexive	Irreflexive
isFulfilledBy		X					
hasTransformationDimension	X				X		
hasTransformationEffect	X				X		
hasTransformationFunction	X				X		
hasTechnicalFunction	X		X				
triggers		X	X				X
isBearerOf	X				X		
affects	X				X		
enables	X				X		X
uses	X				X		
isProcessedBy	X				X		
isManufacturedBy	X				X		

- **isA**: It is an object property useful to model heritage relations between parent and children classes, it is indeed functional because it contributes to the definition of the children class; there is only one parent to each children class and transitive because it passes all the characteristics of the parent class to the children class without any restriction.
- **has**: It is an object property expressing possession either of a class or a data property. It is indeed functional and irreflexive because it contributes to the definitions of the class, and it can be only one outgoing relationship with this property: a one-way property. It is used in some properties in the ontology: `Object has Transformation_function`, and `Voxel has Color`.
isComposedOf: It is a functional object property and denotes the constituents of such a class; it is indeed used in the following properties in the ontology: `Product isComposedOf Hybrid_part`, `Transformation_process isComposedOf Transformation_step`, `Homogeneous_part isComposedOf Voxel`.
- **hasSpatialRelation**: It is an object property denoting the mereotopological relationships between some classes. It is a function because it assures only one outgoing relationship, transitive. If a class *a* is spatially connected to *b* and *b* is spatially connected to *c*, then *a* is spatially connected to *c*, symmetric because it is indeed an inverse property and affects both classes. It is used in the following properties in the ontology: `Homogeneous_part hasSpatialRelation Hybrid_part`, `Hybrid_part hasSpatialRelation Embedded_part`.
- **isArrangedIn**: It is inverse functional because the inversed relationship is functional, i.e., if a voxel is arranged in such grid' coordinates, then those coordinates bear only one voxel at a time, and irreflexive because a voxel cannot be arranged in itself. It is in the following property in the ontology: `Voxel isArrangedIn Voxel_grid`.
- **applies**: It is a functional and symmetric object property; it is in the following property in the ontology: `Machine applies Additive_manufacturing_process`.
- **inheritsIn**: It is a functional and asymmetric object property; it is in the following property in the ontology: `Process_condition inheritsIn Additive_manufacturing_process`.
- **fulfils**: It is a transitive reflexive object property; it is in the following property in the ontology: `Process_condition inheritsIn Additive_manufacturing_process`.
- **hasMaterialDistribution**: It is a functional transitive reflexive object property; it is in the following property in the ontology: `Material hasMaterialDistribution Material_distribution`.
- **isTriggeredBy**: It is an inverse-functional asymmetric object property; it is in the following property in the ontology: `Material isTriggeredBy Physical_property`.
- **hasMechanicalProperty**: It is a functional asymmetric object property; it is in the following property in the ontology: `Material hasMechanicalProperty Mechanical_property`.

- `isFulfilledBy`: It is an inverse-functional object property; it is in the following property in the ontology: `Transformation_function isFulfilledBy Transformation_process`
- `hasTransformationDimension`: It is a functional asymmetric object property; it is in the following property in the ontology: `Transformation_function hasTransformationDimension Transformation_dimension.`
- `hasTransformationEffect`: It is a functional asymmetric object property; it is in the following property in the ontology: `Transformation_function hasTransformationEffect Transformation_effect.`
- `hasTransformationFunction`: It is a functional asymmetric object property; it is in the following property in the ontology: `Object hasTransformationFunction Transformation_function.`
- `hasTechnicalFunction`: It is a functional transitive object property it is in the following property in the ontology: `Material hasTechnicalFunction Technical_function.`
- `triggers`: It is an inverse functional transitive object property it is in the following property in the ontology: `Stimulus triggers Material`
- `isBearerOf`: It is a functional asymmetric object property; it is in the following property in the ontology: `Stimulus isBearerOf Physical_property.`
- `affects`: It is a functional asymmetric object property; it is in the following property in the ontology: `Stimulus affects Geometry.`
- `enables`: It is a functional asymmetric irreflexive object property it is in the following property in the ontology: `Stimulus enables Transformation_function.`
- `uses`: It is a functional asymmetric object property it is in the next property in the ontology: `Stimulation uses Stimulus.`
- `isProcessedBy`: It is a functional asymmetric object property it is in the following property in the ontology: `Object_aggregate isProcessedBy Additive_manufacturing_process.`
- `isManufacturedBy`: It is a functional asymmetric object property it is in the next property in the ontology: `Object_aggregate isManufacturedBy Machine.`

3.4.2 DL rules

In this section, the proposed classes, object properties and data properties above are further specified by providing DL rules. The latter is used as a knowledge representation language to define class restrictions. DL rules are essential for inference reasoning mechanisms, such as consistency checking, subsumption, realization, and retrieving. Consistency checking assures the coherence of the presented ontological model concerning this

language. It provides the possibility to reason over it with the appropriate algorithms. The application of DL rules helps structure and classify knowledge and provides a comprehensive machine language that can be further interpretable. Two types of rules were used here:

- Cardinality: The number of elements in a given rule.
- Min Cardinality: Minimum number of entity instances that must participate in a relationship.

Table 2 presents DL rules for the class Product: it is a subclass of Object_aggregate, it must be composed whether of Homogeneous_part or a Hybrid_part, and it can be composed of an Embedded_part.

Table 2 DL rules for Product class

Class name	Rule type	DL rule
Product	Min cardinality	$\text{Product} \sqsubseteq \text{Object_aggregate}$ $\text{Product} \sqsubseteq (\forall \text{isComposedOf.Hybrid_part} \sqcap$ $\exists \text{isComposedOf.Homogeneous_part} \sqcap$ $\forall \text{isComposedOf.Embedded_part})$

Table 3 describes DL rules for the class Homogeneous_part: it is a subclass of Object_aggregate, it can be composed of voxels or not depending on the granularity level of the definition, and it is linked to Hybrid_part.

Table 3 DL rules for Homogeneous_part class

Class name	Rule type	DL rule
Homogeneous_part	Min cardinality	$\text{Homogeneous_part} \sqsubseteq \text{Object_aggregate}$ $\text{Homogeneous_part} \sqsubseteq (\forall \text{isComposedOf.Voxel} \sqcap$ $\text{hasSpatialRelation.Hybrid_part})$

Table 4 presents DL rules for the class Hybrid_part: it is a subclass of Object_aggregate, it can be composed of voxels or not depending on the granularity level of the definition, and it may be linked to Embedded_part.

Table 4 DL rules for Hybrid_part class

Class name	Rule type	DL rule
Hybrid_part	Min cardinality	$\text{Hybrid_part} \sqsubseteq \text{Object_aggregate}$ $\text{Hybrid_part} \sqsubseteq (\forall \text{ isComposedOf.Voxel} \sqcap \forall \text{ hasSpatialRelation.Embedded_part})$

Table 5 defines DL rules for the class Voxel: it is a subclass of Object; it must be arranged in a Voxel_grid and it has a position and a color imperatively.

Table 5 DL rules for Voxel class

Class name	Rule type	DL rule
Voxel	Cardinality	$\text{Voxel} \sqsubseteq \text{Object}$ $\text{Voxel} \sqsubseteq (\text{isArrangedIn} = 1 \text{ Voxel_grid} \sqcap \text{has} = 1 \text{ Position} \sqcap \text{has} = 1 \text{ Color})$

Table 6 presents DL rules for the class Object: it is a subclass of Material_entity, it has a Geometry and a Material, and its existence in this context imperatively must be linked to a Transformation_function, and its realization has to be linked to a Machine and a process.

Table 6 DL rules for Object class

Class name	Rule type	DL rule
Object	Min cardinality	$\text{Object} \sqsubseteq \text{Material_entity}$ $\text{Object} \sqsubseteq (\exists \text{ has.Geometry} \exists \text{ has.Transformation_function} \sqcap \exists \text{ hasMaterial.Material} \sqcap \text{isManufacturedBy} = 1 \text{ Machine} \sqcap \forall \text{ isProcessedBy.Additive_manufacturing_process})$

Table 7 presents DL rules for the class Transformation_function: it is a subclass of Function, its definition is imperatively linked to a Technical_function and a fulfilment by a Transformation_process, and it must have only one dimension and effect.

Table 7 DL rules for Transformation_function class

Class name	Rule type	DL rule
Transformation_function	Min cardinality	$\text{Transformation_function} \sqsubseteq \text{Function}$ $\text{Transformation_function} \sqsubseteq (\exists$ $\text{isComposedOf.Technical_function} \sqcap$ $\text{hasTransformationDimension} = 1$ $\text{Transformation_dimension} \sqcap$ $\text{hasTransformationEffect} = 1$ $\text{Transformation_effect} \sqcap$ $\exists \text{isFulfilledBy.Transformation_process})$

Table 8 defines DL rules for the class Bending: it is a subclass of Transformation_function and it has only one parameter of each kind.

Table 8 DL rules for Bending class

Class name	Rule type	DL rule
Bending	Cardinality	$\text{Bending} \sqsubseteq \text{Transformation_function}$ $\text{Bending} \sqsubseteq (\text{has} = 1 \text{ Bending_torque} \sqcap \text{has} = 1$ $\text{Bending_radius})$

Table 9 formulates DL rules for the class Twisting: it is a subclass of Transformation_function and it has only one parameter of each kind.

Table 9 DL rules for Twisting class

Class name	Rule type	DL rule
Twisting	Cardinality	$\text{Twisting} \sqsubseteq \text{Transformation_function}$

$\text{Twisting} \sqsubseteq (\text{has} = 1 \text{ Twisting_angle})$

Table 10 shows DL rules for the class `Folding`: it is a subclass of `Transformation_function` and it has only one parameter of each kind.

Table 10 DL rules for `Folding` class

Class name	Rule type	DL rule
<code>Folding</code>	Cardinality	$\text{Folding} \sqsubseteq \text{Transformation_function}$ $\text{Folding} \sqsubseteq (\text{has} = 1 \text{ Folding_torque} \sqcap \text{has} = 1 \text{ Folding_angle})$

Table 11 presents DL rules for the class `Transformation_process`: it has imperatively one or more `Transformation_step`.

Table 11 DL rules for `Transformation_process` class

Class name	Rule type	DL rule
<code>Transformation_process</code>	Cardinality	$\text{Transformation_process} \sqsubseteq (\text{isComposedOf} \geq 1 \text{ Transformation_step})$

Table 12 describes DL rules for the class `Stimulation`: it is a subclass of `Transformation_step`, and it uses precisely one `Stimulus`.

Table 12 DL rules for `Stimulation` class

Class name	Rule type	DL rule
<code>Stimulation</code>	Cardinality	$\text{Stimulation} \sqsubseteq \text{Transformation_step}$ $\text{Stimulation} \sqsubseteq (\text{uses} = 1 \text{ Stimulus})$

Table 13 presents DL rules for the class `Stimulus`: it is a subclass of `Occurent`, and all its connections to other classes are mandatory.

Table 13 DL rules for Stimulus class

Class name	Rule type	DL rule
Stimulus	Min cardinality	$\text{Stimulus} \sqsubseteq \text{Occurent}$ $\text{Stimulus} \sqsubseteq (\exists \text{ triggers.Object_aggeregate} \sqcap \exists \text{ affects.Geometry} \sqcap \text{enables} = \text{Transformation_process} \sqcap \exists \text{ triggers.Material} \exists \text{ isBearerOf.Physical_property} \exists \text{ affects.Mechanical_property})$

Table 14 shows DL rules for the class Material: it is a subclass of Material_entity, it must have mechanical properties, it must be fulfilled by a Technical_function, it has only one Material_distribution, and it must be triggered by one Physical_property.

Table 14 DL rules for Material class

Class name	Rule type	DL rule
Material	Min cardinality	$\text{Material} \sqsubseteq \text{Material_entity}$ $\text{Material} \sqsubseteq (\exists \text{ fulfils.Technical_function} \sqcap \exists \text{ hasMechanicalProperty.Mechanical_property} \sqcap \text{hasMaterialDistribution} = 1 \ 1 \ \text{Material_distribution} \sqcap \text{isTriggeredBy} = 1 \ 1 \ \text{Physical_property})$

Table 15 presents DL rules for the class Machine: it is a subclass of Material_entity, it has some Process_condition, it applies an AM process, and it manufactures an Object.

Table 15 DL rules for Machine class

Class name	Rule type	DL rule
Machine	Min cardinality	$\text{Machine} \sqsubseteq \text{Material_entity}$

$$\text{Machine} \sqsubseteq (\forall \text{has.Process_condition} \sqcap \text{applies} = \text{Additive_manufacturing_process} \sqcap \forall \text{manufactures.Object})$$

Table 16 formulates DL rules for the class `Process_condition`: it is a subclass of `Quality` and is inhered in specific AM processes.

Table 16 DL rules for `Process_condition` class

Class name	Rule type	DL rule
<code>Process_condition</code>	Cardinality	$\text{Process_condition} \sqsubseteq \text{Quality}$
		$\text{Process_condition} \sqsubseteq (\text{inheresIn} = \text{Additive_manufacturing_process})$

Table 17 presents DL rules for the class `Additive_manufacturing_process`: it is a subclass of `Process`, it is applied with exactly one `Machine`, and it manufactures an `Object`.

Table 17 DL rules for `Additive_manufacturing_process` class

Class name	Rule type	DL rule
<code>Additive_manufacturing_process</code>	Cardinality	$\text{Additive_manufacturing_process} \sqsubseteq \text{Process}$
		$\text{Additive_manufacturing_process} \sqsubseteq (\text{isAppliedWith}=1 \text{ Machine} \sqcap \forall \text{creates.Object})$

3.5 Conclusion

This third chapter underlines a pioneering effort dedicated to formalizing and representing 4D printing knowledge relating AM processes and techniques, SMs, stimuli, and transformation issues to design and engineering objects. It has highlighted the usefulness of an ontology to federate the scattered knowledge related to the emerging 4D printing technology. Hence, this contribution addresses an entire understanding and description of the complexity of perdurant objects and represents a pioneering effort towards knowledge formalization and representation for multiple purposes. To do so, an ontological framework has been beforehand established with the underlying philosophical and scientific hypotheses, along with the use of 4D printing knowledge in design. This has led to the construction of the HERMES ontology around several views

(aligned with stakeholders concerns), namely design and engineering, material, AM process, and transformation process. Considered a domain ontology, the HERMES ontology has been built upon the upper ontology BFO, and therefore, provides a significant contribution to the IOF community regarding the 4D printing paradigm. Such a formal ontology enables the concurrent consideration of design, materials, process, and transformation aspects, which may become complex and inaccessible to a novice actor of the community and even to a domain expert. This statement is reinforced with the significant research advances of this emerging field; in such a context, one may assume that the underlying body of knowledge will evolve accordingly. It is imperative to integrate ontology change management procedures to provide an active and living ontology, able to check, update and add new knowledge related to AM techniques, smart materials, or even product models. Nevertheless, one can assume that the proposed development may have some limitations. Case studies are introduced in Chapter 6 to illustrate the relevance of the proposed ontology.

Chapter 4 Formalization of the multi-representation of a 4D printed object

“No models are [true]—not even the Newtonian laws. When you construct a model, you leave out all the details which you, with the knowledge at your disposal, consider inessential.... Models should not be true, but it is important that they are applicable, and whether they are applicable for any given purpose must of course be investigated. This also means that a model is never accepted finally, only on trial.”

Georg Rasch (1960), Probabilistic Models

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4.1 Introduction

From the numerous proofs-of-concept proposed in the literature, which show the broad spectrum of shape/property/functionality change capabilities, emerging academic interests are tackling 4D printing from a design perspective. The previous chapter has set up the fundamental pillars on which 4D printing technology is built. It mainly introduces a specific stimulus to such a part manufactured with AM processes and SMs. This definition of 4D printing impacts how product architects, product designers, and mechanical engineers can design and develop their products. From a design point of view, 4D printing opens up the design space by enabling dynamic products, however, designers are not entirely free to provide any random geometry since this technology has its own limitations and constraints like SMs and stimuli selection and materials' distribution in such a part.

This change in the design space requires designers to move away from the traditional design rules for manufacturing and adopt new design guidelines that can leverage the opportunities of 4D printing. Toward this direction, product architect, product designer, mechanical engineer, and experts must have the necessary knowledge and tools to make informed decisions about the product, SMs usage, materials' distribution, and many other stakeholders. It is needed to anticipate considering SMs and stimuli constraints and limitations in the CDS phase. In other words, design for 4D printing deals with revisiting and adopting the multiple representations of the objects (i.e., covering geometric change, transformation process simulation, etc.) in the CDS phase. In the previous chapter, the object is formalized with the composition of three main parts: `Homogeneous_part`, `Embedded_part`, and `Heterogenous_part`. These parts coupled with the notion of materials' distribution and allocation should formalize and represent an object.

Thus, the scientific contribution in this chapter consists in describing and formalizing the multiple representations of a 4D printed object. To do so, Section 4.2 proposes a design process for 4D printing and the general interaction between multiple involved stakeholders. Section 4.3 describes the multiple representations of a 4D printed object. Then, Section 4.4 formalizes semantically these multiple representations as an ontology fragment to be integrated in HERMES ontology.

4.2 Design for 4D printing process

To describe the 4D printed object representation, proposing a design for 4D printing process seems crucial. The missing product development process for 4D printing is a remarkable gap [8]. Considering the basic design process proposed by Pahl and Beitz [146][147], a design for 4D printing process is presented in Figure 61.

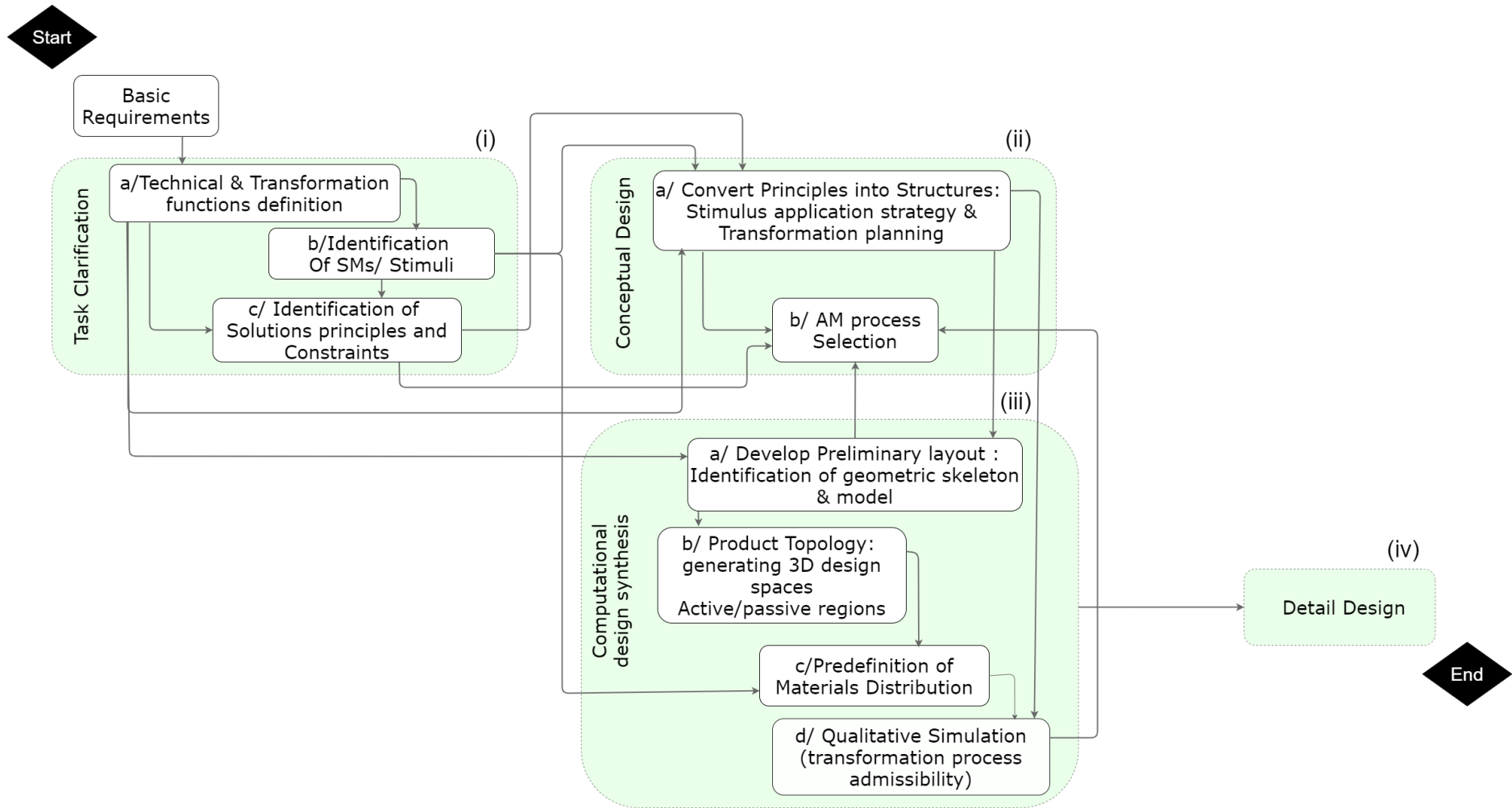


Figure 61. Proposed design for 4D printing process

It has mainly four concurrent phases: (i) task clarification, (ii) conceptual design, (iii) computational design synthesis, and (vi) detail design; as such, every phase is composed of further steps.

- As for (i) task clarification phase, it is about:
 - a/ Technical & transformation function definitions are defined in the ontology presented in Chapter 3.
 - b/ Identification of smart materials and stimuli, i.e., according to the above-fixed functions and user's requirements, the smart and inert materials will be assigned as well as the appropriate stimuli for the smart and inert materials.
 - c/ Identification of solutions principles and constraints: gathering information about the criteria that must be met by the product/part/structure and the constraints that are already in place and their significance.

- As for (ii) conceptual design phase, it englobes:
 - a/ Convert design principles into structures: the basic problem is abstracted by establishing functional solutions like suggesting the transformation planning (process and steps) and the stimulus application strategy: internal/external (i.e., if it is an electric field, for example, it must be integrated into the part/product).
 - b/ AM process selection: this decision is approximatively taken in the conceptual design phase, but it can be updated in many other steps, as shown in Figure 61 by the external connections between phases.

- As for (iii) computational design synthesis (CDS) phase expands the classical steps of the embodiment design phase and involves fast exploration of shape variation or shape optimization. It integrates the allocation of materials and simulation early to assume the dynamic and spatiotemporal aspects of 4D printing technology. This design phase has primarily three axes (i.e., representation - generation - evaluation) and can be captured in four steps as detailed below:
 - a/ Develop preliminary layout: identification of geometrical skeleton respecting the findings and the constraints/solutions of the preceding steps. It is a representation step in which the product designer establishes the basic layout of his product/part/structure.
 - b/ Product topology - 3D design spaces: it is about generating the active/ passive regions. Since the transformation sequence is approximatively structured as the initial product drawing is stated, the topology (i.e., form) can be formed by suggesting the parts and/or regions that will be triggered and the other parts that will remain inert during the transformation.
 - c/ Predefinition of materials distribution: the allocation and assignment of active/passive material in such a part/product - geometrically defined – facilitates the simulation, detail design and multi-material printing tasks. In this step, the distribution can be recommended and suggested to the designer by some computational tools or generated independently.

d/ Qualitative simulation (transformation process admissibility): this step tests if the above material distribution serves to carry out or not the desired performance of such a structure. It is an evaluation step that couples the eligibility of the above material distribution to the transformation process admissibility.

- As for (vi) detail design phase can be further subdivided into: (a) multi scales voxel-based product model where the voxels' distribution, forms, dimensions are laid out, and then manufacturing possibilities are assessed. All the CAD models are produced: the phase of the design process in which the final design is completed. (b) quantitative simulation: since the 4D printed object is dynamic, a rough simulation must be run to assess the design and suggested multi-material distribution; as such, the proposed drawings will be achieved by respecting the initials and final states of the product.

Nevertheless, this design for 4D printing process is concurrent; many steps and solutions can be updated or changed along the process, as presented by the rows between multiple phases and steps in Figure 61. For example, identifying the technical and transformation functions opens up four other steps simultaneously. The CDS leverages profit from identifying materials and stimuli, technical and transformations function, AM process selection, and conversion of principles into solutions. This process presented almost all design building blocks for 4D printing; it can be further extended by completing detailed design and production specifications.

Indeed, many stakeholders ensure that a 4D printing process of such a part/structure is correctly maintained, as presented in the unified modeling language (UML) diagram in Figure 62. Firstly, the product architect plans the transformation and the ultimate changing behavior by clarifying needed tasks and defining several inputs (e.g., stimuli, material, transformation function) customized within the project requirements. Then, the product designer predefines and redefines the geometry and receives a recommendation about material distribution accordingly in conceptual design and CDS phases. Moreover, the material expert approves the selection of materials. The process planner is responsible for AM process selection and AM planning. Finally, the mechanical engineer assumes modeling different tasks in real-time like the transformation process or the manufacturing operations. Accordingly, the consequences of various decisions taken along the design for 4D printing process of such a product/system are evaluated and measured, and the failure risk reduces moderately. In other words, 4D printing is an interdisciplinary technology that compasses multiple experts and influences the upstream design of such a product.

This section introduced a design for 4D printing process - highlighting CDS phase in particular - with the interaction of different job profiles all along this process. Still, the focus – in this PhD – is roughly about the product designer activities in the CDS phase. But introducing other phases, stakeholders, and aspects is still valuable and crucial to appreciate more what this 4D printing technology alleviates in terms of interdisciplinary research. Next section describes the multiple representations of an object in the CDS phase.

4.3 Multi-representation of the 4D printed object

Since 4D printing involves several materials usage inside a single part intended to transform over time, designers must rethink and modify how they envision and create their products. We can propose the hypothesis that the product/part/structure can be defined in four basic representations: graph (i.e., kinematic/topological), skeleton, form (i.e., design space), and region/voxel-based structure [159] (see Figure 63). These representations are developed within a top-down approach (considering the level of abstraction of each representation).

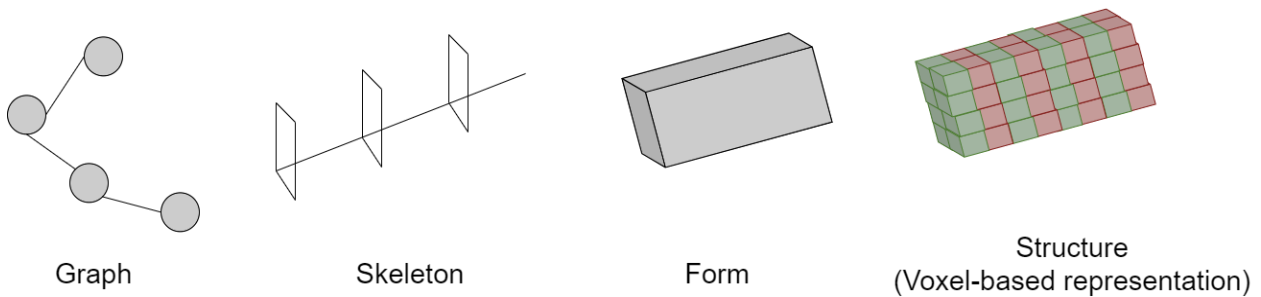


Figure 63. Multi-representation of a 4D printed object

Each representation corresponds to a specific step in the CDS phase; the product moves from one representation to another as the CDS phase progresses:

- Graph- and skeleton-based representations correspond to the development of a preliminary layout.
- Form-based representation corresponds to the generation of the object topology, in which the active and passive regions will be specified.
- Region/voxel-based representation corresponds to the predefinition of materials distribution for further qualitative simulation.

Graph-based representation can be extracted from the function-behavior-structure definitions of such an object for describing the connection between its components (i.e., parts). Skeleton-based representation consists in describing the product/part/structure with few geometrical entities (i.e., plane, line, curve, point, etc.) to build the trusses for the next representation. This representation displays the transformation function specifications and may respect any early dimensioning (e.g., distance, angle). Its key usage is describing the transformation process at early design phase. Those planes outline, therefore, functional surfaces that delimit regions. Hence, one can affirm that the transformation function affects the object from its skeleton-based representation (i.e., the skeleton can be represented in initial and final states).

Form-based representation may be generated with skinning, volume generation or flow creation methods [159]. This gives the part/product/structure its 3D shape, which establishes a first connection between the

aforementioned representations. A form-based representation follows the skeleton-based representation and volume generation methods. Further specifications might be revealed in this representation, such as stimuli usage, high/low heat transfer regions, or opaque/transparent regions, etc. The transition from the skeleton-based representation to the form-based representation highlights different parametric and topological rules (i.e., must not have gaps, boundaries must be covered by, must not overlap with, must be larger than cluster tolerance, must not intersect or touch interior, etc.) for volume generation purpose. Some information is hidden in the graph- and skeleton-based representations and shows up only when the product is at its form-based representation, like, for instance, an integrated stimulus (internal electric field, see Figure 64 below). This Figure overlaps the form-based representation on the skeleton-based representation.

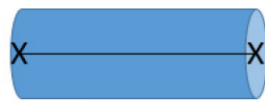


Figure 64. A form-based representation of a beam intended to transform later with an electric charge thanks to the usage of an integrated electric field as a stimulus

Region/voxel-based representation is valuable and crucial for different job profiles. But the interest is only about the product designer profile, this representation allows to test and control the proposed materials distribution eligibility before passing to definitive layout and quantitative simulations. This representation helps define and design complex structures by pattern repetition and orientations, to cite a few. Voxels are arranged and stored in a voxel grid, allowing quick transformation simulation. The voxel grid allows the storage of the voxels coordinates in their initial and final states (i.e., before and after a specific transformation function). Voxels define such a region with single or mixed materials, then dispersed either within a pattern or not to fulfil a transformation function based on smart and inert materials characteristics.

These representations grant capturing object evolutions and further specifications likewise: stimulus, material, transformation function, transformation process, etc. Each representation has its own advantages and parameters to be respected. They promote flexibility in designing for 4D printing with different abstraction levels. Each abstraction level reveals specific information depending on the progress in the CDS. As for twisting, bending, and folding transformation functions, the shape change will be visible in the skeleton-based representation. But, for contraction and expansion transformation functions, the shape change will be noticeable at the form-based representation.

The multiple representations of a 4D printed object in the CDS phase use extensive parametric models and consistent families of geometries. It remains essential to mention within the skeleton-based representation – which may look simple – that it allows significant deal of generalizations like transformation functions

prediction and transformation processes proposition (this is mainly treated with data/knowledge processing research field). They are indeed advantageous because they reduce the design space and make future computations and simulations more efficient.

In a traditional design process, the material - corresponding to the product requirements - is not selected at preliminary design phases. As for 4D printing technology, this step is integrated early in the process. Several loops must be made to adapt the geometry according to the material specifications. Indeed, the materials distribution drives the product geometry and structure. In the next example, let be four parts each performs a given transformation. Figure 65 presents the initial state of the four parts - represented geometrically in a parallelepiped - with skeleton-based and form-based representations. We evoke that a part is split into several sections at the level of skeleton in order to be able to control a change of forms. The skeleton is introduced with four parallel planes and an orthogonal line. This customized skeleton is proposed as input of the second step (i.e., product topology generation) in the CDS phase.



Figure 65. The part in its initial state with two representations: (a) skeleton and (b) form

Figures 66 and 67 present folding and bending transformations respectively in both representations skeleton and form. We can notice with the naked eye that there are active regions in which the transformations are centralized and passive regions that do not move at all, or move without changing the shape, just pulled by the effect of the active regions.

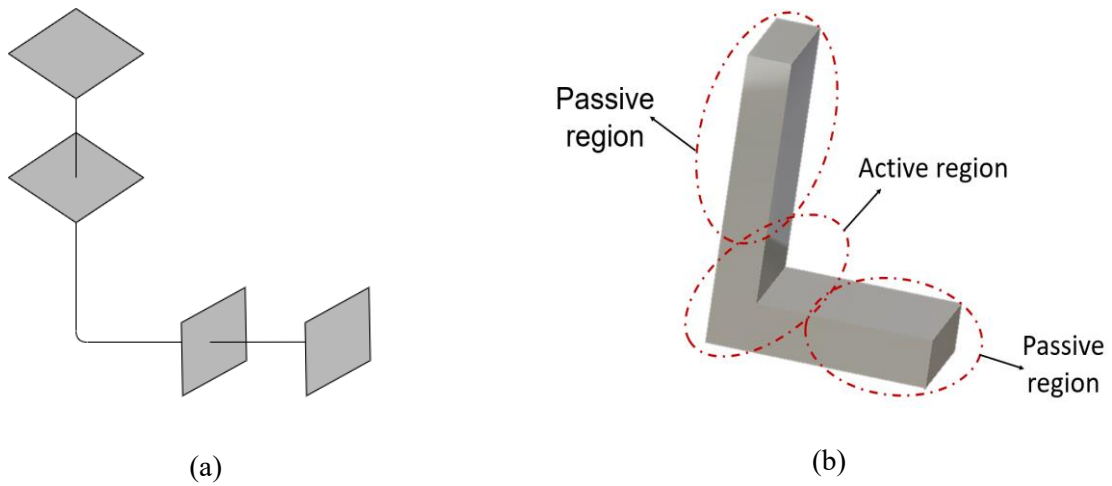


Figure 66. *Folded part, (a) skeleton-based representation, (b) form-based representation with a specification of active/passive regions*

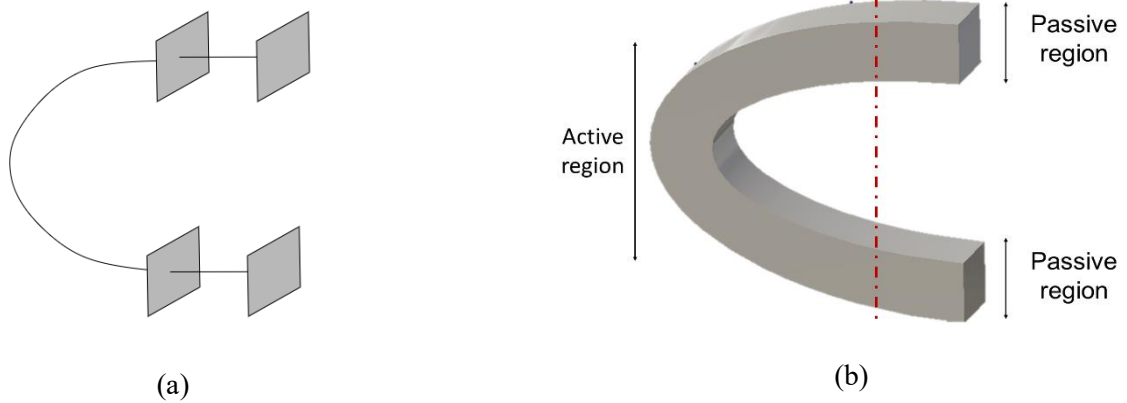


Figure 67. *Bending part, (a) skeleton-based representation, (b) form-based representation with a specification of active/passive regions*

Figures 68 and 69 present twisting and buckling transformations, respectively, with their skeleton-based and form-based representations. The shape change affects indeed both of the representations as schematized in Figures 68 and 69. Like the previous transformations, twisted and buckled beams present a central active region with two passive ones at the extremums. The planes delimit the active and passive regions in the final state of the skeleton-based representation.

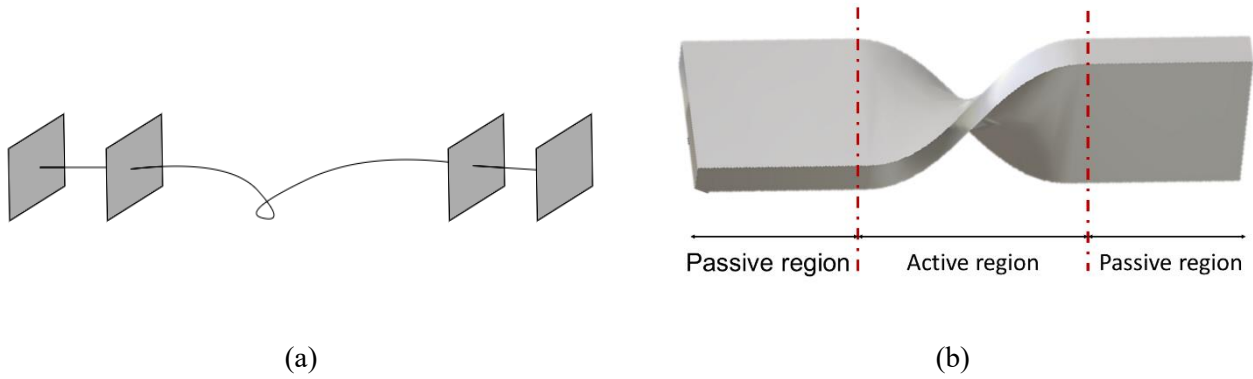


Figure 68. Twisted part, (a) skeleton-based representation, (b) form-based representation with a specification of active/passive regions

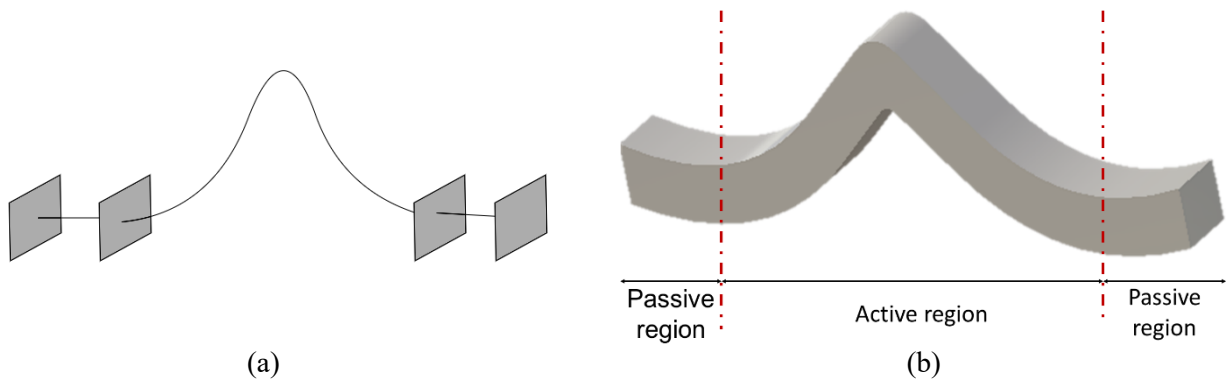


Figure 69. Buckled part, (a) skeleton-based representation, (b) form-based representation with a specification of active/passive regions

To develop different representations and states of the 4D printed product, it is necessary to provide the possibility of several visualizations. Figures 70 and 71 present a drawing sheet (top, face, right and perspective views) for skeleton in an initial state and a skeleton in a final state performing a bending transformation respectively. Both drawings (i.e., drawing of initial state and drawing of final state) of all the representations are needed in the future to capture material distribution aspect in regard of multi-material printing for the building of the part (as initial state) in order to enable machine / process selection, and a visualization of this part after its triggering (as final state), to illustrate the shape or property change of the part during time.

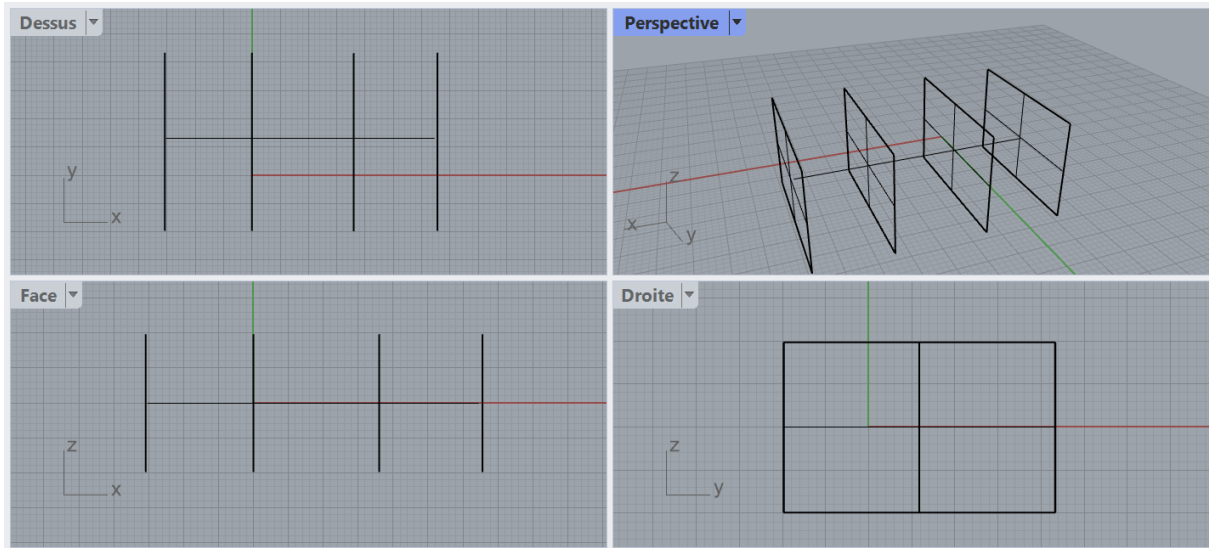


Figure 70. A skeleton-based representation of a part - intended to effectuate a bending function - in its initial state

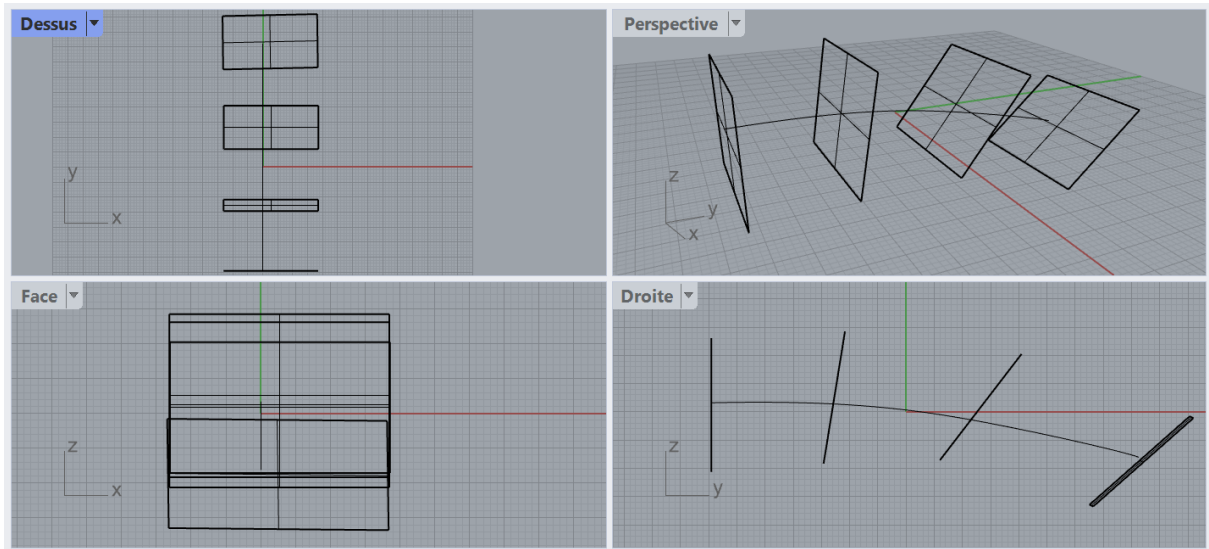


Figure 71. A skeleton-based representation of a part- intended to effectuate a bending function – in its final state

In conclusion, each active region includes and encompasses a specific materials' distribution that has permitted a particular function of transformation. As proposed in the design process, integrating the materials specifications should be at the early stages of CDS. Using this integrated design paradigm, the CAD models of a 4D printed part/product will be driven by the distribution of the smart and inert material or the distribution of active and passive regions at a more abstracted level. The combination of many insights (materials' distribution, transformation functions, stimulus selection, AM process/technique selection, etc.) while designing a 4D printed product from the graph, skeleton, form, and structure representations falls indeed under design for 4D printing. The concept of integrated multi-representations with materials distribution aid the product designer in thinking concurrently and "out of the box". CAD models (representations) and SMs are

thus considered two critical variables of the product designer here. The SMs material should often satisfy the desired transformability and reactivity to such stimulus. In order to finalize the CDS design phase, two major outputs can be pointed out. The first output is the topology of the future product, and the second, its final state (transformed state), which is itself based on the defined topology. These outputs will also be the input of the detail design phase. Now the design problem in CDS phase can be formulated as: determining the product skeleton and form in the initial and final states and satisfying a specific transformation function under multiple other constraints (i.e., the different top classes listed in the HERMES ontology).

4.4 Formalization of the multi-representation within the HERMES ontology

The above-mentioned representations in the previous section are federated here in the subclasses of the Representation class as shown in Figure 72. Representation is a subclass of the Spatiotemporal_region class of BFO because a representation occurs in a laps of time and encompasses the three geometric dimensions. Sequencing the presentations one after the other in the CDS phase affirms that a representation is both a temporal and spatial regions. This part of ontology will be integrated further in HERMES ontology.

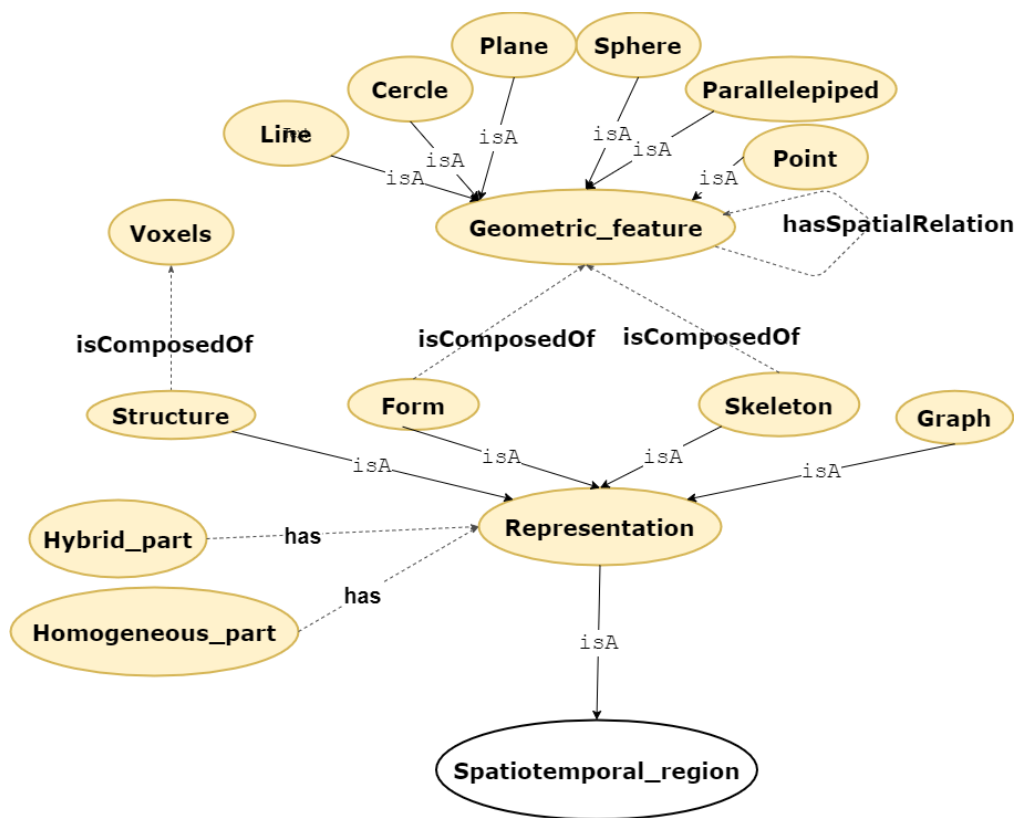


Figure 72. Part of the ontology formalizing the multi-representations of a 4D printed object

The previous section states that the **Skeleton** and **Form** classes are **ComposedOf Geometric_features** (i.e., **Plane**, **Line**, **Point**, etc.), which composes in their turn the **Geometry** class defined in the HERMES ontology. As for the **Structure** class **isComposedOf Voxel(s)**. Each representation has, indeed, initial, and final states, which endeavors the fact that each geometric feature that defines this representation also has initial and final states. Finally, the **Homogeneous** and **Hybrid_part(s)** are linked to the **Representation** class trivially by the object property **has** in order to have a solid link and integration with the HERMES ontology.

Section 4.3 describes a multi representations of the 4D printed object, this section is about defining constraints on this multi representations so as to guide the designer in order to avoid errors. This add-on within HERMES ontology is presented in the next Figure 73.

Next paragraphs present the integration and its verification in the HERMES ontology and some logical axioms formalizing the multiple representations of a 4D printed object. To do so, a pseudo-code in Karlsruhe language [196] is proposed to verify the constraints of integration of this add-on in the ontology. It starts by describing all the classes and axioms; and then, defining the constraints related to the classes to be integrated (e.g., **Representation**); finally verify them.

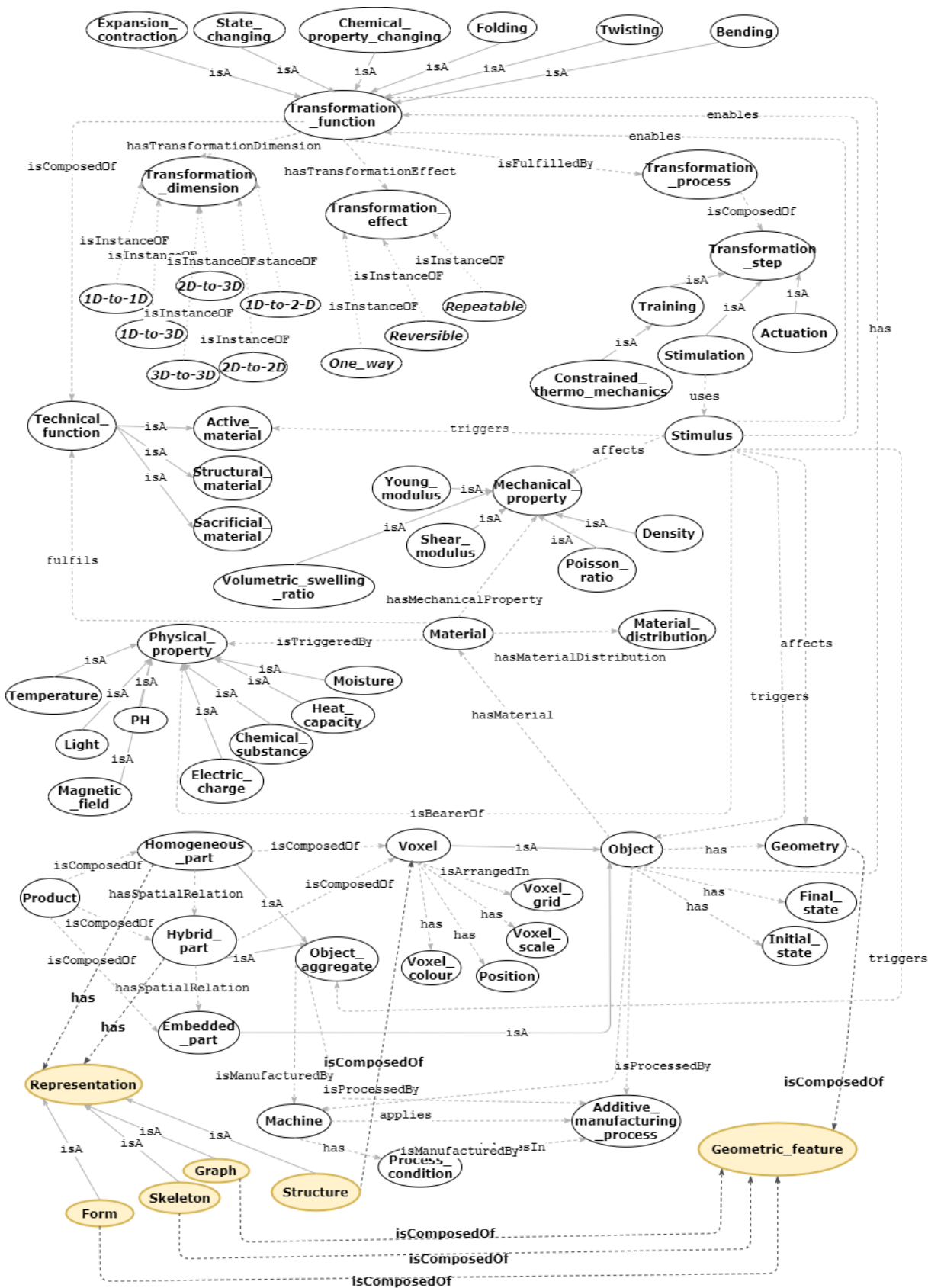


Figure 73 Integration of the part of ontology describing multi representations of 4D printed object in HERMES ontology

4.4.1 Verification of the integration

In this sub-section, a pseudo-code in Karlsruhe language is developed for constraints verification purpose of the integration of the part of ontology presented in Figure 72 in HERMES ontology. It starts by describing all the classes and axioms in HERMES as detailed below. Set of top classes defines all the top classes in HERMES and Concept Subsumption defines all the subclasses in HERMES and states some of the object properties existing in HERMES ontology. Object properties set is intended to list all the object properties figuring as well in HERMES.

Ontology Definition:

Set of top concepts $s_c = \{ \text{TopConcept, Transformation_function, Transformation_process, Transformation_step, Transformation_effect, Transformation_dimension, Material, Machine, AM_process, Process_condition, AM_operation, Stimulus, Physical_property, Material_distribution, Technical_function, Mechanical_property, Product, Voxel, Voxel_grid, Homogeneous_part, Hybrid_part, Embedded_part, Geometry} \}$

Concept Subsumption $\leq_c = \{ (\text{Top_concept, Transformation_function}), (\text{Top_concept, Transformation_process}), (\text{Top_concept, Transformation_step}), (\text{Top_concept, Transformation_effect}), (\text{Top_concept, Transformation_dimension}), (\text{Transformation_function, Bending}), (\text{Transformation_function, Folding}), (\text{Transformation_function, Twisting}), (\text{Transformation_function, Expansion/Contraction}), (\text{Transformation_function, Chemical_property_change}), (\text{Transformation_function, State_change}), (\text{Bending, Buckling}), (\text{Transformation_step, Training}), (\text{Transformation_step, Stimulation}), (\text{Transformation_step, Actuation}), (\text{Training, Constrained_thermo_mechanical}), (\text{TopConcept, Stimulus}), (\text{TopConcept, Material}), (\text{TopConcept, Machine}), (\text{TopConcept, Material_distribution}), (\text{TopConcept, Technical_function}), (\text{TopConcept, Mechanical_property}), (\text{TopConcept, Physical_property}), (\text{TopConcept, Geometry}), (\text{TopConcept, AM_process}), (\text{TopConcept, Process_condition}), (\text{TopConcept, Voxel}), (\text{TopConcept, Voxel_grid}), (\cap_c (\text{Transformation_function, } \rho_R(\text{isFulfilledBy, Transformation_process}))), (\cap_c (\text{Transformation_function, } \rho_R(\text{hasTransformationEffect, Transformation_effect}))), (\cap_c (\text{Transformation_function, } \rho_R(\text{hasTransformationDimension, Transformation_dimension}))), (\cap_c (\text{Transformation_function, } \rho_R(\text{isComposedOf, Technical_function}))), (\cap_c (\text{Transformation_process } \rho_R(\text{isPartOf, Transformation_step}))), (\cap_c (\text{Stimulation } \rho_R(\text{uses, Stimulus}))), \}$

Object Properties Set $s_A = \{ \text{TopDataProperty, isPartOf, uses, isFulfilledBy, isComposedOf, hasTransformationDimension, hasTransformationEffect, etc.} \}$

The following Data Type Set defines the data types and their associated classes.

Data Type Set $s_T = \{ \text{Bending_Torque, Bending_radius, Twisting_angle, Folding_angle, Folding_torque, } (\rho_T(\text{Bending_torque, xsd: decimal}), \text{Bending}), (\rho_T(\text{Bending_radius, xsd: decimal}), \text{Bending}), (\rho_T(\text{Twisting_angle, xsd: decimal}), \text{Twisting}), (\rho_T(\text{Folding_angle, xsd: decimal}), \text{Folding}), (\rho_T(\text{Folding_torque, xsd: decimal}), \text{Folding}) \}$

The following set of instances lists the defined instances in HERMES ontology, and the set of instantiation defines each class associated to each instance.

Set of Instances $S_I = \{ \langle \langle 1D_to_1D \rangle \rangle, \langle \langle 1D_to_2D \rangle \rangle, \langle \langle 1D_to_3D \rangle \rangle, \langle \langle 2D_to_2D \rangle \rangle, \langle \langle 2D_to_3D \rangle \rangle, \langle \langle 3D_to_3D \rangle \rangle, \langle \langle One_way \rangle \rangle, \langle \langle Reversible \rangle \rangle, \langle \langle Repeatable \rangle \rangle \}$

Set of Concept Instantiation $i_c = \{ (Transformation_dimension, 1D_to_1D), (Transformation_dimension, 1D_to_2D), (Transformation_dimension, 1D_to_3D), (Transformation_dimension, 2D_to_2D), (Transformation_dimension, 2D_to_3D), (Transformation_dimension, 3D_to_3D), (Transformation_effect, One_way), (Transformation_effect, Reversible), (Transformation_effect, Repeatable) \}$

These listed functions below allow to add new concept (i.e., class), intersection of concepts, union of concepts, new instances, new object properties, their restrictions, new data properties, and as well their restrictions with F1, F2, F3, F4, F5, F6, F7, and F8 respectively. These functions take in input parameters the elements to add or to verify they already exist (case of F5 in the application below). The algorithms of these functions are detailed in this reference [225].

Functions to apply for verification purpose:

F1 : add Concept	F2 : add ConceptIntersection
F3 : add ConceptUnion	F4: InstanceEnumeration
F5: add ObjectProperty	F6: add ObjectPropertyRestrictions
F7: add DataProperty	F8: add DataPropertyRestrictions

In order to add the classes Representation, Skeleton, Graph, Form, Structure, and Geometric_features in HERMES ontology respecting object properties isComposedOf, has, isA, we use the functions F1 and F5 for adding concept and linking them to object properties defined in Set of Subsumptions.

Application

F1 (Representation, Skeleton, Graph, Form, Structure, Geometric_features)
 F5 (isComposedOf, has, isA)

The idea is to check the logical description rules and the characteristics of the object properties defined in the previous chapter. The results must affirm that the object properties for example are respected in terms of their restrictions

- has used in the relationships: “ Hybrid_part has Representation ; Homogeneous_part has Representation “ is indeed functional asymmetric and irreflexive.
- isComposedOf used in the relationships: “ Skeleton isComposedOf Geometric_features ;

Form isComposedOf Geometric_features ;
 Structure isComposedOf Voxel “ is indeed functional.
 - isA used in the relationships: “ Graph isA Representation ;
 Skeleton isA Representation ;
 Form isA Representation ;
 Structure isA Representation “ is indeed functional and transitive.

4.4.2 Logic Axioms

Let’s take the bending transformation function as an example. One can state that logical axioms can be defined to formalize and restrict these concepts:

- There are at least two Plane(s) in the Skeleton representation in its initial state.
- There are at least two Plane(s) and an angle different from 0° in the Skeleton representation in its final state.

It serves to verify normalities and abnormalities at the Skeleton level. In general, reverse engineering can help to recreate the skeleton-based representation from other experiences presented in a form-based or structure-based representations by reducing the volume, so that a population is further possible for these representations in the future.

4.5 Illustrative case

Figure 74 presents a bending skeleton with four planes and a line connecting them; thus, three regions are defined. Changes between initial positions and final positions are highlighted in with the angles in red. It will be formally described within the ontology mentioned above. We try to show the formalization of the transition from the initial state to the final state for the skeleton-based representation.

Assuming the fact that:

Product isA Object
 Product hasTransformationFunction Transformation_function
 Product has Representation
 {Graph, Skeleton, Form, Structure} isA Representation

If the Transformation_function is defined in a Bending as Figure 74, then:

Skeleton has Initial_skeleton
 Skeleton has Final_skeleton
Initial_skeleton isComposedOf 4 *Initial_plane* (s) & *Line*
Final_skeleton isComposedOf 4 *Final_plane* (s) & *Curve*

Line hasFinalState *Curve*
Initial_plane hasFinalState *Final_plane*
Final_plane_4 has 60° angle with *Initial_plane_4*
Final_plane_1 has 0° angle with *Initial_plane_1*
Curve has Equation $x^2 + 2 * x + 6$

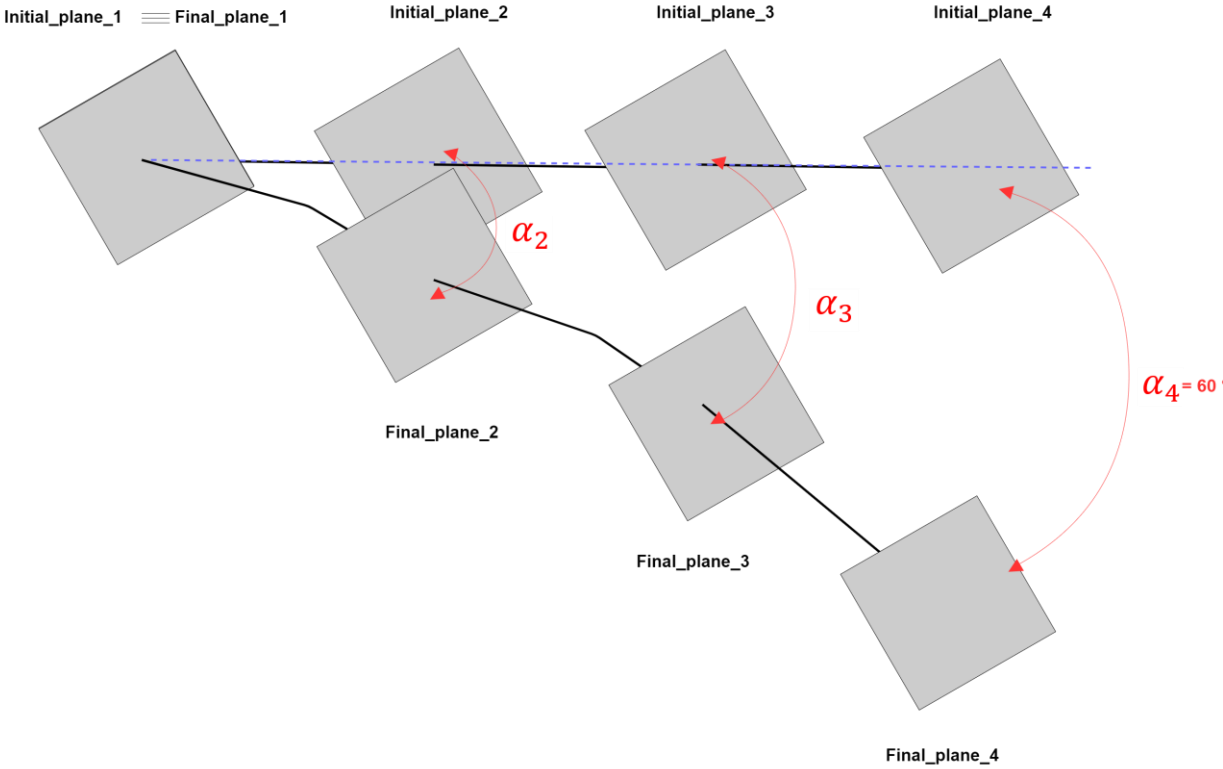


Figure 74. Bending skeleton

Figure 75 presents an expanded cylinder in its form-based representations, assuming that twisting, bending, and folding transformation functions affect the parts' representations in the skeleton-based representation and that expansion and contraction transformations function affect the parts in their form-based representation. That is to say the shape change is visible at the level of the skeleton-based representation for the transformations twisting, bending, and folding; and it is visible at the level of form-based representation for the transformations expansion and contraction.

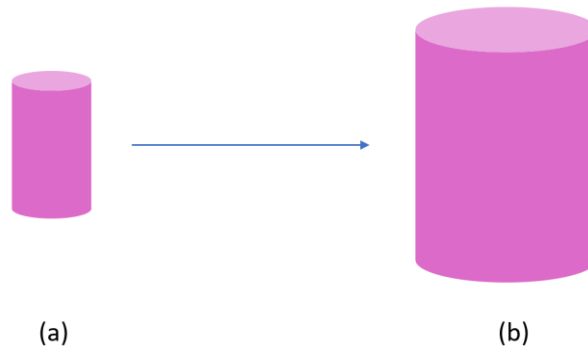


Figure 75. Expanded cylinder

If the Transformation_function is defined in an Expansion as Figure 75, then:

Form has *Initial_form* & *Final_form*

Initial_form has *initial_volume* 16 mm^3

Final_form has *Finall_volume* 64 mm^3

These two illustrations of bending and expansion with respectively skeleton-based representation and form-based representation capitalize the knowledge behind the transformation process for both transformation functions and for both representations. This federation of knowledge is of extreme importance for creating a solid knowledge background replying to the first and the second engineering issue (i.e., formalization with a database and/or a knowledge base and design) and the first scientific issue (i.e., transformation and deformation) stated in the first Chapter.

4.6 Conclusion

This chapter introduced a multi-representation for the 4D printed object. These multiple representations were formalized and described in a sub-ontology with some restriction rules. The built classes are then integrated in the HERMES ontology by verifying the characteristics of the object properties linking new classes to “old” ones. Graph, skeleton, form, and structure are the basis for CAD representations of 4D printed objects. It is possible in CDS to switch from one view to another to better understand the definition of the object to be printed. This knowledge also makes it possible to assist the product designer in defining the product since it considers the transformation process and the materials distribution. Indeed, he can determine the transformation function abstractly, to inform the type of behavior or transformation that they must fulfil, such as bending such an angle in a specific direction, which must be carried out with a precise stimulus. Using the information given, the ontology can provide according to some reasoning rules the materials distributions allowing such a function to be carried out which will be the object of the next chapter.

Chapter 5 Knowledge recommendation supported by case-based and semantic reasoning

“All our knowledge begins with the senses, proceeds then to the understanding, and ends with reason. There is nothing higher than reason.”

Emmanuel Kant, 1790

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5.1 Introduction

The development of an ontology has enabled the capture of multiple perspective knowledge related to SMs, stimuli, AM, and product design. Beyond constructing an interdisciplinary knowledge base, the ontology has to be valuable and useful for the product designer in CDS and has to be integrated into a CAD system. The objective of this chapter is to develop recommendation method in CDS in order to provide suitable knowledge. To do so, case-based reasoning and rules-based semantic reasoning layers are introduced. A specific emphasis is presented on materials distribution prediction within a part design space (including a predefined form). It mainly highlights the passage from the form-based representation to the region/voxel-based structure representation. Section 5.2 introduces how the HERMES ontology is integrated in the CDS. Section 5.3 states the recommendation method using VSM of materials distribution. And section 5.4 introduces some semantic rules-based reasoning.

5.2 Integration of HERMES ontology in the CDS

Considering the framework proposed as the first contribution for ontology building and its future usages, the contribution in this chapter is located in the red rectangle drawn in Figure 76, exactly in the reasoning engine box and the methods that constitute it. As this framework is aligned with many theories (i.e., multi-dimensionalism, BFO, and mereotopology) and *ad hoc* experiments to implement a domain ontology, rules and queries are developed to be integrated into such a reasoning engine (inference engine) and then implemented and visualized to different users (i.e., product architect, material expert, product design, and process planner). As such, this contribution seeks to aid the product designer to determine the materials' distribution by using the knowledge in HERMES ontology aligned with different reasoning methods.

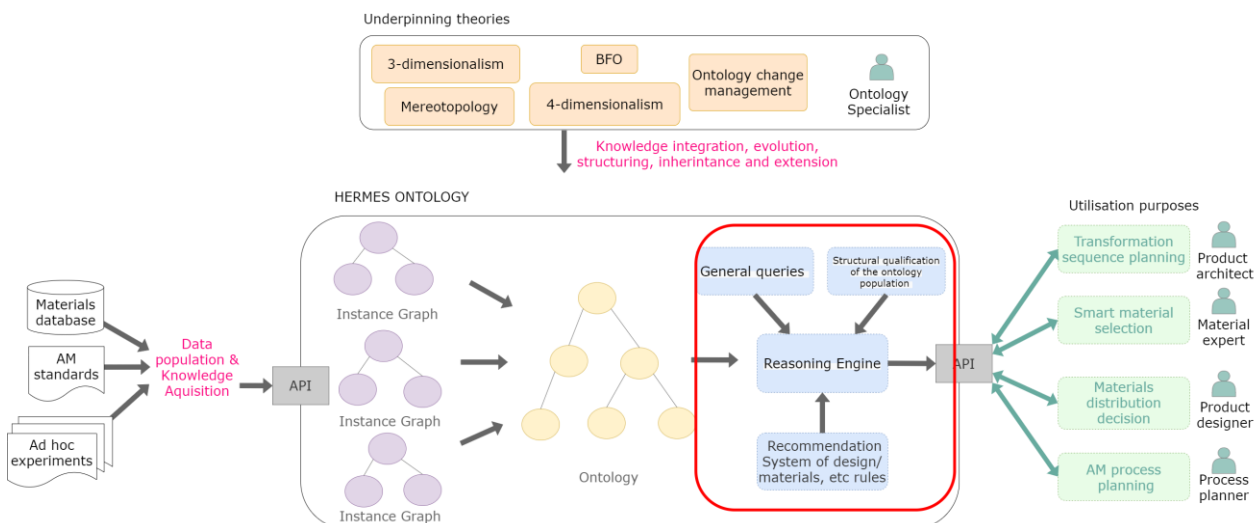


Figure 76. HERMES framework focusing on reasoning layers

Figure 77 presents how the ontology is integrated into CDS for aiding the product designer. This integration uses the two following reasoning procedures that will be detailed in the following sections:

- Case-based reasoning using vector space model (VSM) method because it is useful for retrieval purposes and it is a suitable method to reason over knowledge given by the ontology.
- Semantic reasoning (i.e., semantic, and logical rules to be respected while designing 4D printed structure/part) because it can infer consequences from a set of rules and ontologies and can combine knowledge to draw some conclusions.

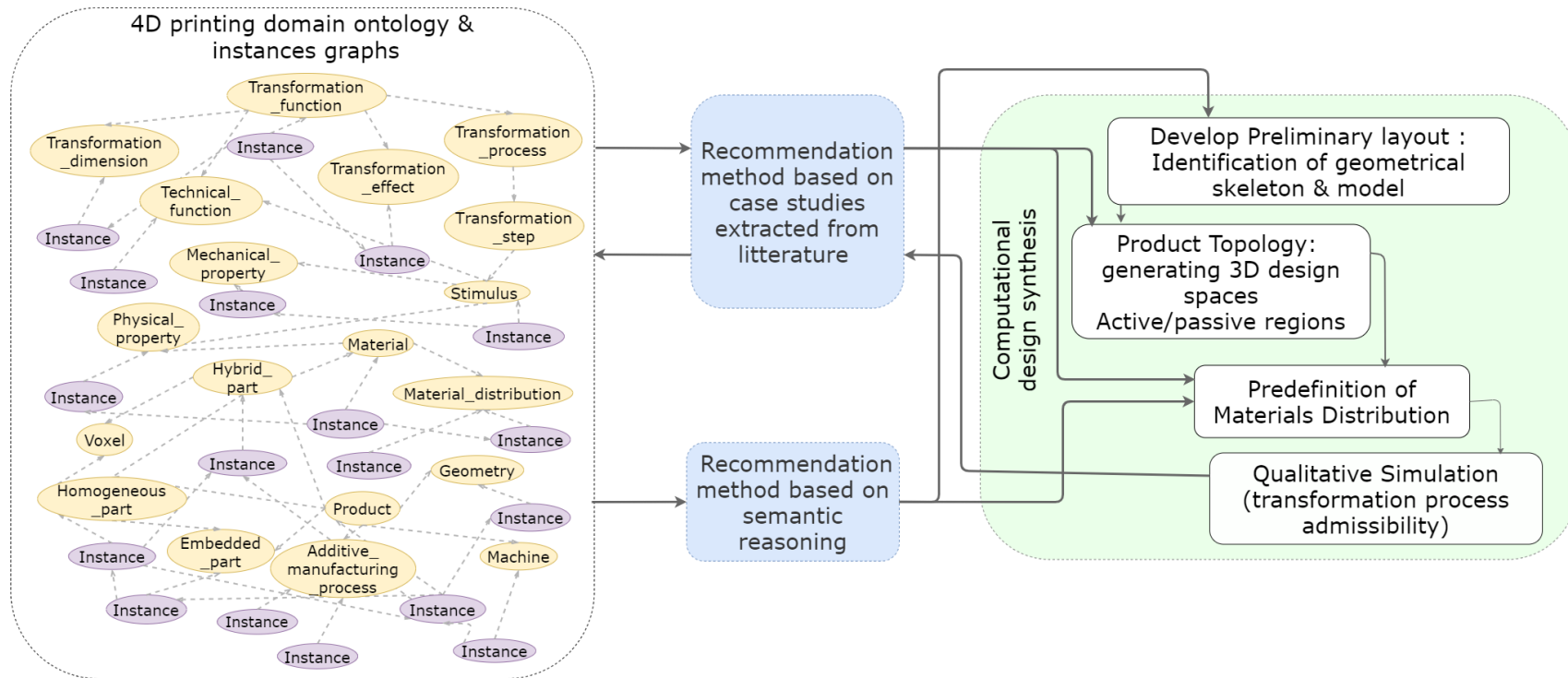


Figure 77. Usability of HERMES ontology in CDS

5.3 Recommendation method of materials' distribution based on case-based reasoning using VSM method

The proposed knowledge recommendation method is built upon the HERMES ontology. It falls under the research domain case-based reasoning since it is based on other case studies (i.e., *ad hoc* experiments extracted from the literature to be considered as the instances for the ontology). This contribution aims to recommend the materials' distribution in the part/object to assure the passage to region-based structure representation. We have mentioned the term region here, it is a set of voxels as an instance of the top-class Voxel. A voxel is a volumetric pixel – as defined in Chapter 3 – with a reduced volume than the region making the simulation of the Transformation_function more accurate: this constitutes a quantitative level of recommendation (i.e., each voxel of each material in specific coordinates). But in this context, we would rather use a set of voxels/region to coordinate with the qualitative context of this work. The product designer cannot roughly decide at the present active/passive regions distribution in such a part, hence it is crucial to support him at this aspect. To do so, VSM is an algebraic method for representing text documents (and any objects in general) as vectors of identifiers. It represents knowledge as vectors in a multidimensional space and serves to apply case-based reasoning approaches for pattern retrieval purpose in this context. The VSM method may be broken down into four steps (see Figure 78) as follows: (i) generate a vector space in accordance with the HERMES ontology classes; (ii) populate the ontology with experiments from the literature, which creates a semantic base (also denoted semantic matrix in Figure 78) by considering each experiment as a vector of knowledge, (iii) create a target vector (i.e., the experience that looks for a material recommendation), and (vi) compute and compare the latter experiment to the others with a qualitative prediction and recommendation of the nearest material distribution. So it is about suggesting and retrieving the nearest and the most similar experiment to the target one. Coupling this method with the usage of the ontology falls under symbolic reasoning¹⁵.

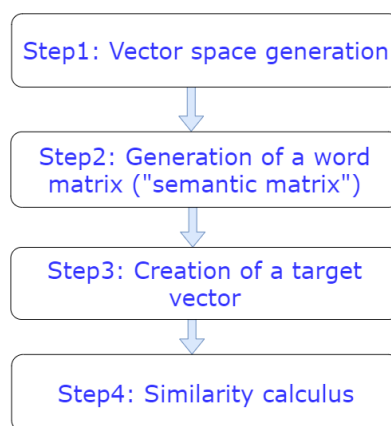


Figure 78. Main steps of the VSM method applied to *ad hoc* experiments extracted from the literature

¹⁵ Symbolic reasoning refers to mathematical logic or more precisely a first-order logic and sometimes higher orders. The reasoning is considered to be deductive when a conclusion is established by means of premises like logical inference rules.

5.3.1 Step 1: Vector space generation

HERMES ontology federates 4D printing knowledge in this relational top classes listed below in Table 18:

Table 18 HERMES top-classes

Transformation_function	Process_condition
Transformation_dimension	Additive_manufacturing_process
Transformation_effect	AM_operation
Transformation_process	Material
Transformation_step	Stimulus
Technical_function	Mechanical_property
Homogeneous_part	Material_distribution
Hybrid_part	Physical_property
Embedded_part	Geometry
Machine	Product
Form	Graph
Skeleton	Structure

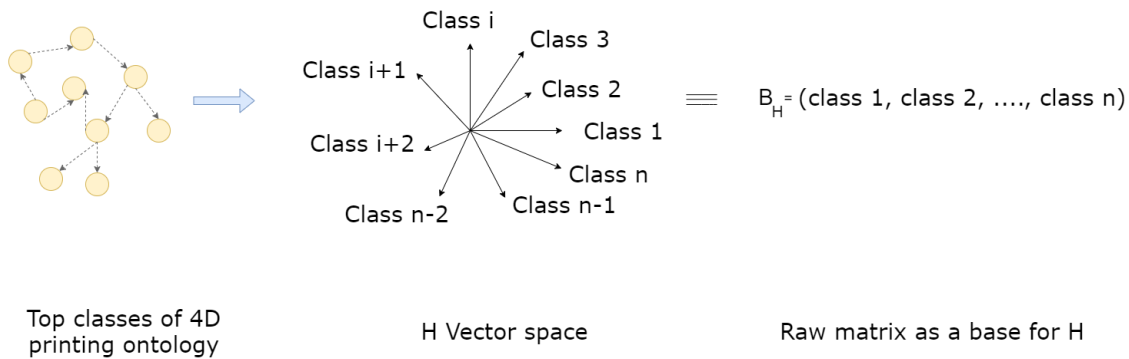
Some classes are created to clarify and precise the knowledge with respect to the theories in the framework presented in Chapter 3. But in practical usage, they may be overlapped with other classes to decrease abstraction level; nevertheless, this overlap would not reduce their descriptive and illustrative roles of the knowledge. Considering the object property: `Stimulus bear(s) the Physical_propety` class, the existence of one of them defines the existence of the other; since a `Stimulus` is viewed as a temporal region that uses and bears – in a specific laps of time – an existing `Physical_propety` such as `Heat`. This stands as the logical and theoretical definition of stimulation in 4D printing. Still in practical use, we consider `Stimulus` as a top-class instantiated with *Temperature*, *Electric field*, etc. We may not use the term `Stimulus` and put `Physical_property` instead. Still, the first proposition seems to be more appropriate for commercial and industrial future usages. Moreover, considering this object property, `Transformation_process isComposedOf Transformation_step` may lead to the hypothesis that a process is defined by a set of steps. Also, the `Form` representation of the `Object` can be abstracted in its `Geometry` since this representation is defined is a volume/skinning step for the product after his skeleton-based representation. As for the `Structure` representation and `Skeleton` representation classes will not be considered in the creation of the vector space because they are missing in the definition of the majority of the experiments, hence the disposed knowledge do not cover all the top classes. In other terms, those *ad hoc* experiments are done without passing through a design process and disposing CAD models. Each experiment or proof-of-concept will be seen as a vector of knowledge having missing elements about the object’s multiple representations at the moment: these classes do not exist in the literature for recent experiments. But in future usage, as the base continues to be populated and gets more enriched, the product designer should be recommended from the skeleton-based representation. Thus, if we omit two classes created

because of contextual clarification and four for the weaknesses of the data found from the listed classes above, there are eighteen (18) top-level classes in the HERMES ontology to be considered as listed in Table 19:

Table 19 HERMES top-classes used to define H vector space

Transformation_function	Process_condition
Transformation_dimension	Additive_manufacturing_process
Transformation_effect	AM_operation
Transformation_step	Material
Technical_function	Stimulus
Homogeneous_part	Mechanical_property
Hybrid_part	Material_distribution
Embedded_part	Geometry
Machine	Product

Figure 79 demonstrates how these top-level classes of HERMES ontology are transformed in a vector space. Let's H be the multi-dimensional vector space with 18 vectors, each one with a top-level class name. H is mathematically defined with the raw matrix $B_H = (\text{Stimulus, Material, Mechanical_property, Technical_function, Transformation_function, Transformation_dimension, Transformation_effect, Transformation_step, Machine, Additive_manufacturing_process, Process_condition, AM_operation, Homogeneous_part, Hybrid_part, Embedded_part, Geometry, Material_distribution, Product})$.



(n : total number of upper classes in the 4D printing domain ontology
i : incremental number)

Figure 79. Vector space generation for the HERMES top classes

5.3.2 Step 2: Generation of the semantic matrix

Once the vector space is set up, the next step consists in instantiating the HERMES ontology and presenting each instance graph as a knowledge vector in H vector space. The first blue arrow in Figure 80 below, going

from scientific publications to instance graphs, constitute an extraction step for *ad hoc* experiences: this stands as populating the ontology by case studies existing in the literature.

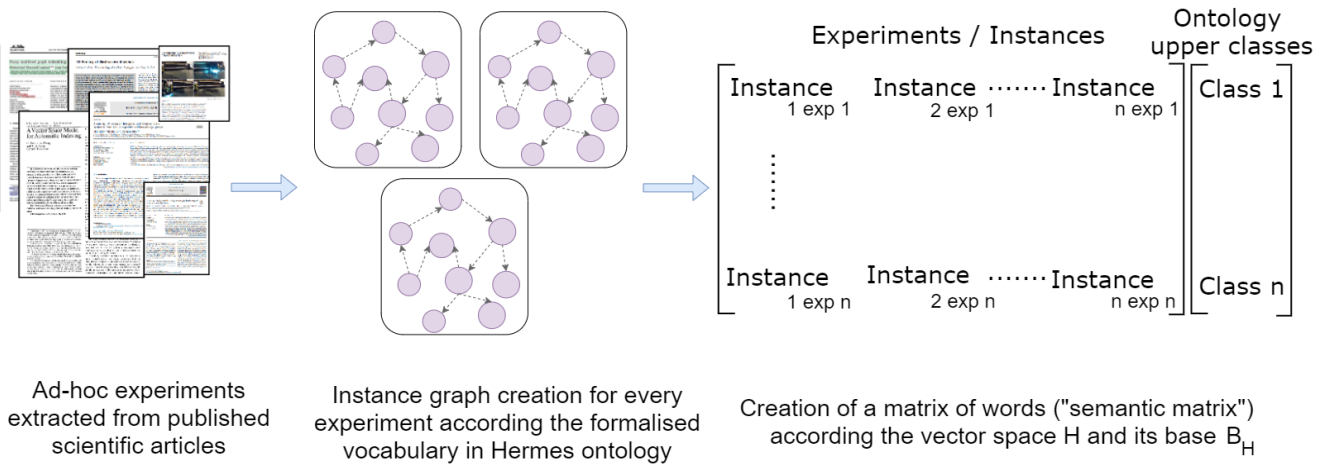


Figure 80. Generation of the semantic matrix

The population is then made manually. The experience may be described in the literature with a vocabulary different from the semantic of HERMES ontology. It is up to the ontology specialist to set it according to the vocabulary specified in HERMES. For instance, it may be found that the Product performs a topological transformation; it could be defined according to the illustrations of that experience in the literature as a Rolling, Multi_bending, or Curling, to cite a few. If some information is missing, for example, a Technical_function of such a Transformation_function, we may complete the instance graph by querying this information from the ontology.

Once the instance graphs are built and ready, each instance graph – representing a specific experiment – is presented as a vector containing ordered elements (i.e., instances); the size of the vector is dynamic: not roughly 18. The section 5.3.5 illustrates four instance graphs - for the usage mentioned above - extracted from different literature research works and formalized according to the ontology concepts presented in Chapter 3. All in all, 30 experiences were extracted in the proposed research work. These instance graphs are transformed in a semantic matrix by considering each experiment as a vector of knowledge. An 18-dimensional vector can be expressed as follows $E_i = (instance_{1exp_i}, \dots, instance_{18exp_i})$ with $instance_{jexp_i}$ is the j^{th} instance of the i^{th} experience. These *ad hoc* experiments extracted from the literature respecting HERMES ontology are the semantic base for the VSM method. Once each experiment is extracted, it will stand as a new vector in the semantic base (i.e., define previous case studies as new vectors to be inserted). This second step is formally defined as the indexing step, which is the initial stage, during which content-bearing words are extracted from the document text.

5.3.3 Step 3: Creation of the target vector

A new vector (new experiment or target experiment) has to be determined in order to be compared to the created semantic base (semantic matrix), as shown in Figure 81. This experiment is defined according to the design for 4D printing process (i.e., given a product requirements, different instances like material, machine, desired transformation function, dimension, etc.). Some classes will be populated (17 as maximum because the materials' distribution is not defined yet at that phase), therefore leading to a new knowledge vector.

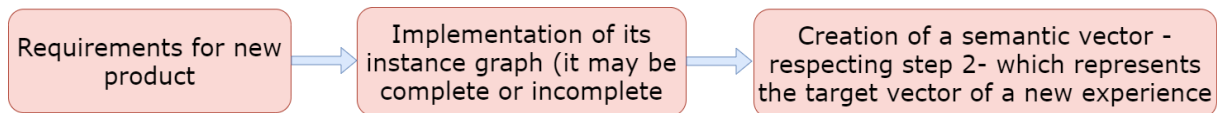


Figure 81. Creation of a target vector

5.3.4 Step 4: Similarity calculus

It is needed at this stage to retrieve and recommend the nearest materials' distribution for the new experience considered as a target vector. This last step scores each vector following a similarity metric (see Figure 82). The above falls under the case-based reasoning domain, which is helpful to recommend active/passive regions (distribution of smart and inert materials in the object) at its form representation to create the structure representation. It is a qualitative prediction of such materials distribution to the designer follows a comparison logic to other similar experiments, which falls under qualitative reasoning before quantitative reasoning (i.e., computation of deformation, degrees of freedom, stiffness, etc.). The materials distribution is the main output to be searched, and all the other classes are considered as inputs. The fourth step of the VSM method starts with a base change (see Step 4-1 in Figure 82). This means the semantic matrix and the target vector must undergo a base change, i.e., from linguistic to numerical. As shown in Figure 82, this step is word embedding: conversion of the word (semantic) matrices to numerical matrices. It is about representing the words for text analysis purposes, typically in the form of a real-valued vector that encodes the meaning of each word.

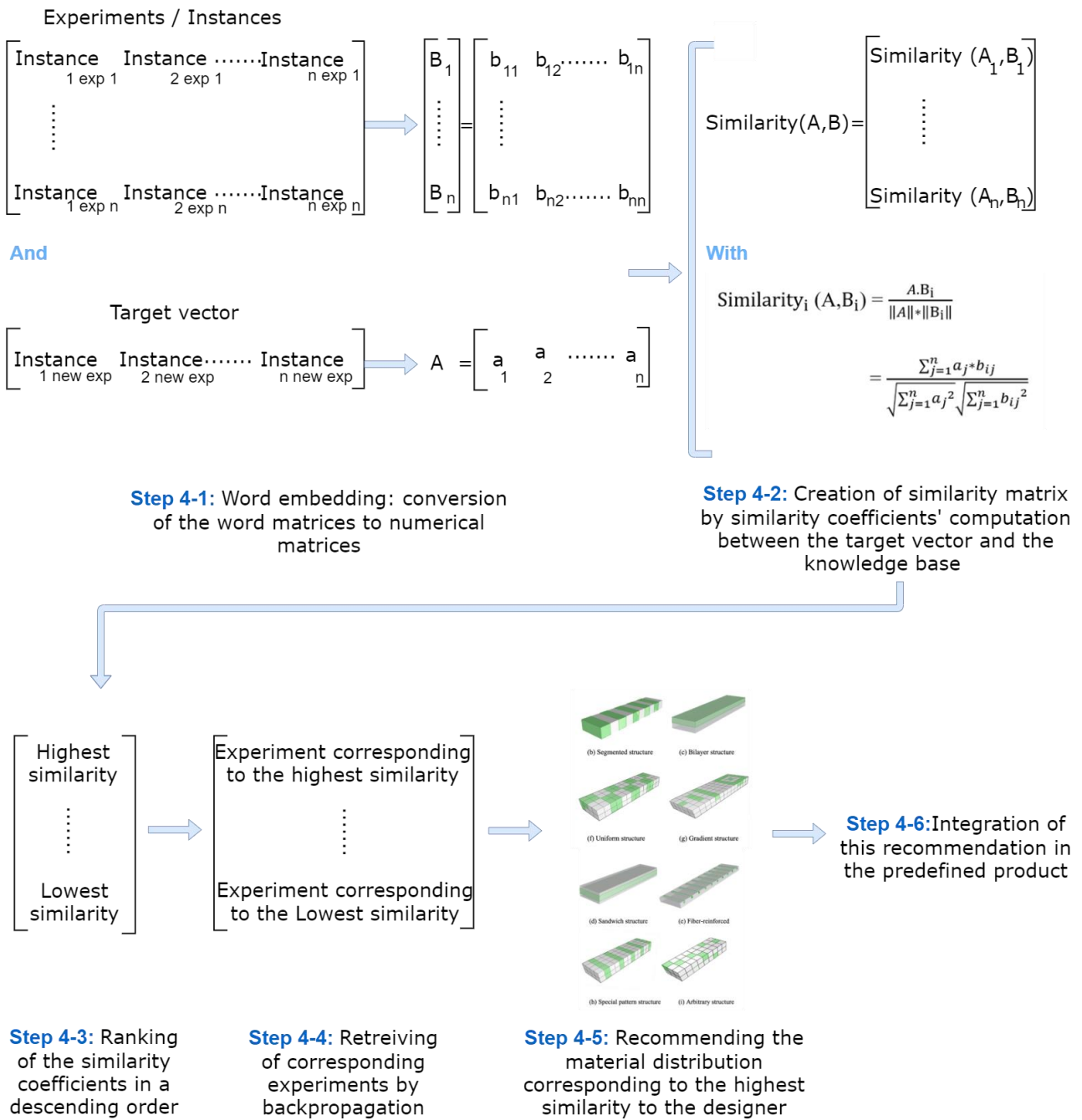


Figure 82. Word embedding and ranking of materials' distribution

At this stage, a computation of similarity between experiences is possible (see Step 4-2 in Figure 82). The research space may be refined if the target vector has fewer elements than the maximum of the semantic base. It is possible also to weigh some classes (i.e., elements in the matrix) to weaken or force their effects on the recommendation results (i.e., weighting the indexed keywords to improve the retrieval of documents relevant to the user). The weights of the terms are not considered in the schematization of Figure 82, but they are considered when implementing the code. Pre-prepared libraries assure the below illustrated transformation

between matrices (1) like word2vec¹⁶ for example, or libraries developed for the bag of words technique¹⁷, the blue arrow denotes the transformation between the two matrices.

$$\begin{array}{ccc}
 \left[\begin{array}{ccc} instance_{1exp1} & \cdots & instance_{17exp1} \\ \vdots & \ddots & \vdots \\ instance_{1exp40} & \cdots & instance_{17exp40} \end{array} \right] & \xrightarrow{\text{blue arrow}} & \left[\begin{array}{ccc} Num11 & \cdots & Num17 - 1 \\ \vdots & \ddots & \vdots \\ Numn1 - 40 & \cdots & Numn17 - 40 \end{array} \right] \quad (1) \\
 \text{Semantic matrix} & & \text{Transformed matrix according to the base change}
 \end{array}$$

Since the experiences are defined into vectors, the calculation measures the angular distance between the target vector and each in the semantic base. The angle between the semantic base's vectors and the target vector (also called query vector) is determined using a standard similarity metric called the cosine measure. The angle between two vectors is regarded as a measure of divergence between the vectors; the cosine angle is used to calculate the numeric similarity between the semantic base's vectors and the target vector when represented in a 17-dimensional vector space. So, this method is an algebraic model representing a text or a semantic knowledge as a vector and distance measurements help determine nearby materials' distribution in the defined space. This ontology-based similarity measure may be used to get similar prior instantiated materials' distribution for a target vector (target experiment) as presented in equation (2):

$$\text{Similarity}_i(A, B_i) = \frac{A \cdot B_i}{\|A\| \cdot \|B_i\|} = \frac{\sum_{j=1}^n a_j \cdot b_{ij}}{\sqrt{\sum_{j=1}^n a_j^2} \sqrt{\sum_{j=1}^n b_{ij}^2}} \quad (2)$$

Let A be the target vector and B_i is the i^{th} vector in the semantic matrix, the similarity coefficient between these two vectors is equal to the inner product of them divided by the product of the two vectors' norms. After computing all the similarity coefficients (30 coefficients), a similarity column matrix is created (3).

$$\begin{bmatrix} Sim(A, B_1) \\ \vdots \\ Sim(A, B_n) \end{bmatrix} \quad (3)$$

The similarity vector

The similarity coefficients are calculated between the semantic vectors based on their index vectors, reflecting the degree of correlation between the experiences. When the term assignment for two vectors is equal, the angle will be zero, yielding the maximum similarity measure. The relative distance between the vectors is pre-

¹⁶ The word2vec algorithm learns word associations from a large corpus of text. Once trained, such a model can detect synonymous words or suggest additional words for a partial sentence.

¹⁷ A text, such as a sentence or a document, is represented as the bag of its words, disregarding grammar and even word order but keeping multiplicity.

served by normalizing all base vector lengths to one, rather than identifying each document by a whole vector originating at the 0-point in the coordinate system (see Step 4-3 in Figure 82). Correlation relations between the results of a new experiment and comparable conditions could generate ideas and solutions. The above was a symbolic learning respecting vector space model method (semantic base creation and application of the VSM method). Each of the instances is searched in a knowledge base, making it possible to link the desired knowledge with a selection of known material distribution ranked from the highest similarity coefficient to the lowest. And by backpropagating, the correspondent experiences are then identified and arranged from the nearest to the farthest (see Step 4-4 in Figure 82).

The designer can then choose among the different proposals and thus replace the property zone with a distribution performing this property (see Step 4-5 in Figure 82). It is also possible not to have a known distribution precisely performing this function in our case. Still, a combination of two distributions carrying out a bending of a specific angle could very well be associated one after the other to meet the objective defined by the designer. When numerous materials and their associated qualities are distributed at the appropriate location in the final geometric specification of a product or part, the transformation function that must be devised and executed, as well as its needed performances, distribution challenges arise. Applying well-known distribution patterns to a primitive form can also be used to implement a basic behavior in a primitive shape.

The six kinds of distributions (i.e., uniform, gradient, special pattern, bilayer, sandwich, and computed) defined in Chapter 3 are the principal classes for the materials' distribution. But that does not prevent them from being populated into subclasses (sub distributions) to be much more precise in terms of prediction and to widen the space search of results. If the experience found does not use a basic distribution, but a particular one generally defined in the ontology as a special pattern, it will be expressed precisely in the semantic base as a distinctive pattern of type 'i' (1 to n) and by referring to it by this taxonomy. Other references have merged a few distributions to deliver a combination of basic materials distribution [129][226]. Figure 84 illustrates the above (grey color stands for passive material, blue and green colors stand for two different active materials).

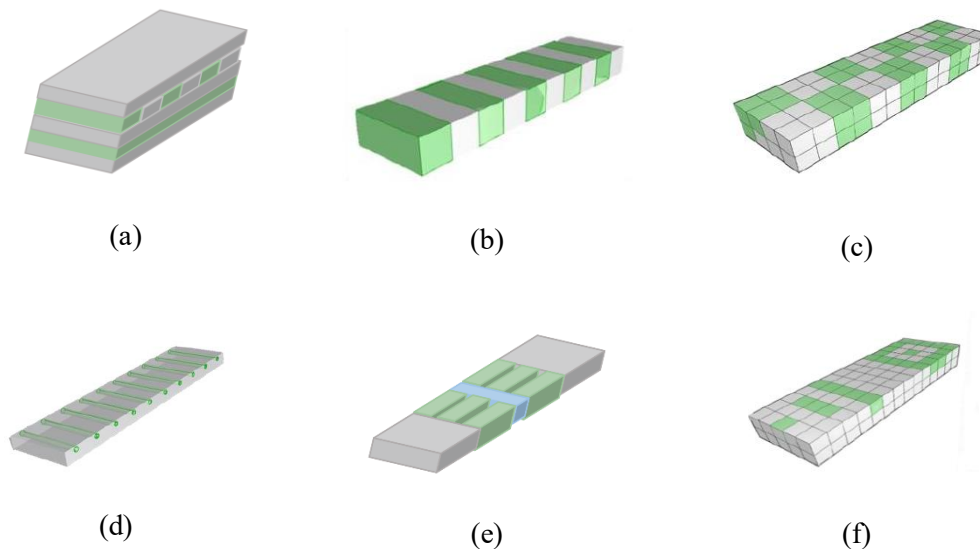


Figure 83 Illustrations of some sub-distributions, (a) combination of the distributions sandwich and segmented, (b) segmented distribution defined under the basic distribution special pattern, (c-f) sub classes of the distribution special pattern

5.3.5 Illustrative cases

This section will illustrate some of the instance graphs used to populate the semantic matrix created in the previous section. Practically, we have collected 30 experiences. Next Figures illustrate four instance graphs corresponding to four different experiences. Figures 84 illustrates the first experience [54]. It is about a bending composite strip manufactured with two types of SMP arranged in a bilayer distribution with material jetting process, and Stratasys objet connex 260 machine. The transformation function bending performs a 3D-to-3D dimension and a repeatable effect. It is triggered by heat as well. The correspondent instance graph is presented in Figure 85 and knowledge vector is presented in Table 20.

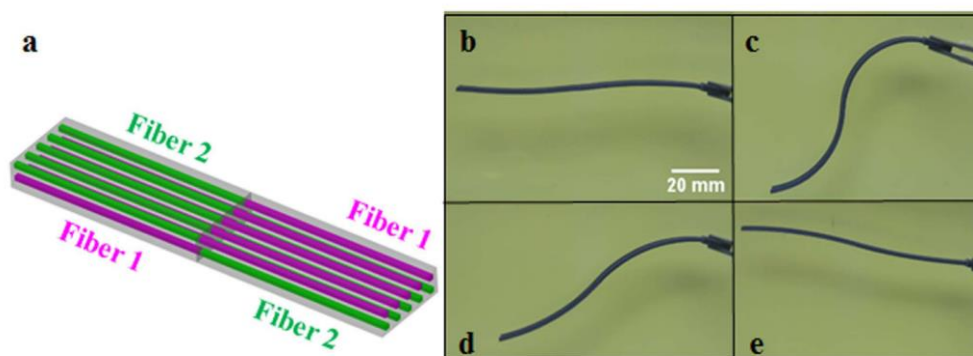


Figure 84. (a) The design of the structure and (b–e) the deformation behavior [54]

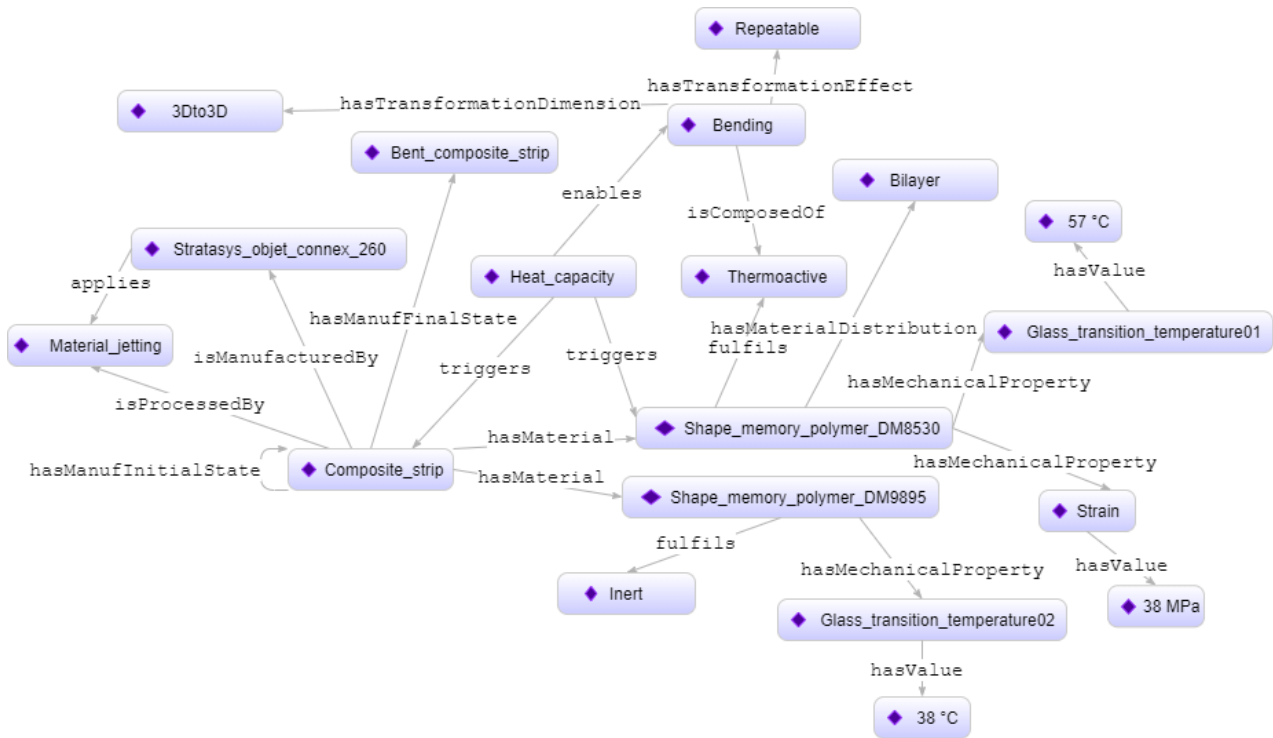


Figure 85. The first instance graph is extracted from the ad hoc experience in this reference [54]

Temperature degree 57°C and strain value 38 MPa are here data properties and not instances.

Table 20 Creation of the first vector in the semantic matrix

<i>Instances</i>	Correspondent classes (Base of the space vector)
<i>3D_to_3D</i>	Transformation_dimension
<i>Repeatable</i>	Transformation_effect
<i>Bent_composite_strip</i>	Product
<i>Bending</i>	Transformation_function
<i>Bilayer</i>	Material_distribution
<i>Glass_transition_temperature01</i>	Mechanical_property
<i>Strain</i>	Mechanical_property
<i>Thermoactive</i>	Technical_function
<i>Shape_memory_polymer_DM8530</i>	Material
<i>Shape_memory_polymer_DM9895</i>	Material
<i>Inert</i>	Technical_function
<i>Heat_capacity</i>	Stimulus
<i>Composite_strip</i>	Product
<i>Material_jetting</i>	Additive_manufacturing_process
<i>Bent_composite_strip</i>	Product
<i>Stratasys_objet_connex_260</i>	Machine

Figure 86 below illustrates the second experience [227]. It is about a folding origami box triggered by an electric field, manufactured with Verowhite and liquid crystal elastomer materials, DIW process, and Stratasys objet connex 260 machine. Those materials are arranged in a bilayer distribution. The active material fulfills an electroactive function and acquires change in terms of rigidity. Figure 87 presents the correspondent instance graph and Table 20 defines the correspondent knowledge vector.

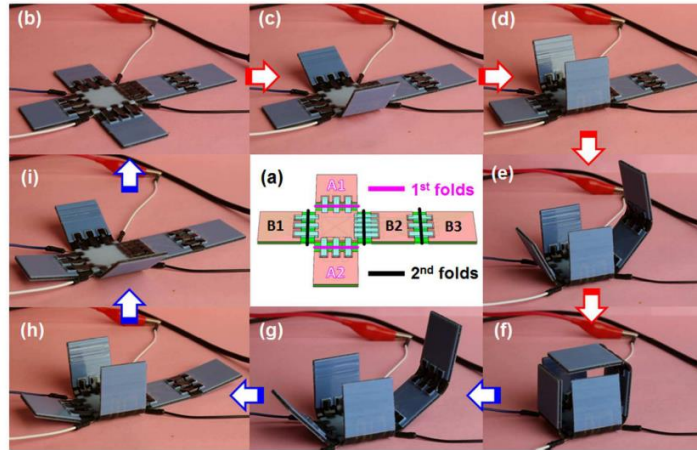


Figure 86. (a) Design schematics of the sequential folding box, (b-i) snapshots of the folding and unfolding process of the box [227]

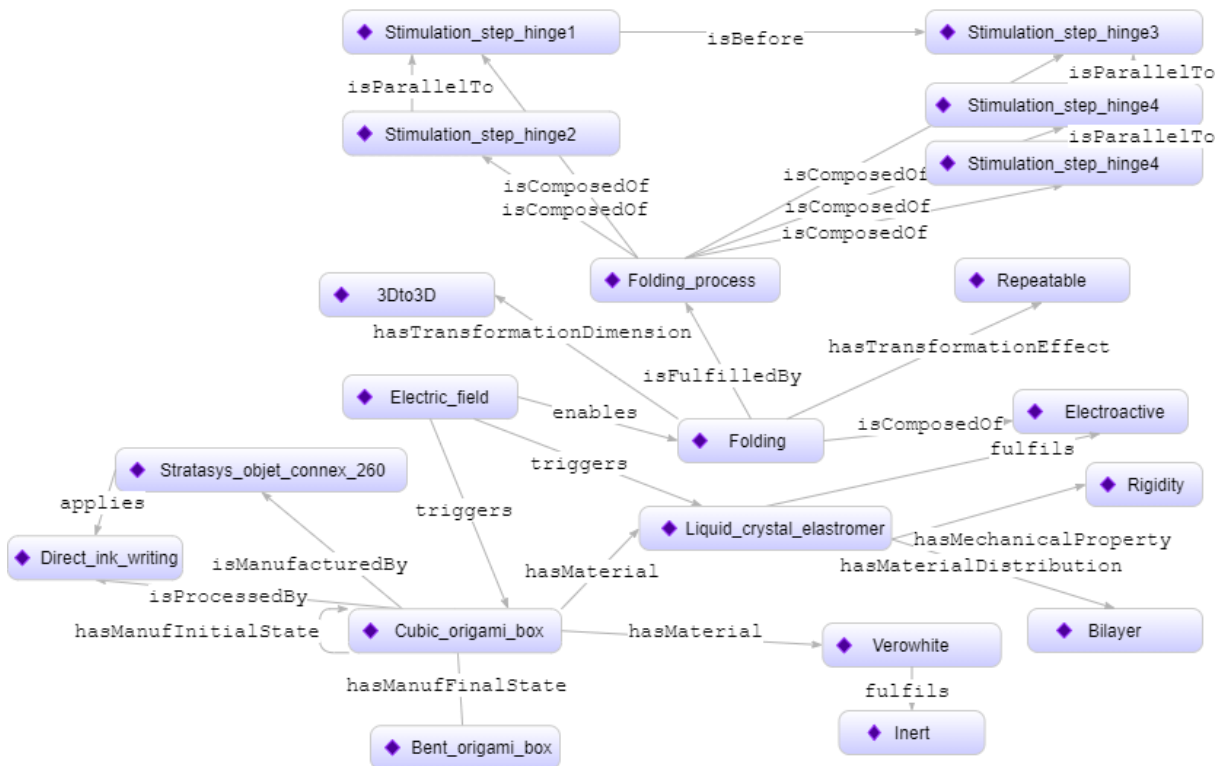


Figure 87. The second instance graph is extracted from the ad hoc experience in this reference [227].

Table 21 Creation of the second vector in the semantic matrix

<i>Instances</i>	Correspondent classes (Base of the space vector)
<i>3D_to_3D</i>	Transformation_dimension
<i>Repeatable</i>	Transformation_effect
<i>Folding</i>	Transformation_function
<i>Bilayer</i>	Material_distribution
<i>Rigidity</i>	Mechanical_property
<i>Electroactive</i>	Technical_function
<i>Verowhite</i>	Material
<i>Liquid_crystal_elastomer</i>	Material
<i>Inert</i>	Technical_function
<i>Electric_field</i>	Stimulus
<i>Cubic_origami_box</i>	Product
<i>Direct_ink_writing</i>	Additive_manufacturing_peocess
<i>Bent_origami_box</i>	Product
<i>Stratasys_objet_connex_260</i>	Machine
<i>Stimulation_step_hinge1 ... 5</i>	Tranformation_step
<i>Folding_process</i>	Transformation_process

Figure 88 below illustrates the third used experiments [23]. It is a bending structure in the form of MIT manufactured with hydrophilic polymer with a special pattern distribution with material jetting process, and Stratasys objet connex 260 machine. The material fulfills a thermoactive function and is triggered by temperature. The transformation function (i.e., bending) performs a 1D-to-3D dimension and a repeatable effect. Figure 89 presents the correspondent instance graph and Table 22 defines the creation the knowledge vector.



Figure 88. MIT structure [23]

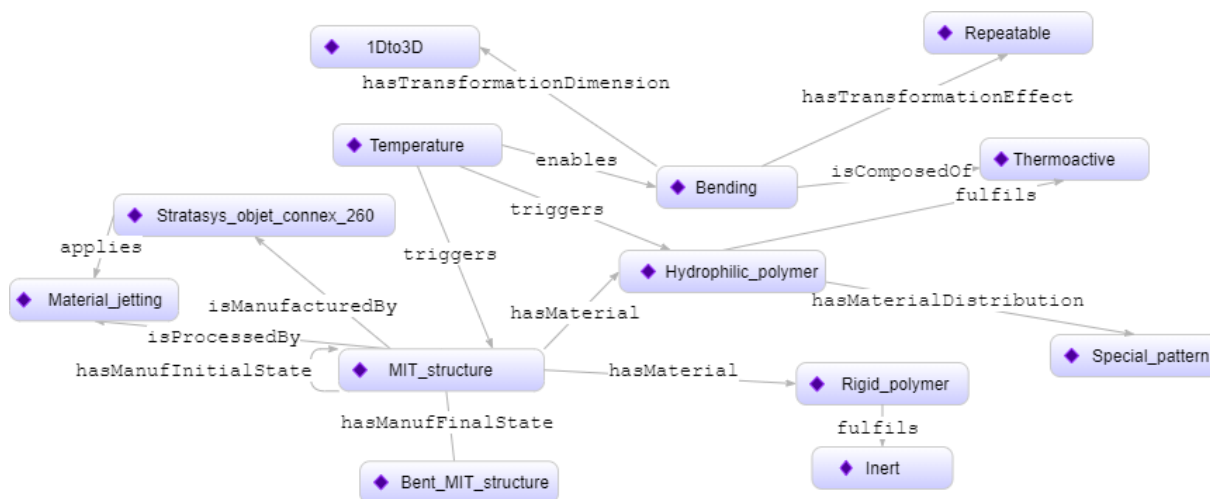


Figure 89. The third instance graph is extracted from the ad hoc experience from [23].

Table 22 Creation of the three vector in the semantic matrix

<i>Instances</i>	Correspondent classes (Base of the space vector)
<i>ID_to_3D</i>	Transformation_dimension
<i>Repeatabe</i>	Transformation_effect
<i>Bending</i>	Transformation_function
<i>Special_pattern</i>	Material_distribution
<i>Thermoactive</i>	Technical_function
<i>Rigid_polymer</i>	Material
<i>Inert</i>	Technical_function
<i>Temperature</i>	Stimulus
<i>MIT_struture</i>	Product
<i>Material_jetting</i>	Additive_manufacturing_process
<i>Bent_MIT_structure</i>	Product
<i>Stratasys_objet_connex_260</i>	Machine

Figure 90 presents the printed sample of the fourth experience [104]. It is a printed flower like structure performing a bending function. It is manufacturing with SLA process, a customized machine, and SMP in a uniform distribution, and triggered with temperature. The material fulfills a thermoactive function and the transformation function performs a 3D-to-3D dimension and a reversible effect. Figure 91 presents the correspondent instance graph and Table 23 presents the creation of a knowledge vector.



Figure 90. Printed flower like structure [104]

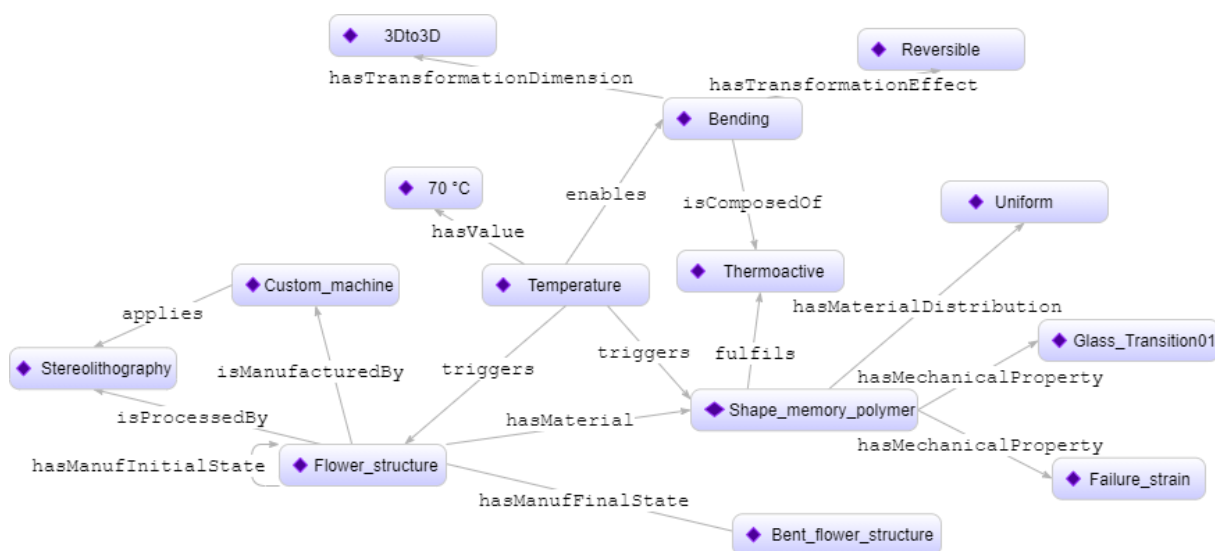


Figure 91. The fourth instance graph is extracted from the ad-hoc experience from [104].

Table 23 Creation of the fourth vector in the semantic matrix

Instances	Correspondent classes (Base of the space vector)
<i>3D_to_3D</i>	Transformation_dimension
<i>Reversible</i>	Transformation_effect
<i>Flower_structure</i>	Product
<i>Bent_flower_structure</i>	Product
<i>Bending</i>	Transformation_function
<i>Uniform</i>	Material_distribution
<i>Glass_transition_temperature01</i>	Mechanical_property
<i>Failure_strain</i>	Mechanical_property
<i>Strain</i>	Mechanical_property
<i>Thermoactive</i>	Technical_function

<i>SMP</i>	Material
<i>Temperature</i>	Stimulus
<i>Sterolithography</i>	Additive_manufacturing_process
<i>Custom_machine</i>	Machine

Some experiences are formulated in lesser classes than predefined classes in the knowledge base; this is mainly due to the fact that these missing classes are not defined in the scientific article. In order to cover this gap, we proceed in two different ways: either we put “none” in the adequate element of the vector or we request the ontology (e.g., given that a machine is not mentioned in such an article, we may request the ontology about which machine applies the specific AM process mentioned in the reference). But it should not have the same value as the other real instances, it must be penalized with a coefficient lowering its value.

Other experiences have more than one instance under the same class. In this case, we will consider the instances as a concatenated string of characters and each bag of words is corresponding to another instance of another class by a particular object property. Thus, we could make a difference between two instances (e.g., the materials defined in the first instance graph: *Shape_memory_polymer_DM8530* and *Shape_memory_polymer_DM9895* are differentiated by the Technical_function fulfilled by them: *Inert* and *Thermoactive*).

Let’s be a new experience that will be formulated in via a target vector requiring a prediction of the material distribution. The requirement is to design and manufacture a deployable satellite hinge, as presented in Figure 92, performing an unfolding Transformation_function that has to be repeatable. Following the design for 4D printing process defined in Chapter 4, multiple other instances can be defined. Figure 93 presents the instance graph for this experience. Each word will be processed and converted by the adequate predefined functions in the language C# for the VSM algorithms and word embedding problematics.

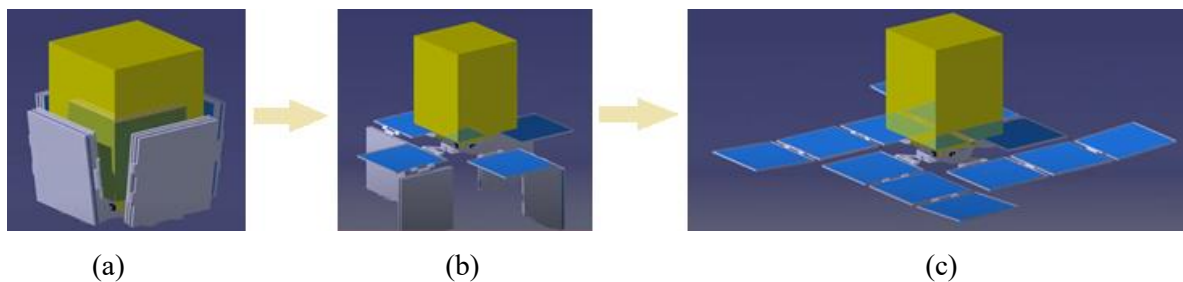


Figure 92. Deployable satellite: (a) initial state, (b) intermediary state, and (c) final state

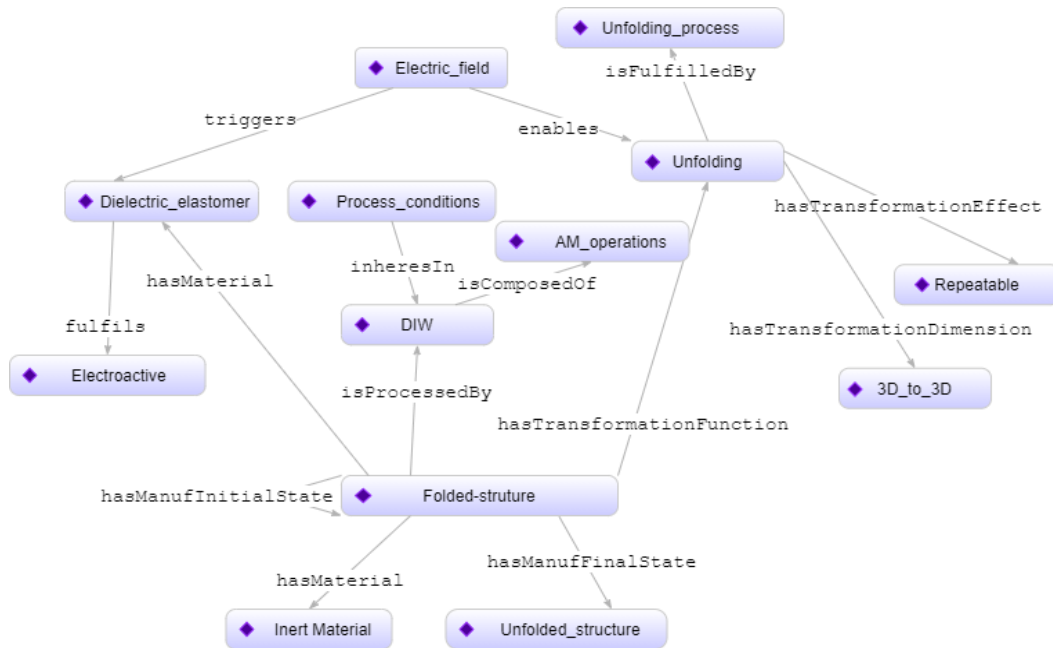


Figure 93. Instance graph for a satellite hinge

The results have to list the second experience [227] as the nearest one, followed consecutively by the first [54], the third [23], and the fourth experiences [104], so the predicted materials' distribution will be a bilayer. After receiving the recommendation about materials' distribution, the new experience can be returned to the ontology to populate it more; thus the CAD model for this new experience with all its representations can be stored in the ontology to cover the present gap of missing knowledge about multiple representations. The limited number of the experiences in the semantic base constitutes a cold start for the VSM method also.

5.4 Semantic reasoning

Proposing semantic reasoning-based rules is crucial for verifying some principles, solutions, and constraints while designing such 4D printed object. The product designer will verify his design consistency while evolving in the design process. Let's Y be the stimulus and X be the object, Figure 95 illustrates multiple mereotopological relationships between stimuli and parts. For example, if the stimulus is an electrical field, it must be overlapped by the part: either a proper tangential part or not but still in an internal part or as defined in the ontology: embedded part. When the stimulus is a magnetic field, heat, pH, chemical substance, light, and moisture, the stimulus can overlap or partially overlap or be in external contact with the part. Which means the stimuli can be external or internal part in the structure.

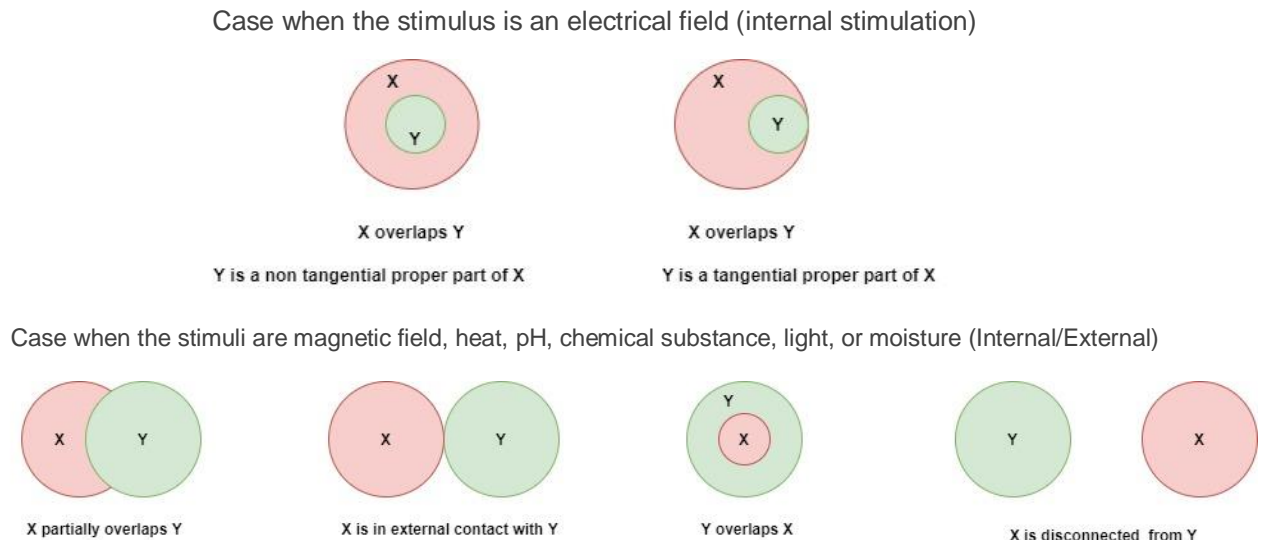


Figure 94. Mereotopological relations between stimuli and parts

If the active/smart region was about to be put as an internal part in such a structure and overlapped by more than two passive regions, then some tangent regions in a lattice structures seem to be a convenient design solution for reducing the required trigger timing.

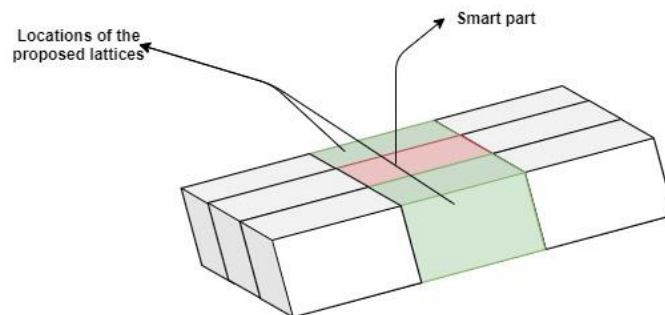


Figure 95 Position of the proposed lattice structures in the 4D printed part in its region-based representation

Some other assertions seem to be crucial to define and constitute further semantic rules:

- If only one material was used, then the material distribution is imperatively uniform;
- If the transformation function is bending, folding, or twisting then the technical function is shape changer;
- If the transformation function is bending, folding, or twisting and the stimulus is temperature, electrical field, light, or magnetic field then the technical function is respectively thermoactive, electroactive, photoactive, magnetoactive.
- If the stimulus is electric field, then the materials can be carbon-based composites, metal nanoparticles, polyelectrolyte hydrogel, conductive inks. SMP (to cite a few), and the AM processes can be DIW, FFF, SLA, and SLS [128].

5.5 Conclusion

The objective of this chapter is to propose a recommendation method to guide designers in the CDS phase. To do so, case-based reasoning and semantic reasoning-based rules layers, are introduced to reason with the knowledge captured in the HERMES ontology. This stands as the third scientific contribution of the PhD. It introduces a symbolic method in order to aid the designer while reasoning with analogy to other case studies. The prediction is mainly about the distribution of the active and passive regions in such a part/structure in its form-based representation to create a structure-based representation. An implementation of the recommendation mechanisms is made within a dedicated computational design for 4D printing plugin in a CAD environment, and a case study are introduced to illustrate the relevance of the proposal in the next chapter.

Chapter 6 Case Studies and implementation

*“Knowledge without application
is simply knowledge. Applying the
knowledge to one’s life is wisdom
– and that is the ultimate virtue”*

Kasi Kaye Iliopoulos

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6.1 Introduction

Previous chapters have established the main theoretical background for the three proposed contributions, this chapter will present the implementation and the practical use of the ontology, its usability, and the recommendation method. The implementation will be carried out by considering multi-abstraction layer (i.e. foundational, domain, and instance) and semantic application architecture with reasoning units (i.e., knowledge base, logic reasoning, and interface application) [228]. Such development will be based on specific languages – such as OWL-DL, SWRL (Semantic Web Rule Language) to name a few – in Protégé 5.5 Ontology software. Additional development will be addressed to integrate the multi-layer ontology and the envisioned CAD system (Rhino/Grasshopper 7 and its plugin Grasshopper). This will improve the knowledge representation abilities of Rhino/Grasshopper tools in the architectural definition of smart products/systems. Since Grasshopper is a .NET plugin from CAD Rhinoeros3D environment, it will be strategically interesting to use C# as critical technology development of programming language for developing an appropriate add-on within the Grasshopper plugin. An implementation of the recommendation method is made within a dedicated computational design for 4D printing plugin, and four case studies were introduced to illustrate the relevance of the proposal in this chapter.

6.2 Case studies implemented in Protégé 5.5

To demonstrate the applicability of the developed HERMES ontology, an implementation has been made in Protégé software 5.5, and two use cases are introduced. The consistency of the ontology is checked by using Pellet reasoner and DL rules for classes restrictions have been set up. This section describes a folding function fulfilled by an origami cube [17] and also a multi-bending actuator similar to the case presented in [221]. Therefore, it shows 2D-to-3D and 3D-to-3D transformation dimensions, respectively.

6.2.1 Folding cube

The objective here is to capture relevant 4D printing knowledge ensuring the transformation from a 2D origami precursor to a cube as illustrated in Figure 96. In its actual shape, the HERMES ontology has then been manually populated, leading to an instance graph represented in Figure 97.

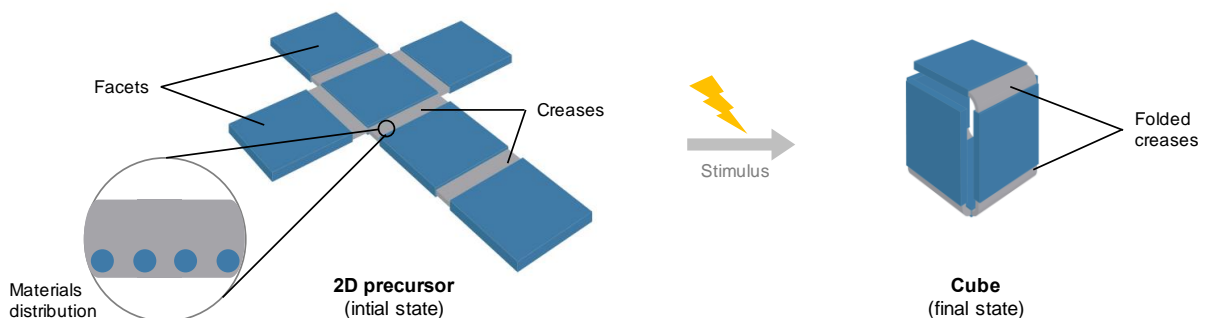


Figure 96. Folding Cube

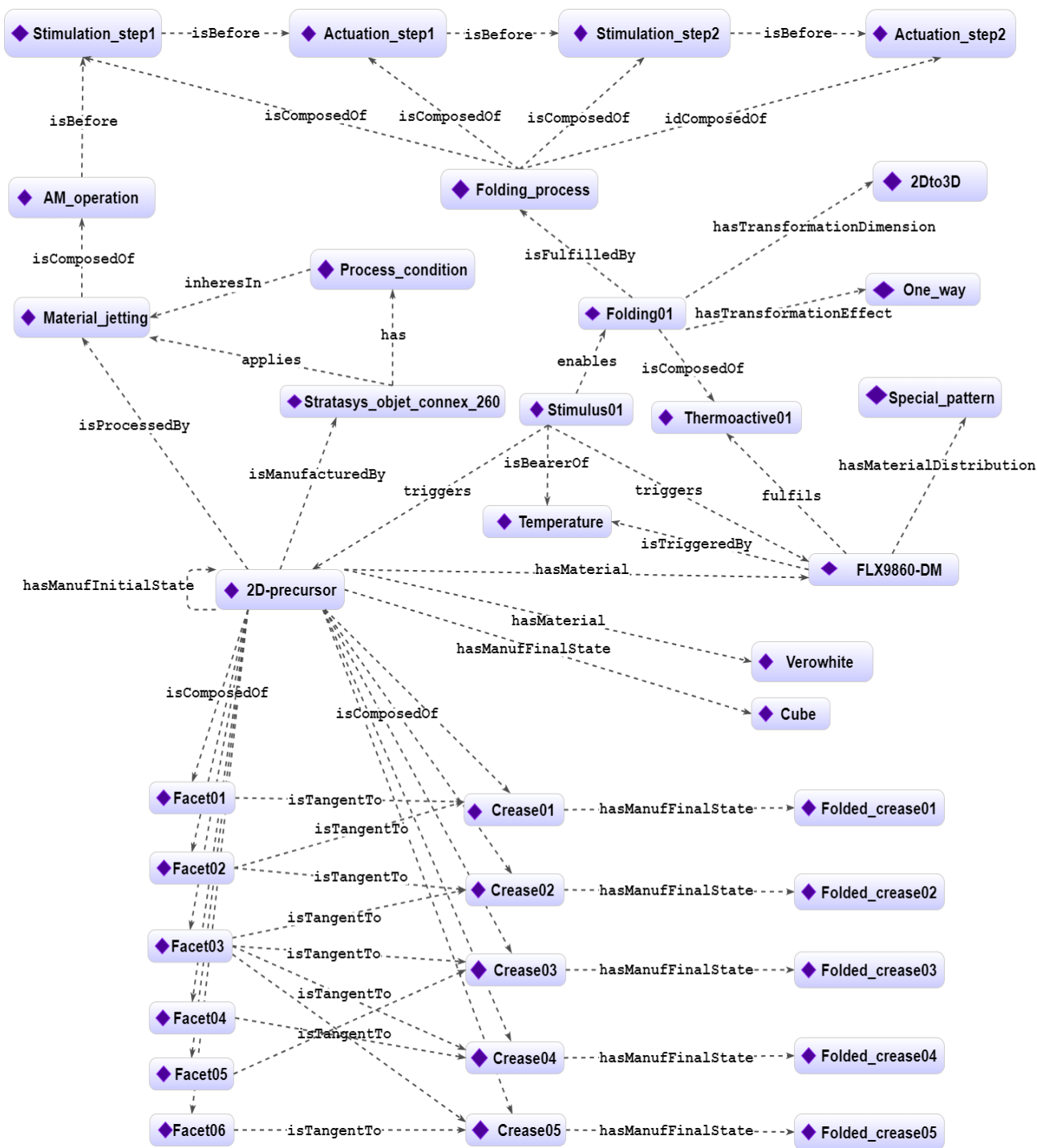


Figure 97. Instance graph for 4D printed cube using multiple folding transformation

For the sake of clarity, a few features have been selected to show how HERMES ontology represents knowledge from a logical and functional point of view. For instance, voxels and geometry have not been considered here. Still, some standard classes in the design and transformation views are illustrated to demonstrate the suitability of the ontology in preliminary design phases. The property `isComposedOf` fully covers information about the 2D precursor composition in to describe facets and creases, which are allocated

to homogeneous and hybrid parts, respectively. These parts are topologically connected with `isTangentTo` relation (as part of the mereotopological theory). Each crease is transformed to a specific folded crease; hence the confusion while affecting these instances to their transformation steps is avoided. The AM and the material views have also been built to have a comprehensive knowledge description from the conceptual design stage. In the present case study, a 2D precursor has two different materials: FLX9860 and VeroWhite [17]. It exhibits a thermoactive function via a particular patterned materials distribution. This multi-material 2D precursor is printed through the Stratasys Objet Connex 260 machine using the material jetting process and particularly the PolyJet technique [17] respecting the main conditions and following a set of universal and agreed operations. These AM operations are the first step in defining the folding sequence of the cube followed by two consecutive stimulations and actuations; as the creases from 01 to 04 are simultaneously folded, and then the fifth crease is actuated in a separate step (as illustrated in Figures 96 and 97). For consistency checking purpose and to assure the coherence of the presented instance graph, some DL descriptive rules are explicitly defined below:

1) The population of the HERMES top classes is as follows:

$$\begin{aligned}
 &2D_precursor \sqsubseteq \text{Product} \\
 &Cube \sqsubseteq \text{Product} \\
 &\{Crease01, Crease02, Crease03, Crease04, Crease05\} \sqsubseteq \text{Hybrid_part} \\
 &\{Facet01, Facet02, Facet03, Facet04, Facet05, Facet06\} \sqsubseteq \text{Homogeneous_part} \\
 &Stratasys_Objet_Connex_260 \sqsubseteq \text{Machine} \\
 &Verowhite \sqsubseteq \text{Material} \\
 &FLX9860-DM \sqsubseteq \text{Material} \\
 &Material_jetting \sqsubseteq \text{Additive_manufacturing_process} \\
 &Folding01 \sqsubseteq \text{Folding} \\
 &Thermoactive01 \sqsubseteq \text{Thermoactive} \\
 &Special_pattern \sqsubseteq \text{Material_distribution} \\
 &Temperature \sqsubseteq \text{Physical_property} \\
 &Stimulus01 \sqsubseteq \text{Stimulus} \\
 &Folding_process \sqsubseteq \text{Transformation_process} \\
 &AM_operation \sqsubseteq \text{AM_operation} \\
 &Process_condition \sqsubseteq \text{Process_condition} \\
 &\{Stimulation_step1, Actuation_step1, Stimulation_step2, Actuation_step2\} \sqsubseteq \text{Transformation_step}
 \end{aligned}$$

2) The population of the object properties is as follows:

$$\begin{aligned}
 &isTangentTo \sqsubseteq \text{hasSpatialRelation} \\
 &hasManufInitialState \sqsubseteq \text{has} \\
 &hasManufFinalState \sqsubseteq \text{has} \\
 &hasTransformationFunction \sqsubseteq \text{has}
 \end{aligned}$$

3) The restriction rules are as follows:

- Composition of the *2D_precursor*:

$$2D_precursor \sqsubseteq (\text{isComposedOf.Crease01} \sqcap \text{isComposedOf.Crease02} \sqcap \text{isComposedOf.Crease03} \sqcap \text{isComposedOf.Crease04} \sqcap \text{isComposedOf.Crease05} \sqcap \text{isComposedOf.Facet01} \sqcap \text{isComposedOf.Facet02} \sqcap \text{isComposedOf.Facet03} \sqcap \text{isComposedOf.Facet04} \sqcap \text{isComposedOf.Facet05} \sqcap \text{isComposedOf.Facet06})$$

- Meretopological relationships between *facets* and *creases*:

$$\text{Facet01} \sqsubseteq (\text{isTangentTo.Crease01})$$

$$\text{Facet02} \sqsubseteq (\text{isTangentTo.Crease01} \sqcap \text{isTangentTo.Crease02})$$

$$\text{Facet03} \sqsubseteq (\text{isTangentTo.Crease02} \sqcap \text{isTangentTo.Crease03} \sqcap \text{isTangentTo.Crease04} \sqcap \text{isTangentTo.Crease05})$$

$$\text{Facet04} \sqsubseteq (\text{isTangentTo.Crease04})$$

$$\text{Facet05} \sqsubseteq (\text{isTangentTo.Crease03})$$

$$\text{Facet06} \sqsubseteq (\text{isTangentTo.Crease05})$$

- Property assertions:

2D_precursor has only one initial state and one final state:

$$2D_precursor \sqsubseteq (\text{hasManufInitialState} = 1 \ 2D_precursor)$$

$$2D_precursor \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Cube})$$

Each *crease* has only one final state:

$$\text{Crease01} \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Foldel_crease01})$$

$$\text{Crease02} \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Foldel_crease02})$$

$$\text{Crease03} \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Foldel_crease03})$$

$$\text{Crease04} \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Foldel_crease04})$$

$$\text{Crease05} \sqsubseteq (\text{hasManufFinalState} = 1 \ \text{Foldel_crease05})$$

Each *step* of the *Folding_process* is preceded by only one precise *step*:

$$\text{AM_operation} \sqsubseteq (\text{isBefore.Stimulation_step1})$$

$$\text{Stimulation_step1} \sqsubseteq (\text{isBefore.Actuation_step1})$$

$$\text{Actuation_step1} \sqsubseteq (\text{isBefore.Stimulation_step2})$$

$$\text{Stimulation_step2} \sqsubseteq (\text{isBefore.Actuation_step2})$$

Definition of the instance *2D_precursor*:

$$2D_precursor \sqsubseteq (\text{hasMaterial.Verowhite} \sqcap \text{hasMaterial.FLX9860-DM} \sqcap \text{hasTransformationFunction.Folding01} \sqcap \text{isManufacturedBy.Sratasys_Object_Connex_260} \sqcap \text{isProcessedBy.Material_jetting})$$

Definition of the instance *FLX9860-DM*:

$$\text{FLX9860-DM} \sqsubseteq (\text{fulfils.Thermoactive01} \sqcap \text{hasMaterialDistribution.Special_pattern} \sqcap \text{isTriggeredBy} = 1 \ \text{Temperature})$$

Definition of the instance *Stimulus01*, see Figure 99:

$$\text{Stimulus01} \sqsubseteq (\text{triggers.FLX9860-DM} \sqcap \text{triggers.2D-precursor} \sqcap \text{isBearerOf} = 1 \ \text{Temperature} \sqcap \text{enables} = 1 \ \text{Folding01})$$

Definition of the instance *Folding01*:

$$\text{Folding01} \sqsubseteq (\text{isComposedOf} . \text{Thermoactive01} \sqcap \text{hasTransformationDimension} . \text{2Dto3D} \sqcap \\ \text{hasTransformationEffect} . \text{One_way} \sqcap \text{isFulfilledBy} = 1 \text{ Folding_process})$$

Definition of the instance *Folding_process*:

$$\text{Folding_process} \sqsubseteq (\text{isComposedOf} . \text{Stimulation_step1} \sqcap \text{isComposedOf} . \text{Actuation_step1} \sqcap \\ \text{isComposedOf} . \text{Stimulation_step2} \sqcap \text{isComposedOf} . \text{Actuation_step2})$$

Definition of the instances *Sratasys_Object_Connex_260*, *Process_condition*, and *Material_jetting*:

$$\text{Sratasys_Objet_Connex_260} \sqsubseteq (\forall \text{has} . \text{Process_condition} \sqcap \text{applies} = 1 \text{ Material_jetting})$$

$$\text{Process_condition} \sqsubseteq (\text{inheritsIn} = 1 \text{ Material_jetting})$$

$$\text{Material_jetting} \sqsubseteq (\forall \text{isComposedOf} . \text{AM_operation})$$

To demonstrate the applicability of the developed HERMES ontology, an implementation has been made in Protégé software 5.5 with the folding cube as case ad denoted in Figure 98. It displays the properties assertions for the instance *Stimulus01*.

The screenshot shows the Protégé 5.5 ontology editor interface. The top menu bar includes File, Edit, View, Reasoner, Tools, Refactor, Window, Ontop, and Help. The main window displays the ontology 'hermes_v8_article1_cas1' with the following components:

- Class hierarchy:** A tree view showing the hierarchy of classes. The root is 'Thing', which includes 'Entity', 'Continuant', 'Occurent', and 'Process'. Under 'Process', there are several subclasses: 'Additive_manufacturing_operation', 'Additive_manufacturing_process', 'Liquid_raw_material_based_process', 'Powder_raw_material_based_process', 'Solid_raw_material_based_process', 'Transformation_process', and 'Transformation_step'. The 'Simulus' class is highlighted in blue.
- Annotations:** A panel showing 'Annotations: Stimulus01' with a plus sign to add more annotations.
- Property assertions:** A panel showing 'Property assertions: Stimulus01'. Under 'Object property assertions', there are three assertions: 'isBearerOf Temperature', 'triggers 2D_precursor', and 'triggers FLX9860-DM'. Under 'enables', there is one assertion: 'enables Folding01'.
- Direct instances:** A panel showing 'Direct instances: Stimulus01' with a plus sign to add more instances.
- For:** A panel showing 'For: Simulus' with a plus sign to add more instances.

Figure 98. Implementation of the HERMES ontology with protégé 5.5 with a display of properties assertions for the instance *Stimulus01*

6.2.2 Bending actuator

A beam is considered a second illustrative case to realize a bending resulting from multiple contractions. This beam is represented in various ways in Figure 99 [221]. Starting from a geometric definition, this actuator is then voxelized in order to describe mechanical properties within the 3D structure, enabling the determination of passive and active materials and then simulated via VoxSmart [123], a Grasshopper plugin within Rhinoceros3D environment. The adopted decomposition is based on the concepts of homogeneous and hybrid parts, then describing the active and passive elements with material knowledge of the actuator, respectively.

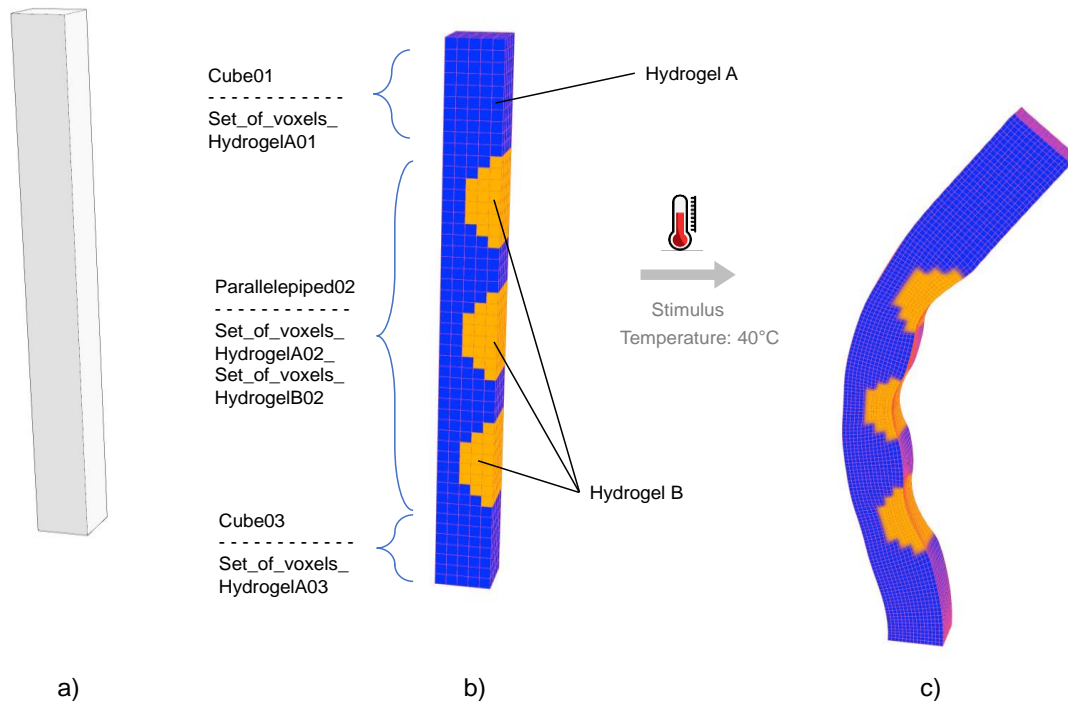


Figure 99. Bending actuator through (a) form-based representation and (b) voxel-based structure representation

(c) bending voxel-based structure

Among the three identified parts of the actuator, both extremum sides can be considered as Homogeneous_part(s) composed of a *HydrogelA* with the following parameters: young modulus $E = 10$ MPa, shear modulus $G = 5.2$ MPa, relative swollen ratio limit_min = 0.01 and close collapsed ratio limit_max = 0.4). The internal zone refers to the Hybrid_part with a *Special_pattern* distribution of two different materials *HydrogelA* and *HydrogelB*. The latter has similar characteristics but exhibits different swelling ratios such as min = 0.4 and max = 0.8. While triggered by its appropriate Stimulus (i.e., Lower Critical Solution Temperature (LCST) around 40°C), the thermoactive *HydrogelB* shrinks in volume; hence the multiple contracted sections created will enable the bending of the whole structure. It is mainly about having different transformation functions via a single triggering.

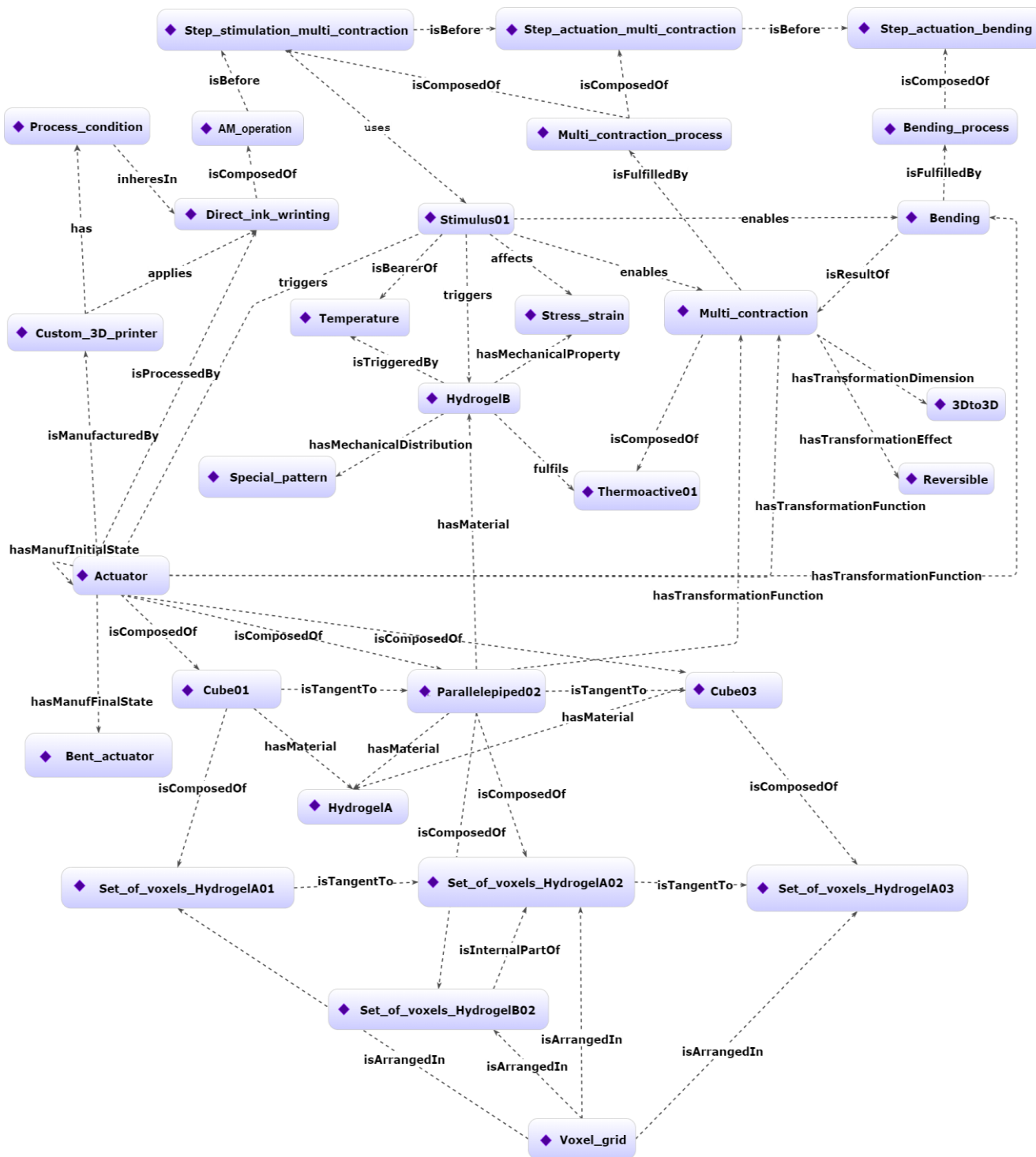


Figure 100. Instance graph of the bending actuator

This use case illustrates a physical point of view with some mereotopological relations. For instance, cubes 01 and 03 are composed of *HydrogelA* voxels on one side. On the other side, the parallelepiped is composed of two combined sets of voxels of hydrogels (A and B); in such case, both sets are spatially connected with ‘is InternalPartOf’ mereotopological connection. In a same way, cubes 01 and 03 are tangentTo the middle space of the actuator. Furthermore, the spatiotemporal aspect of the HERMES ontology is

captured in the two presented sequences (see the instance graph in Figure 100), the first defines the contraction steps, and the second is for the bending function. It starts as usual by the AM operations, then a stimulation step, and ends with an actuation step. As a result, the multi-contraction actuation leads to a bending actuation; they are two steps in parallel. Both use cases demonstrate how the HERMES ontology perceives interlinked concepts and formalizes scattered knowledge of the 4D printing domain. For consistency checking purpose and to assure the coherence of the presented instance graph, some DL descriptive rules are explicitly defined below:

1) The population of the HERMES top classes is as follows:

$$\begin{aligned}
 & \textit{Actuator} \sqsubseteq \textit{Product} \\
 & \textit{Bent_actuator} \sqsubseteq \textit{Product} \\
 & \textit{Paralleliped02} \sqsubseteq \textit{Hybrid_part} \\
 & \{ \textit{Cube01}, \textit{Cube 03} \} \sqsubseteq \textit{Homogeneous_part} \\
 & \textit{HydrogelA} \sqsubseteq \textit{Material} \\
 & \textit{HydrogelB} \sqsubseteq \textit{Material} \\
 & \textit{Voxel_grid} \sqsubseteq \textit{Voxel_grid} \\
 & \textit{Custom_3D_printer} \sqsubseteq \textit{Machine} \\
 & \textit{Direct_ink_jetting} \sqsubseteq \textit{Additive_manufacturing_process} \\
 & \textit{Bending} \sqsubseteq \textit{Bending} \\
 & \textit{Multi_contraction} \sqsubseteq \textit{Contraction} \\
 & \textit{Thermoactive01} \sqsubseteq \textit{Thermoactive} \\
 & \textit{Special_pattern} \sqsubseteq \textit{Material_distribution} \\
 & \textit{Temperature} \sqsubseteq \textit{Physical_property} \\
 & \textit{Stress_strain} \sqsubseteq \textit{Mechanical_property} \\
 & \textit{Stimulus01} \sqsubseteq \textit{Stimulus} \\
 & \textit{Multi_contraction_process} \sqsubseteq \textit{Transformation_process} \\
 & \textit{Bending_process} \sqsubseteq \textit{Transformation_process} \\
 & \textit{AM_operation} \sqsubseteq \textit{AM_operation} \\
 & \textit{Process_condition} \sqsubseteq \textit{Process_condition}
 \end{aligned}$$

2) The population of the object properties is as follows:

$$\begin{aligned}
 & \textit{isTangentTo} \sqsubseteq \textit{hasSpatialRelation} \\
 & \textit{isInternalPartOf} \sqsubseteq \textit{hasSpatialRelation} \\
 & \textit{hasManufInitialState} \sqsubseteq \textit{has} \\
 & \textit{hasManufFinalState} \sqsubseteq \textit{has} \\
 & \textit{hasTransformationFunction} \sqsubseteq \textit{has}
 \end{aligned}$$

3) The restriction rules are as follows:

- Composition of the *Actuator* :

$$\begin{aligned}
 \textit{Actuator} \sqsubseteq & (\textit{isComposedOf.Cube01} \sqcap \textit{isComposedOf.Paralleliped02} \\
 & \sqcap \textit{isComposedOf.Cube 03})
 \end{aligned}$$

$$\{Set_of_voxels_HydrogelA01, Set_of_voxels_HydrogelA02, Set_of_voxels_HydrogelA03, \\ Set_of_voxels_HydrogelB02\} \sqsubseteq \text{Voxel}$$

$$Set_of_voxels_HydrogelA01 \sqsubseteq (\text{isArrangedIn}.Voxel_grid)$$

$$Set_of_voxels_HydrogelA02 \sqsubseteq (\text{isArrangedIn}.Voxel_grid)$$

$$Set_of_voxels_HydrogelA03 \sqsubseteq (\text{isArrangedIn}.Voxel_grid)$$

$$Set_of_voxels_HydrogelB02 \sqsubseteq (\text{isArrangedIn}.Voxel_grid)$$

$$Cube01 \sqsubseteq (\text{isComposedOf}.Set_of_voxels_HydrogelA01)$$

$$Parallelepiped02 \sqsubseteq (\text{isComposedOf}.Set_of_voxels_HydrogelA02 \sqcap \\ \text{isComposedOf}.Set_of_voxels_HydrogelB02)$$

$$Cube\ 03 \sqsubseteq (\text{isComposedOf}.Set_of_voxels_HydrogelA03)$$

$$\{Step_stimulation_multi_contraction, Step_actuation_multi_contraction, Step_actuation_Bending\} \sqsubseteq \\ \text{Transformation_step}$$

- Meretopological relationships between *facets* and *creases*:

$$Cube01 \sqsubseteq (\text{isTangentTo}.Parallelepiped02)$$

$$Parallelepiped02 \sqsubseteq (\text{isTangentTo}.Cube\ 03)$$

$$Set_of_voxels_HydrogelA01 \sqsubseteq (\text{isTangentTo}.Set_of_voxels_HydrogelA02)$$

$$Set_of_voxels_HydrogelA02 \sqsubseteq (\text{isTangentTo}.Set_of_voxels_HydrogelA03)$$

$$Set_of_voxels_HydrogelB02 \sqsubseteq (\text{isInternalPartOf}.Set_of_voxels_HydrogelA02)$$

- Property assertions:

Actuator has only one initial state and one final state:

$$Actuator \sqsubseteq (\text{hasManufInitialState} = 1\ Actuator)$$

$$Actuator \sqsubseteq (\text{hasManufFinalState} = 1\ Bent_actuator)$$

Definition of materials:

$$Cube01 \sqsubseteq (\text{hasMaterial}.HydrogelA)$$

$$Parallelepiped02 \sqsubseteq (\text{hasMaterial}.HydrogelA \sqcap \text{hasMaterial}.HydrogelB)$$

$$Cube\ 03 \sqsubseteq (\text{hasMaterial}.HydrogelA)$$

Definition of the instance *Parallelepiped02*:

$$Parallelepiped02 \sqsubseteq (\text{hasTransformationFunction}.Multi_contraction)$$

Definition of the instance *Actuator*:

$$Actuator \sqsubseteq (\text{hasTransformationFunction}.Bending \sqcap \\ \text{hasTransformationFunction}.Multi_contraction \sqcap \\ \text{isManufacturedBy}.Custom_3D_printer \sqcap \text{isProcessedBy}.Direct_ink_jetting)$$

Definition of the instance *HydrogelB*

$$HydrogelB \sqsubseteq (\text{fulfils}.Thermoactive01 \sqcap \text{hasMaterialDistribution}.Special_pattern \\ \sqcap \text{isTriggeredBy} = 1\ Temperature \sqcap \text{hasMechanicalproperty}.Stress_strain)$$

Definition of the instance *Stimulus01*:

$$Stimulus01 \sqsubseteq (\text{triggers}.HydrogelB \sqcap \text{triggers}.Actuator \sqcap \text{isBearerOf} = 1\ Temperature \\ \sqcap \text{enables}.Bending \sqcap \text{enables}.Multi_contraction \sqcap \text{affects}.Stress_strain)$$

Definition of the instance *Multi_contraction*:

$$\text{Multi_contraction} \sqsubseteq (\text{isComposedOf}.\text{Thermoactive01} \sqcap \text{hasTransformationDimension}.\text{3Dto3D} \sqcap \text{hasTransformationEffect}.\text{Reversible} \sqcap \text{isFulfilledBy} = 1 \text{ Multi_contraction_process})$$

Definition of the instance *Bending*:

$$\text{Bending} \sqsubseteq (\text{isResultOf}.\text{Multi_contraction} \sqcap \text{isFulfilledBy} = 1 \text{ Bending_process})$$

Definition of the processes:

$$\begin{aligned} \text{Multi_contraction_process} &\sqsubseteq (\text{isComposedOf}.\text{Step_stimulation_multi_contraction} \sqcap \\ &\quad \text{isComposedOf}.\text{Step_actuation_multi_contraction}) \\ \text{Bending_process} &\sqsubseteq (\text{isComposedOf}.\text{Step_actuation_Bending}) \end{aligned}$$

Definition of the steps:

$$\begin{aligned} \text{Step_stimulation_multi_contraction} &\sqsubseteq (\text{uses}.\text{Stimulus01}) \\ \text{AM_operation} &\sqsubseteq (\text{isBefore}.\text{Step_stimulation_multi_contraction}) \\ \text{Step_stimulation_multi_contraction} &\sqsubseteq (\text{isBefore}.\text{Step_actuation_multi_contraction}) \\ \text{Step_actuation_multi_contraction} &\sqsubseteq (\text{isBefore}.\text{Step_actuation_Bending}) \end{aligned}$$

Definition of the instance *Custom_3D_printer*, *Process_condition*, *Direct_ink_jetting*:

$$\begin{aligned} \text{Custom_3D_printer} &\sqsubseteq (\forall \text{ has}.\text{Process_condition} \sqcap \text{applies} = 1 \text{ Direct_ink_jetting}) \\ \text{Process_condition} &\sqsubseteq (\text{inheritsIn} = 1 \text{ Direct_ink_jetting}) \\ \text{Direct_ink_jetting} &\sqsubseteq (\forall \text{ isComposedOf}.\text{AM_operation}) \end{aligned}$$

As far as HERMES ontology is established, two case studies have been set up to show its applicability from different design points of view. Besides the limitation of the knowledge domain to product/part design, the folded-2d-precursor is presented with the omission of some classes that introduce geometry specification and voxel identification. This is due to the objective of capturing 4D printing-related knowledge that is aligned with CDS. In our opinion, presenting the second case study with further formalization compared to the first one supports the usefulness of the proposed method and the capacity of the ontology to capture 4D printing-related knowledge for different design matters. In complementarity with Figure 99, Figure 101 presents the actuator's skeleton, the three representation will be integrated in the instance graph. The multi representation classes of 4D printed object is implemented in HERMES ontology as shown in Figure 102. Each plane in the skeleton has specific final plane as a final state linked to it with a precise data properties, see Figure 103.

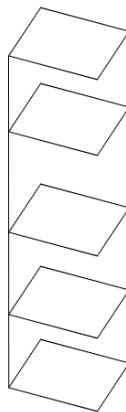


Figure 101. Illustrative figure of the actuator skeleton

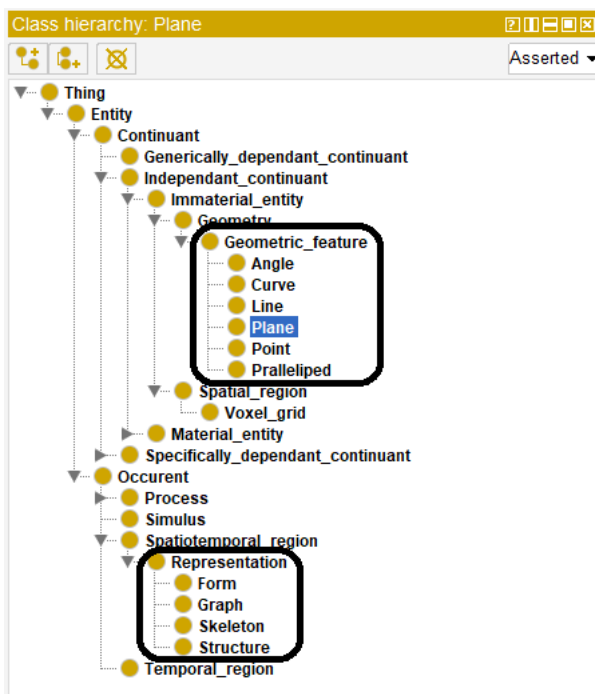


Figure 102. Integration of the add-on built in Chapter 4 in the HERMES ontology

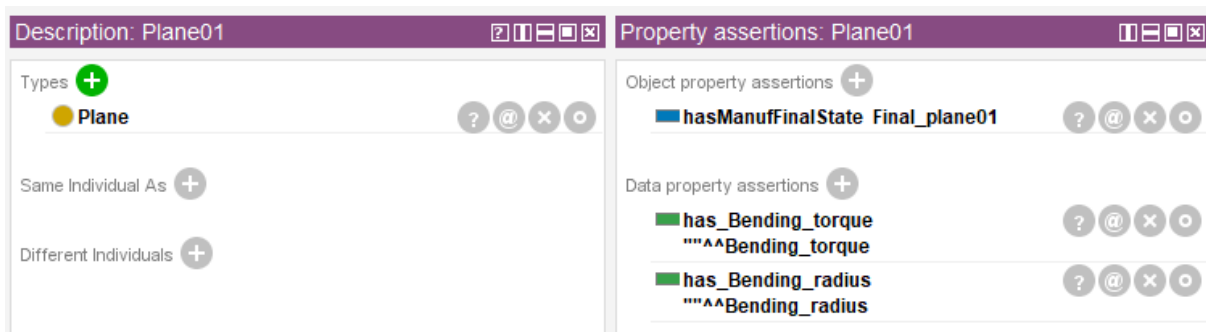


Figure 103. Visualization of the description of the instance Plane01

The screenshot displays the Protégé 5.5 interface for SHACL constraint verification. On the left, a class hierarchy for 'Plane' is shown, including 'Entity', 'Continuant', 'Immaterial_entity', 'Geometry', and 'Geometric_feature'. The 'SHACL editor' in the center contains the following code:

```

@prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#> .
@prefix sh: <http://www.w3.org/ns/shacl#> .
@prefix xsd: <http://www.w3.org/2001/XMLSchema#> .
@prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#> .
@prefix owl: <http://www.w3.org/2002/07/owl#> .
@prefix hermes: <https://icb.u-bourgogne.fr/HERMES/ontologies/2020/03/hermes_v8_article1_cas2_v2#> .

hermes:RepresentationShape
  a sh:NodeShape ;
  sh:targetClass hermes:Representation ;
  sh:property [
    sh:path hermes:isComposedOf ;
    sh:maxCount 1 ;
    sh:functional ;
  ] ;
hermes:SkeletonShape
  sh:property [
    sh:targetClass hermes:Skeleton ;
    sh:path hermes:isComposedOf ;
    sh:instance Plane:string ;
    sh:pattern "~^Plane d{1}\\d{2}-\\d{3}-\\d{4}\\d{5}-\\d{6}-\\d{7}-\\d{8}$" ;
    sh:severity sh:Warning ;
  ] ;
  sh:closed true ;
  sh:ignoredProperties ( rdf:type owl:topDataProperty owl:topObjectProperty ) ;
  .

##### add SHACL vocabulary #####
    
```

At the bottom right, the 'SHACL constraint violations' table is empty, indicating no violations:

Severity	SourceShape	Message	FocusNode	Path	Value
no constraint violations					

Figure 104. Constraints verification in SHACL language in Protégé 5.5

The Karlsruhe pseudo code proposed in Chapter 4 is verified with SHACL language as demonstrated in Figure 104. The results show that there is no constraints violation respecting the characteristics defining the object property “isComposedOf” – as explicited in Chapter 3 – and the instantiation of Plane class.

6.3 General logic axioms verification

Querying the ontology for retrieval purpose is always a valid usability of the ontology. Qualifying the inputs in the first phase for example (i.e., task clarification) is an information retrieval step using SPARQL queries according to task requirements in always a valid usability for the ontology. The structure of queries and their applications will be illustrated in this section. The queries have been created using a Resource Description Framework (RDF) query language: SPARQL, a plugin for different environments: Protégé, Jena, Ontorion, etc. SPARQL is a semantic query language that is able to retrieve and manipulate data stored in the RDF format

where the entities and its relations are expressed in the form of subject-predicate-object. For each query, the namespaces and its binded prefixes were used to identify the URI of the classes, besides the URI of the ontology itself “hermes” as follows:

- rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
- owl: <http://www.w3.org/2002/07/owl#>
- rdfs: <http://www.w3.org/2000/01/rdf-schema#>
- xsd: <http://www.w3.org/2001/XMLSchema#>
- hermes: http://www.semanticweb.org/sdimassi/ontologies/2021/8/Hermes_29_Sep#

The qualification of inputs can be an identification of the materials, stimuli, AM, transformation function of the product, or the technical function of the material. Two different queries are proposed as follows:

Query1: Identification of the technical function corresponding to the transformation function bending respecting the semantic rule defined in the previous chapter, the result is presented in Figure 105.

```
SELECT ?Bending ?x
WHERE {
  ? Bending rdf: type: Transformation_function.
  rdfs: label: Bending.
  : isComposedOf? x.
  rdfs: label?x
}
```

x
Shape_changer

Figure 105. Result of the first query

Query2: Identification of the materials that can be triggered by temperature, Figure 106 show the results for this query:

```
SELECT ?x
WHERE {
  ? x rdf: type: Material.
  ?x hermes: isTriggeredBy? Temperature. }
```


x
Epoxy_based_UV_curable
Methacrylate_based_copolymer
Methyle_cellulose_hydrogel
Poly_acrylic_acide_and_ceramic_powder
Poly_ether_amide_grafting_with_PNIPAA_and_PEG
Poly_lactic_acide
Poly_lactide_co_glycolide
Polyethylene_oxide
Hybrid_inorganic_polymer_system
Nylon_ABS
Onyx
PETG
PLA
PVA

Figure 106. Results of the second query

6.4 Case studies implemented in the Grasshopper plugin

This section introduces two case studies for material distribution recommendation purpose using VSM method and applying the steps described in Chapter 5.

6.4.1 Developed Component

In order to apply the VSM method, a code has been developed and stored in a component developed in the Grasshopper environment (see Figure 107).

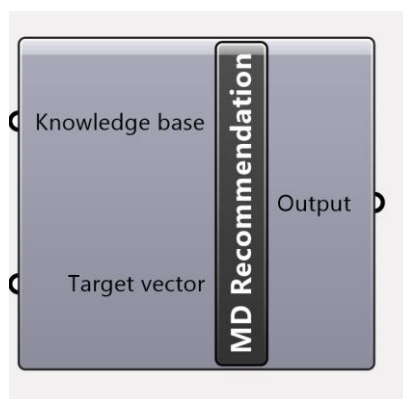


Figure 107 Component for material distribution recommendation

The component is named material distribution (MD) recommendation, it gets the knowledge base and the target vector as inputs and delivers the experiences ranked as expressed in Step 4-4 of Figure 82 in Chapter 5.

6.4.2 Bending Beam

This use case is about recommending the material distribution for a bending beam. Assuming that the instance graph for this aim has led to the target vector { Repeatable, 3D_to_3D, Bending, Thermoactive, Heat_capacity, SMP, Stratasys_objet_connex_260, Material_jetting, Glass_transition}. The “MD Recommendation” component will be connected to the semantic base created with 30 experiences defined in the component path (see Figure 108), and to the knowledge vector written manually in a panel. The output displays the nearest experiences ranked in descending way. The display is roughly for the experiences having a cosine value more than 0.1. The output panel displays the whole knowledge vector of those experiences to facilitate the selection of other missing elements for the designer (this stands as a future use). The number of experiences is extracted from the knowledge vector displayed in the output panel using the component cluster, and therefore it is concatenated to the expression ‘Exp’. Exp ‘i’ (i denotes the number of the experience extracted) is searched as a name of a .png file in a file directory in which the photos of the corresponding materials distribution are. Finally, the component IMG displays the found image in the Rhinoceros3D environment as shown in Figure 109. The corresponding material distribution is bilayer.

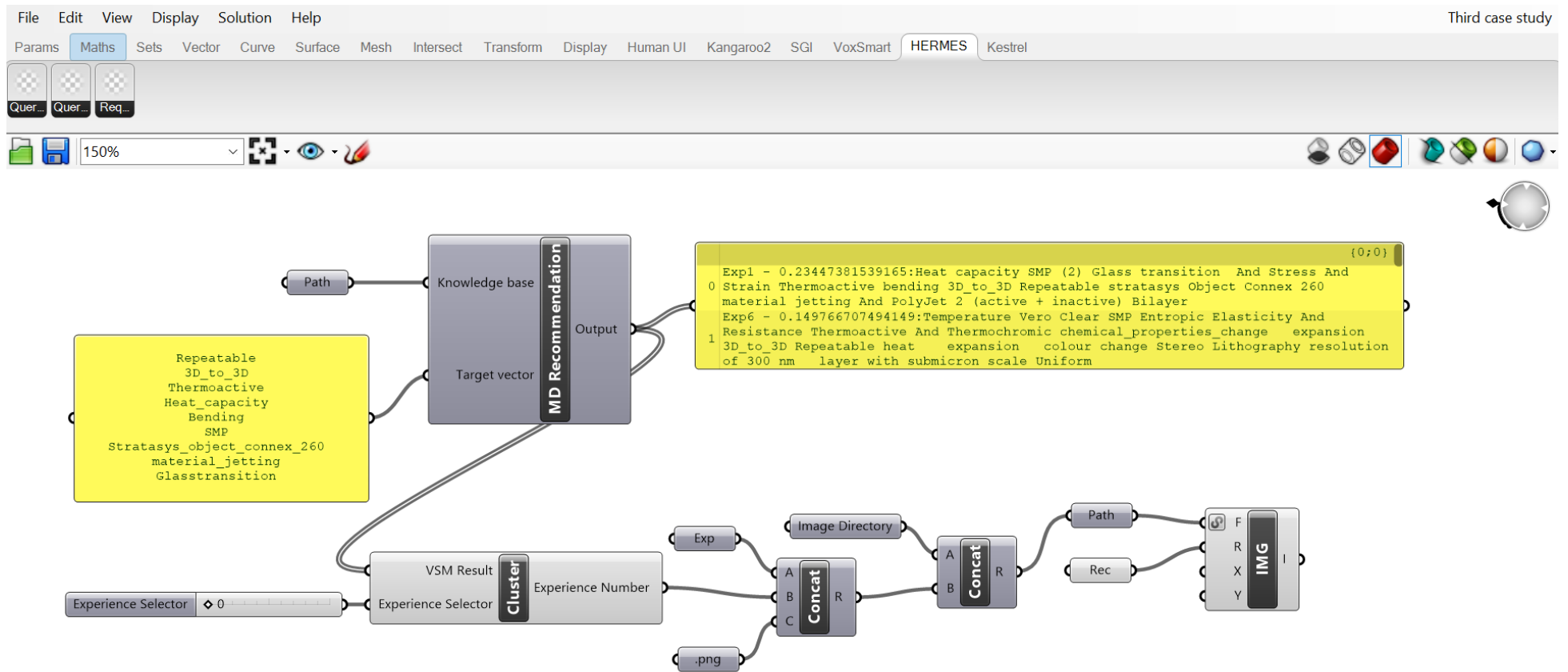


Figure 108. Visual programming on Grasshopper plugin of the material distribution recommendation for the third case study

Figure 109 illustrates the visualization of the material distribution in the Rhinoceros3D as a support approach to assist the product designer. Figure 110 shows the manual definition of two B-Rep (Boundary representation) to delimit active and passive regions for a beam.

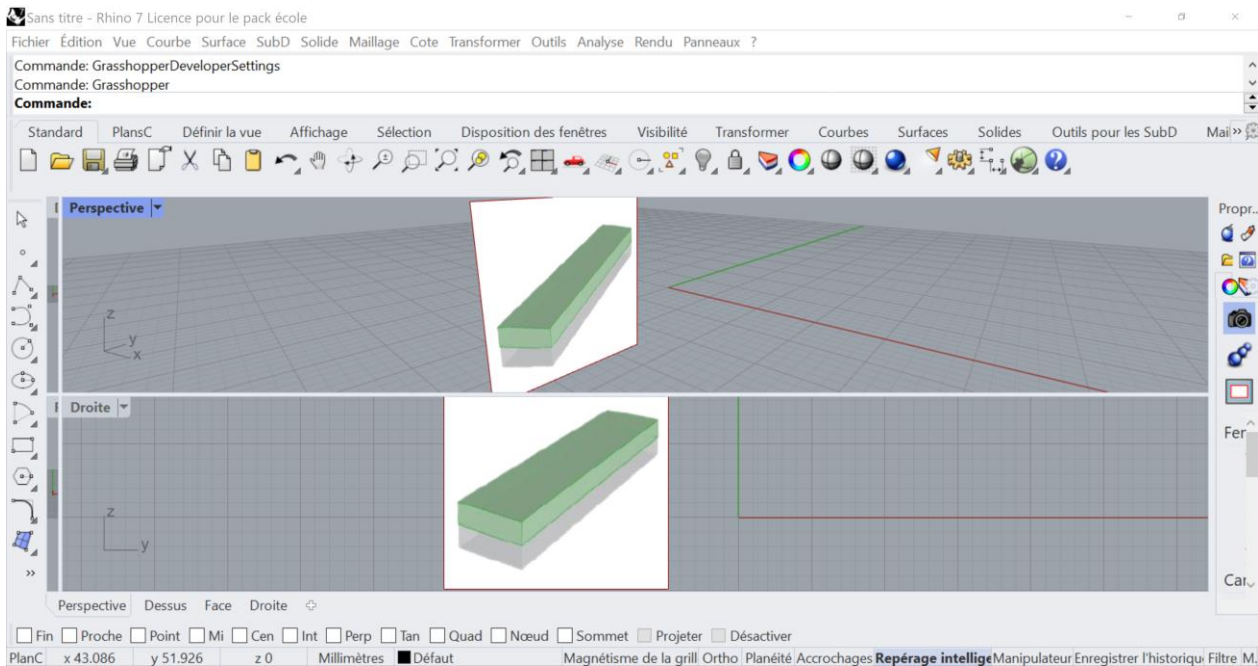


Figure 109. Illustration of the material distribution in Rhinoceros3D

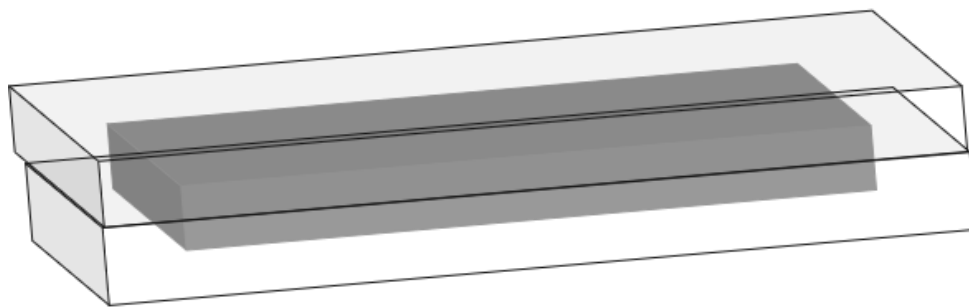


Figure 110. B-Rep definition of the beam

One of the B-Rep will be defined as an active region connected to the component of smart material in the plugin VoxSmart¹⁹ and the other as a passive region connected to the component inert material. There is another B-Rep not displayed, fixing the beam for simulation purpose. Figure 111 demonstrated the initial and final state of the bending beam considering the recommended material distribution.

¹⁹ Voxsmart is a plugin defined in a previous PhD in ICB-COMM lab, defined in Chapter 2 and uses genetic algorithm to simulate few transformation functions for 4D printing technology.

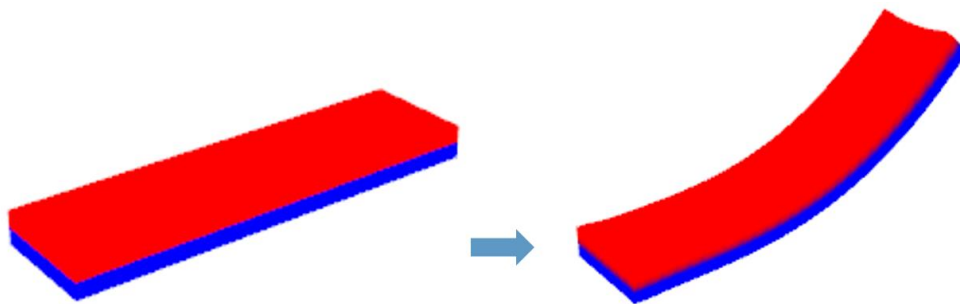


Figure 111. Simulation results from VoxSmart add-on using hydrogel material and heat as stimulus

6.4.4 Multi-bending (wrinkles) in a humanoid face

The fourth case study aims at integrating wrinkles in a humanoid face (exactly at the front) to give natural aspects for future robots as shown in Figure 112. A functional analysis is beforehand done in Figure 113, in order to reply for this requirement in the CDS phase.

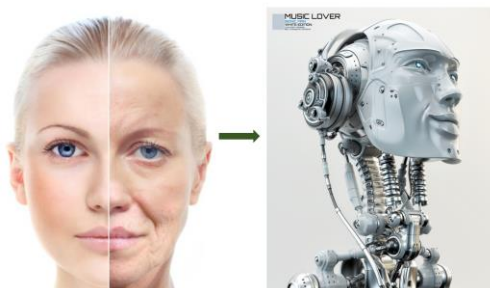


Figure 112. Instruction given to the designer: the purpose is the integrate the wrinkles in the lady face in the humanoid face²⁰

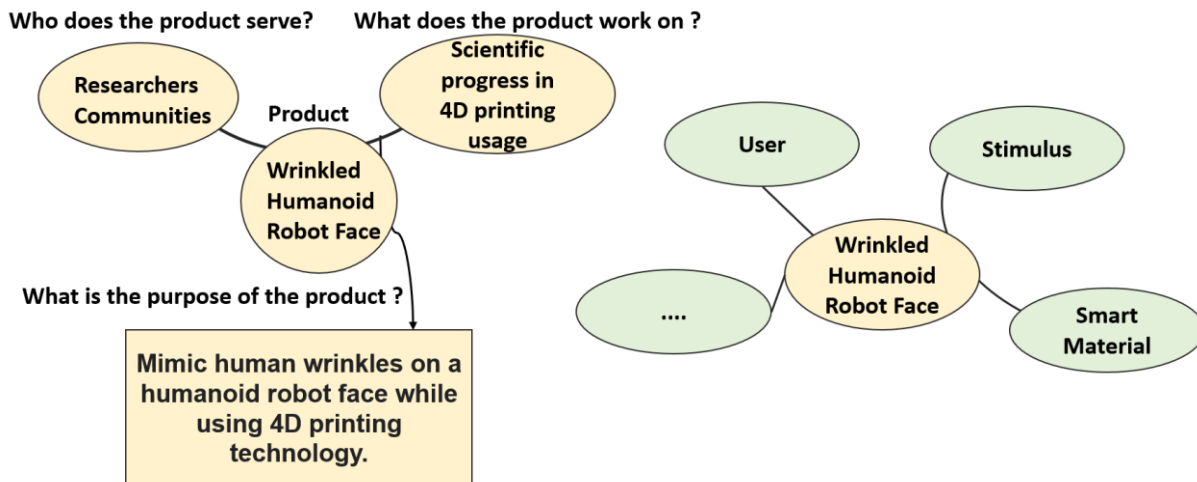


Figure 113. Functional analysis

²⁰ Photos extracted from <https://www.medicalnewstoday.com/articles/307383> and <https://www.artstation.com/artwork/music-lover-white-version>

The Transformation_function is defined as *Multi_bending* as instance of bending. The Stimulus is fixed as *Electric_field*, the Transformation_dimension as *3D_to_3D*, and the Transformation_effect as *Repeatable*. The Machine is also fixed to *Stratasys_objet_connex_260* These are the fixed and well-defined classes by the product designer and product architect after getting through task clarification and conceptual design phases. Knowledge can be generated also by using SPARQL queries. An API was developed to communicate externally with the ontology and integrate it into Rhinoceros3D. The ontology will be stored in triple store (i.e., Jena apache fuseki) with further semantic rules, and then connected to the API for retrieval and reasoning purposes in the CAD system as illustrated in Figure 114.

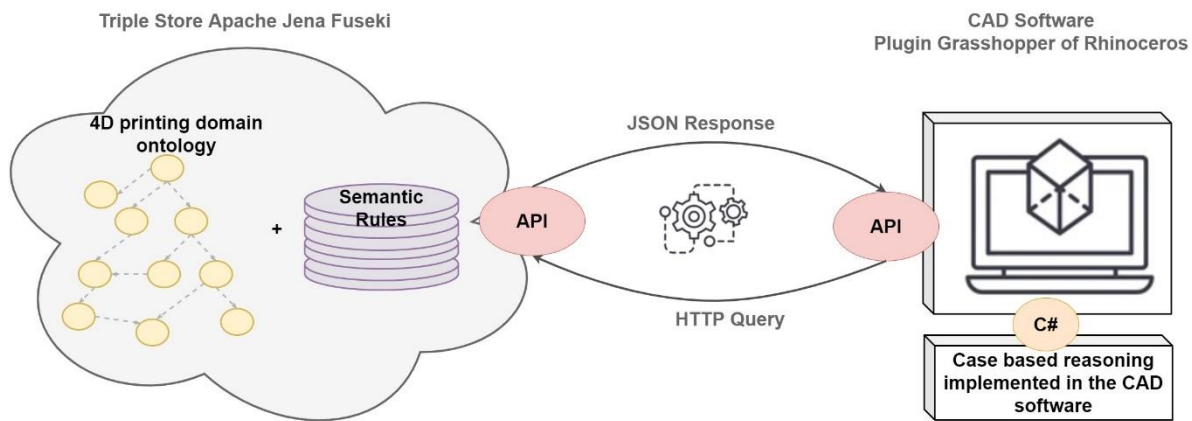


Figure 114. The main architecture for connecting the ontology to a CAD system

The transformation functions are associated set by set to a technical function, then it is crucial to determine the technical functions associated to this case study. Knowing the fact that *Multi_bending* isComposedOf *Shape_changer*, *Electric_field* is the Stimulus, and Stimulus triggers Technical_function. The query will query the ontology which subclass of the *Shape_changer* is triggered by an *Electric_field*: it is indeed *Electroactive* as shown in Figure 115.

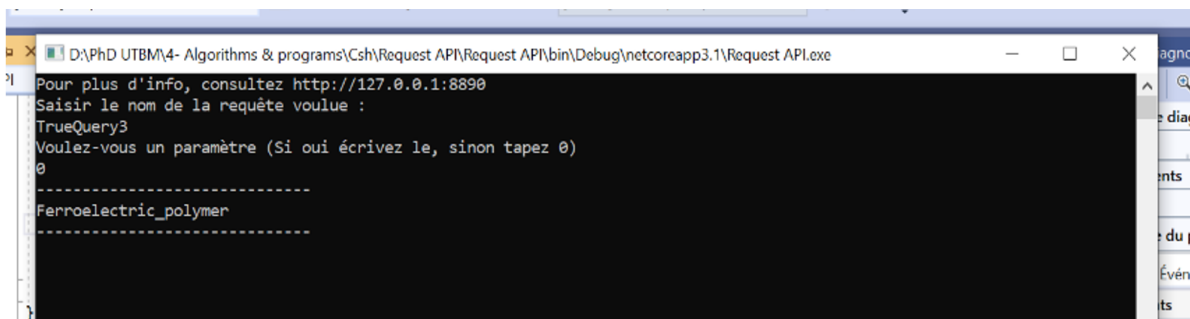


Figure 115. First query returned by interrogating the developed API

Along with the relation **Material** fulfills **Technical_function**, the suggested **Material** is *Ferroelectric_polymer* (see Figure 116). The ontology will be requested which **Material**'s subclasses is triggered by an *Electric_field*, fulfills an *Electroactive* function, and has a **Transformation_effect** *Repeatable*).

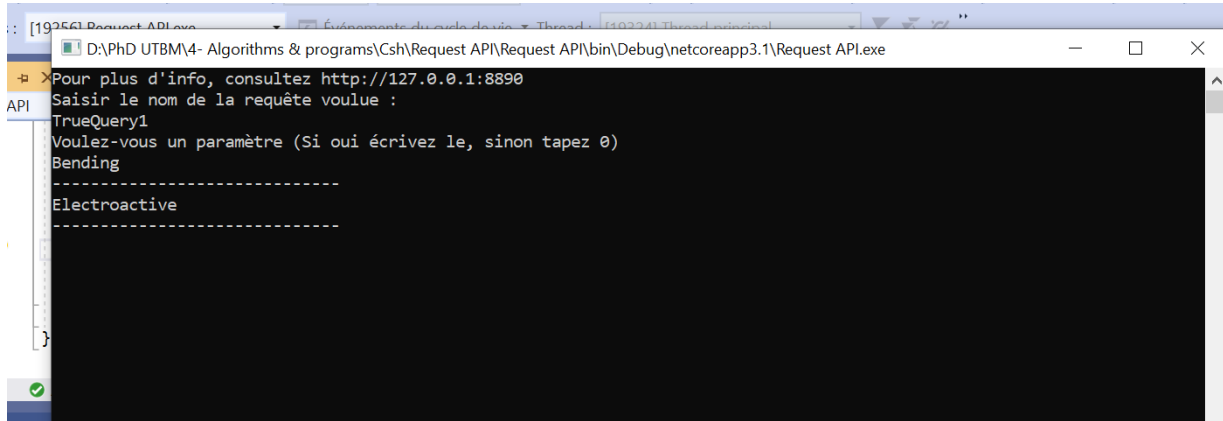


Figure 116. Second query returned by interrogating the API

Hence the target vector is defined as: {Repeatable, 3D_to_3D, Multi_bending, Electroactive, Electric_field, Ferroelectric_polymer, Stratasys_objet_connex_260}. As stated in the previous case study, the “MD Recommendation” component will be connected to the semantic base and to the target vector written manually in a panel. The output displays the nearest experiences ranked in descending way. The display is roughly for the experiences having a cosine value more than 0.1 (see Figure 117). In addition, with the same concept, the figure of the material distribution is displayed in Rhinoceros3D (as shown in Figure 118). The nearest material distribution in this case is a combination of multi-sandwich and segmented. The experience selector lift serves to change the number of the experience if the product designer want to display the materials distributions for other near experiences.

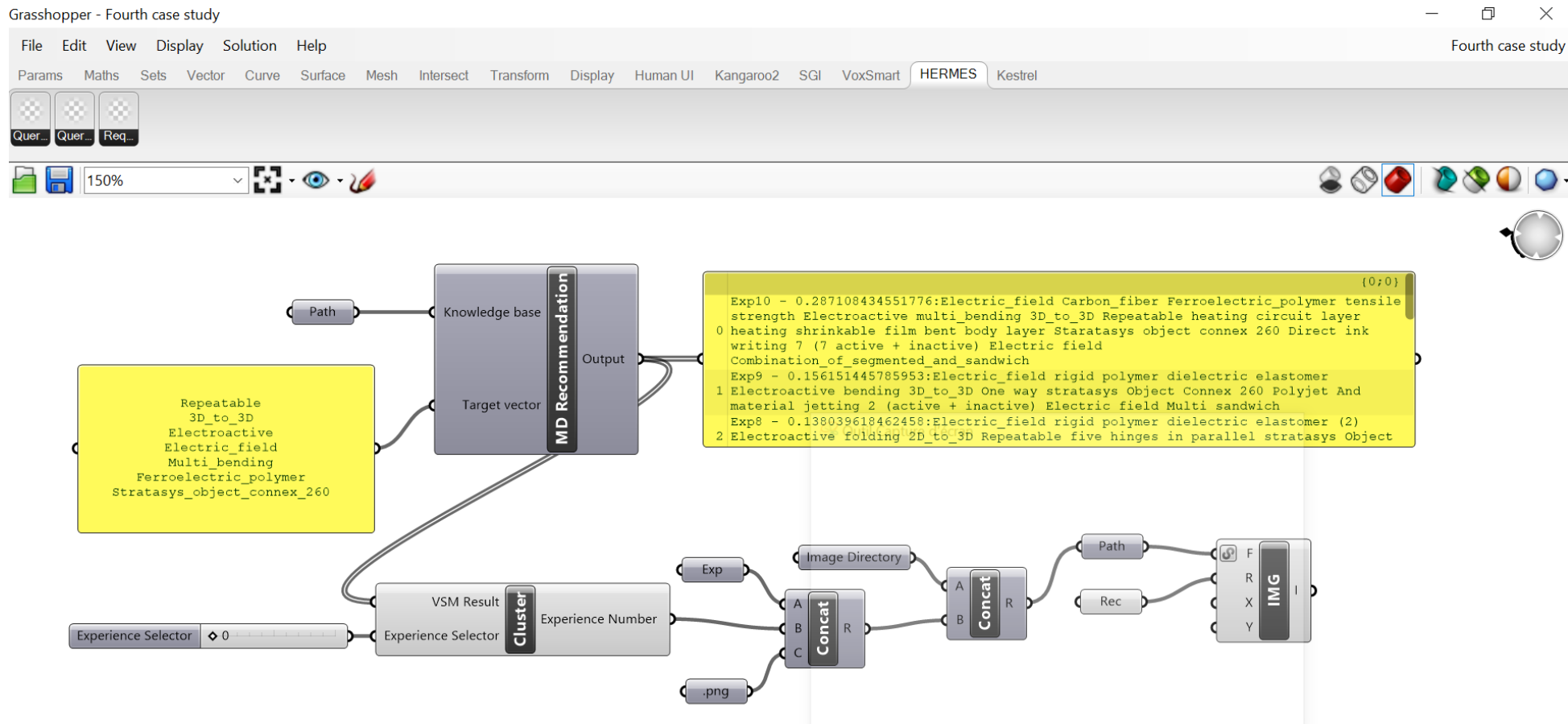


Figure 117. Visual programming on Grasshopper plugin of the material distribution recommendation for the fourth case study

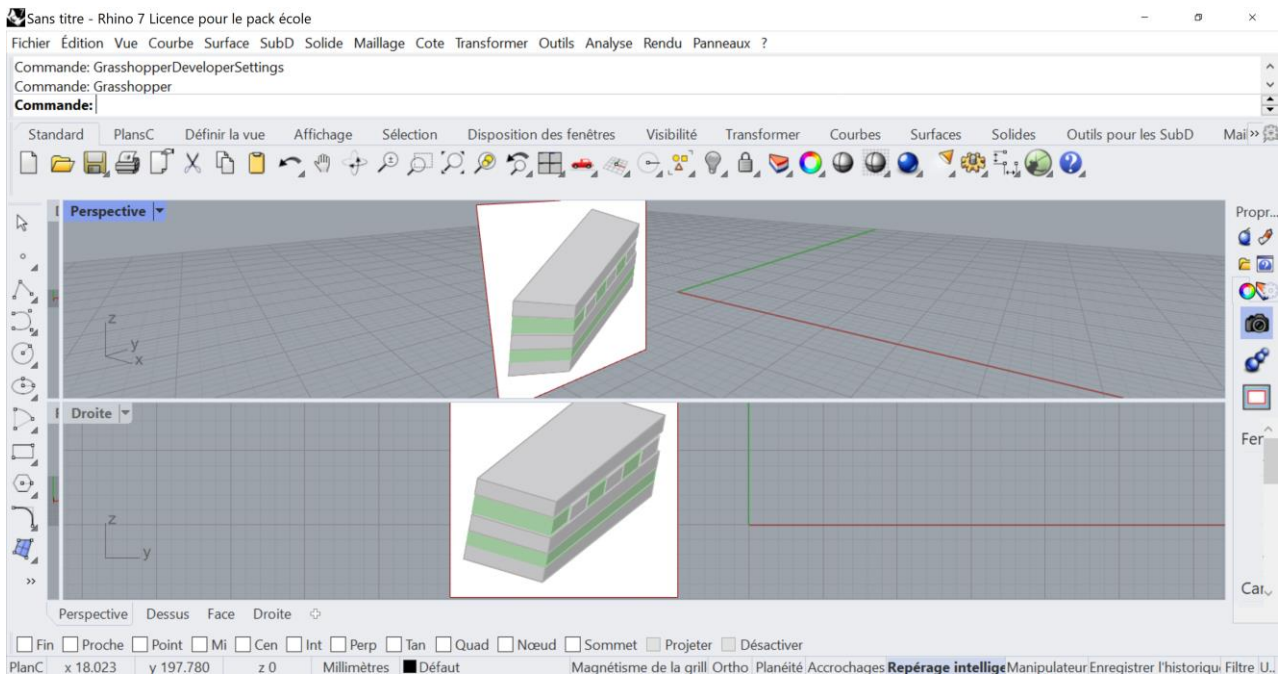


Figure 118. Illustration of the material distribution in Rhinoceros3D

Figure 119 shows the manual definition of B-Reps to delimit active and passive regions for the front of the face.

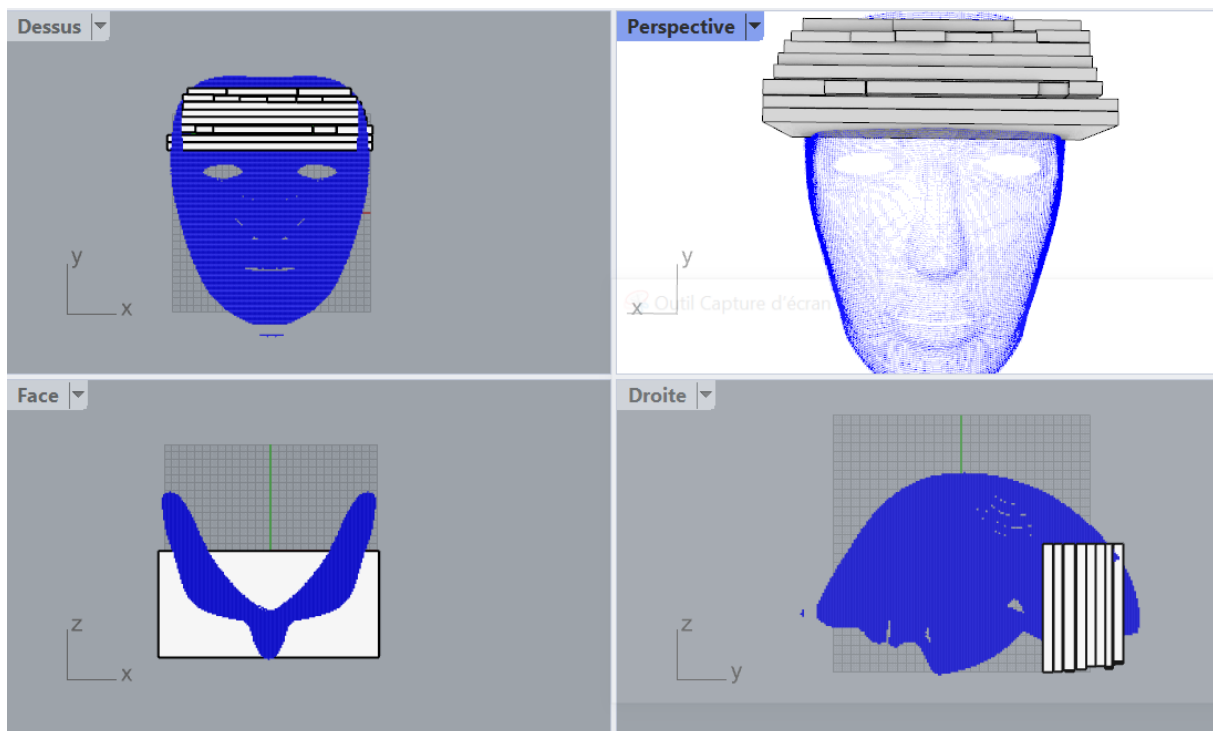


Figure 119. Manual definition of recommended active/passive regions in Rhinoceros3D:

B-Rep definition

The B-Reps will be associated to active and passive regions connected to components defining smart and inert material in the VoxSmart add-on. Figure 120 demonstrates the final state of the wrinkled front considering the recommended materials distribution. The surface is meshed and voxelized due to VoxSmart computing algorithm.

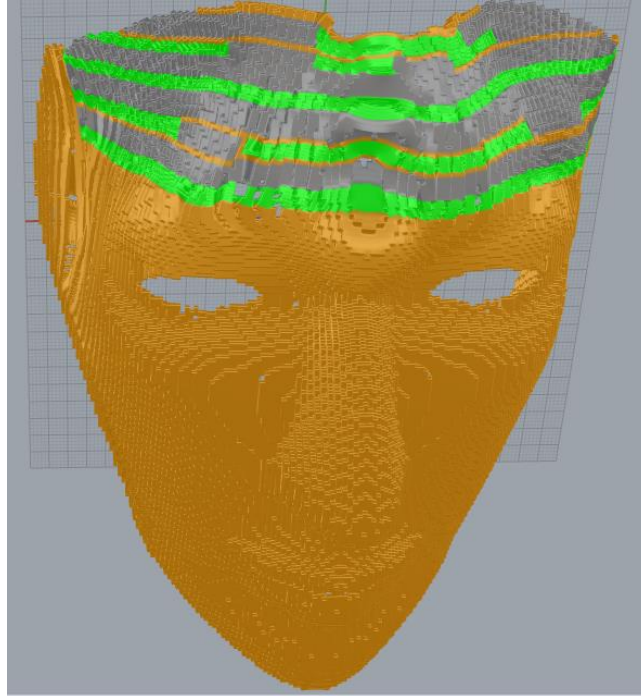


Figure 120. Simulation results from VoxSmart using piezoelectric material and electric field as stimulus

6.5 Conclusion

This chapter has illustrated the usability and the relevance of the three contributions proposed in this PhD (an ontology-based framework, a multi-representation of 4D printed object, and a recommendation method based on semantic-based reasoning and case-based reasoning using VSM for materials distribution prediction. An implementation of the latter is made within a dedicated computational design for 4D printing plugin into a CAD environment.

Chapter 7 Conclusions and future work

"It is always important to know when something has reached its end: closing circles, shutting doors, finishing chapters [...]."

Paulo Coelho

"Things don't always happen like that, clearly for specific reasons: they settle down, slip away, they arrive on their own and often unwittingly to a conclusion that is gradually being accepted."

Hervé Bazin

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7.2 Perspectives 160

This thesis is the first research work formalizing 4D printing with an ontology. The goal of this PhD project was to put forth a framework, ontology, methods, and tools to design for 4D printing. So, as highlighted in the introduction and literature review, there was a lack of design tools and methodologies to help designers considering this innovative technology in manufacturing. This chapter summarizes the contributions proposed to achieve the aforementioned goal and it presents the work that still need to be achieved for a better 4D printing establishment.

7.1 Conclusions

The key research questions stated in the introductory Chapters were mainly about how to formalize and represent the knowledge behind 4D printing technology, how to represent a printed object, and how to recommend a specific knowledge: materials distribution to the designer in the CDS phase?

This research work has started with building a domain ontology as a pioneer effort dedicated to formalizing and representing 4D printing knowledge relating AM processes and techniques, SMs, stimuli and transformation issues to design and engineering objects. To do so, an ontological framework has been beforehand established with the underlying scientific hypotheses, along with the use of 4D printing knowledge in design. Then, formal description of objects' relationships and formal description of spatiotemporal objects with description logic (first order logic) were defined. This contribution addresses an entire understanding and description of the complexity of 4D printing technology. Then, a multi representation of the object is suggested to enhance the limits for the design for 4D printing. This was considered as an add-on to be formalized and integrated in HERMES ontology. The knowledge issued from the above-mentioned ontology is integrated in CDS phase. To do so, semantic and case-based reasoning layers are suggested to aid the product designer. A recommendation method was proposed on one hand using VSM algebraic method to predict such a material distribution that has to be adequate to specific requirements. On the other hand, semantic reasoning-based rules are suggested to reason with the knowledge federated in the HERMES ontology. An implementation of the recommendation method is made within a dedicated computational design for 4D printing plugin in a CAD environment, and a four case studies were illustrated in Chapter 6.

7.3 Perspectives

The work undertaken in this research provides a large spectrum of perspectives in short, mid, and long terms. A development of remaining work and opportunities is introduced hereafter.

7.3.1 Short-term perspectives

Considering the framework established in Chapter 3, different research work can be recommended at a short term. In this thesis, we have only considered some of the limits that the product designer is facing; but many efforts should be put to enhance the recommendation of a contextual knowledge for him. It is also important to consider other experts like materials expert, AM expert and mechanical engineer. It needed to populate the ontology in advantage of material selection and AM process planning purposes. Also, the simulation of the transformation process has to be considered from a quantitative level. To do so, further population is needed for the multi-representations of the 4D printed object to recommend pertinent initial and final states at different level of abstraction. Also, the connection between HERMES ontology and Grasshopper plugin is done manually until now, which means the .json file is integrated manually in the C# editor of grasshopper. Thus an automatic connection is strongly needed; to do so, two components are about to be developed “ontology reader” for query purposed and “get instances” for creating the semantic base automatically with .json files received from the triple store, as illustrated in Figure 121.

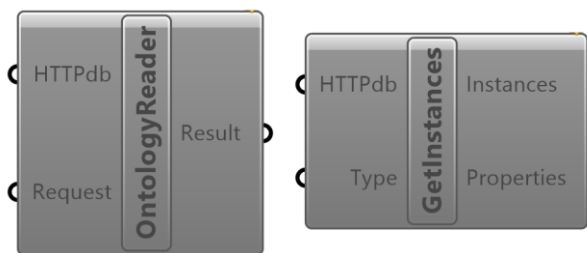


Figure 121. Dedicated components for envisioned connection of the ontology to Grasshopper

As for recommendation method using the VSM method, it is envisioned to automatically create the target vector using components representing the top classes of the ontology, see Figure 122 where some components: “Machine” and “AM process” are being developed.

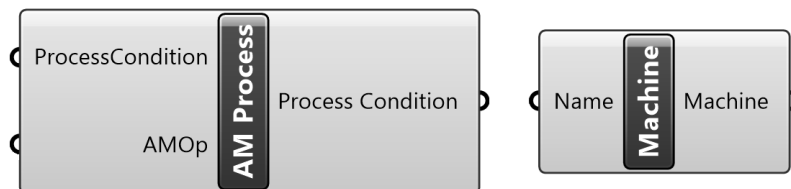


Figure 122. Example of components denoting HERMES top classes

7.3.2 Mid-term perspectives

The proposed ontology includes reasoning capabilities supported by DL rules; however, additional reasoning layers will be needed to fully capture 4D printing knowledge over views and scales. For instance, among the opportunities and alignment issues between HERMES and EMMO ontology to tackle the material design aspect. Several APIs and reasoning-based requests – dedicated to specific purposes like transformation sequence planning, smart material selection and distribution, AM process planning can be developed to increase its operational level. Such foundational and computational layers will be considered to specify means for developing the next generation of CAD systems dedicated to the geometric definition of products capable of changing their configuration and shape over time. This will ensure the capture and reuse of appropriate knowledge with appropriate semantic to the right person at the right time. This will be critical for product architects and designers to make the right decision during the design process of alive and transforming products/objects.

7.3.3 Long-term perspectives

As the primary purpose of framework proposed in Chapter 3 is to unlock all the potential of 4D printing, the use of HERMES ontology [229] as a knowledge base as well as neural networks for the generation and the evaluation of solutions has been planned at ICB-COMM lab. By this way, the designer will have a complete toolbox to design and generate complex part without wondering about inner matter distribution that he needs to realize a defined transformation behavior or property changing. On one hand, considering the integration of new knowledge in the ontology is crucial in order to assure a continually updated dynamic HERMES ontology. As a fact, this may consider a closed-loop system for ontology implementation, which can assure continued data collection. On the other hand, having a complete understanding of the overall conceptualization provided by such an ontology is often illusory and delicate. Therefore, it is essential to provide customized access to a portion of the corresponding ontology based on their assumptions to the involved stakeholders (i.e., product architect, product designer, material expert, and process planner). Such a performance could be produced by the proposed views as reported in previous sections and by considering a stakeholders-based view respecting their different design needs. To ensure the construction of comprehensive knowledge base in this research field, further efforts have to be conducted to address other abstraction levels such as material design and system design.

It is also possible to constitute complex patterns of materials distribution formed from other described patterns in this PhD, thus allowing the easy and optimized realization of complex structures such as metamaterials. Voxels may be interpreted by neural networks, the very structure of an object represented by voxels resembles a three-dimensional matrix where each component is a voxel. Also, if the product is composed of multiple parts, then the skeleton will be defined by lines, planes and points representing the “main structure” of the part,

but and a collection of mechanical links or joints between the different parts and subparts, that can be realized in fine by conventional means or specific matter distribution, in order to represent the main structure and articulation of an object. As for the skeleton-based representation, it can serve for deep learning-based design for manufacturability.

The ultimate and long-term objective is to propose models, methods, and tools for the design of more intelligent, more sensitive, more obedient, and more transformable structures at various hierarchical levels, imbuing them with properties that will make them act nearly like living objects, like matter aware of its own. The recommendation is not limited to predicting materials' distribution, it could be any other specific knowledge contained in the ontology in general to enhance the quality of the delivered object by this technology.

To sum up: many perspectives can be proposed based on the above work:

- Knowledge extraction from scientific articles to populate the knowledge base using natural language processing;
- Knowledge extraction from physical experiments;
- Knowledge extraction from numerical simulation;
- Knowledge reuse;
- Management of the knowledge base;
- Defining the object (meretopological level).

Research work publications

Journal Papers

- [1] S. Dimassi, F. Demoly, C. Cruz, H. Jerry Qi, K. Kim, J-C. André, S. Gomes, “An ontology-based framework to formalize and represent 4D printing knowledge in design,” *Computers in Industry*, volume 126, 2021.
- [2] S. Dimassi, H. Belkebir, F. Demoly, C. Cruz, J-C. André, S. Gomes, “Ontology-based design for 4D Printing: Recommendation system via semantic and case-based reasoning” *Artificial Intelligence for Engineering Design, Analysis and Manufacturing*, *Submitted*.

Conference paper

S. Dimassi, F. Demoly, C. Cruz, and S. Gomes, “From dispersed knowledge to Ontology : A proposal for formalising and integrating 4D printing in design,” in *IFIP PLM*, 2021, pp. 1–18.

Promotion of this thesis’ works in other international events

✓ Communications in Congresses

- GDR Macs, Nantes, France, Feb 2020 “4D printing related knowledge representation with ontology: importance and usability”.
- GDR Macs, Online, December 2020 “Distributed knowledge issued from HERMES ontology for design for 4D printing purpose”.

✓ Poster in ISITE UBFC conference, Besançon, France, October 2020: “Theory, model and approach to the design of dynamic objects in the era of 4D printing and smart materials”.

✓ Summer schools: Integrated product development

- Presentation subject: “State of the art: 4D printing, smart materials and relational bases domains” University of Malta, May 2019.
- Presentation subject: “4D printing: concrete challenges nowadays and what is missing” University of Magdeburg, Germany, September 2019.

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